

A Thesis Submitted for the Degree of PhD at the University of Warwick

Permanent WRAP URL:

<http://wrap.warwick.ac.uk/111554/>

Copyright and reuse:

This thesis is made available online and is protected by original copyright.

Please scroll down to view the document itself.

Please refer to the repository record for this item for information to help you to cite it.

Our policy information is available from the repository home page.

For more information, please contact the WRAP Team at: wrap@warwick.ac.uk

THEORY OF SUPERFLUIDITY

by

Rafael F. Angulo G.
B.Sc., M.Sc.

A Dissertation submitted to the University
of Warwick for the admission to the degree
of Doctor of Philosophy.

April, 1983.

MEMORANDUM

This dissertation is submitted to the University of Warwick in support of my application for admission to the degree of Doctor of Philosophy. It contains an account of my own work performed at the Department of Physics of the University of Warwick in collaboration with Dr. G. J. Hyland. No part of this dissertation has been used previously in a degree thesis submitted to this or any other University. The work described in this thesis is the result of my own independent research, except where specifically acknowledged in the text. Parts of this thesis are to be submitted for publication.

Rafael F. Angulo

April 1983

Acknowledgements

The author wishes to thank a number of persons for their direct, or indirect, participation towards the completion of this work. First and foremost to Dr. G. J. Hyland for his continued support and advice; for taking the risk of accompanying me into research in a field outside of his immediate expertise, and offering to me the benefit of his experience. To Professor P. N. Butcher for his hospitality during my stay at the University of Warwick. To Dr. G. Rowlands for helpful discussions and for offering to me the benefit of his sharp and accurate criticism. To all the members of staff and Research Students of the Theoretical Group for continued and valuable discussions. To my wife, Mireya, for her loving support, to my son J.J. for being my source of inspiration, and to Misses Sandra Callanan and Nada Gvero for typing the manuscript: to all my sincere thanks.

I would also like to thank C.O.N.I.C.I.T. (Venezuela) for financial support, and - finally - my appreciation to those physicists of my own regional scientific community who listened and cared, and to those who did not; for, in either case, they provided me with renewed sources of encouragement and determination.

ABSTRACT

A theory of superfluidity (S.F.) is developed from first principles using two novel concepts, (1) that of a 'superfluid Ensemble' (S.E.) i.e. a 'Restricted Ensemble' constructed from a 'Separable Phase Space' (S.P.S.) admitting *independent* configurations, at least one set of which are statistically equivalent. (2) The notion of 'Dynamical Equivalence' (D.E.), satisfied if and only if (i) *all* dynamical symmetries are *rearranged* (*not broken*) for two Lagrangian formulations of the same problem and if (ii) the expectation values of *all* the constants of motion are the same, even if their functional expressions are *not*. The dynamical variables (d.v.) of the S.P.S. are defined from the ('q' and 'c' number) fields of the most general 'Linear Coherent State Representation', more general than those of Glauber and Bogoljubov-Valatin combined. *Three independent* pairs of d.v. are obtained.

D.E. is proven for the Ideal Bose Gas and for a non-linear, interacting zero order Bose problem (I.Z.O.P.). An exact relation is obtained from the action principle, ensuring the cancellation of 'low and high order dangerous diagrams'. From this it follows that D.E. for the exact interacting problem must be demonstrable at infinite order of perturbation, in the *finite* volume limit. The I.Z.O.P. is posed in the Random Phase Approximation (R.P.A.), free from 'anomalous averages' and solved for the *three* branches of the excitation spectrum in a pure state description; the lowest branch is gapless, whilst the upper two coincide and show a gap. The standard strategy of linearization is found to be faulty.

The partition functions for both superfluid and non-superfluid ensembles are obtained for the I.Z.O.P. in the R.P.A. The coincident upper two branches (in a pure state description) split into a band in thermal equilibrium for the superfluid ensemble, in agreement with an upper band recently observed experimentally. O.D.L.R.O. is found in the *second* reduced density matrix, but ruled out in the *first*. Integral equations are obtained in thermal equilibrium - for the I.Z.O.P. in the R.P.A.; which differ, however, from those of existing approaches for the same problem. Most existing theories of S.F. are in fact shown *not* to predict superfluid behaviour. The present theory is applicable to arbitrary Bose or Fermi systems, whether superfluid or *not*. O.D.L.R.O. is found to be sufficient for SF. No *a priori* assumption is made as to the occurrence of Bose-Einstein condensation, its existence being here contingent on the solution of the integral equation; in any case, it is *not* to be associated with O.D.L.R.O. or S.F.

INDEX

CHAPTER ONE: INTRODUCTION	1
§1.1. Introduction	1
§1.2. Theoretical survey of existing literature	5
A. Bogoljubov's Theory of superfluidity	8
B. Valatin and Butler's Pairing Theory	14
C. Girardeau and Arnowitt's Pair Theory	26
D. Hugenholtz and Pines' Field Theoretic Approach ..	29
E. Luban's Thermodynamically Equivalent Hamiltonian Method	31
F. Etters, Hierarchy of Linear Equations of Motion ..	36
G. Cummings and Johnston, Theory of Superfluidity ...	41
H. Coniglio and Marinaro, Coniglio, Mancini and Manturi. On Umezawa's Physical Representation.	48
I. Evans and Imry. Self-consistent Pairing Theory .	56
§1.3. Overview of the proposed new theory of superfluidity.	62
A. Preliminaries	62
B. Statistical Characterization of a Superfluid	70
C. Equivalent Formulations of Dynamics from Variables of Separable and Non-seperable Phase Spaces	73
D. Resolution of the unperturbed Problem in the Random Phase Approximation	81
CHAPTER TWO: BASIC DEFINITIONS AND NOTATION	85
§2.1. Introduction	85
§2.2. Definition of Separable Phase Space and the Notion of Dynamical Equivalence	86
A. Separable Phase Space	86
B. Dynamical Equivalence	91
§2.3. Definition of Linear Coherent State Representation (L.C.S.R.)	96
§2.4. Definition of Separable Phase Space Variables in Terms of Fields of L.C.S.R.	104

CHAPTER THREE: DYNAMICS IN A SEPARABLE PHASE SPACE (S.P.S.)	108
§3.1. The Problem of the Ideal Bose Gas (I.B.G.)	108
§3.2. The Interacting Problem: A model for ^4He	122
§3.3. Mean Field Approximation for the Zeroth Order Problem	130
CHAPTER FOUR: REARRANGEMENT OF GAUGE INVARIANCE, O.D.L.R.O. AND STATISTICAL MECHANICS IN A SEPARABLE PHASE SPACE. 154	
§4.1. Introduction	154
§4.2. Rearrangement of Gauge invariance	156
§4.3. O.D.L.R.O.	165
§4.4. Statistical Counting in the S.P.S.	175
§4.5. Further Developments	205
CHAPTER FIVE: SUMMARY AND CONCLUSIONS	225
§5.1. Summary	225
§5.2. Conclusions	232
APPENDIX A	238
APPENDIX B	243
APPENDIX C	245
REFERENCES	247

... 'The world was so recent that things lacked names, and to mention them they had to be pointed with the finger' ...

Gabriel Garcia-Marquez, from "Hundred years of solitude"
(free translation)

§1.1. INTRODUCTION

The theoretical understanding of the phenomena exhibited by ^4He below the lambda transition temperature can be separated into three broad levels, each of which corresponds to particular periods in a chronological sequence of developments.

The first level, corresponding to the early days of investigations on 'Quantum Fluids', was characterized by phenomenological studies - at a macroscopic scale - of the hydrodynamic properties of superfluid ^4He . Representative works at this level are those of London (52), Feynman (26), Landau (47a) and Penrose (57). These works may be briefly summarized by the statement that a superfluid system is one whose dynamic and thermodynamic properties in equilibrium must be described in terms of 'macroscopic wave functions'. Among the consequences of this fact are the existence of additional thermodynamic variables, such as the superfluid density and velocity, also that of quantized vortices. One of the main objectives at this level was to develop a Two-fluid Model capable of giving a complete hydrodynamic description of ^4He II in terms of variables potentially connected with microscopic quantities.

The second level is a semi-phenomenological one. It relates macroscopic, thermodynamic properties - such as the temperature dependence of the specific heat, the entropy, the thermal conductivity, etc. - observed experimentally, to microscopic properties susceptible to independent measurement (and also derivable from microscopic first principles), such as the excitation spectrum for instance. The most outstanding representative works at this level are those by Landau (47b). This author initially conjectured a two-branch excitation spectrum; the low lying branch was envisaged as gapless and linear at small wave vector, k ; the upper branch - on the other hand - was thought to show a gap at $k=0$, being essentially flat at small k and continuing quadratically at higher wave vector values. This initial

conjecture was modified in a later work by the same author proposing a single-branch spectrum instead. This was assumed gapless and linear in the long-wave limit, but showed a relative minima at some finite wave vector value. Two different types of 'quasi-particles' were postulated by this author, namely 'phonons' and 'rotons'; associated respectively, with excitations in the linear region and in the relative minima region. Remarkably accurate predictions were obtained for the magnitudes of various thermodynamic quantities; the qualitative dependence of the excitation spectrum on k was confirmed years later by direct neutron scattering experiments (54).

The third level on which the properties of ^4He are discussed is a fully microscopic one. The objectives at this level are to derive and confirm the *ad hoc* premises of phenomenological and semi-phenomenological theories from microscopic and statistical first principles, and ideally to construct a unified microscopic theory capable of explaining superfluid behaviour - not only in the Bose superfluid, namely ^4He II, - but in arbitrary superfluids. The work reported in this thesis belongs to this microscopic level.

The era of strictly first principle microscopic theories was initiated in 1947 by the pioneering work of Bogoljubov (6), followed shortly after by the works by Beliaev (5), Valatin and Butler (68), Hugenholtz and Pines (40), Zubarev (73), Girardeau and Arnowitt (29), Hohenberg and Martin (38) and by many others^(*). The theory of superfluidity was thereby turned into a broad body of theory which successfully predicted a large variety of phenomena in all three fronts - dynamical, hydrodynamical and thermodynamical; furthermore, it validated to a large extent the propositions and conjectures of the phenomenological level.

During the sixties there seemed to be an almost universal consensus as to the fact that the fundamentals of the problem of the Bose superfluid

(*) see Refs. 10-12, 18, 20, 22, 23, 32, 35, 38-40, 45, 51, 55, 56, 58-60, 62, 65, and ref. therein.

were already understood, despite the existence of the conceptual, methodological and practical difficulties encountered. It was thought that it was only a matter of time until the remaining loose ends could be tied up. But the difficulties remained and gradually became worse.

A brief comment on these difficulties will, for the present, suffice to illustrate their extent. Firstly, a central element of the theory of superfluidity is the assumption of the existence of macroscopic Bose-Einstein condensation (B.E.C.) in the interacting liquid. The relative magnitude of B.E.C. has reduced through the years and even its very occurrence is now being questioned. But in any event the association of the condensate with the superfluid is dubious, for nothing prevents particles in the condensate from being scattered individually or collectively, resulting in disorder and dissipation. On the other hand the occurrence of a fractionally small condensate invalidates the Goldstone linked cluster expansion theorem (32a,40) and the condensate mode ($k=0$) must be completely eliminated - in an *ad hoc* way - from the dynamical and statistical scene if significant results are to be obtained. But even then, if realistic interactions (12) are employed and the excitation spectrum is chosen as to fit experimental values, a non-condensed fraction larger than one is found! (56).

A second difficulty has become intolerable with the passage of time. The initial simple work of Bogoljubov predicted a gapless spectrum - in agreement with experimental observation - and this was confirmed by Beliaev using infinite order perturbation techniques and by Hugenholtz and Pines using Green's function methods; on the other hand however, a large number of authors using a variety of different approaches (18,20, 29, 32,45,46,51,55,60,65) consistently obtained a gap in the excitation spectrum in a self-consistent Random Phase Approximation (R.P.A.). Hence, the theory seems doomed to infinite order perturbative calculation and out of

the reach of simple techniques. A review of self-consistent, mean field theories is given in the following section. A similar difficulty does not arise in the theory of superconductivity (4,34) developed very much on the same lines - except for the non-occurrence of B.E.C. For, the observed excitation spectrum for most superconductors does indeed show a gap.

A third difficulty of the theory of superfluidity, shared by the theory of superconductivity, is that the gauge symmetry present in the normal phase description is broken in the superfluid phase; that is the total number of atoms is not a good quantum number below the transition temperature. This is not only a conceptual nonsense (in the absence of massless bosons carrying away the gauge symmetry) (33b,42) but is also against experimental observation.

A fourth conceptual difficulty is the fact that the very origin of superfluid behaviour is not clear. The usual argument from which superfluid behaviour is predicted is that the entropy is independent of some parameter which contributes fractionally to the total average ensemble density. However, it happens that the ensemble is constructed such that the *only* configurations are those associated with *normal* elementary excitations, and *not* with (would-be) superfluid variables; hence the notion of entropy does not apply to the latter, which accordingly cannot be used as an order parameter. Consequently most existing theories of superfluidity (4,6,15,18,20,22,23,29,32,40,43,46,51,55,60,62,65,59,68,73) do *not predict* superfluid behaviour, but *impose* it *a priori*.

This thesis is concerned with a non-conventional theory of superfluidity free from *all* the above mentioned difficulties and some others that will become clear in due course. The main element of our strategy here is that superfluid behaviour should arise - from a theoretical view point - solely from statistical considerations, applicable to arbitrary

superfluids, and *not* from dynamical considerations. It is argued that in order to be able to characterize a superfluid both the statistical and dynamical problems should be *reformulated* on the basis of a separable phase space (Ch. 2), such that a restricted ensemble description is always possible. This will entail a profound change of viewpoint in the formulation of dynamics. In particular, it will be seen that the appropriate hamiltonian and number operators are *not* the usual *particle* functionals, but different operators. It follows from this alone that the gauge symmetry is rearranged, *not* broken. This also results in an excitation spectrum which possesses several (three) branches; one branch is manifestly gapless, whilst the two upper branches are identical in a pure state description and correspond to that repeatedly obtained before, showing a gap. Averaged over the *superfluid ensemble*, however, these two branches split into a band observed in a recent experiment (19, 43).

§1.2. THEORETICAL SURVEY OF EXISTING LITERATURE

This section contains a detailed account of a number^(*) of fundamental works on the theory of the Bose superfluid, selected on the basis of conceptual content, proximity to microscopic first principles and operative simplicity.

The objectives aimed at in this incomplete review section are:

- (i) To provide the non-specialized reader with a fairly complete survey of the basic conceptual elements and methods necessary for the appreciation of the novel features of the non-conventional theory of superfluidity proposed in this thesis.

(*) To give a complete account of the present state of theory is a major task, well outside the scope of this modest work. Several compendia already embody a number of such theories and the reader is referred to them for further information. (see list of compendia references.)

- (ii) To emphasize the sequence of development of existing ideas.
- (iii) To point out and analyse the unresolved difficulties encountered by existing microscopic theories, avoiding technical complexity, however, in so far as it does not obscure conceptual understanding.

The theoretical knowledge on superfluid ⁴He has grown so much in the last forty years - both from fundamental developments and as to their implications - in so many different directions, that a list of references would fill an entire volume. Significantly new fundamental innovations have seldom appeared in the literature in recent years; on the other hand, however, works on further implications of existing theories are still overwhelming in number. As to the conceptual aspect of the theoretical understanding, the present state of affairs on superfluidity has been compared to the calm of a cemetery. On the other hand, Ph.D. theses have been described as the transposition of bones from one cemetery to another. A personal aim in this work is to try to prove these analogies wrong; to show - in particular - that conceptual growth on superfluidity is alive and well.

This review is confined to self-consistent, mean field theories, as these already involve all conceptual features involved in more elaborate theories, and also because a measure of the failure of these theories is more markedly revealed by them. The omission of more elaborate approaches, making use of perturbation techniques (5) and/or Green's function methods (40,73) or 'S' matrix techniques (4) is regretted, but well documented reviews on these already exist (*). To include these approaches here would greatly increase the mathematical complexity and far from clarifying the basic concepts would obscure them; besides, they would take considerable space.

(*) (see compendia references)

The unification of notation of the works reviewed here poses a linguistic problem; it is a compromise which would be resented by both the authors and the reader. For this reason the original notation is kept with minor modifications, e.g. the Fourier transforms of the interaction potential is assumed to exist and is denoted by $V(k)$ instead of V_k . It should be noted that creation and annihilation operators in the work by Valatin and Butler are denoted oppositely to the conventional notation; i.e. for V-B ξ_k, ξ_k^+ are creation and annihilation operators, respectively. The name "coherent state representation" is used for both Glauber (first order) and Bogoljubov-Valatin (pair) second order representations, whilst the names first and second order coherent fields refer to the c-number fields involved in these two representations, respectively; however, no *a priori* association of either of these fields with superfluid variables is implied. Furthermore no association is (or should be) made between Bose-Einstein condensation (either simple or generalized) and the first order coherent field.

A. Bogoljubov's (B) Theory of Superfluidity (1947)

The treatment of the many boson system by B (6) at very low temperatures is the earliest and - perhaps - the most influential microscopic work on superfluidity in ^4He . The two basic elements of his theory, namely the occurrence of macroscopic Bose-Einstein condensation (B.E.C.) and the pairing of particles of zero overall momentum, are incorporated - in some form or another - in almost all subsequent approaches, either *ab initio* or obtained as a consequence. Basic to B is the assumption that B.E.C. occurs in the interacting system, a proposition originally due to London (52). This assumption justifies what has been called the "Bogoljubov prescription" - namely the replacement of quantum creation and annihilation operators for the condensed mode, a_0^+ , a_0 , by real c-numbers of the order of $N^{1/2}$, where N is the total number of atoms; symbolically,

$$a_0^+ = a_0 = N_0^{1/2} \quad (1.2.1)A,$$

where

$$\lim_{N \rightarrow \infty} (N_0/N) \neq 0 \quad (1.2.2)A.$$

The above prescription is introduced into the exact equations of motion obtained from the second quantized hamiltonian

$$\hat{H} = \sum_k \epsilon_k a_k^+ a_k + \frac{1}{2} \sum_{p, \ell, q} V(\ell) a_{p+\ell}^+ a_{q-\ell}^+ a_p a_q \quad (1.2.3)A^{(*)}$$

where $\epsilon_k \equiv \frac{\hbar^2}{2m} k^2$ and $V(\ell)$ is the Fourier transform of the two-body local potential, $V(|\underline{r}|)$. It is argued that the number of particles not in the condensed mode (the depletion) is rather small at sufficiently low temperatures and low density, for essentially repulsive interactions, i.e. $V(0) > 0$;

(*) The notation as to \hat{H} differs from the original work and is consistent with that used in the present work; the volume dependence is not displayed.

in this case interactions among depletion particles is negligible compared with their kinetic energy. Within this approximation - known as Bogoljubov's weakly excited state approximation - the resulting eqs. of motion for condensed and depletion modes are:

$$i\hbar \partial_t a_0 = E_0 a_0 \quad (1.2.4.)A$$

and

$$i\hbar \partial_t a_k = [\epsilon_k + E_0 + N_0 V(k)] a_k + (a_0)^2 V(k) a_{-k}^* ; \text{ for } k \neq 0 \quad (1.2.5.)A,$$

respectively, where $E_0 = N_0 V(0)$.

The time dependence of both condensate and depletion variables is *rescaled* by this author; in such a way that the condensed mode is time-independent; i.e. new fields b_k are defined as follows:

$$a_k = \exp(-iE_0 t/\hbar) b_k, \text{ for } k \neq 0 \quad (1.2.6.)A$$

$$a_0 = \exp(-iE_0 t/\hbar) b \quad (1.2.7.)A.$$

The equations at motion for the new re-scaled depletion operators then become

$$i\hbar \partial_t b_k = [\epsilon_k + N_0 V(k)] b_k + b^2 V(k) b_{-k}^* \quad (1.2.8.)A$$

$$-i\hbar \partial_t b_{-k}^* = (b^*)^2 V(k) b_k + [\epsilon_k + N_0 V(k)] b_{-k}^* \quad (1.2.9.)A.$$

Mutually conjugate operators ξ_k and ξ_k^* and then defined by

$$\xi_k = (b_k - L_k b_{-k}^*) / (1 - |L_k|^2)^{1/2} \quad (1.2.10.)A^{(*)}$$

$$\xi_k^* = (b_k^* - L_k^* b_{-k}) / (1 - |L_k|^2)^{1/2} \quad (1.2.11.)A,$$

where the complex c-numbers L_k and L_k^* are chosen as

(*) The notation here is that of the original paper; a more modern notation for elementary excitations and c-number fields will be adopted later on.

$$L_k = \frac{b^2}{N_0 V(k)} [W_k - E_k - N_0 V(k)] \text{ (and similarly for } L_k^*) \quad (1.2.12.)A ,$$

where

$$W_k = \{E_k [E_k + 2N_0 V(k)]\}^{\frac{1}{2}} \quad (1.2.13.)A .$$

Inverting (1.2.10,11)A, i.e.

$$b_k = (\xi_k + L_k \xi_{-k}^+) / (1 - |L_k|^2)^{\frac{1}{2}} \quad (1.2.14.)A$$

$$b_k^+ = (\xi_k^+ + L_k^* \xi_{-k}) / (1 - |L_k|^2)^{\frac{1}{2}} \quad (1.2.15.)A ,$$

and inserting these relations into (1.2.8,9)A, the eqs. of motion for the new "elementary excitation" operators are obtained, namely

$$i\hbar \partial_t \xi_k = W_k \xi_k ; \quad -i\hbar \partial_t \xi_k^+ = W_k \xi_k^+ \quad (1.2.16.)A .$$

This Bogoljubov claims - together with the fact that ξ 's satisfy the same Bose commutation relations, implies that the excited states of an ensemble of atoms can be treated as a perfect gas of elementary excitations, with an excitation spectrum given by (1.2.13.)A and whose number distribution operator is given by:

$$\hat{n}_k = \xi_k \xi_k^+ \quad (1.2.17.)A .$$

Expression (1.2.13.)A is the celebrated Bogoljubov excitation spectrum. It is manifestly gapless and linear in the long-wave limit, in agreement with experimental evidence⁽⁵⁴⁾.

Bogoljubov goes on to point out (i) that the overall momentum of the ensemble of atoms is the same as the overall momentum of elementary excitations, even though (ii) the overall number of excitations is not invariant (but a function of temperature, $\beta \equiv 1/K_B T$, where K_B is Boltzmann's constant and T is the absolute temperature); accordingly, the average number of elementary excitations is given by

$$\bar{n}_k = \{A \exp \beta (W_k - \vec{k} \cdot \vec{u}) - 1\}^{-1} \quad (1.2.18.)A ,$$

where $A=1$ is a normalization constant. (iii) The positiveness of $\bar{\eta}_k$ entails that the modulus of the average velocity u has maximal critical value, i.e.

$$|u| \leq \min(W_k/|k|) \quad (1.2.19.)$$

The latter argument holds for a frame of reference at rest with the centre of mass of the whole system (condensate plus depletion). Selecting now another frame at rest with the elementary excitations - making up the depletion in this approximation - one finds that the condensate moves with velocity u . Bogoljubov then adds:

'This relative motion goes on stationarily in the state of statistical equilibrium without any external forces. Hence we see that it is not accompanied by friction and thus represents the property of superfluidity.'

The final part of Bogoljubov's classic paper is concerned with the evaluation of the condensate fraction and with the establishment of conditions, necessary to ensure the validity of his method. These important matters are, however, not relevant for the present work. It suffices to emphasise that the latter conditions require a lower density than that of real ^4He in typical experimental conditions, and also strong repulsive interactions. It is finally concluded by the author that while repulsive interactions enhance the condensed fraction; the existence of an attractive part in the potential, on the other hand, inhibits condensation.

Bogoljubov's simple microscopic theory has been commented on and analysed by very many authors, but a number of questions have not found a satisfactory answer. It is appropriate to comment upon some of these here.

The first criticism which can be raised concerns the actual population of the condensed mode. A theoretical estimate of the condensed fraction by Penrose and Onsager⁽⁵⁷⁾ gives about 10% and several analysis of inelastic

neutron scattering measurements⁽⁵⁴⁾ yield a rather smaller fraction of about 3%⁽⁴⁴⁾. It has even been argued⁽⁴⁴⁾ that the data are consistent with the complete *absence* of Bose-Einstein condensation. Also on the theoretical side Evans⁽²⁴⁾ has given an argument ruling out the existence of BEC within the hierarchy of self-consistent equations for the one-body propagator of the interacting system. More recently, however, Hyland, Rowlands and Cummings^(21a) have proposed a different method of measuring the condensate fraction; a number of experiments have been performed on such a basis yielding - again - a condensate fraction of a few percent (*).

The present situation as to the existence of an overwhelming condensate fraction is clear, ruling it out, and with it Bogoljubov's weakly excited state approximation. As to the occurrence of B.E.C. at all, however, there is no conclusive, uncontroversial, evidence. This state of things has moved workers in the field to develop self-consistent theories free from Bogoljubov's approximation, but yet displaying either simple or smeared condensation⁽³⁰⁾ of some form. Some of these approaches will be examined latter on in this section, but before that let us comment upon two other features of Bogoljubov's theory. One is Bogoljubov's derivation of the excitation spectrum and the other is the resort to Landau's criterion of superfluidity^(47b).

It has been noted repeatedly (1,18,20,29,32,36,40,43,45,46,50,60,62,66) that conservation of total number of atoms is *not* satisfied in Bogoljubov's work, due to both Bogoljubov's prescription (1.2.1.)A and the resort to elementary excitation operators associated with a representation of states such that the number operator $\hat{N} = \sum_k a_k^\dagger a_k$ is *not* diagonal. A discussion of this matter will be given later on in this section; for the present let us point out that the chemical potential (in a grand canonical ensemble formulation) or the Lagrange multiplier (in a canonical ensemble formulation)

(*) See references 1-5 of Ref. 21b.

are not present in Bogoljubov's work. On the other hand the rescaling of the time dependence of operators - given by relations (1.2.6,7)A - has the effect of removing the contribution E_0 from the square bracket of (1.2.5.)A yielding the square bracket of (1.2.8)A. Such a rescaling is the main reason why Bogoljubov's spectrum is gapless. In fact had it not been introduced, and the operator $\hat{H}' = \hat{H} - \mu \hat{N}$ used in the place of \hat{H} , the result obtained for W_k would be

$$W_k = \{(\epsilon_k - \mu + E_0)[\epsilon_k - \mu + E_0 + 2N_0 V(k)]\}^{\frac{1}{2}} \quad (1.2.20)A,$$

μ should be evaluated from the normalization condition fixing the average value of \hat{N} (in the G.C.E.), or from the auxiliary condition $\mu = \partial \hat{H} / \partial \hat{N}$ (in the C.E.), before anything can be said about the existence or not of a gap. It is noted, on the other hand, that gapless solution is obtained if μ takes the value

$$\mu = E_0 \equiv N_0 V(0) \quad (1.2.21)A,$$

which is the value obtained by Hugenholtz and Pines⁽⁴⁰⁾ for the chemical potential corresponding to Bogoljubov's approximation. The above result makes us feel, with Galaziewicz⁽²⁸⁾ and others⁽³⁶⁾, that even though the result obtained by Bogoljubov is essentially correct, the method by which it was produced is invalid.

Finally it is interesting to point out that it is not clear from Bogoljubov's work why and how an ensemble of condensed particles moving with velocity u are prevented from getting *disordered* by collisions with other condensed particles and elementary excitations. And in the last analysis - *if that is the case*, why not resort to a criterion stating this explicitly in the first place, instead of resorting to such an indirect criterion as Landau's, which is so dependent on the shape of the spectrum and therefore not directly applicable to other superfluids, such as bi-excitons⁽¹⁴⁾ for instance.

B. Valatin and Buttler's (V-B) Pairing Theory (1958)

The first self-consistent theory of the Bose superfluid was the pairing model of V-B⁽⁶⁸⁾, developed in close analogy to the theory of superconductivity⁽⁴⁾. The method proposed by these authors is also based on the introduction of collective variables - as in the case with Bogoljubov's work - but without introducing the same approximation, nor resorting to Bogoljubov's prescription (1.2.1.)A.

The starting point of this approach is the proposal of a *trial* representation of state amplitudes, whose ground state amplitude is formally defined as

$$|\phi_0\rangle = C \exp[\hat{A}] |0\rangle \quad (1.2.1.)B,$$

$$\hat{A} = \frac{1}{2} g_0 a_0^2 + \sum_k g_k a_k a_k \quad (1.2.2.)B^{(*)},$$

where $|0\rangle$ is the vacuum of the particle representation, i.e. the state of no particles. In the summation each pair is to be counted once. It is shown [see Ref. (67)] that Bogoljubov elementary excitation operators are the appropriate creation and annihilation operators for $|\phi_0\rangle$, i.e. ξ_k and ξ_k^+ defined as

$$\xi_k = (a_k - g_k a_{-k}^+) / (1 - g_k^2)^{\frac{1}{2}} \quad (1.2.3.)B$$

$$\xi_k^+ = (a_{-k}^+ - g_k a_k) / (1 - g_k^2)^{\frac{1}{2}} \quad (1.2.4.)B,$$

where $g_k = g_{-k}$, and satisfy

$$\xi_k^+ |\phi_0\rangle = 0;$$

an orthogonal set of states is obtained by operating successively with ξ_k on $|\phi_0\rangle$, i.e.

$$|\phi_{k_1 \dots k_j}\rangle = (m_{k_1}! \dots m_{k_j}!)^{-\frac{1}{2}} \xi_{k_1}^{m_{k_1}} \dots \xi_{k_j}^{m_{k_j}} |\phi_0\rangle \quad (1.2.5.)B$$

(*) It is noted that V-B denote creation & annihilation operators by a_k & a_k^+ respectively, i.e. differently from the current notation, where a_k^+ is the creation operator. Similarly for ξ 's

The only two differences from Bogoljubov's work with respect to the introduction of the variables ξ_k and ξ_k^+ are (i) that g_k is *real* (Γ_k in Ref (6) is a complex number) and (ii) that state amplitudes $|\phi\rangle$ are *explicitly introduced*. With the help of the inverse of (1.2.3,4)B the averages of all particle operators can be evaluated in the ground state $|\phi_0\rangle$ (or in any other excited state $|\phi_m\rangle$, for that matter). The ground state average of the number distribution, for instance, is given by

$$\langle \phi_0 | a_k a_k^\dagger | \phi_0 \rangle \equiv h_k = g_k^2 / (1 - g_k^2) \quad (1.2.6.)B ;$$

this is the average number of *particles* in the vacuum of *elementary excitations*, similarly the average for the pair operator is given by

$$\langle \phi_0 | a_k a_{-k} | \phi_0 \rangle \equiv x_k = g_k / (1 - g_k^2) \quad (1.2.7.)B$$

$$= \langle \phi_0 | a_k^\dagger a_k^\dagger | \phi_0 \rangle \quad (1.2.8.)B$$

$$= \{h_k(1+h_k)\}^{1/2} \quad (1.2.8.)B ;$$

$$(1.2.6,9)B \text{ entail } (1+2h_k)^2 - (2x_k)^2 = 1 \quad (1.2.10.)B .$$

It is noted by V-B that both the hamiltonian and particle number operators, \hat{H} and \hat{N} , can be written as $\hat{H}_0 + \hat{H}_1$ and $\hat{N}_0 + \hat{N}_1$, where \hat{H}_1 and \hat{N}_1 have vanishing expectation values over pair states (1.2.5.)B; hence the diagonal part $\hat{H}_0 - \lambda \hat{N}_0$ - where λ is the chemical potential - can be written as

$$\hat{H}_0 - \lambda \hat{N}_0 = W_0 + \sum_k \tilde{E}_k \eta_k + \sum_{k \neq k'} V_{kk'} \eta_k \eta_{k'} + F ,$$

where $\eta_k = \xi_k \xi_k^\dagger$ is the distribution number of elementary excitations and W_0 is the ground state energy given by

$$W_0 = \langle \phi_0 | \hat{H} | \phi_0 \rangle \quad (1.2.11.)B$$

$$= \frac{1}{2} \sum_k \{ (\epsilon_k - \lambda) h_k + h_k h_{-k} - \mu_k x_k \} \quad (1.2.12.)B .$$

(1.2.12.)B is the energy of the *particle* system in the vacuum of *elementary excitations*, where

$$\nu_k \equiv \epsilon_k - \lambda + \sum_{k'} [V(0) + V(k-k')] h_{k'} \quad (1.2.13.)B^{(*)}$$

and

$$\mu_k \equiv - \sum_{k'} V(k-k') x_{k'} \quad (1.2.14.)B$$

and F are fluctuations about mean field averages.

For the excitation energy \tilde{E}_k they obtain

$$\tilde{E}_k = \nu_k (1 + 2h_k) - \mu_k^2 x_k \quad (1.2.15.)B$$

As to the evaluation of the c-number field, g_k , involved in the definition of elementary excitation operators, V-B proceed differently from B, but obtain an equivalent result. g_k is determined in V-B's work from the condition that the ground state energy, W_0 , is minimal respect to variations of g_k ; this yields the following quadratic equation:

$$\mu_k g_k^2 - 2\nu_k g_k + \mu_k = 0 \quad (1.2.16.)B,$$

which is, in fact, an integral equation admitting the solution

$$g_k = (\nu_k - \omega_k) / \mu_k \quad (1.2.17.)B;$$

where

$$\omega_k = \{\nu_k^2 - \mu_k^2\}^{\frac{1}{2}} \quad (1.2.18.)B$$

Solution (1.2.17)B gives the following expression for h_k and x_k

$$h_k = \frac{1}{2} [(\nu_k / \omega_k) - 1] \quad (1.2.19.)B$$

$$x_k = \mu_k / 2\omega_k \quad (1.2.20.)B$$

The ground state energy and the excitation spectrum, then, become

$$W_0 = \frac{1}{2} \sum_k \{ (\epsilon_k - \lambda) h_k + \frac{1}{2} (\omega_k - \nu_k) \} \quad (1.2.21.)B$$

and

$$\tilde{E}_k = \omega_k \quad (1.2.22.)B,$$

(*) The volume dependence has been omitted and the Fourier transform of the interaction potential V_k is written as $V(K)$.

respectively. The integral equations for the Hartree-Fock energy, v_k , and the 'pairing energy', x_k , are obtained from (1.2.13,14.)B and (1.2.19, 20.)B and are given by

$$v_k = \bar{\epsilon}_k + h_0 V(k) + \frac{1}{2} \sum_{k'} V(k-k') v_{k'} / (v_k^2 - \mu_k^2)^{\frac{1}{2}} \quad (1.2.23.)B$$

$$\mu_k = x_0 V(k) - \frac{1}{2} \sum_{k'} V(k-k') \mu_{k'} / (v_k^2 - \mu_k^2)^{\frac{1}{2}} \quad (1.2.24.)B,$$

$$\text{where } \bar{\epsilon}_k \equiv \epsilon_k - \lambda + NV(0) - \frac{1}{2} \sum_{k'} V(k-k') \quad (1.2.25.)B ;$$

where the summations over k' exclude the contribution $k'=0$ which has been written separately.

Up to this point no assumption whatsoever has been introduced as to the occurrence of BEC. The chemical potential λ is determined from the condition $\omega_0=0$, i.e. the assumption of a gapless spectrum, and the condensate population from

$$N = N_0 + \sum_{k \neq 0} h_k .$$

It is argued that if in the infinite volume limit, a singularity occurs in h_k at $k=0$ yielding a finite condensate fraction - not necessarily large compared with the non-condensed fraction, there will be a non-trivial solution for μ_k due to the inhomogeneous contribution in (1.2.24.)B proportional to x_0 for predominantly repulsive interactions $\approx h_0$.

The latter conclusion has been critically examined by Kobe⁽⁴⁶⁾ who has shown that the treatment of the condensed mode as a special case of the pairing states leads to inconsistencies; in addition a trivial solution, $\mu=0$, is found for purely repulsive interactions. Let us comment, now, upon some *conceptual* features of the V-B approach which are particularly related with the main strategy of this thesis.

The V-B approach to superfluidity is perhaps the simplest of all self-consistent pairing models, and as such, is the best candidate for investigating

and commenting upon some deep conceptual propositions - other than those related to the involvement of Bose condensation - present in nearly all first principle approaches to superfluidity and also to superconductivity. These propositions are not always put explicitly, but rather introduced in an implicit fashion.

The first observation concerns a premise commonly employed involving quantum averages in two non-equivalent representations; particle and pair representation, for instance. It is often stated that some operators, such as the particle number and the particle hamiltonian operators, \hat{N} and \hat{H} have the same quantum average in their natural-particle representation as in the pair representation, i.e.

$$N = \langle n | \hat{N} | n \rangle = \langle \phi_m | \hat{N} | \phi_m \rangle \quad (I)$$

$$E = \langle n | \hat{H} | n \rangle = \langle \phi_m | \hat{H} | \phi_m \rangle \quad (II),$$

where $|n\rangle$ is a N-particle state and $|\phi_m\rangle$ is a pair state of m elementary excitations. (I,II) can be regarded to hold either for the ground state of the N-particle state, $|n_0\rangle$, and the ground state of the pair representation, $|\phi_{m,0}\rangle$ - which may or may not be the vacuum state $|\phi_0\rangle$ - or for every N-particle state and every pair state.

Propositions (I,II) are not both consequential statements; that is, are not both derived from other premises of a more general (or equivalent) logical status, but one is a *postulate* from which the other follows (or should follow, rather).

It might be thought that (I,II) are a consequence of the fact that the trace is invariant under cyclic permutation, and the fact that particle and pair states are related through a canonical transformation, $\tau_p^\dagger = \tau_p^{-1}$; that is

$$(N=) \text{Tr}(\hat{N}) = \text{Tr}(N_p \tau_p^{-1}) = \text{Tr}(\tau_p^{-1} N_p) ;$$

hence taking the trace over particle states one finds

$$\langle n | \hat{N} | n \rangle = \langle n | \tau_p^\dagger \hat{N} \tau_p | n \rangle = \langle \phi_m | \hat{N} | \phi_m \rangle \quad (I)$$

and similarly for \hat{H} and, in fact, for every operator.

On the other hand, however,

$$\begin{aligned} \text{Tr}(\hat{N}) &= \text{Tr}(\tau_p^{-1} \tau_p \hat{N} \tau_p^{-1} \tau_p) \\ &= \text{Tr}(\tau_p^{-1} \hat{\eta} \tau_p) \end{aligned}$$

where $\hat{\eta} \equiv \tau_p \hat{N} \tau_p^{-1} = \sum_k \xi_k \xi_k^\dagger$ is the operator for the number of elementary excitation. Taking now the traces over particle states one obtains

$$\langle n | \hat{N} | n \rangle = \langle \phi_m | \hat{\eta} | \phi_m \rangle \quad (III),$$

that is, the number of particles equals the number of excitations! It can be shown very simply that relations (I and II) are *incompatible* in the non-trivial case $\tau_p \neq \hat{1}$. In effect, from (1.2.3,4)B it follows that

$$\langle \phi_m | \hat{N} | \phi_m \rangle = \sum_k (1 - g_k^2)^{-1} [g_k^2 + (1 + g_k^2) \langle \phi_m | \xi_k \xi_k^\dagger | \phi_m \rangle];$$

$$\text{while } \langle \phi_m | \hat{\eta} | \phi_m \rangle = \sum_k \langle \phi_m | \xi_k \xi_k^\dagger | \phi_m \rangle,$$

hence (I,II) are consistent only if $g_k \equiv 0$ or $\tau_p \equiv \hat{1}$.

The above result is a general feature of two non-equivalent representations of quantum states. Nothing of the kind happens for equivalent representations. For the latter representations both sets of elementary operators differ by a multiplicative phase only, while for the former representations both sets of elementary operators differ by an additive contribution and/or a real factor, as is the case for particle operators and elementary excitation operators of the pair representation, see (1.2.3,4)B.

The dilemma can be paraphrased in terms of phase spaces, after normalizing the particle phase space $\Gamma_p \equiv \{a_k, a_k^\dagger\}$ and the phase space of elementary excitations $\Gamma_e \equiv \{\xi_k, \xi_k^\dagger\}$ to be number of particles and the number of excitations

respectively. While (III) entails that the volume of r_p is the same as the volume of r_e , (I) implies that the volume of r_p is different (larger) than that of r_e .

The dilemma is resolved by *postulating* that (I) *holds* - as is, in fact, done implicitly in most microscopic theories - and also postulating that (III) *does not* hold; for, a re-scaling of the volume of r_e is introduced to satisfy (I). Consequently, pair states are normalized so as to satisfy (I).

As to the relation involving the hamiltonian, it will become clear later that (II) needs not to be postulated in addition, but it can be obtained as a consequence of (I). As a matter of fact (II) *must* be derivable from (I), for there is only one elementary excitation phase space to normalize. Should that not be the case, i.e. $\langle n | \hat{H} | n \rangle \neq \langle \phi_m | \hat{H} | \phi_m \rangle$, one would conclude that pair states are good to give average number but not average energy and such states should then have to be abandoned. The same argument holds for all other *constants of motion*.

Now, as to any particle operator, other than the constants of motion, the averages over particle and pair states need not be the same, there being no physical reason why they should; as a matter of fact they are *not* the same. The pair of particle operator $a_k a_{-k}$, for instance, has zero average over particle states, but finite average, x_k , over pair states. Should these averages be the same, i.e. zero, then - again - one must have $g_k = 0$.

Summarizing, proposition (I) is a postulate, (II) is (or should be) a consequence of (I).

Another premise implicit in all microscopic theories of superfluidity - and of superconductivity for that matter - is that the introduction of elementary excitation operators of the pair representation, or any other coherent state representation (non-equivalent to the particle representation^(*)) is nothing more than a change to "normal mode" variables - a practical tool

(*) Two representations related by canonical transformations are non-equivalent if their number operators do not commute.

for readily achieving diagonalization, but which does not affect the (hamiltonian) formulation of dynamics, in the sense that the constants of motion are considered to be the same functionals but in terms of different variables.

The energy and number functionals, for instance, are regarded to be \hat{H} and \hat{N} either in terms of a 's or ξ 's. In the particular case of ${}^4\text{He}$ $\hat{H}(a^+, a)$ and $\hat{N}(a^+, a)$ commute. After replacing particle by elementary excitation operators, however, and introducing the diagonalization condition (either explicitly, as in B's work, or through the minimal ground state energy condition, as in the present approach of V-B) the *remaining* part of $\hat{H}(\xi^+, \xi)$ and \hat{N} no longer commute; in fact, \hat{N} is non-diagonal in the pair representation, but \hat{H} has been 'successfully' diagonalized.

This feature is referred to as 'breakdown of the gauge invariance'. It is generally believed to be an inherent feature arising from the involvement of non-equivalent representations of the particle representation, such as the pair representation. As a consequence of this, one is led to the conclusion that the number of particles, whose quantum average could be measured with an error of 'less than one particle' (say, for a unique system, not an ensemble of systems) in the normal phase (described by particle states) cannot be accurately measured in the superfluid phase (described, say, by pair states).

The reason why a breakdown of symmetry is brought about in the successful event of the particle hamiltonian being diagonalizable in the pair representation, for instance, (or any other non-equivalent representation of the particle picture) is that no similar cancellation of the non-diagonal part of \hat{N} is introduced.

The overall breakdown of the gauge symmetry^(*) is quite an unsatisfactory

(*) here we are not considering a massless boson carrying away the lost gauge symmetry

conceptual feature of nearly all microscopic theories of superfluidity (with the exception of that by Girardeau and Arnowitt to be considered shortly). The difficulty is not diminished by the fact that one should, in fact, consider an ensemble of identical systems involving a large number of replicas; in this condition one is bound to get normal deviations - of order $N^{-1/2}$ - about the mean average number. For, even if the deviations of quantum origin are of the order of the statistical deviations and negligible in the infinite number of particles, the conceptual difficulty remains (as 'large' as before). Disqualifying the trouble can never resolve it.

This conceptually big (but practically small) trouble will be finally and conclusively resolved in this thesis. It will be shown that the spurious breakdown of the gauge symmetry is just but the tip of the iceberg, the remainder of which will be exposed later on. For now it suffices to point out that the paradox arises from the erroneous assumption that the hamiltonian and number functionals have the same expressions irrespective of the variables employed.

Let us now turn to comment upon an even bigger conceptual difficulty shared by most existing microscopic theories of superfluidity (5,6,18,20, 22,23,29,35,40,51,55,60,62,65,59,68,70,73)≡(REF) (and of superconductivity (4, 34)), which threatens the very foundations of their whole theoretical construct. This difficulty, which is very simply expressed within the present simple framework of V-B's approach, concerns the supposed origin of superfluidity itself.

Nothing in the results quoted so far permits any conclusion to be drawn as to whether the system under consideration in fact behaves as a superfluid. As a matter of fact no reference to an *ensemble* of pair states describing a collection of elementary excitations in thermal equilibrium has been introduced. The statistical considerations in V-B's paper are relegated to a final brief section, as these follow fairly closely the same lines as the

superconducting case, developed in more detail in a previous paper by Valatin⁽⁶⁷⁾. These considerations seemingly give a clear idea of how superfluidity comes about, which is shared by nearly all subsequent approaches to superfluidity from microscopic principles (REF).

The statistical operator associated with an ensemble of states of the pair representation in thermal equilibrium at low temperature T is regarded by V-B to be given by

$$\hat{U}_0 = C_0^{-1} \sum_{j=0}^{\infty} \sum_{k_1 \leq \dots \leq k_j} \omega_{k_1} \dots \omega_{k_j} P_{k_1 \dots k_j} \quad (1.2.26.)B.$$

$P_{k_1 \dots k_j}$ is the projection operator of a pair state occupied by elementary excitations in modes k_1, \dots, k_j ; $\omega_{k_1}, \dots, \omega_{k_j}$ are the statistical weights corresponding to a Grand Canonical Ensemble, as yet unspecified. C_0^{-1} is a normalization constant introduced to satisfy $\text{Tr}\{\hat{U}_0\} = 1$, and given by

$$\begin{aligned} C_0 &= \text{Tr} \left\{ \sum_{j=0}^{\infty} \sum_{k_1 \leq \dots \leq k_j} \omega_{k_1} \dots \omega_{k_j} P_{k_1 \dots k_j} \right\} \\ &= \prod_k (1 - \omega_k)^{-1} \end{aligned} \quad (1.2.27.)B.$$

The sub index (o) denotes that at low temperature the elementary excitations are 'nearly' free; hence \hat{U}_0 is an approximation to the exact statistical operator for strongly interacting excitations.

The ensemble average of the excitations (called by them "phonons" due to the fact that they believed the spectrum \bar{E}_k to be gapless and linear) is

$$\langle n_k \rangle_{\text{Th}} = \text{Tr} \{ \eta_k \hat{U}_0 \} = \omega_k (1 - \omega_k)^{-1} \equiv f_k \quad (1.2.28.)B,$$

where f_k is to be determined from the condition that the free energy is minimal respect to variations of f_k . The free energy is given by

$$F_0 = W_0^{(T)} - TS_0 \quad (1.2.29.)B,$$

where $W_0^{(T)}$ is the internal energy obtained as the quantum and statistical average of H , a function of f_k and of the c-number g_k . The entropy is taken to be

$$S_0 = -k_B^{-1} \sum_k [f_k \log f_k - (1+f_k) \log(1+f_k)] \quad (1.2.30.)B.$$

The expression above for the entropy is the usual expression for an ensemble of bosons, for which the only configuration is f_k (48), obtained from purely combinational considerations. The entropy is independent of the family of c-number functions g_k , so these c-numbers do not contribute to the disorder; they do, however, contribute to the total number of particles, thus:

$$\langle \hat{N} \rangle_{Th} = \sum_k (1-g_k^2)^{-1} [g_k^2 + (1+g_k^2)f_k] \quad (1.2.31.)B,$$

i.e. not only through an additive contribution, but also through a factor in the remaining part. Hence, it seems clear that such a system is a superfluid since a fraction of the total average number of particles does not contribute to the entropy, i.e. is fully ordered. Thus, by construction, the above ensemble describes a superfluid.

Minimizing the free energy (or equivalently, $W_0(T)$) with respect to g_k the diagonalization condition is brought about at ensemble level. In addition, minimizing F_0 respect to f_k , the following solution is obtained:

$$f_k = (\exp \beta \tilde{E}_k^{(T)} - 1)^{-1} \quad (1.2.32.)B;$$

whence ω_k is given - via (1.2.28.)B - by

$$\omega_k = \exp(-\beta \tilde{E}_k^{(T)}) \quad (1.2.33.)B,$$

$$\text{with } \tilde{E}_k^{(T)} = \frac{\partial W_0^{(T)}}{\partial f_k} = v_k^{(T)} (1+2h_k) - \mu_k^{(T)} 2x_k \quad (1.2.34.)B$$

The origin of superfluidity is now clear - well, almost clear. The trouble with the above mechanism for superfluid behaviour is rather subtle, but demolishing. The superfluid phase is characterized by the existence of an *order parameter* associated with a finite fraction of the total average number of particles. But $g_k^2/(1-g_k^2)$ cannot be an order parameter. For, if it was it should have to be included into the ensemble configurations - if not as an independent additive configuration, then at least as a factor of a generic configuration - which is not the case for V-B. In fact the expression (1.2.30.)B for the entropy corresponds to an ensemble for which the *only* configurations are configurations of elementary excitations.

In consequence relation (1.2.31.)B cannot be read as: "A fraction of the ensemble of particles is fully ordered" - as was advanced before, but instead must be read as: "The ensemble average distribution of elementary excitations times some quantity $[(g_k^2+1)/(1-g_k^2)]$ plus some quantity $[g_k^2/(1-g_k^2)]$ is normalized to the total number of particles". This only points out at the fact that the volume of the phase space $\Gamma_e = \{\xi_k^+, \xi_k\}$, namely $\text{Vol}(\Gamma_e) = \text{Tr}\{\xi_k^+ \xi_k\}$, is different (smaller) than the volume of $\Gamma_p = \{a_k^+, a_k\}$, namely $\text{Vol}(\Gamma_p) = \text{Tr}\{a_k^+ a_k\} = N$, and *not* to the existence of an ordered part in the ensemble of elementary excitations, which is the only one involved here. So the physical system described above *is not a superfluid*.

N.B.: No new information is given in the following paragraphs (C) to (I); these are included here only for the sake of completeness, as these approaches involve either conceptual elements, methods or arguments which are either employed or criticized in this thesis. The specialized reader may well by-pass them and continue in section 1.3. without loss of continuity. The non-specialist reader, however, may find this further review helpful to appreciate the novel approach contained in this work.

C. Girardeau and Arnowitt's (G-A) Pair Theory (1959)

The theory proposed by G-A⁽²⁹⁾ starts by recognizing the fact that states of the pair representation introduced by B and V-B are not eigenstates of the number operator \hat{N} . They regard this as a *defect*, which - on the other hand - can be easily remedied. They find that B's elementary excitation operators ξ_k^+ and ξ_k can be obtained by canonical transformation from particle operators, i.e.

$$\xi_k^+ = U_B a_k^+ U_B^{-1} \quad (1.2.1.)C$$

$$\xi_k = U_B a_k U_B^{-1} \quad (1.2.2.)C$$

where

$$U_B = \exp\left[\frac{1}{2} \sum_{k \neq 0} (a_{k-k}^+ a_{-k} - a_{k-k} a_{-k}^+) \tanh^{-1} L_k\right] \quad (1.2.3.)C,$$

and propose new elementary excitation operators - also related to particle operators by a canonical transformation U - whose natural states are exact eigenstates of \hat{N} and which are given by

$$\xi_{k(G-A)}^+ = U a_k^+ U^{-1} \quad (1.2.4.)C$$

$$\xi_{k(G-A)} = U a_k U^{-1} \quad (1.2.5.)C,$$

and the ground state by

$$|\phi(G-A)\rangle = U|n\rangle \quad (1.2.6.)C,$$

where U is given by

$$U \equiv \exp\left[\frac{1}{2} \sum_{k \neq 0} \psi(k) (\beta_0^{-1} a_{k-k} a_{-k} - \beta_0 a_{k-k}^+ a_{-k}^+)\right] \quad (1.2.7.)C.$$

$\psi(k)$ is a real and even c-number function of k , to be determined by the variational principle - as in the case of V-B, and β_0 is an unitary operator defined by

$$\beta_0^{\frac{1}{2}} = a_0 N_0^{-\frac{1}{2}}, \quad \beta_0^{-\frac{1}{2}} = \hat{N}_0^{-\frac{1}{2}} a_0^+ = (\beta_0^{\frac{1}{2}})^+ \quad (1.2.8.)C,$$

satisfying the following properties

$$\begin{aligned}
 \beta_0 |n\rangle &= |n-2\rangle \quad (n>2) \\
 \beta_0^+ |n\rangle &= \beta_0^{-1} |n\rangle = |n+2\rangle \\
 [\beta_0, N_0] &= 2\beta_0, [\beta_0^{-1}, N_0] = 2\beta_0^{-1} \\
 [\beta_0, a_k] &= [\beta_0, a_k^+] = 0 \text{ for } k \neq 0
 \end{aligned}
 \tag{1.2.9.)C}$$

The resort to a representation of states such as (1.2.4-6)C is *necessary* - they argue - since total number and total linear momentum must be conserved in the many boson problem and *must be good quantum numbers*.

G-A consider a pair hamiltonian, \hat{H}_p , given by the segment of the full hamiltonian \hat{H} [as given by (1.2.3.)A] giving finite average over states $|\phi(G-A)\rangle$, but like Bogoljubov do not introduce the chemical potential (or a lagrange multiplier, for that matter). They then work out the ground state energy

$$E_0 \equiv \langle \phi_0(G-A) | \hat{H}_p | \phi_0(G-A) \rangle \tag{1.2.10.)C}$$

by replacing particle operators in \hat{H}_p by $\xi_k^+(G-A)$ and $\xi_k(G-A)$ and making use of normal ordering properties, and going to the thermodynamic limit $n \rightarrow \infty$, $\text{vol} \rightarrow \infty$, $n/\text{vol} = \rho(\text{finite})$.

The relationship between particle and G-A's elementary excitations resembles very much relations (1.2.10,11)A and (1.2.3,4.)B; for the annihilation operator this relation is

$$\xi_k(G-A) = (a_{k-\phi(k)} \beta_0 a_{-k}^+) / (1 - \phi^2(k))^{1/2} \tag{1.2.11.)C}$$

$$\text{where } \phi(k) = \tanh \psi(k) \tag{1.2.12.)C}.$$

The ground state energy is the same function of ϕ as V-B's is of g_k , except for the fact that the chemical potential is now absent and that summations over wave vector are replaced by integrals appropriate to the infinite volume limit. The function $\phi(k)$ is determined by minimizing E_0 respect to $\phi(k)$. This leads to a quadratic equation whose solution is an

integral equation for $\phi(k)$, for which they find limiting solutions as $k \rightarrow 0$ and $k \rightarrow \infty$.

The energy of excited states is then evaluated in the usual way and in particular, its limiting behaviour as $k \rightarrow 0$ and $k \rightarrow \infty$; the former is given by

$$\omega_k^{(G-A)}|_{k \rightarrow 0} = 2\epsilon^{\frac{1}{2}}\rho_0 V(0) + O(k) \quad (1.2.13.)C$$

where $\epsilon \equiv I_1(0)/\rho_0 V(0)$ (1.2.14.)C,

$$I_1(0) \equiv (2\pi)^{-3} \int V(k) [\phi(k)/(1-\phi^2(k))] d^3k \quad (1.2.15.)C$$

$$\rho_0 \equiv \rho - (2\pi)^{-3} \int [\phi^2(k)/(1-\phi^2(k))] d^3k \quad (1.2.16.)C$$

and ρ is the total density.

For $k \rightarrow 0$ the excitation spectrum $\omega_k^{(G-A)}$ (1.2.13.)C exhibits a gap proportional to the condensate density ρ_0 . However, as in the case of Bogoljubov's work the chemical potential was not introduced, and even though the G-A state amplitudes are exact eigenstates of the total number operator the eigenvalues correspond to precise but *unspecified* number of particles. Some condition must thus be brought in to discard all eigenstates associated which particle numbers different from the *real* total number N - in the canonical ensemble; alternatively, a normalization condition must be included involving the chemical potential to ensure that the ensemble of states with different number of particles yield the correct ensemble average number $\langle N \rangle_{Th} = N$. In either case a further unknown, μ , and a further condition (involving μ) must be introduced before any conclusive result as to the spectrum can be reached.

G-A consider the unphysical result (1.2.13.)C as a *defect* of the pair approximation and suggest that an improved trial representations of states involving clusters of three particles might perhaps resolve the difficulty; a calculation by Takano⁽⁶²⁾ confirms this.

The strategy of G-A as to this problem offers an opportunity to comment again on the question of conservation of number. These authors argue - with reason - that total number must be rigorously conserved in the superfluid phase provided it is conserved in the normal phase - as it is, in view of the fact that the exact hamiltonian \hat{H} commutes with the total number operator \hat{N} . It is questionable, however, whether in order to satisfy this property it is *necessary* to describe the dynamical behaviour in terms of a representation of states which are eigenstates of \hat{N} .

The fact that the resort to a set of eigenstates of \hat{N} for the purpose of describing the dynamical behaviour of ^4He is *not* necessary for number conservation, is proven in §3.1 by means of a counter example. The general idea is that the constants of motion (associated with the energy and number of particles, say) required for a formulation of the dynamical problem in terms of a representation of states non-equivalent to the particle representation (V-B's pair representation, for instance) are *not* \hat{H} and \hat{N} , as in the particle representation formulation, but are *different* functionals \hat{H}' and \hat{N}' . As it turns out \hat{H}' and \hat{N}' are time independent, commute^(*) and are diagonal in the new representation of states; the pair states, say, then need *not* be eigenstates of \hat{N} but of \hat{N}' .

D. Hugenholtz and Pines' (H-P) Field Theoretic Approach (1959)

The problem of interacting bosons at zero temperature was first studied by Beliaev⁽⁵⁾ using perturbation techniques based on a 'S' matrix formalism, to take into account the depletion effect rigorously. Shortly after H-P⁽⁴⁰⁾ applied the Green's function method to calculate the zero temperature properties of a low-density boson gas, obtaining essentially the same results.

It is recalled that the interest of this thesis is in reformulating the many boson problem - originally posed in terms of the fields of the particle representation - in terms of a non-equivalent representation⁽³⁾ and to propose a physically meaningful self-consistent approximation. Our interest

(*) both properties may not necessarily be equivalent.

in field theoretic calculations is thus marginal, and for this reason only the latter work is briefly examined; for it is simpler and conceptually more transparent than Beliaev's. Our main interests in H-P's work is in connection with their treatment of the condensed mode and on the elements that eventually led them to the evaluation of the chemical potential and to the conclusion that the excitation spectrum is gapless.

H-P start by noting that the ground state for the non-interacting Bose system is not a 'good vacuum' with respect to the operators a_0^+ and a_0 , unlike for the Fermi system. For the latter system the non-interacting ground state is such that no particle (hole) can be annihilated above (below) the Fermi level. For bosons, on the other hand, particles and holes can always be annihilated from the fully condensed mode ($k=0$). i.e. $a_0|n\rangle_{gr} \neq 0$, $a_0^+|n\rangle_{gr} \neq 0$, for there is no upper limit to the occupancy of any mode.

The above feature - these authors argue - renders invalid the Goldstone linked cluster theorem^(33a) in the sense that the various disconnected diagrams cannot be expressed in terms of their connected counterparts, (in the infinite volume and number limit) except in the extremely low density limit - that is, within Bogoljubov's approximation. But the presence of a large depletion population at higher density spoils the validity of both Bogoljubov's approximation and the Goldstone theorem.

As to the elimination of the condensed mode from the dynamical problem, H-P proceed as follows. They first replace $a_0^+\Omega^{-1/2}$ and $a_0\Omega^{-1/2}$ by $n_0^{1/2}$, where Ω is the volume. The resulting hamiltonian $\hat{H}(n_0)$ does not commute with $\sum_{k \neq 0} a_k^+ a_k$ (though the commutator is of order Ω^{-1}). They thus consider the problem of finding the eigenvalue of $\hat{H}(n_0)$ subject to the subsidiary condition $\langle N' \rangle = N - n_0 \Omega$ (1.2.1.)D, or alternatively the problem posed by Hamiltonian $\hat{H}^*(n_0) = \hat{H}(n_0) - \mu \hat{N}$ (1.2.2.)D without any further condition, where n_0 is to be determined as to minimize the ground state energy, i.e.

$$\frac{d}{dn_0} \left(\frac{E_0}{\Omega} \right) = 0 \quad (1.2.3.)D$$

The ground state $|\psi_0(n_0, \mu)\rangle$ and the ground state expectation values of \hat{H} and \hat{N} , namely $E_0(n_0, \mu)$ and $N(n_0, \mu)$ depend upon μ , which is determined from (1.2.1.)D

$$n(n_0, \mu) = n - n_0 \quad (1.2.4.)D.$$

This gives, in turn, an expression for μ as a function of n_0 for a given density n .

E. Luban (L) (1962) Thermodynamically Equivalent Hamiltonian Method

The model developed by L⁽⁵¹⁾ in great mathematical detail is based on a method proposed by Wentzel⁽⁷⁰⁾, known as the thermodynamically equivalent hamiltonian method, successfully applied by the latter author to the theories of superfluidity and superconductivity.

The main feature of this method is that the thermodynamic properties derived from the free energy - obtained from a *four linear* segment of the full hamiltonian^(*) - are the same as derived from a different but thermodynamically equivalent free energy functional, obtained from a *quadratic* hamiltonian⁽⁷⁰⁾. The latter hamiltonian can easily be diagonalized - again, by resorting to elementary operators of the pair representation, leading to a solvable model, though the solutions are often not unique.

The hamiltonian segment, \hat{H}_p , considered by L (and Wentzel) is the so called pair hamiltonian, obtained by neglecting from the full hamiltonian (1.2.3)A all interactions; except for direct, indirect and pair scattering terms associated with the contributions $l=0$, $p+l=q$ and $p=-q$, respectively. The general idea of the method is as follows;

(i) Introduce first new operators B_{k1} and B_{k2} defined as

$$B_{k1} \equiv a_k^\dagger a_k - \epsilon_k \quad (1.2.1.)E$$

$$B_{k2} \equiv a_{-k} a_k - \eta_k \quad (1.2.2.)E,$$

where ϵ_k and η_k are *real* c-number functions.

(*) namely, the pair hamiltonian

(ii) Express \hat{H}_p as

$$\hat{H}_p = \hat{H}^0 + \hat{H}' \quad (1.2.3.)E,$$

where

$$\hat{H}^0 \equiv \hat{U} + \sum_k [f_k a_{k,k}^+ a_{k,k} + \frac{1}{2} h_k (a_{k,k}^+ a_{-k,k}^+ + a_{k,k} a_{-k,k})] \quad (1.2.4.)E;$$

and \hat{U} , f_k and h_k are defined as

$$\begin{aligned} \hat{U} \equiv & -(2V)^{-1} V(0) \sum_{k,p} \xi_k \xi_p - (2V)^{-1} \sum_{k,p \neq \pm k} V(p-k) \xi_k \xi_p \\ & - (2V)^{-1} \sum_{k,p \neq k} V(p-k) \eta_k \eta_p \end{aligned} \quad (1.2.5.)E,$$

$$\begin{aligned} f_k \equiv & \left(\frac{\hbar^2}{2m} \right) k^2 - \mu + V^{-1} V(0) \left[\left(\sum_p \xi_p \right) - \frac{1}{2} \right] + \\ & + V^{-1} \sum_{p \neq \pm k} V(p-k) \xi_p \end{aligned} \quad (1.2.6.)E,$$

$$h_k \equiv V^{-1} \sum_{p \neq k} V(p-k) \eta_k \quad (1.2.7.)E,$$

where V is the volume and $\hat{H}' = \hat{H}_p - \hat{H}^0$ (1.2.8.)E.

The thermodynamic potentials (free energy functionals) associated with \hat{H}^0 and \hat{H}_p are

$$\Omega^0 = -\beta^{-1} \ln \text{Tr} \{ \exp(-\beta \hat{H}^0) \} \quad (1.2.9.)E$$

$$\text{and} \quad \Omega_p = -\beta^{-1} \ln \text{Tr} \{ \exp(-\beta \hat{H}_p) \} \quad (1.2.10.)E,$$

respectively.

(iii) In the infinite volume limit ($V \rightarrow \infty$, $N \rightarrow \infty$, $N/V = \rho$ finite) Wentzel has shown that the thermodynamic properties of Ω_p are given by Ω^0 alone, provided that ξ_k and η_k are chosen to satisfy

$$\partial \Omega^0 / \partial \xi_k = \partial \Omega^0 / \partial \eta_k = 0 \quad (1.2.11.)E,$$

or equivalently if

$$\xi_k = \langle a_k^\dagger a_k \rangle \quad (1.2.12.)E$$

$$\eta_k = \langle a_k^\dagger a_{-k} \rangle \quad (1.2.13.)E,$$

where the symbol $\langle \dots \rangle$ stands for quantum and thermal average.

The power of this method is notable, for it reduces the statistical mechanics of (certain) non-linear problems to that corresponding to a linear problem.

Hamiltonian \hat{H}^0 is brought to a diagonal form by introducing Bogoljubov-Valatin-Buttler elementary excitation operators (denoted here by α_k^\dagger and α_k)

$$\left. \begin{aligned} a_k &= u_k \alpha_k + v_k \alpha_{-k}^\dagger \\ a_k^\dagger &= u_k \alpha_k^\dagger + v_k \alpha_{-k} \end{aligned} \right\} \quad (1.2.14.)E,$$

for real c-numbers u_k, v_k satisfying

$$u_k^2 - v_k^2 = 1 \quad (1.2.15.)E,$$

so that α 's are also Bose operators. These c-numbers are determined by the diagonalization condition

$$f_k u_k v_k + \frac{1}{2} h_k (u_k^2 + v_k^2) = 0 \quad (1.2.16.)E,$$

which has the solution

$$\left. \begin{aligned} u_k^2 &= \frac{1}{2} [(f_k/\epsilon_k) + 1] \\ v_k^2 &= \frac{1}{2} [(f_k/\epsilon_k) - 1] \end{aligned} \right\} \quad (1.2.17.)E,$$

$$\text{where } \epsilon_k = (f_k^2 - h_k^2)^{\frac{1}{2}} \quad (1.2.18.)E.$$

In consequence \hat{H}^0 becomes

$$\hat{H}^0 = \hat{U}^0 + \sum_k \epsilon_k \alpha_k^\dagger \alpha_k \quad (1.2.19.)E,$$

where

or equivalently if

$$\epsilon_k = \langle a_k^\dagger a_k \rangle \quad (1.2.12.)E$$

$$n_k = \langle a_k^\dagger a_{-k} \rangle \quad (1.2.13.)E,$$

where the symbol $\langle \dots \rangle$ stands for quantum *and* thermal average.

The power of this method is notable, for it reduces the statistical mechanics of (certain) non-linear problems to that corresponding to a linear problem.

Hamiltonian \hat{H}^0 is brought to a diagonal form by introducing Bogoljubov-Valatin-Buttler elementary excitation operators (denoted here by α_k^\dagger and α_k)

$$\left. \begin{aligned} a_k &= u_k \alpha_k + v_k \alpha_{-k}^\dagger \\ a_k^\dagger &= u_k \alpha_k^\dagger + v_k \alpha_{-k} \end{aligned} \right\} \quad (1.2.14.)E,$$

for *real* c-numbers u_k, v_k satisfying

$$u_k^2 - v_k^2 = 1 \quad (1.2.15.)E,$$

so that α 's are also Bose operators. These c-numbers are determined by the diagonalization condition

$$f_k u_k v_k + \frac{1}{2} h_k (u_k^2 + v_k^2) = 0 \quad (1.2.16.)E,$$

which has the solution

$$\left. \begin{aligned} u_k^2 &= \frac{1}{2} [(f_k/\epsilon_k) + 1] \\ v_k^2 &= \frac{1}{2} [(f_k/\epsilon_k) - 1] \end{aligned} \right\} \quad (1.2.17.)E,$$

$$\text{where } \epsilon_k = (f_k^2 - h_k^2)^{\frac{1}{2}} \quad (1.2.18.)E.$$

In consequence \hat{H}^0 becomes

$$\hat{H}^0 = \hat{U}^0 + \sum_k \epsilon_k \alpha_k^\dagger \alpha_k \quad (1.2.19.)E,$$

where

$$\hat{U}^0 \equiv \hat{U} + \frac{1}{2} \sum_k (\epsilon_k - f_k) \quad (1.2.20.)E.$$

Hence the free energy Ω^0 becomes

$$\Omega^0 = U^0 + \beta^{-1} \sum_k \ln[1 - \exp(-\beta \epsilon_k)] \quad (1.2.21.)E^{(*)}$$

From this thermodynamic potential it follows that the average number of excitations is given by the well-known relation

$$\langle \alpha_k^* \alpha_k \rangle = [\exp(\beta \epsilon_k) - 1]^{-1} \quad (1.2.22.)E.$$

Similarly using (1.2.12 -17) he finds that

$$\xi_k = \frac{1}{2} [(f_k/\epsilon_k) \coth(\frac{1}{2} \beta \epsilon_k) - 1] \quad (1.2.23.)E$$

$$\eta_k = -\frac{1}{2} (h_k/\epsilon_k) \coth(\frac{1}{2} \beta \epsilon_k) \quad (1.2.24.)E ;$$

or from (1.2.6,7)E he finally obtains the coupled set of integral equations characterizing this model, namely

$$f_k = \left(\frac{\hbar^2}{2m} \right) k^2 - \mu + \rho V(0) + V^{-1} \xi_0 V(k) + \\ + (2V)^{-1} \sum_{p \neq 0} V(p-k) [(f_p/\epsilon_p) \coth(\frac{1}{2} \beta \epsilon_p) - 1] \quad (1.2.25.)E,$$

and

$$h_k = V^{-1} \eta_0 V(k) - (2V)^{-1} \sum_{p \neq 0} V(p-k) (h_p/\epsilon_p) \coth(\frac{1}{2} \beta \epsilon_p) \quad (1.2.26.)E,$$

$$f_0 = -\mu + \rho V(0) + (2V)^{-1} \sum_{p \neq 0} V(p) [(f_p/\epsilon_p) \coth(\frac{1}{2} \beta \epsilon_p) - 1] \quad (1.2.27.)E,$$

$$h_0 = -(2V)^{-1} \sum_{p \neq 0} V(p) (h_p/\epsilon_p) \coth(\frac{1}{2} \beta \epsilon_p) \quad (1.2.28.)E.$$

This set of equations is completed by the normalization condition

$$\rho = (\xi_0/V) + (2V)^{-1} \sum_{k \neq 0} (f_k/\epsilon_k) [\coth(\frac{1}{2} \beta \epsilon_k) - 1] \quad (1.2.29.)E.$$

(*) It is noted that the *only* configurations considered to construct such an ensemble are the various distributions of elementary excitations, c-number distributions *not* being taken into account, as in V-B's work.

The main concern of this author was in deriving the above set of equations and to *search for a solution of it*. Our concern however - as mentioned before - is *not* with the actual solution of a corresponding set of equations - to be found in §4.4 - but rather in elucidating some conceptual matters concerning the formulation of the many body problem itself. For the purpose of comparison the information already quoted from L's work suffices; however, it is interesting to summarize briefly the main conclusions of this work, which is one of the most complete and elegant in the field of ^4He models.

Firstly L shows that for a positive definite excitation spectrum ϵ_k , equation (1.2.26.)E admits the trivial solution $h_k \equiv 0$ for temperatures $T > T_c$. At some temperature $T \leq T_c$ the subsidiary condition is no longer satisfied. Secondly, if the kernel, J , of the integral equation for h_k has only positive eigenvalues- i.e. is a J_+ kernel in L's notation

$$\text{i.e.} \quad \int_0^\infty dp \int_0^\infty dk \theta(k) J(k,p) \theta(p) > 0 ,$$

$$\text{where} \quad \theta(k) \equiv k^2 (h_k / \epsilon_k) \coth(\frac{1}{2} \beta \epsilon_k) ,$$

$$\text{and} \quad J(k,p) = (8\pi^2)^{-1} \int_{-1}^{+1} ds V[(k^2 + p^2 - 2kps)^2] -$$

then the only solution for (1.2.26.)E is $h_k \equiv 0$; hence the hypothesis of $\epsilon_k > 0$ is untenable i.e. ϵ_k must have a zero (at $k=0$). He illustrates his idea by showing that a Lee, Huang and Yang hard sphere pseudopotential and a V-B separable potential both yield a zero in ϵ_k .

Thirdly, B.E.C. is shown to take place for temperatures $T \leq T_c$ if $\epsilon_0 = 0$ for J_+ kernels. This leads him to the conclusion that Bogolubov's approximation is valid (for the pair hamiltonian) for $T < T_c$. Fourthly, in the limit $k \rightarrow 0$ the excitation spectrum does *not* tend to zero, but to $[4SV(0)(f_0 + 0(k^2))]^{\frac{1}{2}}$ where S is the condensate density, i.e. $\lim_{k \rightarrow 0} \epsilon_k \neq \epsilon_0 = 0$, but is separated by a gap of the same magnitude as that of G-A. The

remaining part of Luban's paper is concerned with the resolution of the system of integral equations below and above the transition temperature, characterized by the onset of B.E.C., and with the evaluation of thermodynamic quantities. These - Luban admits - do not resemble the real experimental curves. He concluded by wondering whether the lambda transition can be explained on the basis of an independent excitation description.

F. Etters (E) (1966) Hierachy of Linear Equations of Motion

The work of E⁽²²⁾ on the many boson problem is based upon a generalization of the standard Random Phase approximation due to Suhl and Werthamer⁽⁶¹⁾.

The strategy underlying this method consists in devising an iterative procedure leading to a transformation of variables, i.e. from particle variables a_k^+, a_k to some others b_k^+, b_k satisfying the *same* commutation relations; such that the equations of motion are linear; that is

$$[H, b_k^+] = \omega_k b_k^+ \quad (1.2.1.)F$$

The canonical equation (1.2.1.)F corresponds to a stationary state $b_k^+(t) = b_k^+(0) \exp(i\omega_k t/\hbar)$ and makes reference to a set of states $\{|s\rangle\}$ for which b^+ and b are creation and annihilation operators, and which possess a good vacuum; i.e. $b_k|0\rangle = 0$ for all k .

Eq. (1.2.1.)F is, in fact, never satisfied⁽⁶¹⁾. The problem is to devise a suitable succession of operators $b_k^{+(i)}$, $b_k^{(i)}$ such that (1.2.1.)F is approximately satisfied to an increasing degree of accuracy.

For the zeroth order approximation one can take single particle operators, i.e. $b_k^{+(0)} \equiv a_k^+$, $|s\rangle^0 \equiv |n\rangle$; the zeroth order equation is then

$$\begin{aligned} [H, a_p^+] &= [T_p + K_p] a_p^+ + \sum_{p,k} V(k) a_{p-k}^+ a_{q+k} a_q \\ &+ \sum_k V(k) [a_{p-k}^+ a_{p-k} - N_{p-k}] a_p^+ \end{aligned} \quad (1.2.2.)F$$

$$\text{where } \hat{H} = \sum_k T_k a_k^\dagger a_k + \frac{1}{2} \sum_{k,p,q} V(k) a_{p-k}^\dagger a_q^\dagger a_p a_q \quad (1.2.3.)F,$$

$$T_k \equiv \frac{\hbar^2}{2m} k^2 \quad (1.2.4.)F,$$

K_p is the exchange term of the Hartree-Fock approximation. The direct term contribution is a constant energy and "can be removed" - Etters argues - by *shifting the zero point energy* (an argument similar to Bogoljubov's rescaling of the depletion operator's time dependence).

$$K_p = \sum_k V(k) N_{p-k} \quad (1.2.5.)F,$$

and N_k is the expectation value of $a_k^\dagger a_k$ in the correct ground state $|n\rangle_{gr}$. Linearization is achieved in the usual way by discarding the summation \sum over the rest of the scattering terms (other than $k=0$ and $p-k=q$) and neglecting fluctuations about the ground state expectation average of the number operator; i.e. only the first term of (1.2.2.)F is kept; the linearized equation then becomes

$$[H, a_p^\dagger] = (T_p + K_p) a_p^\dagger \quad (1.2.6.)F;$$

this is the usual standard R.P.A.

Etters continues and argues that: 'A potentially more exact procedure ... is formulated by performing the most general linearization of [(1.2.2.)F] consistent with conservation of momentum'. This he realizes as including the pair scattering term $p=-q$ - neglecting the remaining contributions - and rewriting (1.2.2.)F as:

$$\begin{aligned} [H, a_p^\dagger] = & [T_p + K_p] a_p^\dagger + \sum_k V(k) \langle a_{k-p}^\dagger a_{p-k}^\dagger \rangle a_{-p}^\dagger + \\ & + \sum_{p,k} V(k) a_{p-k}^\dagger a_{q+k}^\dagger a_q + \sum_k V(k) [a_{p-k}^\dagger a_{p-k} - N_{p-k}] a_p^\dagger \\ & + \sum_k V(k) [a_{k-p}^\dagger a_{p-k} - \langle a_{k-p}^\dagger a_{p-k} \rangle] a_{-p}^\dagger \end{aligned} \quad (1.2.7.)F,$$

where $\langle a_{p-p}^{+} a_{-p}^{+} \rangle$ is the average between states of different number of particles - $\langle n+2 | a_{p-p}^{+} a_{-p}^{+} | n \rangle (!)$, \sum'' indicates, now, the omission of scattering contributions *other than* direct, indirect and pair scattering. Again, fluctuations about N_k and $\langle a_k^{+} a_k^{+} \rangle$ are neglected resulting in the linearized equation

$$[H, a_p^{+}] = [T_p + K_p] a_p^{+} + \sum_k V(k) \langle a_{k-p}^{+} a_{p-k}^{+} \rangle a_{-p}^{+} \quad (1.2.8.)F.$$

For eq. (1.2.8.)F - E says - one can construct an operator

$$b_p^{+(1)} = \alpha_p a_p^{+} + \beta_p a_{-p} \quad (1.2.9.)F$$

where α_p and β_p are c-numbers, so that (1.2.1.)F is satisfied. E points out that eq. (1.2.1.)F for b_p^{+} - given by (1.2.9.)F "makes sense" only if the hamiltonian is a particle *non conserving* operator (!). Hence one should consider state amplitudes containing a mixture of states with a 'slight' spread in particle number (!) which is small compared with N ; only in this way can the existence of finite (non-zero) values of $\langle a^{+} a^{+} \rangle$ be admitted. Furthermore - he adds - for large systems the number operator may still be an *approximate* good quantum number, since it 'approximately' commutes with the hamiltonian.

The above formulation^(*) of a generalized version of the R.P.A. is not, however, the main aspect of interest in Etter's work. The main feature of the work under consideration is the setting up of an extended *hierachy* of R.P.A.'s⁽⁶¹⁾, initiated either by the standard or the generalized version^(1,2) of R.P.A. The general idea is this: instead of neglecting trilinear contributions in (1.2.2.)F (as in the standard R.P.A.) these contributions are included in the first order iteration by defining first order operators $b^{+(1)}$ as

$$b_p^{+(1)} = a_p^{+} + \sum_{q,k} g(q,k) a_{p-k}^{+} a_{q+k}^{+} a_q \quad (1.2.10.)F$$

where $g(q,k)$ are c-numbers to be determined.

(*) A more precise and consistent formulation of such an approximation is given by Anderson (1,2) in connection with the theory of superconductivity.

The first order eq. of motion is then

$$[H, b_p^{+(1)}] = [H, a_p^+] + \sum_{q,k} g(q,k) [H, a_{p-k}^+ a_{q+k}^+ a_q] \quad (1.2.30)F.$$

The tri-linear term coming from $[H, a_p^+]$ is then transferred to the second term on the R.H.S. of (1.2.30.)F as 'linear in $a^+ a^+ a$ '. The commutator $[H, a^+ a^+ a]$ when expanded contains tri-linear and five-linear contributions. The latter are 'contracted' to a tri-linear form by neglecting fluctuations about the average of N_k , and the 'irreducible' five-linear contributions are neglected at first order of the hierarchy; they are, however, included in second order, and so on.

Suhl and Werthamer point out that finding the solution of (1.2.1.)F for, say, $b_p^{+(2)}$ given by

$$b_p^{+(2)} = a_p^+ + \sum_{q,k} g(q,k) a_{p-k}^+ a_{q+k}^+ a_q + \sum h a^+ a^+ a a \quad (1.2.31)F$$

is equivalent to solving the coupled system of equations

$$\left. \begin{aligned} [H, a_p^+] &= \omega_p a_p^+ \\ [H, a_{p-k}^+ a_{q+k}^+ a_q] &= \omega_p a_{p-k}^+ a_{q+k}^+ a_q \\ [H, a^+ a^+ a a] &= \omega_p a^+ a^+ a a \end{aligned} \right\} \quad (1.2.32.)F,$$

whose simultaneous solution yields the excitation spectrum ω_p and values for g , h , etc.

The method just described yields essentially exact results in the infinite limit, provided that there is a finite region where fluctuations are indeed negligible. The only problem with such an approach is that beyond the first few orders of approximation it already becomes very cumbersome, not to say in the infinite limit of the hierarchy; thus, its practical use is rather limited. A similar iterative method was proposed by Umezawa et al^(50,66) to deal with a different but somewhat related

problem, to be discussed later on in this section. Etters' simple formulation of Suhl and Werthamer method is included here for the sake of comparison. The remainder of Etters' work is devoted to showing that the excitation spectrum for operators (1.2.28)F is *gapless* and linear in the extreme weak-coupling limit, so reproducing Bogoljubov's result but without actually introducing the assumption of macroscopic condensation, but only a weaker statement $N_k \gg 1$ for $k < \delta$, with δ macroscopically small, [generalized condensation⁽³⁰⁾]. However his result is questionable for the same reason as Bogoljubov's - namely the *a priori* neglect of the direct scattering energy and the independence of the result from the normalization condition. Etters finds for the excitation spectrum

$$\omega_p = \mu_p^2 - \eta_p^2 \quad (1.2.33.)F,$$

where

$$\mu_p \equiv T_p + K_p \quad (1.2.34.)F,$$

$$\eta_p \equiv \sum_k V(p-k) \langle a_k a_{-k} \rangle \quad (1.2.35.)F;$$

provided that α_p and β_p in (1.2.28.)F satisfy

$$\alpha_p^2 - \beta_p^2 = 1 \quad (1.2.36.)F$$

$$\alpha_p^2 = \frac{1}{2} \left(\frac{\mu_p}{\omega_p} + 1 \right) \quad (1.2.37.)F,$$

$$\beta_p^2 = \frac{1}{2} \left(\frac{\mu_p}{\omega_p} - 1 \right) \quad (1.2.38.)F.$$

Etters argues that if

$$T_k \ll K_k \quad (1.2.39.)F$$

for $k < \delta$, for some macroscopically small δ , then

$$\lim_{k \rightarrow \delta} \frac{\omega_k}{\mu_k} = \lim_{k \rightarrow \delta} \left| 1 - \frac{K_k^2}{(T_k + K_k)^2} \right| \ll 1 \quad (1.2.40.)F.$$

Rewriting $\langle a_k a_{-k} \rangle$ as

$$\langle a_k a_{-k} \rangle = - \frac{\alpha_k}{\beta_k} N_k \quad (1.2.41.)F$$

and substituting this into η_p one obtains

$$\eta_p = - \sum_k V(p-k) N_k \frac{\alpha_k}{\beta_k} \quad (1.2.42.)F.$$

Finally from (1.2.40.)F it follows that $\frac{\alpha_k}{\beta_k} \approx 1$, where $\eta_p \approx -K_p$; thus if (1.2.39.)F is satisfied

$$\omega_k \rightarrow 0 \text{ for } k \rightarrow 0 ;$$

in fact the spectrum becomes

$$\omega_p = \{T_p(T_p + 2K_p)\}^{\frac{1}{2}} \quad (1.2.43.)F$$

for $p < \delta \rightarrow 0$, i.e. in the extreme weak coupling limit of Bogoljubov.

G. Cummings and Johnston (C-J) Theory of Superfluidity (1966, 1968)

The works by C-J⁽²⁰⁾ and Johnston⁽⁴⁵⁾ introduced a new element into the theory of superfluidity. These authors proposed the notion of *first order coherence* for the Bose superfluid in analogy with the quantum theory of radiation, developed by Glauber and Glauber and Tituelar⁽³¹⁾ in 1963. Similar approaches incorporating first order coherence have been proposed by a number of authors (13,45,49,59,60,65) in connection with superfluid ⁴He and by Casher and Revzen⁽¹⁵⁾ for the ideal Bose gas.

C-J found the notion of first and second order coherence deeply related to the notion of Off-Diagonal-Long-Range-Order (O.D.L.R.O.) in the first and second order reduced density matrices, respectively. It was known - from the works of Penrose and Onsager⁽⁵⁷⁾, Yang⁽⁷¹⁾ and (later) Fröhlich⁽²⁷⁾ - that a characterization by means of O.D.L.R.O. encompasses a variety of superfluid phenomena in systems of diverse nature, such as fermions (i.e.

superconductors, ^3He , etc) and bosons (^4He , laser radiation, masers, etc). Suspecting a common underlying description for all these systems - particularly between coherent electromagnetic radiation and ^4He - they proposed a new set of trial eigenstates obtained from particle states by canonical transformation. The ground state of the trial coherent state representation was defined as

$$|\psi_0\rangle = DT|0\rangle \quad (1.2.1.)G,$$

where T and D are Bogoljubov-Valatin's and Glauber's transformations respectively, given by

$$T \equiv \prod_k \exp\{\gamma_k a_k^\dagger a_{-k}^\dagger - \gamma_k^* a_k a_{-k}\} \quad (1.2.2.)G$$

$$D \equiv \prod_k \exp[\sigma_k a_k^\dagger - \sigma_k^* a_k] \quad (1.2.3.)G.$$

σ_k is a complex, c-number field (as γ_k) and $|0\rangle$ in (1.2.1.)G is the vacuum of particles. Particle operators transform ($T^\dagger = T^{-1}$, $D^\dagger = D^{-1}$) according to

$$Ta_k T^\dagger = (a_k - g_k a_{-k}^\dagger) / (1 - |g_k|^2)^{\frac{1}{2}} \quad (1.2.4.)G$$

$$Da_k D^\dagger = a_k - \sigma_k \quad (1.2.5.)G,$$

where $g_k \equiv (\gamma_k / |\gamma_k|) \tanh(|\gamma_k|) = g_{-k}$. The c-number functions g_k , σ_k and their c.c. are determined from the condition that the ground state energy be minimal with respect to variations of g_k and σ_k (and their c.c.), i.e.

$$\frac{\delta}{\delta g_k} \langle \psi_0 | \hat{H} | \psi_0 \rangle = 0 \quad (1.2.6.)G$$

$$\frac{\delta}{\delta \sigma_k} \langle \psi_0 | \hat{H} | \psi_0 \rangle = 0 \quad (1.2.7.)G,$$

and similarly for g_k^* and σ_k^* . \hat{H} is the usual hamiltonian for a collection of bosons. The solution of (1.2.6,7.)G are

superconductors, ^3He , etc) and bosons (^4He , laser radiation, masers, etc). Suspecting a common underlying description for all these systems - particularly between coherent electromagnetic radiation and ^4He - they proposed a new set of trial eigenstates obtained from particle states by canonical transformation. The ground state of the trial coherent state representation was defined as

$$|\psi_0\rangle = DT|0\rangle \quad (1.2.1.)G,$$

where T and D are Bogoljubov-Valatin's and Glauber's transformations respectively, given by

$$T \equiv \prod_k \exp\{[\gamma_k a_{k-}^{*+} - \gamma_k^* a_k a_{-k}]\} \quad (1.2.2.)G$$

$$D \equiv \prod_k \exp[\sigma_k a_k^{*+} - \sigma_k^* a_k] \quad (1.2.3.)G.$$

σ_k is a complex, c-number field (as γ_k) and $|0\rangle$ in (1.2.1.)G is the vacuum of particles. Particle operators transform ($T^+ = T^{-1}$, $D^+ = D^{-1}$) according to

$$T a_k T^+ = (a_k - g_k a_{-k}^{*+}) / (1 - |g_k|^2)^{1/2} \quad (1.2.4.)G$$

$$D a_k D^+ = a_k - \sigma_k \quad (1.2.5.)G,$$

where $g_k \equiv (\gamma_k / |\gamma_k|) \tanh(|\gamma_k|) = g_{-k}$. The c-number functions g_k , σ_k and their c.c. are determined from the condition that the ground state energy be minimal with respect to variations of g_k and σ_k (and their c.c.), i.e.

$$\frac{\delta}{\delta g_k} \langle \psi_0 | \hat{H} | \psi_0 \rangle = 0 \quad (1.2.6.)G$$

$$\frac{\delta}{\delta \sigma_k} \langle \psi_0 | \hat{H} | \psi_0 \rangle = 0 \quad (1.2.7.)G,$$

and similarly for g_k^* and σ_k^* . \hat{H} is the usual hamiltonian for a collection of bosons. The solution of (1.2.6,7.)G are

$$g_k = (\Omega_k - E_k) / P_k \quad (1.2.8.)G$$

$$\begin{aligned} \sigma_k = & -(E_k / \Omega_k^2) \sum_{p,r} V(p) \sigma_r^* \sigma_{r-p} \sigma_{k+p} \\ & + (P_k / \Omega_k^2) \sum_{p,r} V(p) \sigma_r \sigma_{r-p}^* \sigma_{-k+p} \end{aligned} \quad (1.2.9.)G,$$

and similarly for their c.c. (The dash on the summatoria symbol indicates the omission of the terms $p=0$, $k=-r$ and $p=r-k$). E_k , P_k and Ω_k are the Hartree-Fock energy, the pairing self-energy and the excitation spectrum, respectively, and are given by

$$\begin{aligned} E_k = & (\hbar^2 k^2 / 2m) - \mu + nV(0) + \\ & + \sum_{k' \neq k} V(k'-k) \langle n_{k'} \rangle \end{aligned} \quad (1.2.10.)G$$

$$P_k = \sum_{k' \neq k} V(k'-k) \langle a_{k'} a_{-k} \rangle = P_{-k} \quad (1.2.11.)G$$

and

$$\Omega_k = \{E_k^2 - |P_k|^2\}^{1/2} \quad (1.2.12.)G,$$

respectively, where $n = \sum_k \langle n_k \rangle$ and $\langle \dots \rangle$ denotes averages taken over vacuum state amplitudes $\langle \psi_0 | \dots | \psi_0 \rangle$ (and not over particle states).

The ground state energy is found to be given by

$$\begin{aligned} \langle \hat{H} \rangle_0 = & \langle \psi_0 | \hat{H} | \psi_0 \rangle = - \sum_k [1/2 (E_k - \Omega_k) + \\ & + \Omega_k |\sigma_k - g_k \sigma_{-k}^*|^2 / (1 - |g_k|^2)] , \end{aligned}$$

from which it is clear that a non-zero value of σ_k lowers $\langle \hat{H} \rangle_0$. The integral eqs. for this model are obtained as usual by working out the average values of $\hat{N}_k = a_k^\dagger a_k$ and $a_k a_{-k}$ as functionals of E_k, P_k and Ω_k , and replacing these in (1.2.10-12.)G, i.e.

$$\langle n_k \rangle = |\sigma_k|^2 + |g_k|^2 / (1 - |g_k|^2) = |\sigma_k|^2 + (E_k - \Omega_k) / P_k \quad (1.2.13.)G$$

$$\langle a_{k-k_0}^{\dagger} a_{-k_0} \rangle = \sigma_k \sigma_{-k} + g_k / (1 - |g_k|^2) = \sigma_k \sigma_{-k} - P_k / 2\Omega_k \quad (1.2.14.)G.$$

Introducing these values into (1.2.10,11)G, the eqs. for the Hartree-Fock and pairing energy become

$$E_k = (\hbar^2 k^2 / 2m) - \mu + nV(0) + \sum_{k' \neq k} V(k' - k) |\sigma_{k'}|^2 + \sum_{k' \neq k} V(k' - k) (E_{k'} - \Omega_{k'}) / 2\Omega_{k'} \quad (1.2.15.)G$$

and

$$P_k = \sum_{k' \neq k} V(k' - k) \sigma_{k'} \sigma_{-k'} - \sum_{k' \neq k} V(k' - k) P_{k'} / 2\Omega_{k'} \quad (1.2.16.)G.$$

These eqs. together with the normalization condition

$$N = \sum_k \langle n_k \rangle = \sum_k [|\sigma_k|^2 + |g_k|^2 / (1 - |g_k|^2)] \quad (1.2.17.)G$$

and eq. (1.2.9.)G - together with the complex conjugate eqs. of (1.2.9,16)G - constitute a set of six eqs. for the six variables involved, namely E_k , μ , P_k , P_k^* , σ_k and σ_k^* . The involvement of complex variables, g_k and g_k^* , does not affect much the structure of the integral eq. for the pairing energy (as given by V-B, say) and affects nothing in the normalization condition, whence a drastic modification of the excitation spectrum is *not* expected from this source. The involvement of an extra pair of functions, σ_k and σ_k^* , however, *does* affect $\langle n_k \rangle$ and $\langle a_{k-k}^{\dagger} a_{-k} \rangle$ and hence the normalization condition, as well as the eqs. E_k and the P_k 's. It is also noted that the eqs. for the newly introduced variables σ_k 's are linearly coupled to E_k and the P_k 's; hence the spectrum might be changed from that obtained in other approaches *not* involving first order coherent fields such as V-B's and Luban's.

The hope that the inclusion of first order coherent fields might render the spectrum continuous, i.e. $\lim_{k \rightarrow 0} \Omega_k = \Omega_0 (=0)$, has moved a number of authors

to pursue further this approach, in spite the immediate failure - in the sense that the gap remains, as shown next - and the strong criticisms which follow below.

The occurrence of a gap in this model, and in similar ones (18,45,46, 59,60,65), follows in a quite simple way. The eq. of motion for the first order coherent function, $\sigma(x)$ - i.e. the Fourier transform of σ_k - is given by

$$\frac{\partial \langle \hat{H} \rangle_0}{\partial \sigma(x)} = \langle [\psi(x), \hat{H}] \rangle_0 = 0 \quad (1.2.18.)G,$$

where $\psi(x)$ is the particle annihilation operator in the coordinate basis, i.e. $\sigma(x) = \langle \psi(x) \rangle_0$. From eq. (1.2.18.)G together with the assumption that $\sigma(x)$ is a constant, $\sigma(0)$, the following relation is obtained:

$$[-\mu + nV(0) + \bar{K}_0] \sigma(0) + \bar{P}_0 \sigma^*(0) = 0 \quad (1.2.19.)G$$

and similarly for its c.c., where \bar{K}_k and \bar{P}_k are defined as

$$\bar{K}_k \equiv \sum_{k'} V(k'-k) \langle a_k^\dagger a_{k'} \rangle_T = \sum_{k'} V(k'-k) \frac{|g_{k'}|^2}{1 - |g_{k'}|^2} \quad (1.2.20.)G$$

$$\bar{P}_k \equiv \sum_{k'} V(k'-k) \langle a_{k'} a_{-k} \rangle_T = \sum_{k'} V(k'-k) \frac{g_{k'}}{1 - |g_{k'}|^2} \quad (1.2.21.)G,$$

where $\langle \dots \rangle_T$ means $\langle 0 | T^\dagger \dots T | 0 \rangle$, i.e. the average over the ground state amplitude of the pair representation. From (1.2.19.)G a solution exists if

$$-\mu + nV(0) + \bar{K}_0 = \pm |\bar{P}_0| \quad (1.2.22.)G.$$

Now, the phases of σ_0 and \bar{P}_0 are related through (1.2.19.)G, i.e. if $\bar{P}_0 = |\bar{P}_0| \exp(2i\phi)$, then $\sigma_0 = (\pm 1)^{\frac{1}{2}} |\sigma_0| \exp(i\phi)$. In consequence they find

$$\lim_{k \rightarrow 0} P_k = \left[\sum_{k'} (\pm 1) V(k') \sigma_k \sigma_{-k'} + |\bar{P}_0| \right] e^{2i\phi} \quad (1.2.23.)G$$

$$\lim_{k \rightarrow 0} E_k \rightarrow [\sum_{k'} V(k') |\sigma_{k'}|^2 |\tilde{p}_0|] \quad (1.2.24.)G,$$

if σ_k is symmetric in k , and using

$$\langle 0 | T^+ D^+ \dots D T | 0 \rangle = \langle 0 | T^+ \dots T | 0 \rangle + \langle 0 | D^+ \dots D | 0 \rangle$$

to relate P_k and \tilde{P}_k .

The limiting value, $k \rightarrow 0$, for the excitation spectrum, Ω_k , can now be worked out using (1.2.22.)G for the chemical potential; from (1.2.23, 24.)G these authors obtain

$$\lim_{k \rightarrow 0} \Omega_k \rightarrow \{4 \sum_{k'} V(k') |\sigma_{k'}|^2 |\tilde{p}_0|\}^{1/2} \quad (1.2.25.)G$$

which is *the same* gap found by G-A and L. Whilst this puts an end to the hope of a simple successful derivation of a gapless spectrum, it has not deterred further developments of the same model (18,45,46,59,60,65).

More fundamental criticisms, however, can be raised against the very involvement of first order coherent states in the Bose problem. A brief mention of two of these is appropriate at this stage, in view of the fact that the model proposed in this thesis involves such a representation of states.

The first criticism against using first order coherent fields to describe (at least part of) the order parameter is that it inevitably entails a breakdown of the gauge invariance linked to particle conservation - in the sense that the system is no longer invariant under gauge transformations of the q -number variables, even though it *is* invariant under gauge transformations of the c -number variables, $\langle a_k \rangle = \sigma_k$ say. This feature, however, is not peculiar to first order coherent fields; it also applies to the second order coherent fields $\langle a_k a_{-k} \rangle = g_k / (1 - |g_k|^2)$. However, the phase of σ_k - unlike that of g_k - is an observable, whence the gauge trans-

formation $\sigma_k + \sigma_k \exp(is_k)$, for arbitrary c-numbers s_k , alters the observable properties of the system.

A second criticism due to Evans and Imry⁽²³⁾ is somehow related to the first but goes much deeper. These authors noted that random collisions over a long period of time change randomly the phases of the particle amplitudes, so that its time average is identically zero. On the other hand, the ergodic hypothesis equates this temporal average with an ensemble average; hence $\langle a_k \rangle$ can hardly be finite! The same conclusion as to the average of pair amplitudes, however, can be easily avoided since the phases of a_k and a_{-k} are thought to be linked; hence a random collision changing the phase of a_k , say, will also change the phase of a_{-k} so that the overall phase of $a_k a_{-k}$ is *not* changed at random. In consequence both temporal and ensemble averages of $a_k a_{-k}$ may be non-zero.

As to the first criticism it will be shown later in this work that the gauge invariance is *not* in fact broken but rearranged. The phase of σ_k will be shown to be related to an *external* velocity field. The observable phase of σ is thus *not* arbitrary but is determined by the coupling to this field.

As to the second criticism it will be shown in §4.4 that σ is *not defined* as the ensemble average of the particle operator $\langle a_k \rangle$ but by different means. The phase of σ will be shown *not* to change at random by collisions *if* σ is associated with the superfluid - due to a *global* property of the fields associated with the order parameter of the superfluid phase. However, as it will turn out the first order coherent field σ is *not* a good candidate to be associated with the order parameter of the superfluid phase; in consequence it will be shown that the ensemble average of σ is, in fact, identically zero, as follows from the argument of Evans and Imry.

H. Coniglio and Marinaro (C-M) (1967), Coniglio, Mancini and Manturi (C-M-M) (1969). On Umezawa's physical representation.

The model proposed by C-M⁽¹⁸⁾ - based upon a first order self-consistent method developed by Umezawa⁽⁶⁶⁾ and Umezawa et al⁽⁵⁰⁾ - resembles that of C-J and also that of Kobe⁽⁴⁶⁾.

The strategy of the self-consistent method of Umezawa is rather simple, even though the algebraic development of the method becomes rather cumbersome. The general idea is to devise a relationship between particle operators and elementary operators α^*, α of another representation in the form

$$a_k = c \delta_{k,0} + d_k \alpha_k + e_k \alpha_{-k}^* + \dots \quad (1.2.1.)H,$$

such that α 's are also Bose operators and the particle hamiltonian \hat{H} - given by (1.2.3.)A, as usual - takes the form

$$\hat{H} = \sum_k E_k \alpha_k^* \alpha_k + Q_V(\alpha) + W_0 \quad (1.2.2.)H$$

after replacing (1.2.1.)H, W_0 is a constant and $Q_V(\alpha)$ is a quantity that vanishes in the infinite volume limit.

In order to determine the c-number coefficients c, d_k, e_k, \dots of (1.2.1.)H one proceeds by iteration. Initially one devises a zeroth order trial in the form of a relation between particle operators and elementary operators $\bar{\alpha}_k^*, \bar{\alpha}_k$ of an *intermediate* representation. Let us write this relation symbolically as

$$(\text{zeroth order}) \quad a_k = \bar{a}_k(\bar{\alpha}) \quad (1.2.3.)H.$$

After replacement of a 's by \bar{a} 's in \hat{H} , an expression of the following form is obtained

$$\hat{H}(\bar{\alpha}) = W_0 + \sum_k E_k \bar{\alpha}_k^* \bar{\alpha}_k + :H_I(\bar{\alpha}): \quad (1.2.4.)H,$$

where $:H_I(\bar{\alpha}):$ involves cubic and quartic terms in $\bar{\alpha}$, provided that (1.2.3.)H is a *linear* relation.

The diagonalization is effected⁽⁶⁶⁾ in terms of *new* elementary operators α_k^+, α_k , of the so-called 'physical' representation if these operators are defined as

$$\bar{\alpha}_k = S^{-1} \alpha_k S \quad (1.2.5.)H,$$

where

$$S = 1 + (-i) \int_{-\infty}^0 :H_I(s): ds,$$

and

$$H_I(s) \equiv \exp(-\epsilon|s|) H_I(\alpha_k \exp[iE_k s]) \quad (1.2.6.)H,$$

for

$$\epsilon \sim V^p, \quad -\frac{1}{3} < p < 0 \text{ for large volume } V.$$

The approach just described is just a perturbative expansion of an integral equation⁽⁶⁶⁾.

C-M take for the zeroth order trial

$$\begin{aligned} a_k &= u_k \bar{\alpha}_k - v_k \bar{\alpha}_{-k}^{\dagger} + V^{\frac{1}{2}} \chi \delta_{k,0} \\ a_k^{\dagger} &= u_k \bar{\alpha}_k^{\dagger} - v_k \bar{\alpha}_{-k} + V^{\frac{1}{2}} \chi \delta_{k,0} \end{aligned} \quad (1.2.7.)H,$$

where u_k , v_k and χ are c-numbers, u and v satisfying $u_k^2 - v_k^2 = 1$. The first order correction to (1.2.7.)H is taken by neglecting powers of $:H_I(s):$ higher than the first in the exact expression $a_k = a_k(\alpha)$, they find

$$\begin{aligned} \text{(first order)} \quad a_k &= u_k \alpha_k - v_k \alpha_{-k}^{\dagger} + V^{\frac{1}{2}} \chi \delta_{k,0} - \\ &\quad - i u_k \int_{-\infty}^0 [\alpha_k, :H_I(s):] ds + i v_k \int_{-\infty}^0 [\alpha_{-k}^{\dagger}, :H_I(s):] ds \end{aligned} \quad (1.2.7.a)H,$$

which, after replacement into \hat{H} , yields

$$\hat{H} = W_0^{\dagger} + \sum_k E_k \alpha_k^{\dagger} \alpha_k + Q_V^{\dagger}(\alpha) \quad (1.2.8.)H,$$

where $Q_V^{\dagger} \rightarrow 0$ as $V \rightarrow \infty$. At infinite order of perturbation Umezawa shows

that $W_0^* \rightarrow W_0$, $E_k^* \rightarrow E_k$ and $Q_V^* \rightarrow Q_V$ where, again, Q_V goes to zero in the infinite volume limit.

The beauty of this method can be grasped from the fact that the hamiltonian expressed in terms of elementary operators of the limiting physical representation is such that non-diagonal contributions vanish in the bulk limit ($N \rightarrow \infty$). Furthermore such contributions also vanish in the same limit ($V \rightarrow \infty$) for the first order trial representation. In consequence, these contributions - unlike for V-B or C-J - do *not* contribute to the thermodynamic properties in the bulk limit. The ugliness of this method, however, is apparent from the difficulty of developing the expansion series for selected topologies; this is perhaps one of the reasons why this method has not made much impact amongst workers in the theory of superfluidity (or superconductivity, for that matter).

It is noted that the first order correction does not affect the constant W_0^* , nor the excitation spectrum, E_k^* , as given in the zeroth order correction, hence there is no need, to this approximation, to go beyond (1.2.7.)H. It is also noted that this relation is the same as C-J, except for a change of sign (for v_k) and the fact that the c-number field shift is only introduced for the $k=0$ mode, which is proportional to $V^{1/2}$ and hence is rather large. C-M proceed to evaluating the excitation spectrum to first order in the self-consistent method and eventually find a gap - the same one as found before - for the same reasons as in the case of C-J.

Replacing (1.2.7.)H into \hat{H} they find

$$\begin{aligned} \hat{H} = & W_0^* + A(\bar{\alpha}_0 + \alpha_0^*) + \sum_k B_k (\bar{\alpha}_k \bar{\alpha}_{-k} + \alpha_k^* \alpha_{-k}^*) + \\ & + \sum_k E_k \bar{\alpha}_k \alpha_k^* + :H(\bar{\alpha}): \end{aligned} \quad (1.2.9.)H$$

The contribution $:H(\bar{\alpha}):$ can be neglected, since in first order it yields zero in the bulk limit. The coefficients u_k , v_k , and χ are determined from the conditions

$$\left. \begin{aligned} A &= 0 \\ B_k &= 0 \end{aligned} \right\} \quad (1.2.10.)H,$$

which lead to the following relations

$$(u_0 - v_0) V^{\frac{1}{2}} \chi (-\mu + V(0) \chi^2 - J_0 + V(0) + I_0) = 0 \quad (1.2.11.)H$$

$$\left. \begin{aligned} u_k^2 &= \frac{1}{2} \left(\frac{f_k}{E_k} + 1 \right) \\ v_k^2 &= \frac{1}{2} \left(\frac{f_k}{E_k} - 1 \right) \end{aligned} \right\} \quad (1.2.12.)H$$

$$u_k v_k = \frac{1}{2} \frac{g_k}{E_k} \quad (1.2.13.)H,$$

where $g_k = \chi^2 V(k) - J_k \quad (1.2.14.)H$

$$f_k = \frac{\hbar k^2}{2m} - \mu + \chi^2 [V(k) + V(0)] + V(0) K + I_k \quad (1.2.15.)H$$

and

$$K \equiv \frac{1}{V} \sum_p v_p^2, \quad I_k \equiv \frac{1}{V} \sum_p v(p-k) v_p^2, \quad J_k \equiv \frac{1}{V} \sum_p V(p-k) u_p v_p \quad (1.2.16.)H.$$

From these the excitation spectrum takes the form:

$$E_k = \{f_k^2 - g_k^2\}^{\frac{1}{2}} \quad (1.2.17.)H,$$

which can be simply shown to be the same expression obtained by several authors before, for the appropriate definition of χ , v_k and u_k .

For non-zero χ , the chemical potential is given from (1.2.11.)H, introducing this value of μ into (1.2.17.)H, these authors obtain

$$\omega_0 = 2\chi V(0) J_0^{\frac{1}{2}} \quad (1.2.18.)H$$

for the $k=0$ mode.

It is interesting to observe that C-M obtain the chemical potential, μ , from the diagonalization condition involving the - newley introduced - (first-order) c-number field χ - or σ_0^* , σ_0 for C-J. These conditions are

$A = 0$ for C-M and $\partial \langle H \rangle_0 / \partial \sigma_0 = 0$, $\partial \langle H \rangle_0 / \partial \sigma_0^* = 0$ for C-J. It is noted that while the latter conditions yield and homogeneous set of two coupled equations for σ_0 and σ_0^* , the former gives only one linear equation - also homogeneous - for the only real variable χ ; in both cases, however the chemical potential is the same, and the resulting spectrum turns out to have the same gap.

This way of evaluating the chemical potential is familiar in the context of the theories of superfluidity; however, it is rather unusual in other statistical mechanical theories. In fact, μ is evaluated without resorting explicitly to the subsidiary condition, fixing the *average* number of particles (in the physical representation) to N in the grand canonical ensemble formulation. This method of C-J and C-M cannot be used if χ or σ_0 , σ_0^* are not introduced, or if they turn out to be zero; for, A would be identically zero (and $\langle H \rangle_0$ independent of σ 's). Another case in which this method cannot be employed is in the event of χ (or σ 's for C-J) being time-dependent dynamical variables. In this event the linear eqs. resulting in either approach will *not* give the chemical potential as a function of known quantities, but rather a *dispersion relation* for the (first order) c-number fields in terms of μ , similar to the case of the excitation spectrum.

In the event of (first order) c-number fields being time dependent the inversion of the normalization condition - to obtain μ - cannot be avoided, unless at least one point on the dispersion relation for the excitation spectrum is known by other means. Against this argument it might be argued that, all c-number fields of the theories considered so far are time independent; and that there is no immediate reason to think differently. The best answer to this counter-argument is that one just gets what one has put in - in the first place, and in the present case what one has put in is a time independent c-number field and one accordingly gets a gap. The idea of c-number time *dependence* is a central part of this thesis; a justification for

it is most important and will be given in the final section of the present chapter.

The possibility of non-trivial solutions for the pairing field for $\chi \neq 0$ and $\chi = 0$ respectively, is investigated by these authors, who conclude that if only repulsive interactions $V(o) > 0$ are taken into account, the solution corresponding to $\chi \neq 0$ - which they associate with the occurrence of Bose-Einstein condensation - is the only possible one. However, if sufficiently strong *attractive* interactions are taken into account both solutions, $\chi = 0$ and $\chi \neq 0$, can exist. The 1969 paper by C-M-M considers the possibility of two forms of condensation - Bose condensation (in C-M sense of the word) - and pair condensation, in the sense of a non-trivial solution of the pairing equation for the quantity

$$\sum_k V(k-k') \ll a_k^+ a_k^+ \gg_{Q\&th} .$$

A more modern treatment of these matters - due to Evans and Imry - will be given later in this section.

C-M's paper introduces still another element of interest for the developments to be reported in this thesis later on. This has to do with the relationship between a gap in the excitation spectrum and a breakdown of symmetry. These authors start by emphasising that the invariance satisfied by the exact particle hamiltonian - under transformation to normal coordinates (8,9,37,51,69) of the form $a_k + a_k - i(a_{k+q} + a_{k-q})\delta\epsilon$, where $\delta\epsilon$ is an arbitrarily small c-numbers parameter and q is an arbitrary wave vector, entails - in general - that the excitation spectrum is gapless and linear in the limit $k \rightarrow 0$. Hence the erroneous prediction of a gap is not only against experimental evidence but also indicates that a (hamiltonian) invariance has been broken in the process of derivation of the spectrum. C-M show that the particle current is not conserved for their model (exhibiting Bose condensation) and also that particle number is not a well-defined

it is most important and will be given in the final section of the present chapter.

The possibility of non-trivial solutions for the pairing field for $\chi \neq 0$ and $\chi = 0$ respectively, is investigated by these authors, who conclude that if only repulsive interactions $V(o) > 0$ are taken into account, the solution corresponding to $\chi \neq 0$ - which they associate with the occurrence of Bose-Einstein condensation - is the only possible one. However, if sufficiently strong *attractive* interactions are taken into account both solutions, $\chi = 0$ and $\chi \neq 0$, can exist. The 1969 paper by C-M-M considers the possibility of two forms of condensation - Bose condensation (in C-M sense of the word) - and pair condensation, in the sense of a non-trivial solution of the pairing equation for the quantity

$$\sum_k V(k-k') \ll a_k^+ a_k^+ \gg_{Q\&th} .$$

A more modern treatment of these matters - due to Evans and Imry - will be given later in this section.

C-M's paper introduces still another element of interest for the developments to be reported in this thesis later on. This has to do with the relationship between a gap in the excitation spectrum and a breakdown of symmetry. These authors start by emphasising that the invariance satisfied by the exact particle hamiltonian - under transformation to normal coordinates (8,9,37,51,69) of the form $a_k \rightarrow a_k - i(a_{k+q} + a_{k-q})\delta\epsilon$, where $\delta\epsilon$ is an arbitrarily small c-numbers parameter and q is an arbitrary wave vector, entails - in general - that the excitation spectrum is gapless and linear in the limit $k \rightarrow 0$. Hence the erroneous prediction of a gap is not only against experimental evidence but also indicates that a (hamiltonian) invariance has been broken in the process of derivation of the spectrum. C-M show that the particle current is not conserved for their model (exhibiting Bose condensation) and also that particle number is not a well-defined

quantum number, and accordingly conclude that a gapless spectrum can only be obtained through a theory in which current is conserved, number is well defined (i.e. no hamiltonian symmetry is broken) and condensation - in either of the two forms single particle or pairs - takes place.

C-M commence their argument by recalling a formal characterization - due to Umezawa - of a broken (hamiltonian) invariance. In the coordinate basis the density and current are defined (in terms of particle field operators) as

$$\rho(x) = \phi^+(x)\phi(x) \quad (1.2.19.)H$$

$$\vec{j}(x) = -i\{\phi^+(x)\text{grad}_x\phi(x) - [\text{grad}_x\phi^+(x)]\phi(x)\} \quad (1.2.20.)H,$$

ρ and j satisfy the continuity equation

$$\partial_t \rho(x) + \text{div } j = 0 \quad (1.2.21.)H.$$

Following Umezawa new operators are defined

$$\left. \begin{aligned} A_1 &\equiv \phi^+(x) + \phi(x) \\ A_2 &\equiv \phi^+(x) - \phi(x) \\ B_1 &\equiv \phi^+(x)\phi^+(x) + \phi(x)\phi(x) \\ B_2 &\equiv \phi^+(x)\phi^+(x) - \phi(x)\phi^+(x) \end{aligned} \right\} \quad (1.2.22.)H,$$

where $\phi^+(x)$, $\phi(x)$ are the Fourier transforms of the particle operators a_k^+ and a_k , respectively.

For these, one finds the following result

$$\left. \begin{aligned} \langle 0 | [\rho(x), A_2(y)] | 0 \rangle &= \langle 0 | A_1(y) | 0 \rangle \delta(x-y) \\ \langle 0 | [\rho(x), B_2(y)] | 0 \rangle &= \langle 0 | B_1(y) | 0 \rangle \delta(x-y) \end{aligned} \right\} \quad (1.2.23.)H,$$

where $\langle 0 |$ is the vacuum of the physical representation; it also follows that

$$\langle 0 | \phi^+(x) | 0 \rangle = \langle 0 | \phi(x) | 0 \rangle = C_A \neq 0 \quad (1.2.24.)H,$$

$$\langle 0 | \phi^+(x) \phi^+(y) | 0 \rangle = \langle 0 | \phi(x) \phi(y) | 0 \rangle = C_B \neq 0$$

where C is a constant for - they argue - the system must be invariant under displacement of the origin of coordinates. Hence from (1.2.23,24.)H upon integration over space they find.

$$\langle 0 | [N, A_2] | 0 \rangle = 2C_A \quad (1.2.25.)H,$$

$$\langle 0 | [N, B_2] | 0 \rangle = 2C_B$$

these relations they regard as the most compact (and formal) definition of (hamiltonian) breakdown of symmetry. It indicates that while the hamiltonian is invariant under transformations generated by the number operator, the ground state $|0\rangle$ changes (is not invariant), or similarly, $|0\rangle$ is not an eigenstate of \hat{N} .

Now taking the commutator of (1.2.21)H with A_2 or B_2 , and calling $g(k, \omega)$ and $h(k, \omega)$ the Fourier transform in space and time of $\langle 0 | [j, A_2] | 0 \rangle$ and $\langle 0 | [\rho, A_2] | 0 \rangle$, or similarly for B_2 , they obtain:

$$k \cdot g(k, \omega) - \omega h(k, \omega) = 0 \quad (1.2.26.)H$$

$$\frac{1}{2\pi} \int h(k, \omega) \delta^3(k) d^3k d\omega = 2C_A \quad (1.2.27.)H.$$

From these it follows that if

$$\lim_{k \rightarrow 0} h \cdot g(k, \omega) = 0 \quad (1.2.28.)H,$$

$$\text{then } \lim_{k \rightarrow 0} h(k, \omega) = 2C\delta(\omega).$$

This last relation guarantees the existence of a gapless spectrum⁽⁶⁶⁾.

The condition (1.2.28.)H means that no flux of particles crosses the boundaries, hence current must be conserved to obtain a gapless spectrum,

however, an explicit calculation of $g(k, \omega)$ shows that

$$\lim_{k \rightarrow 0} k \cdot g(k, \omega) \neq 0$$

which entails that particles are lost or gained through the boundaries (infinitely remote). C-M argue that this explains the reason why a gap occurs in their approximation.

The rather formal approach of the last part of C-M's paper is very interesting for it links - in an elegant fashion - current conservation, breakdown of hamiltonian symmetry and the gapless spectrum. On the other hand, the occurrence of a symmetry breakdown and non conservation of current (as a whole) can be tested by simpler means from $\int \text{div } \mathbf{j}(\mathbf{x}) d^3\mathbf{x} \neq 0$, and $\langle 0 | \phi | 0 \rangle \neq 0$ or $\langle 0 | \phi \phi | 0 \rangle \neq 0$.

The conclusion reached by C-M indicates that one is doomed to obtain a gap unless the symmetry is rearranged and total current conserved, regardless of the type of condensation, which must take place - in the opinion of C-M - to explain superfluidity.

I. Evans and Imry (E-I) Self-Consistent Pairing Theory

The self-consistent theory of E-I⁽²³⁾ is the latest of the pairing models for the Bose superfluid; it is also one of the simplest and conceptually perhaps the clearest of them all. In addition, it is free from contradiction - unlike V-B approach - and travels the entire road from first principles to the numerical solution of the resulting integral equations characterizing the pairing model, for a solvable pseudopotential.

The model proposed by these authors does *not* incorporate first order coherence - nor Bogoljubov's prescription - and the equations of motion are reduced to a linear form through the method of linearization of Anderson⁽²⁾; as such it escapes free of the difficulties that arise when first order

coherence is employed in conjunction with Anderson's Random phase Approximation (see §3.3). As to the prediction of superfluid behaviour, however, E-I's approach is open to the same criticism as V-B's work; in the sense that would-be order parameter configurations are not involved in the statistical ensemble. The only configurations involved in the statistical ensemble are those associated with elementary excitations; this is a conceptual defect of nearly all theories of superfluidity (6,18,20,22,23,29,68) and also of superconductivity (4,34)

The strategy of these authors is to develop anew a pairing model devoid of unnecessary *ad hoc* assumptions as to the occurrence of B.E.C., emphasizing the role of attractive interactions which - unlike for superconductors - arise naturally from the local potential. Indeed, they find that the involvement of the attractive interactions is necessary for a non-trivial solution for the pairing fields, which these authors identify with the order parameter. It is to be noted that E-I do *not* identify the condensate with the order parameter. They do find, however, that the existence of a non-trivial solution for the pairing fields does not *additionally* require the occurrence of B.E.C.; should this occur, however, it ensures a gapless linear spectrum.

The standard technique of linearization should be familiar by now, hence it is not repeated here; it will suffice to point out that these authors take the following distribution of elementary excitations of the pair representation in thermal equilibrium

$$\langle \eta_k \rangle_{Th} = (\exp \beta E_k - 1)^{-1} \quad (1.2.1.) I,$$

where the excitation spectrum is

$$E_k = \{ \tilde{\epsilon}_k^2 - |\Delta_k|^2 \}^{\frac{1}{2}} \quad (1.2.2.) I;$$

$\tilde{\epsilon}_k$ is the Hartree-Fock energy

$$\tilde{\epsilon}_k = \frac{\hbar^2}{2m} k^2 + NV(0) + \epsilon_k - \mu \quad (1.2.3.) I,$$

$$\xi_k = \sum_q V(q) \langle a_{k+q}^+ a_{k+q} \rangle \quad (1.2.4.) I,$$

and Δ_k is the coherence parameter

$$\Delta_k = \sum_q V(q) \langle a_{-k-q} a_{k+q} \rangle \quad (1.2.5.) I;$$

the averages are taken over pair states whose elementary operators are related to particle operators through

$$\left. \begin{aligned} a_k^+ &= u_k a_k + v_k^+ a_{-k}^+ \\ a_k &= u_k a_k^+ + v_k a_{-k} \end{aligned} \right\} \quad (1.2.6.) I.$$

Hence the averages of number and of pairs are given by

$$\left. \begin{aligned} n_k &= \frac{\bar{\epsilon}_k}{2E_k} \operatorname{ctgh} \left(\frac{\beta E_k}{2} \right) - \frac{1}{2} \equiv \langle a_k^+ a_k \rangle_{Th} \\ x_k &= - \frac{\Delta_k}{2E_k} \operatorname{ctgh} \left(\frac{\beta E_k}{2} \right) \equiv \langle a_k a_{-k} \rangle_{Th} \end{aligned} \right\} \quad (1.2.7.) I,$$

where the following solution for the c-number fields u_k, v_k has been used

$$u_k = \frac{1}{2} \left\{ \frac{\bar{\epsilon}_k}{E_k} + 1 \right\}^{\frac{1}{2}}; \quad |v_k| = \frac{1}{2} \left\{ \frac{\bar{\epsilon}_k}{E_k} - 1 \right\}^{\frac{1}{2}} \quad (1.2.8.) I$$

$$\arg(u_k) - \arg(v_k) + \arg(\Delta_k) = 2\pi n \quad (1.2.9.) I.$$

From these results the following set of integral equations is obtained:

$$\xi_k = \sum_{k'} V(k-k') \left\{ \frac{\bar{\epsilon}_{k'}}{2E_{k'}} \operatorname{ctgh} \left(\frac{\beta E_{k'}}{2} \right) - \frac{1}{2} \right\} \quad (1.2.10.) I$$

$$\Delta_k = - \sum_{k'} V(k-k') \frac{\Delta_{k'}}{2E_{k'}} \operatorname{ctg} \left(\frac{\beta E_{k'}}{2} \right) \quad (1.2.11.) I,$$

subject to the normalization condition

$$N = \sum_k \left\{ \frac{\tilde{\epsilon}_k}{2E_k} \operatorname{ctgh} \left(\frac{\beta E_k}{2} \right) - \frac{1}{2} \right\} \quad (1.2.12.)I.$$

In order to reduce this set of equations to a soluble form E-I introduce a hypothesis (to be tested *a posteriori*) involving the occurrence of a macroscopic B.E.C. In order for n_0 to be an extensive quantity E_0 must be macroscopically small - they argue; hence $\operatorname{ctgh} \frac{\beta E_0}{2}$ should be approximately equal to $(2/\beta E_0)$, whence the population of the condensed mode should satisfy

$$n_0 = \tilde{\epsilon}_0 / \beta E_0^2 \quad (1.2.13.)I,$$

and from (1.2.2-7.)I the chemical potential should satisfy the following relation

$$NV(0) + \xi_0 - \mu = |\Delta_0| \quad (1.2.14.)I,$$

which yields the following excitation spectrum

$$E_k = \left\{ \left(\frac{\hbar^2}{2m} + \xi_k - \xi_0 + |\Delta_0| \right)^2 - |\Delta|^2 \right\}^{\frac{1}{2}} \quad (1.2.15.)I,$$

which is manifestly gapless.

After introducing the chemical potential (obtained from (1.2.14.)I) into the integral equations, (1.2.10,11.)I, the following pair of equations are obtained.

$$\xi_k = NV(k) + \sum_{k' \neq 0} [V(k-k') - V(k)] n_{k'} \quad (1.2.16.)I,$$

$$\Delta_k = -V(k) \operatorname{Sign}(\Delta_0) \left\{ N - \sum_{k' \neq 0} n_{k'} \right\} -$$

$$- \sum_{k' \neq 0} V(k-k') \frac{\Delta_{k'}}{2E_{k'}} \operatorname{ctgh}(\beta E_{k'}/2) \quad (1.2.17.)I.$$

Bogoljubov's solution for a repulsive local potential ($V_k =$ positive constant, say) is now impossible, as is seen from (1.2.17.)I, due to the presence of the first term which arises naturally here. However, for

attractive potentials (or rather pseudopotentials) eqs. (1.2.16,17.)I - together with the normalization condition - admit non-trivial solution for Δ_k .

Evans and Imry then proceed to obtain an expression for the specific heat which is in qualitative agreement with Landau's except for a numerical factor. Finally, E-I obtain numerical solutions for (i) the excitation spectrum for several potentials amenable to numerical analysis, and (ii) for the superfluid fraction and the specific heat as functions of temperature, both of which show fairly good qualitative agreement with experiment.

A further analysis by Evans and Harris⁽²³⁾ considered the question of coexistence of B.E.C. and pairing, taking the hard core radius of the potential as a numerical variable; they find that condensate-less solutions for the pairing fields are possible.

It is noted that E-I do *not* identify B.E.C. with first order coherence - in the sense of a non-zero average for the particle amplitudes. It is argued that first order coherent fields should have identically zero ensemble average - according to the argument considered before, concerning the ergodic hypothesis. Furthermore, the introduction of these fields entails a gap in the excitation spectrum,^(**) as in Refs.(20,46). It will be shown later in this work that this is indeed the case. The *ensemble* average of the *first* order coherent field *amplitudes*, $\langle \phi_k \rangle_{\text{Thermal}}$ say, will be shown to vanish for the "most realistic" superfluid ensemble, constructed in §4.4. The ensemble average of $|\phi_k|^2$, however, is shown to be *finite*. This turns out to be the case for *the particular* system under consideration, namely superfluid ^4He ; in general, however, the theoretical possibility of $\langle \phi_k \rangle_{\text{Th}} \neq 0$ will be shown to be an admissible one, from an argument that circumvents E-I's indictment. As to the statement that the involvement of first order coherent fields entails a gap in the excitation spectrum *for elementary excitations*^(*), it will be shown here that this is indeed the

(*) of the pair representation

(**) this though is not a phonon spectrum

case! In addition to that, however, the very presence of first order coherent fields brings about *another branch* of the spectrum which is gapless and linear. This changes the entire view of the pairing model, in that what was a gapless spectrum before now turns out to show a gap, and corresponds to an upper branch of the spectrum discovered - by accident - in an experiment (19,43) performed *after* the appearance of E-I's paper.

As to E-I's identification of the pairing fields with the order parameter it will turn out here to be *correct*. It will be shown that the condensed mode - if it exists at all - is *not* to be identified with the superfluid nor with the first order coherent fields, nor the latter with the superfluid. Attractive interactions should also play a central role in the theory to be developed in what follows, but the strategy underlying the standard method of linearization will be shown to be defective, particularly when first order coherence is involved.

§1.3. Overview of the proposed new theory of superfluidity

A. Preliminaries

The discussion on dynamics and on thermodynamics - for physical systems undergoing a phase transition - has been centred around two deep rooted *paradigms*. The first of these regards *all* phase transitions as signalled by a spontaneous breakdown of *dynamical* symmetry. The other is concerned with the way in which *statistical* ensembles - describing both low and high temperature phases - should be constructed, and the nature of the superfluid phase's order parameter. Most conceptual and practical difficulties encountered by existing theories of superfluidity (6,18,20,22,23,29,32,40,46,51,55,59,60,62,65,68,73) and also of superconductivity (4,34) can be traced back to defects of these two paradigms. It is most important to inspect in some detail these intuitive schemes at this stage, to find the unhappy consequences they bring about; and, eventually, to replace them by others, more suited to developing a *unified* theory of phase transitions - in general - and of super-responsive behaviour, in particular. The most fundamental innovation of the theory of superfluidity proposed in this thesis is a change of the basic underlying paradigms.

Let us consider the dynamical paradigm of a phase transition first. It is almost universally believed that the onset of a phase transition is signalled by a spontaneous breakdown of dynamical symmetry, accompanied or not by the emission of a massless 'object' carrying away the 'lost' symmetry(33b). As far as the superfluid and superconducting transitions are concerned, the alleged broken symmetry is the *gauge symmetry*, closely related to the fact the total number of particles in the low temperature phase is *not* a good quantum number, unlike in the high temperature phase. For the various magnetic transitions (ferromagnetic, antiferromagnetic, spin-glass, etc.), on the other hand, the broken symmetry is associated with

rotational invariance, and for solid-gas transitions with translational invariance.

The breakdown of symmetry is thought to come about - from a microscopic viewpoint - due to the fact that 'the best' spaces of states describing the dynamical behaviour in either phase are non-equivalent^(*). For ^4He and metallic alloys admitting a superconducting phase the normal phase is believed to be best described by states of the (Bose or Fermi) particle representation (P.R.). This representation is given by an orthonormal and complete set of state amplitudes, $\{|n\rangle\}$ for all non-negative integers n , and by creation and annihilation operators, a_k^+, a_k . The low temperature phases, on the other hand, are thought to be best described by generalized coherent state representations (C.S.R.)⁽⁶⁶⁾, or in simple cases by a simplified version of a C.S.R. A formal definition of generalized and simplified (linear) coherent state representations will be given in §2.3.; it suffices, for now, to point out that either version of C.S.R. is given by an orthonormal and complete set of coherent states $\{|C_n\rangle\}$ and elementary excitation creation and annihilation operators, α_k^+ and α_k , related to P.R. by canonical transformation $\tau(\tau^+ = \tau^{-1})$.

Particle representation and coherent state representations are non-equivalent representations of the same commutation relations^(3,25), in so far as both a 's and α 's satisfy the same commutation or anticommutation relations (for bosons or fermions, respectively), and their number operators, namely $N = \sum_k a_k^+ a_k$ and $\hat{n} = \sum_k \alpha_k^+ \alpha_k = \tau N \tau^{-1}$ do not commute in either representation.

Both energy and number are good quantum numbers above the transition; that is \hat{H} and \hat{N} commute in the P.R. Now, the premise embodying the paradigm of a broken symmetry is that: "The constants of motion in either phase - described by non-equivalent representations of states - are the

(*) The notion of non-equivalent spaces of states will become clear shortly.

same functionals, \hat{H} and \hat{N} , for instance". This premise is often stated as: Transformation τ leaves the hamiltonian invariant, while it changes the symmetry of the ground state. In other words, the energy and number functionals are \hat{H} and \hat{N} regardless of whether these are expressed in terms of a 's or α 's.

It is thought that the hamiltonian *must* be diagonal in *both* representations; that is, the *hamiltonian* symmetry must be *rearranged*. For linear - or linearized - problems it has been shown, by the authors reviewed in §1.2 among others, that \hat{H} can be very simply diagonalized (in a simplified version of a C.S.R.) by selecting the c-number fields appearing in τ appropriately, so that low order non-diagonal (dangerous) contributions cancel out exactly. For non-linear problems, however, exact diagonalization of \hat{H} can only be achieved in a highly complex C.S.R.⁽⁶⁶⁾ - the so-called 'physical representation' - in the infinite volume limit.

The main feature of the present argument, however, is that having succeeded in diagonalizing \hat{H} in some C.S.R., the number operator, \hat{N} , remains non-diagonal, in view of the fact that the number of elementary excitation operator \hat{n} is diagonal - by construction - in the C.S.R. and $[N, n] \neq 0$ in the same representation. In consequence, the diagonal segment of \hat{H} in the C.S.R. and \hat{N} do *not* admit the same set of coherent eigenstates. The number of *particles* is *not* a good quantum number and a gauge transformation is not well-defined. The symmetry associated with gauge invariance thus appears broken.

The paradigm just examined, however, is defective, as pointed out before. One can realize this very simply by recalling that one basic *postulate* of dynamics is: *A given physical system is identified by a Lagrange functional, by the group of dynamical transformations (symmetry transformations) leaving the lagrangian invariant, and by the expectation values of all the constants of motion.* In view of this postulate, should two dynamical problems exhibit different overall symmetry groups they *must* correspond to different physical

systems! Should this conclusion be rejected, on the other hand, the postulate just referred to must also be rejected, and one should look for a different means to identify a given physical system. There is, of course, no *reason* why dynamics should be axiomatized as it is, but changing the above postulate is just but changing the subject! Thus one rather leaves the postulate as it is and abandons- if one can - the paradigm of an *overall* breakdown of symmetry.

There is still a well-known^(33b) way in which the postulate and the present paradigm can be reconciled, at least as far as a continuous broken symmetry is concerned. It might be thought that even though the *overall* symmetry is *not* broken, but rearranged, the transition is signalled by the emission of a Goldstone boson, which escapes from the massive system, so carrying away some symmetry (the gauge symmetry, for instance). The massive system is then left with an *effective* broken symmetry.

No logical problem arises in this case; however, in order to support this alternative paradigm on *physical* grounds one must be able to envisage *independent* means of *detecting* the 'flying symmetry wave', and devise an apparatus to measure the massless boson which carries away the symmetry. Until such an independent methods of detection is produced, for every transition explained in this way, the paradigm of an *effective* breakdown of symmetry will remain outside the scope of *physics*. One could find experimental evidence of an effective breakdown of symmetry - in principle - by accurate measurements in both phases of the constant of motion associated with the alleged broken symmetry, and by searching for deviations from the average value *larger* than normal statistical fluctuations. This type of experiment is *not* independent of the above postulates; in fact, it would predict an effective breakdown of symmetry by *defect*. Experiments of this kind have been carried out for the lambda transition of ^4He and for the superconducting transition, showing that deviations in number of quantum -

dynamical origin - if occur at all - are *smaller* than statistical fluctuations - see Ref. (45) and references within - and hence do *not* support the view of the occurrence of a breakdown of the gauge invariance.

The main thesis pursued in this work, as far as dynamics is concerned, is that the overall (and also the effective) symmetry is *rearranged* through the transition, without having to *postulate* or *conjecture* a 'flying symmetry wave'. The strategy here is to exploit the above postulate, not only in the sense that the whole symmetry must be rearranged, but also in regards to the invariance of expectation values for the constants of motion.

It will become clear that a representation of coherent states is *not better* than the particle representation to describe *dynamics* of a superfluid (in a pure state description, say); for it will turn out that both descriptions are, in fact, dynamically equivalent. A C.S.R. description will be shown, however, to be *better suited* for the purpose of *statistical counting*. It will be made clear that C.S. are not necessarily applicable *only* to superfluids, but can also be used to describe non-superfluids. It will be shown also that the involvement of a C.S.R. does *not* entail a breakdown of symmetry. This occurs in existing theories as a direct consequence of the erroneous premise that the constants of motion - \hat{H} and \hat{N} , say, for ${}^4\text{He}$ - are *the same* functionals regardless of the representation of states. It will be made quite clear that the correct energy and number functionals in a C.S.R. description are functionals, \hat{H}' and \hat{N}' , *different* from \hat{H} and \hat{N} . The former operators will be shown to be constants of motion, to commute in the C.S.R. and to yield the same expectation values as \hat{H} and \hat{N} , respectively. Two formulations of the same dynamical problem satisfying the latter properties are referred to here as *dynamically equivalent*. Later in this section the questions on dynamics will be considered further, but now let us examine the other paradigm concerning statistics.

The paradigm to be considered now can be put as a set of heuristic statements giving answers to the questions: How is the statistical ensemble to be constructed from a set of coherent states? what is the order parameter of the low temperature phase?, and, how does it emerge from microscopic and statistical considerations? This paradigm eventually conveys an idea as to what superfluidity (or superconductivity) is.

The statements constituting the statistical paradigm of superfluidity vary in detail - from one approach to the other - particularly as to the nature of the order parameter. That is not so in the theory of superconductivity for which the order parameter is almost universally identified with the 'pairing fields'. As far as the Bose superfluid is concerned the early paradigms of London and Bogoljubov regarded the condensate population fraction as the order parameter of the superfluid phase; later, Valatin and Butler and Evans and Imry identified the order parameter with the fraction of particles normalized by the pairing fields, as in the case of superconductors. Still a third option was proposed by Cummings and Johnston, Coniglio and Marinaro and Kobe, who identified the order parameter with the fraction of particles normalized by the first order coherent fields. It must be noted that the condensate should not be identified with the latter fields. The condensate is a singularity in the distribution function of any fields contributing to the density, not the fields themselves; however, when only the mode $k=0$ is allowed to exist for the first order coherent fields - as is usually the case - the distinction becomes immaterial. Other options combining the former three have also been considered by Coniglio, Mancini and Manturi.

Now, as to the question of how the statistical ensemble is constructed, the idea leading to an answer is the same in all approaches. All authors construct ensembles whose *only* configurations are all possible distributions of *elementary excitations*. The same applies for the theory of superconductivity.

C-number field configurations are *not* considered at all in constructing the ensemble; in fact, c-numbers are regarded as variational parameters, *not* as dynamical variables; hence not even in principle could these fields be considered for the purpose of statistical counting of configurations. This alone suffices to disqualify these fields as acceptable order parameters; for an order parameter is a measure of the number of configurations not contributing to the disorder, i.e. to the entropy. This argument has already been elaborated in §1.2.B and will not be repeated; only the final conclusion will concern us here, namely - none of the theories reviewed in §1.2 predicts superfluid behaviour! The same applies to the theory of superconductivity!

As to the interpretation of Bogoljubov, this seems not to be disqualified by the above argument; for, after all, the condensed mode of elementary excitations is involved in the counting of configurations; however, in Bogoljubov's theory nothing prevents the particles in the condensate - immersed in a thermal bath - to disorder and so dissipate energy, like particles in any other mode. Landau's criterion, on the other hand, does not convey a reason *why* the condensate should keep fully ordered and hence behave as a superfluid.

The key towards a more satisfactory statistical paradigm of superfluidity was proposed by Hohenberg and Martin⁽³⁸⁾, who identified the superfluid order parameter with the condensate fraction. This interpretation turns out *not* to be correct for the reasons given in §1.2A,B, but their approach towards the construction of a Restricted Ensemble (R.E.) opened the way for a formal and satisfactory *characterization* of superfluidity. These authors introduced a partition in the phase space - actually a partition of the wave vector axis, regarding condensate and depletion configurations as *independent*. The *partition function* then turns out to be the product of two summations over two independent sets of configurations. Such a partition function characterizes a Restricted Ensemble. The property of superfluidity then comes about quite

directly and simply, from the *assumption* that configurations differing only by their condensate population are all *statistically equivalent* - that is, cannot be distinguished by their thermal properties. The incorporation of such a *hypothesis* entails superfluidity, in so far as the entropy associated with the condensed mode configurations is identically zero, at all temperatures for which a condensate exists. This, in turn, implies superfluid behaviour of the fraction of the particles in the condensate; for, they cannot dissipate energy without increasing the entropy. So, individual particles in the condensate becomes locked to one another by a global property reflecting their order.

The existence of B.E.C. thus becomes a necessary condition for superfluidity in the work of Hohenberg and Martin, but not sufficient; for, the premise of statistical equivalence must be validated - in turn. This can be shown by proving that the free energy is lower if the condensate is fully ordered; that is, comparing the free energy of the superfluid ensemble thus constructed with another (*comparable*) ensemble, equal to the former except for the fact that statistical equivalence of condensate configurations is *not* imposed.

This paradigm of Hohenberg and Martin will be adopted and fully exploited in this thesis, but free from the special role of Bose condensation as an order parameter, and also from *any* interpretation of the order parameter at initial stages. The order parameter will be identified *at the end*; in the meantime all possibilities will be considered and left open for future decision. The adoption of such an improved paradigm will bring about profound changes in the theory, as to the concepts and methods involved, and - most importantly - as to the prediction of the excitation spectrum. These matters are considered next.

B. Statistical Characterization of a Superfluid

The analysis of dynamics and statistical mechanics in almost all existing theories has been carried out in terms of the fields of the representations involved, either P.R. or the C.S.R. However, the analysis is seen to go deeper, to be richer and more general, if the discussion is shifted into the context of an abstract phase space Γ , i.e. the domain of a set of canonical dynamical variables, without advancing - for now - any reference as to how these variables are defined in terms of the fields of one representation or the other. By keeping the discussion at this level several questions concerning dynamics and statistics can be treated quite generally, and the discussion is seen to apply to either bosons or fermions, as well as for classical systems.

An interesting feature about the phase space is the fact that it is not only the domain of canonical dynamical variables, *but is also* the domain for statistical counting, and hence provides a bridge between dynamics and thermodynamics.

The strategy here is to define a certain *separable phase space*, Γ_S , (see §2.2) as the direct sum of a number of *independent* phase spaces S_i , such that all ensembles constructed from configurations in Γ_S always admit a R.E., *without* having to introduce - *a priori* - a partition of the momentum axis. The partition function of any ensemble constructed from Γ_S will be of the form

$$Z = \sum_{c_k^1} \sum_{c_k^2} \dots \sum_{c_k^j} \Omega \quad (1.3.1.)B$$

where Ω is the statistical operator (to be specified in §4.4) and the summations are over all possible configurations c_k^i in the *independent* spaces S_i . An ensemble whose partition function is given by (1.3.1.)B is called a Restricted Ensemble (R.E.).

A superfluid (non-superfluid) ensemble is defined as a R.E. for which at least one (no) set of configurations c_k^i is statistically equivalent. A superfluid ensemble will be shown to give the properties of a superfluid in agreement with Landau's two fluid model; in addition, the present characterization is analatically refutable (by proving that for a given identification of some set of configurations with the order parameter, the free energy is *not* reduced with respect to that of comparable non-superfluid ensemble); however, it is not verifiable. For it *cannot* be proven that an interpretation of superfluid configurations gives the least conceivable free energy. On the other hand, the present characterization is empirically testable, in so far as the critical temperature, T_c , obtained as the temperature at which the free energies from superfluid and non-superfluid ensembles are the same, can be compared with the actual experimental value of T_c .

Two important features of a separable phase space must be pointed out at this stage. Firstly, the usual dynamical problem - in terms of particle field operators, say - is *not* formulated in terms of a separable phase space, hence the introduction of Γ_s amounts to a change of variables; say from \hat{p}_k, \hat{q}_k - defined in a non-separable phase space $\Gamma_{ns} \equiv \{(\hat{p}_k, \hat{q}_k)\}$ - to \hat{p}_k^i, \hat{q}_k^i defined in $\Gamma_s \equiv \bigoplus_{i=1}^d S_i, S_i \equiv \{(p_{k_i}^i, q_{k_i}^i)\}$. It is noted that even though the number of independent variables in Γ_s is larger than in Γ_{ns} the dimension (i.e. the number of degrees of freedom) is the *same*. It is also noted that if both phase spaces are to be employed to formulate the same dynamical problem, the volumes of Γ_s and Γ_{ns} , must be *the same*; and, to be consistent with the definition of Γ_s , the 'old' and 'new' variables must be *additively* related, i.e. $\hat{q}_k = \sum_i \hat{q}_k^i; \hat{p}_k = \sum_i \hat{p}_k^i$. Secondly, it must be noted that wave-vector labels of *separate* variables $p_{k_i}^i$ and $q_{k_i}^i$ have been specified further by a sub-index i (whenever this is not shown, it is to be read as k_i at k). This indicates that p_k^i, q_k^i are formally defined over different wave-

vector domains though taking the same numerical values; i.e. p^i, q^i and p^j, q^j - for $i \neq j$ - are defined over different domains $k_i \in |K_i, k_j \in |K_j, |K_i \neq |K_j$.

An important consequence of the first observation is that the number branches of the spectrum for a problem formulated in terms of a separable phase space may be *larger* than in terms of a non-separable phase space, if the dispersion relations for all the variables are not identical. This will turn out to be the case here. As to the second observation, the discrimination of wave-vector labels brings about an intrinsic distinguishability among the various *dynamical objects* associated with separate variables. This distinguishability is present in most theories in one form or the other, but - almost invariably - in an implicit fashion. On the other hand, it enables one to end up with a two (distinguishable) fluid model, from an initial problem in terms of indistinguishable ⁴He atoms. Furthermore, this feature establishes a selection rule forcing the various objects "i" to get excited only to the level of their own dispersion relations, ω_k^i , and not to any other level.

One of the advantages of confining the discussion to abstract phase spaces is that it is rather easy to abandon the prejudice that the constants of motion are associated with the same functionals, regardless of the representation of states involved. It becomes clear, for instance, that the number functionals in the S.P.S. and the N.S.P.S. are different, namely $\hat{N} = \sum_{i,k} p_k^i q_k^i$ and $\hat{N} = \sum_k \hat{p}_k \hat{q}_k$, respectively. This without having to specify the representation of states in which the two sets of dynamical variables are defined.

It seems clear also that the hamiltonians for the same dynamical problem as functionals of two sets of canonical variables, defined over domains of *different structure*, should also be different.

An interesting feature of the definition of dynamical variables of separable phase space, in §2.4, is that some of these variables are c-number

fields. In fact, these fields are regarded here as dynamical variables in their own right, not as mere variational parameters, as in existing theories. This feature will bring about a profound change of viewpoint in the sense that the dispersion relations associated with these fields turn out not to be identically zero, but finite and observable. The dynamical implications of introducing c-number variables will be considered next.

C. Equivalent Formulations of Dynamics from Variables of Separable and Non-separable Phase Spaces

Admitting and leaving aside - for now - the conceptual and practical advantages of carrying out the statistical counting in an ensemble defined over a separable phase-space, and in view of the dynamical implications of assigning dynamical character to c-number fields, one must consider the question of whether one is *justified* in thinking that it is possible as all to *reformulate* - on the basis of variables of a separable phase space Γ_s - a (generic) problem originally posed, by means of a Hamilton functional, say, from a non-separable phase space Γ .

As a matter of fact for a dynamical problem to be well defined does not require of the existence of a hamiltonian, but it does require of the existence of a lagrangian. For problems admitting a hamiltonian, both lagrangian and hamiltonian formulations of the action principle are equivalent, in the absence of constraint in the domain of lagrangian variables. The discussion here is confined to such problems.

Now, there is *no* preferred dynamical language to formulate any given problem (of the kind considered here). As a matter of fact any two formulations based upon *the same lagrangian* L , in terms of two *related* sets of variables - defined over domains of the same dimension and hypervolume - are dynamically equivalent if and only if: (i) The symmetry group of *lagrangian* invariances is the same, in the sense that for every unitary transformation

of coordinates (and C.C.) in one domain leaving L invariant, there is another transformation of coordinates in the other domain also leaving L invariant, and associated with the same physical properties, e.g. such as displacements of the zero of the time or space scales, or gauge invariance, etc. (ii) if the number (and nature) of well defined and simultaneously measurable constants of motion is the same and (iii) if the expectation values for these observables are the same.

It is noted that the condition that the hamiltonian (or the number operator) be the same functional for both formulations was not included above, for it is not essential. As a matter of fact if the transformations from lagrangian to hamiltonian variables is not in a one to one correspondence for the variables involved (separable and non-separable) the hamiltonians of both formulations will be different functionals in general.

These defining properties of dynamical equivalence (in the above sense) are satisfied if both domains of lagrangian variables are related via a unitary transformation. The trouble is that separable and non-separable domains are *not* (and *cannot* be) related by canonical, unitary transformation, so these properties must be tested anew.

The main concern here is to investigate whether it is possible to circumvent the trouble raised by the standard formulation of the problem, in the sense that the operators associated with two conserved and *well defined* observables do not commute^(*), namely the hamiltonian and the number operator (and also linear momentum). For simplicity of the argument the attention will be focused here on those invariances associated to conservation of energy and total number, a more extensive analysis as to other lagrangian invariances following a similar path. Similarly for the sake of simplicity a non-relativistic langrangian will be considered. This is justified to some extent - due to the fact that the best known super-responsive phenomena occur in a non-relativistic limit; the treatment,

(*) at least at finite order of perturbation in the finite volume limit

of coordinates (and C.C.) in one domain leaving L invariant, there is another transformation of coordinates in the other domain also leaving L invariant, and associated with the same physical properties, e.g. such as displacements of the zero of the time or space scales, or gauge invariance, etc. (ii) if the number (and nature) of well defined and simultaneously measurable constants of motion is the same and (iii) if the expectation values for these observables are the same.

It is noted that the condition that the hamiltonian (or the number operator) be the same functional for both formulations was not included above, for it is not essential. As a matter of fact if the transformations from lagrangian to hamiltonian variables is not in a one to one correspondence for the variables involved (separable and non-separable) the hamiltonians of both formulations will be different functionals in general.

These defining properties of dynamical equivalence (in the above sense) are satisfied if both domains of lagrangian variables are related via a unitary transformation. The trouble is that separable and non-separable domains are *not* (and *cannot* be) related by canonical, unitary transformation, so these properties must be tested anew.

The main concern here is to investigate whether it is possible to circumvent the trouble raised by the standard formulation of the problem, in the sense that the operators associated with two conserved and *well defined* observables do not commute^(*), namely the hamiltonian and the number operator (and also linear momentum). For simplicity of the argument the attention will be focused here on those invariances associated to conservation of energy and total number, a more extensive analysis as to other lagrangian invariances following a similar path. Similarly for the sake of simplicity a non-relativistic langrangian will be considered. This is justified to some extent - due to the fact that the best known super-responsive phenomena occur in a non-relativistic limit; the treatment,

(*) at least at finite order of perturbation in the finite volume limit

however, can easily be extended to the relativistic case.

In order to test whether a formulation in terms of non-separable variables is dynamically equivalent to another in terms of separable variables, a relationship must exist between these two sets of variables, say

$$\hat{q}_k = \sum_i q_k^i, \quad \hat{p}_k = \sum_i p_k^i \quad (1.3.1.)C.$$

This relationship is - of course - only one of the many conceivable; however, it is a rather simple one, which not only will help to illustrate the method but will eventually be (for different reasons) the one employed here. From (1.3.1.)C one can express the lagrangian

$$L(\hat{q}, \hat{p}) = \frac{1}{2} \sum_k (\hat{p}_k^+ \hat{q}_k - \hat{q}_k^+ \hat{p}_k) - \hat{H}(\hat{q}_k, \hat{p}_k^+) \quad (1.3.2.)C$$

as

$$L(\hat{q}(q^i), \hat{p}(p^i)) \equiv L(q^i, p^i)$$

To prove that $L(q^i, p^i)$ admits a hamiltonian at all one defines generalized momenta as usual by $p_k^i \equiv \partial L / \partial \dot{q}_k^i$ and expresses $L(q^i, p^i)$ as follows

$$L(q, p) = \frac{1}{2} \sum_{k,i} (p_k^i \dot{q}_k^i - C.C.) - \hat{H}^*(p^i, q^i) \quad (1.3.3.)C.$$

From the action principle one can easily prove - from here - that \hat{H}^* is a constant of motion provided, that neither \hat{H} or \hat{H}^* are explicit functions of time, but depend upon it only through $q(t)$, $p(t)$ or $q^i(t)$, $p^i(t)$.

This method is followed in sections 3.1 and 3.2 for the ideal Bose gas and for the interacting problem of ^4He . The results obtained there parallel those of Umezawa⁽⁶⁶⁾ and Coniglio and Marinaro⁽¹⁸⁾ to some extent; even though the formulations here and there are conceptually different. Here it is shown that a hamiltonian, \hat{H}^* , exists^(*) in the separable phase space picture for both problems. For the interacting problem, however, the hamiltonian \hat{H}^* is *not* fully diagonal in the L.C.S.R.; this representation

(*) Different from the particle hamiltonian, \hat{H} , in general.

turns out to be not elaborate enough as to accomplish the exact diagonalization of the newly obtained hamiltonian. This parallels the fact that the *particle* hamiltonian, \hat{H} , is not fully diagonal in the representations adopted in Refs. (18,66); which are particular cases of the more general L.C.S.R. used here.

To achieve diagonalization an iterative scheme must be devised along similar lines as that of Umezawa, but not quite exactly like it. The general idea of this scheme is to use the non-diagonal segment of H' (or of H in Umezawa's method) to generate even more general representations of states. At infinite order of such an iterative procedure Umezawa obtained the 'physical representation', in terms of which \hat{H} was shown to be diagonal - except for some contributions, Q_V , which vanish in the infinite volume limit. Here the proposed strategy is the same^(*) the structure of the separable phase space is *not* changed, by the iterative procedure, but only the definition of dynamical variables in terms of the ever more general fields is. In consequence the expression for \hat{H} as a functional of generalized coordinates and momenta is *not* changed, but the expression in terms of newly obtained fields is. Hopefully one ends up with *another* physical representation, in terms of which \hat{H}' should be diagonal. It is *conjectured* that the diagonalization of \hat{H}' -from the present setting-would be more general than Umezawa's; in the sense that terms of the form of Q_V (i.e. non-diagonal, but negligible in the bulk limit) should *not* arise. This is due to the fact that in Umezawa's approach only *low* order dangerous (diverging) contributions are cancelled out, namely those proportional to *linear* and *quadratic* (non-diagonal) contributions in *elementary excitation operators of the zeroth order trial representation*. Here, on the other hand, an *exact* condition of cancellation is obtained and employed to obtain \hat{H}' . Such a condition is expressed in terms of the dynamical variables - not in terms of elementary excitation operators of

(*) but the hamiltonian are actually different.

the zeroth order trial representation - hence it holds at all orders of iteration. Furthermore, it involves not only *low* order dangerous contributions (proportional to first and second powers in the *dynamical variables*) but *also high* order dangerous contributions (proportional to third and fourth powers). In particular the non-diagonal perturbation is *free* from these dangerous contributions here, unlike in Umezawa's method. For this reason non-diagonal contributions to \hat{H}' such as \hat{Q}_V should *not* arise here, and diagonalization should be proved in the *finite* volume limit.

Now, as to the number operator in the present scheme, it is noted that this functional, \hat{N}' , is determined from the structure of the separable phase space. This functional is given as the local limit, $k' \rightarrow k$, of the most general one-object propagator, $\hat{G}(k', k)$, that can be constructed in Γ_S , namely

$$\left. \begin{aligned} \hat{G}(k', k) &= \sum_i p_k^i q_k^i \\ \hat{N}' &= \sum_k \hat{N}'_k = \sum_{i,k} p_k^i q_k^i \end{aligned} \right\} \quad (1.3.4.)C.$$

It is noted that contributions of the form $p_k^i q_k^j$ (for $i \neq j$) do *not* arise in \hat{G} or \hat{N}' , due to the fact that such contributions make reference to *two* distinguishable objects.

The number functional in the non-separable phase space, Γ_{ns} , is given by

$$\hat{N} = \sum_k \hat{p}_k \hat{q}_k \quad (1.3.5.)C,$$

thus, from $\hat{p}_k = \sum_i p_k^i \hat{q}_k = \sum_i q_k^i$ it follows that \hat{N}' and \hat{N} are *not* the same functionals, i.e.

$$\hat{N} = \hat{N}' + \sum_{\substack{i,j \\ (i \neq j)}} p_k^i q_k^j \quad (1.3.6.)C.$$

This will prove to amount to a very significant difference. When the linear coherent state representation is introduced and canonical variables p^i, q^i are defined in terms of the fields of this representation, it will be possible to appreciate that \hat{N}' is diagonal in L.C.S.R. Furthermore that \hat{N}' is the diagonal part of \hat{N} in this representation. Hence if the hamiltonian in the separable phase space picture is diagonal in the L.C.S.R. (as is the zeroth order hamiltonian \hat{H}_0) the commutativity of \hat{H}_0 and \hat{N}' is ensured.

One can also prove that \hat{N}' is a constant of motion from the canonical equations - properly expressed in terms of generalized poisson brackets - arising from the action principle, i.e. by showing $\{\hat{H}', \hat{N}'\} = 0$ (1.3.7.)C,

where

$$\{A, B\} = \sum_{i,k} \frac{\partial A}{\partial q^i} \frac{\partial B}{\partial p^i} - \frac{\partial A}{\partial p^i} \frac{\partial B}{\partial q^i} \quad (1.3.8.)C,$$

for arbitrary functionals defined in the separable phase space.

Now, some or all of the new variables p^i, q^i may be quantum fields (in general there is a good reason - put forward in Chapter Four - for choosing q^i and p^i to be all quantum fields if \hat{p} and \hat{q} are); hence to prove that \hat{H}', \hat{N}' are simultaneously observable (besides being both constants of motion) one must show

$$[\hat{H}', \hat{N}'] = 0 \quad (1.3.9.)C$$

in addition to $\{\hat{H}', \hat{N}'\} = 0$, where the commutator refers to the Hilbert space of state amplitudes containing a vacuum for the quantum fields in (p^i, q^i) , i.e. $q_k^i |C_0\rangle = 0 = \langle C_0 | p_k^i$ for all k and some i . Both (1.3.7,9)C are proven in Chapter Three.

In order to prove that the expectation values of \hat{N} and \hat{N}' are the same, it will be shown in §2.4 that the normalizing postulate

$$\langle n | \hat{N} | n \rangle = \langle C_n | \hat{N} | C_n \rangle$$

where $|C_n\rangle$ are linear coherent states, entails

$$\langle n|\hat{N}|n\rangle = \langle C_n|\hat{N}'|C_n\rangle,$$

or in terms of the volumes of the phase spaces Γ_{ns} and Γ_s , $\text{Vol}(\Gamma_{ns}) = \text{Vol}(\Gamma_s)$. Similarly, the same normalization postulate is shown to entail

$$\langle n|\hat{H}|n\rangle = \langle C_n|\hat{H}'|C_n\rangle ;$$

proving that both number and energy eigenvalues are the same in both formulations. This together with the fact that the zeroth order hamiltonian, \hat{H}_0' , and \hat{N}' commute and are diagonal in L.C.S.R., and - in addition - are both constants of motion, suffices to entail dynamical equivalence in the present context.

Let us summarize now some of the implications arising in the present theory, in comparison with those of the works reviewed in §1.2.

The general ideal of current dynamical theories is that of diagonalizing the *particle* hamiltonian in a non-equivalent representation of the same commutation relations. Here the idea is different; one aims at *finding* the hamiltonian for *new dynamical objects*, other than particles. In the former case one finds difficulties in diagonalizing the particle hamiltonian - difficulties of the same nature as arise here in diagonalizing \hat{H}' ; one must go to infinite order within a given iterative scheme to get \hat{H} (there) or \hat{H}' (here) diagonal for interacting problems. Eventually one is content - in current theories - with introducing some approximation into the exact \hat{H} (neglecting some non diagonal segment). In this work one neglects some contributions from \hat{H}' in order for this functional to be a diagonal *hamiltonian* (i.e. depending only on generalized coordinates and momenta, but independent of generalized velocities). The main difference is that while the diagonalized *particle* hamiltonian \hat{H}_0 does not commute with the number of *particle* operator. The unperturbed hamiltonian \hat{H}_0' (for the new dynamical objects) *does* commute here with the number operator \hat{N}' .

This entails that from the present view no lagrangian symmetry is broken. The difficulty as to a broken hamiltonian symmetry, and the way in which it is resolved, points out the cause of trouble: Hamiltonian invariance under non-equivalent transformation; once one replaces the statement of hamiltonian invariance by that of Lagrangian invariance no problem arises.

The standard treatment of the problem - given in the works examined in §1.2 - shows two distinctive features: one is that the dynamical objects are *still* regarded as *particles* (of which elementary excitations are just but *convenient* variables); the second feature is entailed by the first and is that the hamiltonian is actually regarded as the same *particle* hamiltonian \hat{H} , which is then diagonalized in a representation other than its natural one. However, no similar compensation can be justified for \hat{N} and leads to the pseudo problem of a broken hamiltonian symmetry. If the problem is properly formulated from the outset, in terms of new dynamical objects, no problems arise at all; furthermore, the notion of anomalous averages does *not* arise, for, the only meaningful averages are those involving variables associated with new objects and anomalous averages for these vanish identically.

The involvement of diagonalization conditions in the standard approach will be seen to have counterparts also in the present approach. The corresponding conditions (enabling here the existence of a hamiltonian) are shown to follow from the fact that action principle is *redundant* in the formulation of the problem in terms of separable phase space. The removal of the redundancy - which is always admissible on logical grounds - will be shown to have the same effect as the diagonalization conditions, i.e. compensating some contributions which prevent the existence of a hamiltonian. The antecedent of the condition of compensation of dangerous diagrams, enabling here the existence of hamiltonian and ensuring in the standard approach diagonalization of \hat{H} , is seen here to arise from the action principle, instead of from the minimal ground state energy, as in existing theories.

The diagonalization conditions in the standard approach involve some conditions concerning the coefficients of non-diagonal contributions in elementary excitation operators. These conditions concern *low* order powers in elementary excitations, namely linear and quadratic. Here the cancellation is an exact one, involving low as well as *high* order contributions (proportional to cubic and quartic contributions).

This amounts to a notable difference; for, now *all* dangerous diagrams cancel out. The unperturbed hamiltonian, H_0' , as well as the perturbation, are free from dangerous contributions (leading to divergencies of the perturbation expansion). For that reason it is believed that Umezawa's result as to hamiltonian symmetry rearrangement should follow in a more simple and general fashion from the present point of view, and also hold in the *finite* volume limit, not only in the bulk limit as it presently stands.

D. Resolution of the Unperturbed Problem in the Random Phase Approximation

The exact hamiltonian, \hat{H} , in the separable phase space is split up here into two parts, one diagonal-defining the unperturbed problem - and the other non-diagonal, regarded as a perturbation, generating a series of representations which hopefully converges to the physical representation. The unperturbed hamiltonian, obtained in §3.2, is four-linear (not bi-linear as in the standard method of Umezawa). From a technical point of view the dynamical problem posed by \hat{H}_0' is as difficult to solve as the exact problem in terms of particle operators. It is recalled that the unperturbed hamiltonian should be chosen not solely with respect to its ready solvability, but also on the basis of it being a good *hamiltonian* and diagonalizable in the C.S.R. To solve exactly the unperturbed problem posed here one should use already infinite order perturbation theory. However, the position here is that if the present approach is to be any good - besides resolving the conceptual difficulties as to symmetry breakdown and the prediction of

superfluid behaviour - it must prove that predictions as to the spectrum in the standard R.P.A. are in good qualitative agreement with experiment.

The unperturbed problem is formulated in the R.P.A. in section §3.3. It will become clear that, due to the fact that the problem is already formulated in terms of elementary excitations and c-number fields, the *standard* version of the R.P.A. suffices, the generalized version of Anderson being not needed at all. In fact the notion of anomalous averages which emerges in Anderson's R.P.A. does not appear in the present formulation.

Three excitation spectra are obtained, corresponding to the three pairs of dynamical variables associated with the fields of the linear coherent state representation employed here (defined in §2.3). The solutions for the spectra, obtained in §3.3, are for a *pure state* description. The effective hamiltonian for one pair of variables (those associated with first order coherent fields) is seen to be invariant under a certain - phonon-like - transformation, proposed by Bogoljubov^(8,9) and discussed by Hohenberg⁽³⁷⁾ and others⁽⁶⁹⁾, which ensures that the dispersion relation for these fields is gapless and linear in the long wave limit. The other two branches, corresponding to the other two pairs of variables, are seen to be the same and to exhibit a gap - the same gap as obtained by many authors before.

The question of rearrangement of gauge invariance and of the coupling of all fields to an external field of velocity is considered in section §4.1. Gauge transformations in the separable phase space are obtained and Lagrangian invariance under gauge transformation is explicitly tested. The transformation laws for all variables involved are also obtained in section 4.2 and the Euler-Lagrange equations of a *complete* Gauge theory of superfluidity are found.

Section §4.3. is concerned with the evaluation of the first two reduced density matrices, for a *unique* system in a *pure state* description. It is shown that for such an ideal system (independent of statistics!) O.D.L.R.O. occurs in both reduced density matrices independently.

The statistical problem is finally posed in section §4.4. A non-superfluid ensemble is constructed first from configurations in the separable phase space. It is shown that the thermal average amplitude of first and second order coherent fields is identically zero in the non-superfluid ensemble. This entails that no O.D.L.R.O. occurs for this ensemble.

Several options of superfluid ensembles are considered, and reduced to only one; the other possibilities being discarded as they do not reproduce experimental results. The remaining option identifies the pairing fields with the order parameter. First order coherent fields are seen to be identified with part of the *normal* fluid. A surprising feature is that as a result of the peculiar statistical counting the upper two branches - which are identical in a pure state description - now *split* into *two separate* branches defining the extremities of an excitation *band*. This band very much resembles the band discovered by Cowley and Woods^(19,43), which they attributed to a multi-phonon (and multi-roton) scattering spectrum, i.e. to optical modes associated with the gapless (one-phonon) acoustic mode. Here, a radically different interpretation - arising naturally - is given.

O.D.L.R.O. is shown to occur in the second reduced density matrix for the superfluid ensemble reproducing best the experimental data. O.D.L.R.O. in the first reduced density matrix, however, is *ruled out*. Finally the integral equations characterizing the present mean field model in thermal equilibrium are given. Due to the difference in statistical counting these equations do not resemble previous integral equations given by Luban and Evans and Imry. Finally, the condition for the existence of a superfluid solution in the above sense is stated.

Further developments are considered in a final section. Firstly, the benefits and difficulties of a more general purely quantum representation are discussed. Secondly, a coherent state representation for fermions is proposed, exhibiting first-order coherence and not open to the indictment put forward by Yang⁽⁷¹⁾. Some conclusions of the theory of the Bose superfluid are extrapolated to the theory of superconductivity.

Finally, a coherent representation appropriate to describe ferromagnetic and spin-glass phases is proposed. It is conjectured that a theory of ferromagnetism, and of spin-glasses, can be constructed along the lines of the present theory of superfluidity, free from a breakdown of rotational symmetry. The elements of a classification of phase transitions is also discussed here.

§2. BASIC DEFINITIONS AND NOTATION

§2.1. Introduction

This chapter is devoted to introducing the definitions of a separable phase space, dynamical equivalence and linear coherent state representation (L.C.S.R.) together with a brief investigation of the properties associated with these definitions. It will also serve the purpose of establishing notation for future use.

The notions of separable phase space and dynamical equivalence are introduced in §2.2. It is shown there that the main properties of separable spaces is that the volume of the whole spaces is the sum of the volumes of separate spaces composing it, and that an ensemble constructed from such separable spaces always admits restricted ensembles.

As to dynamical equivalence, the general idea is that a given physical system is *identified* through its *Lagrangian* operator, *not* by its *hamiltonian* and that a dynamically equivalent formulation of the same problem in terms of an alternative set of variables should leave the group of lagrangian invariances unaltered; the idea that both formulations must possess the same hamiltonian is *abandoned*. A method for demonstrating dynamical equivalence is also given in §2.2.

A L.C.S.R. is formally defined in §2.3. as the canonical mapping from the representation of the number of particles. An explicit expression linking elementary operators of both representations is obtained, some elementary properties of L.C.S.R. are considered and several quantum averages of interest are evaluated. A practical limitation of general coherent state representation beyond the linear case is also noted here.

The canonical variables of the separable phase space - introduced in §2.2. - are explicitly defined in section 2.4. in terms of the fields involved in the L.C.S.R. Finally, the question of interpreting some of these variables with superfluid variables is briefly discussed.

§2.2. Definition of Separable Phase Space and the Notion of Dynamical Equivalence (D.E.)

The present theory of superfluidity is *articulated* by two conceptually different elements. The one is an analytically testable characterization of a superfluid, developed purely on statistical grounds, whilst the other is a reformulation of the dynamical problem free from the occurrence of a breakdown of symmetry. The latter is capable of yielding predictions concerning the excitation spectrum, which - at finite order of perturbation - are in qualitative agreement with experiment, in the finite volume limit. The statistical question, however, will be considered first leaving the discussion on dynamics to the second part of this section.

A. Separable Phase Space

The characterization of a superfluid proposed here stems from the theoretical possibility of discriminating at least two independent sets of configurations, from an ensemble of systems^(*) defined over the phase space. Ensembles admitting such a discrimination are commonly referred to as Restricted Ensembles (R.E.).

A R.E. is said here to characterize a superfluid and accordingly called Superfluid Ensemble (S.E.) if and only if the thermal average of the distribution is an *additive* functional of at least two sets of independent configurations, and if configurations of at least one set are all statistically equivalent.

It is rather simple to see that the above characterization of a superfluid coincides with the paradigmatic view of a superfluid in Landau's two fluid (hydrodynamic) model. In fact, as a result of a statistical equivalence, an additive part of the total density is fully ordered; whilst all particles - in both the ordered and non-ordered parts - are capable of exchanging the available energy, momentum and number; particles in the

(*) of the same or different size

ordered part, however, cannot turn mechanical energy into heat,^(*) for they cannot dissipate energy without increasing their entropy.

It is most convenient to normalize the volume of the phase space to the total number of particles $N^{(**)}$ and to rephrase the necessary and sufficient conditions defining a S.E. in terms of properties of the phase space itself - on the one hand - and as a rule for counting ensemble configurations on the other.

A necessary definitory condition of S.E. is that the ensemble be defined over a *separable phase space*, Γ_S , involving several independent pairs of mutually canonical variables (defined over independent domains S_i), such that the volume of Γ_S is the summation of the volumes of the independent domains, i.e.

$$\text{Vol}(\Gamma_S) = \sum_i \text{Vol}(S_i) \quad (2.2.1.)A.$$

R.E.'s defined over a separable phase space are called *additive* restricted ensembles. A. S.E. is an additive R.E. possessing at least one fully ordered part; otherwise is called Non-Superfluid Ensemble (N.S.E.).

It is noted that it is the property of statistical equivalence which actually incorporates the superfluid properties of the ensemble; the N.S.E. obtained from the elimination of statistical equivalence constitutes a pole of reference to test whether it is energetically favourable for a given system to evolve into a superfluid phase from a normal phase, or - indeed - whether a superfluid solution is possible at all. This question will be considered in Chapter Four.

Throughout this work the following phase space will be considered:

$$\Gamma_S \equiv \bigoplus_{i=1} S_i \quad (2.2.2.)A$$

(*) either individually or collectively

(**) either fix or variable, small or large number.

where S_i are independent phase spaces of the *same* dimension, but whose canonical fields are defined over formally different wave vector domains, symbolically

$$S_i \equiv \{(p_{k_i}^i, q_{k_i}^i)\} \quad (2.2.3.)A^{(*)}$$

where $p^i = (q^i)^+$. It is noted that wave vectors k' and k have been specified further by an index 'i'; this indicates that generalized coordinates and momenta q^i, p^i and q^j, p^j are defined over different domains for $i \neq j$, i.e. $k_i \in K_i \neq K_j$, even though they take the same spectrum of numerical values^(**). This distinguishability has already been mentioned.

It is important to note that definition (2.2.2,3.)A is not restricted to 'q' or 'c'-number variables. In fact, these variables will be associated with both 'q' and 'c' number fields for the most part of this work.

It is rather simple to prove that Γ_S - as defined by (2.2.2,3)A - is a separable phase space. The presence of independent fields is already ensured by construction and it only remains to prove (2.2.1.)A. For this purpose note that the most general one-object functional of both canonical variables that can be constructed from S_i is

$$G_1^i(k', k) \equiv p_{k'}^i q_k^i \quad (2.2.4.)A$$

The number distribution functional in S_i is the local limit, $k' \rightarrow k$, of $G_1^i(k', k)$, i.e.

$$N_k^i = p_k^i q_k^i \quad (2.2.5.)A$$

A generic configuration in S_i is taken - as usual - to be given by the expectation values of generic number distributions in S_i , namely

(*) the symbols $p_{k_j}^i$ etcetera are not defined for $i \neq j$, and p_k^i is $p_{k_i}^i$ at $k_i = k$.

(**) determined by boundary conditions.

$$C_k^i \equiv \text{Tr}\{p_k^i q_k^i\} \quad (2.2.6.)A .$$

The trace is taken over a representation of states obtained as the direct product of the various sets of eigenstates of the number *operator* functionals in S_i , namely: $N^i = \sum_k \hat{N}_k^i$, for the quantum fields involved, or any other representation related to this by canonical transformation.

The volume of S_i is given by the summation over k of configurations C_k^i , i.e.

$$\text{Vol}(S_i) \equiv \sum_k C_k^i \quad (2.2.7.)A$$

$$= \text{Tr}\{\hat{N}^i\} \quad (2.2.8.)A .$$

Now, the most general one-object functional that can be constructed over the whole Γ_S is

$$G_1(k', k) = \sum_i p_k^i q_k^i \quad (2.2.9.)A .$$

It is recalled that a contribution of the form $\sum_{i \neq j} p_k^i q_k^j$ does *not* occur in \hat{G}_1 , since it makes reference to *two* distinguishable objects. The number distribution in Γ_S is

$$N_k = \sum_i p_k^i q_k^i \quad (2.2.10.)A$$

$$= \sum_i N_k^i \quad (2.2.11.)A .$$

A generic configuration in Γ_S is given by

$$\begin{aligned} C_k &= \sum_i \text{Tr}\{p_k^i q_k^i\} \\ &= \sum_i C_k^i \end{aligned} \quad (2.2.12.)A ,$$

and hence the volume of Γ_S is

$$\begin{aligned} \text{Vol}(\Gamma_S) &= \sum_k C_k \\ &= \sum_{i,k} C_k^i = \sum_i \text{Vol}(S_i) , \end{aligned}$$

which is the desired condition (2.2.1.)A; or in terms of the total number expectation values

$$\begin{aligned} N' &= \text{Tr} \left\{ \sum_k N'_k \right\} \\ &= \sum_i N^i \end{aligned} \quad (2.2.13.)A .$$

It is noted that (2.2.1.)A is a consequence of the involvement of distinguishability in (2.2.3.)A. Should this *not* be present additivity would be *lost*.

From the above considerations it follows that the partition function for an ensemble defined over Γ_S , given by

$$Z = \sum_{\vec{C}_k} \text{Tr} \{ \hat{\Omega} \} \quad (2.2.14.)A$$

where $\hat{\Omega}$ is the thermal density operator, is expressible as

$$Z = \sum_{\vec{C}_k^1} \sum_{\vec{C}_k^2} \dots \sum_{\vec{C}_k^l} \dots \text{Tr} \{ \hat{\Omega} \} \quad (2.2.15.)A ,$$

which is the well known expression for a R.E. ^(28,45). The main property of a R.E. is that the (quantum and) thermal average of functionals defined over only one space, S_l , is independent of the weighted counting of configuration over the other separate parts of the ensemble, i.e.

$$\langle \langle \hat{A}_{k_l} \rangle \rangle = \text{Tr} \left\{ \sum_{\vec{C}_k^l} \hat{A}_{k_l} \hat{\Omega} \right\} / \sum_{\vec{C}_k^l} \text{Tr} \{ \hat{\Omega} \} \quad (2.2.16.)A .$$

Should the part of the ensemble-defined over S_l - be fully ordered, then (2.2.16.)A reduces to

$$\langle \langle \hat{A}_{k_l} \rangle \rangle = \text{Tr} \{ \hat{A}_{k_l} \hat{\Omega}(\vec{C}_k^l) \} / \text{Tr} \{ \hat{\Omega}(\vec{C}_k^l) \} \quad (2.2.17.)A ,$$

where the *representative configuration* \vec{C}_k^l is that satisfying the normalization condition (if any).

Consider a *superfluid* ensemble specified by the set of all statistically equivalent configurations, say C_k^i for $i < \ell$. The partition function for such an ensemble is

$$Z_s = \sum_{C_k^{\ell+1}} \sum_{C_k^{\ell+2}} \dots \text{Tr}\{\hat{\Omega}\} \quad (2.2.18.)A.$$

The corresponding *non-superfluid* ensemble, on the other hand, is associated with the partition function

$$Z_{ns} = \sum_{C_k^1} \sum_{C_k^2} \sum_{C_k^{\ell}} \sum_{C_k^{\ell+1}} \dots \text{Tr}\{\hat{\Omega}\} \quad (2.2.19.)A,$$

involving summations over *all* sets of configurations.

A superfluid solution will be energetically favourable if the free energy obtained from Z_s is lower or equal than from Z_{ns} , i.e. if

$$F_n - F_s = -KT \ln(Z_{ns}/Z_s) > 0 \quad (2.2.20.)A$$

$$\equiv -KT \ln Z_o > 0 \quad (2.2.21.)A,$$

where

$$Z_o = \sum_{C_k^1} \dots \sum_{C_k^{\ell}} \text{Tr}\{\hat{\Omega}\} \quad (2.2.22.)A.$$

The equal sign determines the critical temperature, signalling the transition from the normal to superfluid phases or viceversa. Leaving now aside the statistical problem, let us consider next the question of whether a dynamical problem formulated in terms of variables of a non-separable phase space can be *reformulated equivalently* in terms of variables of a separable phase space.

B. Dynamical Equivalence

Consider a quantum system identified by the Lagrange operator $L(\hat{q}, \hat{q})$ functional of one pair of generalized coordinates and velocities,

\hat{q}, \hat{q}^* , defined over a non-separable domain. The dynamical problem is completely specified by the group of lagrangian invariances and by the expectation values of all the commuting constants of motion. For the kind of hamiltonian problem considered here, L can be expressed as

$$L(\hat{q}, \hat{q}^*) = \frac{1}{2} \sum_k [\hat{q}_k^* \hat{q}_k + (\hat{q}_k)^* \hat{q}_k] - \hat{H}(\hat{q}, \hat{q}^*) \quad (2.2.1.)B,$$

where $H(q, q^*)$ is the hamiltonian functional of the generalized coordinates and momenta \hat{q}_k, \hat{p}_k , the latter being defined through

$$\hat{p}_k \equiv \partial \hat{L} / \partial \hat{q}_k = \hat{q}_k^* \quad (2.2.2.)B.$$

The phase space, $\Gamma_{ns} = \{(\hat{p}_k, \hat{q}_k)\}$, is non-separable.

Consider a set of variables of a separable space linearly related to \hat{q}, \hat{q}^* and \hat{p} i.e.

$$\hat{q}_k = \sum_i q_k^i; \hat{q}_k^* = \sum_i q_k^{i*}; \hat{p}_k = \sum_i p_k^i \quad (2.2.3.)B^{(*)}$$

this relation enables us to express \hat{L} as a functional of q^i, q^{i*} . Let us denote by \hat{L}_{ns} and \hat{L}_s the expressions for the same Lagrangian, \hat{L} , in terms of \hat{q}, \hat{q}^* and q^i, q^{i*} , respectively.

The two formulations of dynamics posed by L_{ns} and L_s are dynamically equivalent if and only if (i) the symmetries of L_{ns} and L_s are *rearranged* and (ii) if the expectation values for the constants of motion are the same, irrespective of the domain of definition of the dynamical variables.

The name symmetry rearrangement was coined by Umezawa⁽⁶⁶⁾ to refer to a situation in which the same hamiltonian is diagonal in two non-equivalent representations, i.e. is really *hamiltonian* symmetry rearrangement. Here the connotation of symmetry rearrangement is more general, in that it also incorporates the rearrangement of the gauge symmetry - in particular - and of all Lagrangian invariances, in general. For simplicity the analysis here is confined to two lagrangian invariances, connected with conservation of

(*) The hat ^ on variables p^i, q^i, q^{i*} is not introduced since some of the dynamical variables are c-number fields.

energy and number; the analysis of other invariances - whether related to conservation properties or not - should follow a similar path. The symmetry is rearranged if there is a one-to-one correspondence between unitary transformations in r_{ns} and r_s leaving L_{ns} and L_s invariant, respectively. (*)

L_{ns} is invariant under transformations shifting the zero of the time scale, and under local gauge transformations, amongst other invariances. The generator of two such transformations in the non-separable phase space are

$$U_t \equiv \exp[i\hat{H}(t-t_0)/\hbar] \quad (2.2.4.)B$$

and
$$U_g \equiv \exp[i\int_k S_k \hat{N}_k] \quad (2.2.5.)B,$$

respectively, provided that \hat{p}, \hat{q} are q-numbers and that \hat{H} does not depend explicitly on time; S_k is an arbitrary c-number function, independent of time, and \hat{N}_k is the particle number distribution operator. For the kind of systems considered here, \hat{H} and $\hat{N} = \sum_k \hat{N}_k$ commute in the particle representation (or in any other representation linearly related to it by canonical transformation).

Non-separable variables transform according to

$$\hat{q}_k \rightarrow \bar{\hat{q}}_k = \hat{U} \hat{q}_k \hat{U}^{-1} \quad (2.2.6.)B$$

$$\hat{p}_k \rightarrow \bar{\hat{p}}_k = \hat{U} \hat{p}_k \hat{U}^{-1} \quad (2.2.7.)B,$$

where \hat{U} is either \hat{U}_t or \hat{U}_g ; $\bar{\hat{q}}_k = \hat{q}_k \exp[i\omega_k(t-t_0)]$ for U_t and $\bar{\hat{q}}_k = \hat{q}_k \cdot \exp[iS_k]$ for U_g . The invariance of L_{ns} under gauge transformations can only be shown in the presence in L_{ns} of a compensating vector field, A,

(*) Note that due to the fact that canonical variables are the adjoint of each other, i.e. $p_k^\dagger = (q^\dagger)^\dagger$, $\hat{p}_k = (\hat{q}_k)^\dagger$, symmetry transformations of coordinates (at its canonical conjugate) are, in fact, defined from the phase spaces.

transforming as $A \rightarrow A + \text{const. } k.S_k$ ⁽⁷²⁾.

These invariances are equivalent to the statements

$$(d\hat{H}/dt) = 0, \quad (d\hat{N}/dt) = 0 \quad (2.2.8.)B,$$

or, in view of the fact that the hamiltonian is the evolution operators of canonical variables as indicated by the Heisenberg equations -

$$\begin{aligned} i\hbar \partial_t \hat{p}_k &= [\hat{H}, \hat{p}_k] \\ -i\hbar \partial_t \hat{q}_k &= [\hat{H}, \hat{q}_k] \end{aligned} \quad (2.2.9.)B,$$

it follows that the invariance of L_{ns} under transformations (2.2.6,7.)B is equivalent to the statements

$$(d\hat{H}/dt) = 0, \quad [\hat{H}, \hat{N}] = 0 \quad (2.2.10.)B.$$

To prove symmetry rearrangement one, must show (i) that the expression L_s admits a hamiltonian \hat{H}' , for generalized momenta defined by (2.2.3.)B, i.e. that p_k^i satisfy

$$p_k^i = \partial \hat{L}_s / \partial q_k^i \quad (2.2.11.)B,$$

and that \hat{H}' is a constant of motion, i.e. $(d\hat{H}'/dt) = 0$ and (ii) that the number operator in r_s , namely \hat{N}' , is time independent too, i.e. $(d\hat{N}'/dt) = 0$. It is most important to note that $(d\hat{N}/dt) \neq 0$ is *not* required, for this is *not* the number operator in r_s . The condition of time independence of \hat{N}' can be re-expressed as

$$(\hat{H}', \hat{N}') = 0 \quad (2.2.12.)B,$$

where $\{\hat{A}, \hat{B}\}$ is the generalized Poisson bracket

$$\{\hat{A}, \hat{B}\} = \sum_{i,k} \left(\frac{\partial \hat{A}}{\partial q_k^i} \frac{\partial \hat{B}}{\partial p_k^i} - \frac{\partial \hat{A}}{\partial p_k^i} \frac{\partial \hat{B}}{\partial q_k^i} \right) \quad (2.2.13.)B.$$

This bracket reduces to a commutator if all variables p_k^i, q_k^i are q-numbers.

This is not the case here; hence (2.2.12.)B ensures the time independence of \hat{N}' but does not guarantee that \hat{H}' and \hat{N}' have the same set of eigenstates. This must be proved independently through

$$[\hat{H}', \hat{N}'] = 0 \quad (2.2.14.)B,$$

where the commutator now makes reference to the same set of states mentioned after eq. (2.2.6.)A.

Now, as to the second property required for dynamical equivalence - concerning the same predictions as to expectation values it is noted here that the identity must be a strict one, satisfied by *individual* systems, not only at an ensemble level. In other words,

$$\text{Tr}\{\hat{N}\} = \text{Tr}\{\hat{N}'\} \quad (2.2.15.)B$$

$$\text{Tr}\{H\} = \text{Tr}\{H'\} \quad (2.2.16.)B$$

must be satisfied for every sub-system of an ensemble. It is *not* required that higher momenta of the distribution of energy and number be the same but only their average values.

(2.2.15.)B can be written as

$$\text{Vol}(\Gamma_{ns}) = \text{Vol}(\Gamma_s) \quad (2.2.17.)B$$

this condition cannot be fixed - *a priori* - since the variables of Γ_{ns} and Γ_s are related to each other. One must derive (2.2.17.)B as an identity. As will be made clear in Chapter Three this imposes a limitation on the possible definitions of p^i , q^i in terms of the fields of certain representations. For now, it suffices to point out that (2.2.15,16.)B follow if the quantum field in Γ_s are related to those fields in Γ_{ns} by canonical transformation. One can then prove that taking

$$\text{Tr}\{N\} = \langle n | \hat{N} | n \rangle = \langle C_n | \hat{N} | C_n \rangle = N \quad (2.2.18.)B,$$

as a postulate - where $|C_n\rangle = \pi T_i |n\rangle$ are eigenstates of \hat{N}' - implies

(2.2.15.)B; similarly $\langle n | \hat{H} | n \rangle = \langle Cn | \hat{H} | Cn \rangle$ should entail $\text{Tr}\{\hat{H}\} = \text{Tr}\{\hat{H}^{\sim}\}$.

It is noted that the number of independent symmetry transformations in Γ_s can be larger than in Γ_{ns} . The strategy here is to introduce a link among the transformations in separate spaces, so that the numbers of degrees of freedom are the same in both descriptions and the overall symmetry is rearranged. This matter will be further discussed in §4.2.

§2.3. Definition of Linear Coherent State Representation (L.C.S.R.)

Consider the well known Particle Representation (P.R.), also known as representation of the number of particles. In momentum basis P.R. is characterized by an orthonormal and complete set of state amplitudes, $\{|n_k\rangle\}$, $\sum_k n_k = n$ for all n , and by particle creation and annihilation operators a_k^+ and a_k . The latter satisfy Bose commutation relations

$$[a_k, a_k^+] = \delta_{k,k} \quad (2.3.1.),$$

$$[a_k, a_{k'}] = 0 = [a_k^+, a_{k'}^+] \quad (2.3.2.).$$

Periodic boundary conditions are assumed and volume is taken as unity, momentum is - thus - a discrete label taking any one of the possible values

$$k_n = 2\pi n; \quad n = 0, \pm 1, \dots, \pm N \quad (2.3.3.),$$

where N is the total number of ${}^4\text{He}$ atoms (known as a datum).

Single particle states are eigenstates of the number operator

$$\hat{N} \equiv \sum_k \hat{N}_k \equiv \sum_k a_k^+ a_k \quad (2.3.4.),$$

yielding total number as an eigenvalue, i.e.

$$\hat{N}|n\rangle = N|n\rangle \quad (2.3.5.).$$

The *generalized* version of a C.S.R. is given as the canonical mapping from P.R., according to transformation τ_G , defined as

$$\tau_G \equiv \exp \hat{\theta}_G \quad (2.3.6.),$$

where

$$\hat{\theta}_G \equiv \sum_{p,q,k,\dots} [(\sigma_p a_p^\dagger + \gamma_{p,q} a_p^\dagger a_q^\dagger + \delta_{p,k,q} a_p^\dagger a_q^\dagger a_k^\dagger + \dots) - \text{C.C.} + i \epsilon_{p,q} a_p^\dagger a_q] \quad (2.3.7.),$$

where σ_p , $\gamma_{p,q}$ and $\delta_{p,q,k}$, etc and their complex conjugate (C.C.) are complex, time dependent, abelian c-number fields. These are independent of each other and also of a_k^\dagger, a_k and satisfy the following very important definitory properties; $\epsilon_{p,q}$ is real.

$$|\sigma_p| = |\sigma_{-p}|, \quad \epsilon_{p,q} = \epsilon_{q,p}, \quad \epsilon_{p,p} = 0 \quad (2.3.8.),$$

$$\gamma_{p,q} = \gamma_{q,p} = \gamma_{-p,-q} \quad (2.3.9.),$$

$$\begin{aligned} \gamma_{p,q} \gamma_{p^-,q^-} &= |\gamma_{p,q}|^2 \delta_{p,p} \delta_{q,p} + \\ &+ |\gamma_{p,p}|^2 \delta_{p,q} \delta_{p^-,q} (1 - \delta_{p,p^-}) \end{aligned} \quad (2.3.10.).$$

The dash on the summation in (2.3.7.) indicates that multiple counting is to be avoided. δ 's and other multiple valued c-numbers satisfy similar properties as (2.3.9,10.). Such conditions bring about a remarkable algebraic simplicity without which advance would be impossible. The transformation $\tau_G^{(*)}$ is unitary (in fact $\hat{\theta}^\dagger = -\hat{\theta}$, hence $\tau_G^\dagger = \tau_G^{-1}$). In addition, $\hat{\theta}$ is the most general polynomial of either a_k^\dagger (exclusive) or a_k not commuting with \hat{N} . A simpler transformation will be used throughout this work. This is obtained by neglecting all c-number fields from δ onwards. Such a second order transformation - denoted by $\tau^{(**)}$, comprises and generalizes Glauber's⁽³¹⁾ and Bogoljubov-Valatin's transformations (6,7,67,68) to include also pairs of non-zero overall momentum.

(*) the hat on transformation generators as well as in elementary operators is omitted.

(**) The simpler version of a C.S.R. obtained from the transformation of P.R. according to τ is called L.C.S.R.

The vacuum state amplitude of L.C.S.R. is given by

$$|C_0\rangle = \tau|0\rangle \quad (2.3.11.),$$

and the corresponding creation and annihilation elementary excitation operators by

$$\alpha_k^+ = \tau a_k^+ \tau^{-1} \quad (2.3.12.)$$

$$\alpha_k = \tau a_k \tau^{-1} \quad (2.3.13.).$$

An orthonormal set of C.S. is obtained - as usual - by applying, successively the operator α_k^+ on $|C_0\rangle$ i.e.

$$|C_n\rangle = \prod_k (\eta_k!)^{-1/2} (\alpha_k^+)^{\eta_k} |C_0\rangle \quad (2.3.14.)$$

where $\sum_k \eta_k = n$.

The present version of coherent states differs from that of Glauber in the sense that all states $|C_n\rangle$ are defined for *the same* value of the c-number fields σ_k and $\gamma_{k,q}$; in consequence, the set $\{|C_n\rangle\}$ is orthogonal and *complete*, *not* non-orthogonal and over-complete as for the type of C.S. employed in the theory of lasers. The reason for resorting to the present set - instead of a Glauber-like set - rests on the fact that the kind of statistical counting envisaged here is different from that of the so-called P-representation. A more detailed discussion of this aspect will be given in Chapter Four.

The mathematical complexity of transformations τ_G and τ is enormous. The cumbersome algebra involved in the Baker-Hausdorff-Campbell theorem^(**) prevents their expression as a multiplication for different wave vector modes. In order to evaluate (2.3.12,13) explicitly and exactly, one must devise a method yielding the exact result without factorizing τ ; this is done in Appendix A where the following relations are obtained.

(**) see for instances, A. Messiah, 'Quantum Mechanics' (North Holland Pub. Co., Amsterdam, 1964), Vol. I, p.442.

$$\left. \begin{aligned} \alpha_k^+ &= \sum_q (u_{k,q} a_q^+ - v_{k,q}^* a_q) + \rho_k^* \\ \alpha_k &= \sum_q (u_{k,q}^* a_q - v_{k,q} a_q^*) + \rho_k \end{aligned} \right\} \quad (2.3.15.)$$

where

$$\left. \begin{aligned} u_{k,q} &\equiv \cosh(X_k) \delta_{k,q} + i(\epsilon_{k,q}/X_k) \sinh(X_k) \\ v_{k,q} &\equiv (\gamma_{k,q}/X_k) \sinh(X_k) \\ X_k &= \sum_t |X_{t,k}|; \quad |X_{t,k}|^2 = |\gamma_{t,k}|^2 - (\epsilon_{t,k})^2 \end{aligned} \right\} \quad (2.3.16.)$$

$$\begin{aligned} \rho_k^* &= (\sigma_k \sum_t \gamma_{k,t}^* - i \sigma_k^* \sum_t \epsilon_{t,k}) [\cosh(X_k) - 1] / X_k^2 - \\ &- (\sigma_k^* / X_k) \sinh(X_k) \end{aligned} \quad (2.3.17.)$$

$$\phi_k^* = \sum_q (u_{k,q} \rho_q^* + v_{k,q}^* \rho_q) \quad (2.3.18.)$$

$$\text{From (2.3.16.) it follows that } \sum_q (|u_{k,q}|^2 - |v_{k,q}|^2) = 1 \quad (2.3.19.)$$

which, in turn, enables to show that the α 's are Bose field operators, i.e.

$$[\alpha_k^+, \alpha_{k'}^+] = [\alpha_k, \alpha_{k'}] = 0 \quad (2.3.20.)$$

$$[\alpha_k, \alpha_{k'}^+] = \delta_{k,k'} \quad (2.3.21.)^{(*)}$$

Relations (2.3.15.) are central in this work. From their inspection it is clear that they are the most general linear relations between particle and elementary excitation operators; furthermore, they admit an inverse, namely

$$a_k^+ = \sum_q (u_{k,q} a_q^+ + v_{k,q}^* a_q) + \phi_k^* \quad (2.3.22.)$$

$$a_k = \sum_q (u_{k,q}^* a_q + v_{k,q} a_q^*) + \phi_k \quad (2.3.23.)$$

(*) This result is obvious from (2.3.12,13.)

these relations are obtained by multiplying the upper relation of (2.3.15.) by $u_{k,t}$ and the lower one by $v_{k,t}^*$, summing over k and using the defining properties (2.3.10.), which can be restated more conveniently as follows:

$$v_{p,q} v_{k,q}^* \equiv |v_{k,q}|^2 \quad (2.3.24.)$$

$$v_{p,q} v_{k,q} \equiv (v_{k,q})^2 \quad (2.3.25.)$$

$$u_{p,q} u_{k,q}^* \equiv |u_{k,q}|^2 \quad (2.3.26.) .$$

Should third and/or higher powers of a 's be involved in $\hat{\theta}$ expressions (2.3.15.) would be an infinite series as shown in Appendix A. Even in this case, however, the first three terms of the series would be those of (2.3.15.).

The operator number of elementary excitations is given by

$$\hat{n} \equiv \sum_k \hat{n}_k = \sum_k a_k^* a_k \quad (2.3.27.) .$$

Coherent states $|C_\eta\rangle$ are eigentstates of \hat{n} yielding the number of elementary excitations as eigenvalue, i.e.

$$\hat{n}|C_\eta\rangle = \eta|C_\eta\rangle \quad (2.3.28.) ,$$

as follows from (2.3.5,12-14.).

It can be readily tested that number operators of P.R. and linear C.S.R. do *not* commute, indicating that these two representations are non-equivalent representations of the same (Bose) commutation relations, in the sense of Araki⁽³⁾ and Umezawa⁽⁶⁶⁾. From this, however, one cannot conclude - as will be shown - that the gauge symmetry is inevitably broken.

The notion of normal ordering satisfied by P.R. is also satisfied by linear C.S.R. In effect the properties

$$a_k^+ |n\rangle = (n_k + 1)^{\frac{1}{2}} |n+1\rangle \quad (2.3.29.)$$

$$a_k |n\rangle = n_k^{\frac{1}{2}} |n-1\rangle \quad (2.3.30.)$$

and their conjugate relations, entail (2.3.31.)

$$\alpha_k^+ |C_n\rangle = (\eta_k + 1)^{\frac{1}{2}} |C_{n+1}\rangle \quad (2.3.32.)$$

$$\alpha_k |C_n\rangle = \eta_k^{\frac{1}{2}} |C_{n-1}\rangle \quad (2.3.33.),$$

and their conjugates. In particular, the following relations are satisfied

$$\alpha_k |C_0\rangle = \langle C_0 | \alpha_k^+ = 0 \quad (2.3.34.) ,$$

which defines $|C_0\rangle \equiv |0\rangle$ as the vacuum state amplitude of L.C.S.R.

The average of any operator of P.R. can be easily evaluated over Linear Coherent States (L.C.S.) by replacing particle operators by elementary excitation operators according to (2.3.22,23) and making use of (2.3.32-34.). Some averages of interest are:

(i) the average amplitude of particles

$$\langle C_n | a_k | C_n \rangle = \phi_k \quad (2.3.35.) ,$$

(ii) the average amplitude of pairs

$$\begin{aligned} \langle C_n | a_k a_q | C_n \rangle &= \phi_k \phi_q + \sum_t [u_{k,t}^* v_{q,t} \eta_t + \\ &+ v_{k,t} u_{q,t}^* (\eta_t + 1)] \end{aligned} \quad (2.3.36.)$$

$$\equiv \bar{x}_{k,q} \equiv \phi_k \phi_q + x_{k,q} \quad (2.3.37.),$$

where η_k is the average number of elementary excitations

$$\langle C_n | \alpha_k^+ \alpha_k | C_n \rangle = \eta_k \quad (2.3.38.) .$$

(iii) The average number of particles

$$\langle C_\eta | \hat{N} | C_\eta \rangle = \sum_{k,q} [|\phi_k|^2 + |u_{k,q}|^2 \eta_q + |v_{k,q}|^2 (\eta_q + 1)] \equiv N \quad (2.3.39.)$$

It is important to note that the L.C.S.R. is defined such that the average number of particles is the same when evaluated in the particle representation as in L.C.S.R. This amounts to rescaling the number of elementary excitations (whose number would otherwise equal N).

(iv) The average energy corresponding to the particle hamiltonian

$$\hat{H} = \sum_k \epsilon_k a_k^\dagger a_k + \frac{1}{2} \sum_{p,\ell,q} V(\ell) a_{p+\ell}^\dagger a_{p-\ell}^\dagger a_p a_q \quad (2.3.40.)$$

is given by

$$\begin{aligned} \langle C_n | \hat{H} | C_n \rangle &= \sum_k j_k' N_k - \frac{1}{2} \sum_{p,k} B_{p,k}^* \chi_{p,k} + \\ &+ \frac{1}{2} \sum_{p,\ell,q} V(\ell) \phi_{p+\ell}^* \phi_{q-\ell}^* \phi_q \phi_p + F \end{aligned} \quad (2.3.41.)$$

$$\text{where} \quad j_k' \equiv \epsilon_k + \frac{1}{2} \sum_{\ell} [V(0) + V(\ell)] N_{k+\ell} \quad (2.3.42.)$$

$$B_{p,k}^* = - \sum_p V(\ell) \chi_{p+\ell,k-\ell}^* \quad (2.3.43.)$$

where F involves fluctuations about mean field averages, the dash on the summations denotes the exclusion of terms in $\ell=0$ and $p+\ell = q$.

It can be readily tested that the above average expressions coincide with those of Valatin and Butler⁽⁶⁸⁾ for $\phi_k = \phi_k^* = 0$ and $v_{k,q} = u_{k,q} = 0$ for $k \neq -q$, as they should.

The condition

$$\langle n | \hat{N} | n \rangle = \langle C_\eta | \hat{N} | C_\eta \rangle \quad (2.3.44.)$$

has been used by most authors in the field in a heuristic fashion. It ensures that the (normal) phase space's hypervolume is the same irrespective of the representation of states employed; such a condition is not tautologically satisfied, however; on the contrary its validity - taken here (as elsewhere) as a postulate - entails that the average number of elementary excitations is re-scaled, in the sense that the *identity*

$$\langle n | \hat{N} | n \rangle \equiv \langle C_n | \hat{N} | C_n \rangle \quad (2.3.45.)$$

is no longer valid. In effect the L.H.S. of (2.3.45.) is equal to N - the total number of particles - should (2.3.45.) hold, then $\sum_k \eta_k = N$; hence, according to (2.3.38.) $\langle C_n | \hat{N} | C_n \rangle$ is greater than N (for $|\phi_k|^2$ and $|v_{k,q}|^2$ different from zero). Conversely should (2.3.38.) hold - as is the case here - (2.3.45.) cannot be true. The relevance of this comment will become clear in §3.2.

§2.4. Definition of Separable Phase Space Variables in terms of Fields of L.C.S.R.

There are, in principle, several ways in which dynamical variables p^i , q^i can be defined in terms of the three pairs of canonical fields of L.C.S.R. Most authors employing coherent state representations adopt the viewpoint that the only *dynamical* fields are α_k^+ and α_k ; i.e. they define

$$\hat{p}_k^1 \equiv \alpha_k^+, \quad \hat{q}_k^1 \equiv \alpha_k \quad (2.4.1.),$$

in analogy with \hat{p}_k , \hat{q}_k defined over the particle representation as

$$\hat{p}_k \equiv a_k^+, \quad \hat{q}_k \equiv a_k \quad (2.4.2.).$$

It is clear, however, that the phase space $\Gamma^1 = \{(p_k^1, q_k^1)\}$ is not separable. Furthermore, the number operator in Γ^1 is $\hat{n} \equiv \sum_k \alpha_k^+ \alpha_k$, however, if $\text{Tr}(\eta) = N$; hence from (2.3.39) $\text{Tr}(N) = \langle C\eta | N | C\eta \rangle$ is larger than N . Thus $\text{Tr}(N) \neq \text{Tr}(\eta)$. In consequence the volumes of the phase spaces^(*) are *not* the same.

Presently the following definition is adopted:

$$\left. \begin{aligned} \hat{p}_k^1 &\equiv \sum_q v_{k,q} \alpha_q^+, \quad \hat{q}_k^1 \equiv \sum_q u_{k,q}^* \alpha_q, \quad \hat{q}_k^1 \equiv i\hbar \partial_t q_k^1 \\ \hat{p}_k^2 &\equiv \sum_q v_{k,q}^* \alpha_q, \quad \hat{q}_k^2 \equiv \sum_q v_{k,q} \alpha_q^+, \quad \hat{q}_k^2 \equiv i\hbar \partial_t \hat{q}_k^2 \\ \hat{p}_k^3 &\equiv \phi_k^*, \quad \hat{q}_k^3 \equiv \phi_k, \quad \hat{q}_k^3 \equiv i\hbar \partial_t q_k^3 \end{aligned} \right\} \quad (2.4.3.).$$

Provided that α_k^+ and α_k are defined through (2.3.12,13) the following identities are satisfied

$$\hat{p}_k = \sum_i p_k^i, \quad q_k = \sum_i q_k^i, \quad \hat{q}_k \equiv \sum_i q_k^i \quad (2.4.4.),$$

as anticipated in §2.2.

The number operator in the separable spaces Γ_s is

(*) Normalized to $\text{Tr}(N)$ and $\text{Tr}(\eta)$, respectively.

$$\hat{N}' = \sum_{k,q} |u_{k,q}|^2 \alpha_q^* \alpha_q + |v_{k,q}|^2 (\alpha_q^* \alpha_q + 1) + |\phi_k|^2 \quad (2.4.5.)$$

i.e. \hat{N}' is diagonal in L.C.S.R. It is clear from this that the number operators \hat{N}' and \hat{N} are simply related through

$$\hat{N} = \hat{N}' + \text{non-diagonal terms} ,$$

where the non-diagonal terms are non-diagonal in both P.R. and L.C.S.R.; in other words \hat{N} and \hat{N}' are the diagonal part of each other in the other's representation. From this alone it follows that $\text{Tr}\{N\} = \text{Tr}\{N'\}$. Let us see this in more detail

$$N = \langle n | N | n \rangle = \langle C_n | \hat{N} | C_n \rangle \quad (2.4.6.)$$

and from expression (2.3.39) for $\langle C_n | \hat{N} | C_n \rangle$ it follows that

$$N = \sum_{k,q} [|u_{k,q}|^2 n_q + |v_{k,q}|^2 (n_q + 1) + |\phi_k|^2] \quad (2.4.7.)$$

Finally, (2.4.5,7) imply, $N = \text{Tr}\{N'\} \equiv N'$. It is noted that any other definition - as (2.4.1.) for instance - would render

$$\text{Tr}\{N\} = \text{Tr}\{N'\}$$

and

$$\langle n | N | n \rangle = \langle C_n | N | C_n \rangle$$

in consistent.

One interesting observation as to the canonical variables - as defined in (2.4.3.) - is that neither of them individually is a boson field, in fact

$$[\hat{q}_k^1, \hat{p}_k^1] = \sum_{q,q'} u_{k,q}^* u_{k',q'} - \delta_{q,q'}$$

$$[\hat{q}_k^2, \hat{p}_k^2] = - \sum_{q,q'} v_{k,q} v_{k',q'}^* - \delta_{q,q'}$$

$$[q_k^3, p_k^3] = 0 .$$

The dynamical objects represented in the space $S_1 \otimes S_2$, however, are bosons,

i.e.

$$[(\hat{q}_k^1 + \hat{q}_k^2), (\hat{p}_k^1 + \hat{p}_k^2)] = \sum_{q,q'} u_{k,q}^* u_{k',q'} \delta_{q,q'} - \sum_{q,q'} v_{k,q} v_{k',q'}^* \delta_{q,q'}$$

or from (2.3.30-36)

$$= \sum_q (|u_{k,q}|^2 - |v_{k,q}|^2) \delta_{k,k'} \\ = \delta_{k,k'}$$

To end up this chapter let us consider the question of identifying the superfluid configurations. So far, nothing has been said about this *semantic* question. A common prejudice - shared by the author until fairly late stages in this research - is that the superfluid segment of the total density *must* be identified with the c-number segment of \hat{N} , i.e.

$$\hat{N} \equiv \sum_{\text{normal } k,q} (|u_{k,q}|^2 + |v_{k,q}|^2) n_q$$

$$N \equiv \sum_{\text{superfluid } k,q} (|v_{k,q}|^2 + |\phi_k|^2)$$

It is noted, however, that there is no reason why this *should* be so. In fact, it will become clear in Chapter Four that for the present definition of dynamical variables the first order coherent density segment $\sum_k |\phi_k|^2$ *cannot* be fully ordered, otherwise the thermal properties would not at all resemble those of $^4\text{HeII}$ at low temperatures. Only if another different phase space is envisaged, namely one including a further pair of first order coherent variables i.e.

$$p_k^1 = \sum_q u_{k,q} \beta_q^+, p_k^2 = \sum_q v_{k,q}^* \beta_q^-, p_k^3 = \phi_k^*, p_k^4 = \bar{\phi}_k^*$$

where

$$\beta_k^+ \equiv \tau_1 \alpha_k^+ \tau_1^{-1}, \beta_k^- \equiv \tau_1 \alpha_k^- \tau_1^{-1}$$

$$\tau_1 = \exp \sum_k (\bar{\phi}_k \alpha_k^+ - \phi_k^* \alpha_k^-)$$

satisfying

$$\hat{p}_k = \sum_i p_k^i$$

is it possible to regard either $|\phi_k|^2$ or $|\bar{\phi}_k|^2$ (but not both) as part of the superfluid. This latter possibility will not be considered in this thesis.

§3 Dynamics in a Separable Phase Space (S.P.S.)

This Chapter is concerned with the reformulation, in terms of the dynamical variables of a S.P.S., of the Bose problem originally posed in terms of the variables of a Non-Separable Phase Space (N-S.P.S.).

The problem of the Ideal Bose Gas (I.B.G.) is considered first in §3.1. It is shown that such a problem admits *equivalent* formulations in terms of the variables of both N-S.P.S. and S.P.S. The canonical eqs. of motion in the S.P.S. picture are obtained. The notions of overall and relative equilibrium within the S.P.S. is discussed. Finally, the connection between the present method of reformulation of the dynamical problem and the standard method of Bogoljubov and Valatin and Butler is elucidated.

The interacting problem is considered in §3.2. It is shown that the dynamical problem *cannot* be reformulated *exactly* in the S.P.S. *if* the dynamical variables are defined in terms of the fields of L.C.S.R., but *only if* defined in terms of 'the physical representation'; which is obtained by iteration starting from the L.C.S.R. A zeroth order problem is isolated such that dynamical equivalence holds.

The zeroth order problem for the interacting case obtained in §3.2. is a non-linear problem. This problem is posed in the mean field approximation (M.F.A.) in section 3.3. The three branches of the excitation spectrum are evaluated on the basis of a pure state description. The lowest branch is gapless, and corresponds to the dynamical variables $p_k^3 = \phi_k^*$ and $q_k^3 = \phi_k$. The two upper branches corresponding to the variables p_k^1, q_k^1 and p_k^2, q_k^2 are identical and exhibit a gap.

§3.1. The Problem of the Ideal Bose Gas (I.B.G.)

The dynamical problem of the I.B.G. is of importance here - from a theoretical point of view - because it is *the only* problem which admits *equivalent* formulations in terms of the variables of Non-Separable Phase

space (N-S.P.S.) and separable phase space (S.P.S.), defined in terms of the elementary fields of the P.R. and the L.C.S.R., respectively. In order to produce an equivalent, *exact reformulation* of the interacting problem in terms of variables of the S.P.S., the latter variables *must* be defined in terms of the fields of a certain, very complex, *non-linear* representation of coherent states; and requires of the use of infinite order perturbation techniques in order to prove dynamical equivalence.

An analysis of the problem of the I.B.G. here will help to elucidate the notions of symmetry rearrangement and dynamical equivalence and to expose the conceptual advantages of the present method compared with the standard one. It will also help to lay the foundations to approach the interacting problem.

The problem of the I.B.G. in a non-separable domain is posed by the non-relativistic lagrangian

$$\hat{L}_{ns}(\hat{q}, \hat{q}) = \frac{1}{2} \sum_k (\hat{q}_k^* \hat{q}_k + \text{c.c.}) - \hat{H}_{IBG} \quad (3.1.1.)$$

$$\text{where} \quad \hat{H}_{IBG} = \sum_k \epsilon_k \hat{q}_k^* \hat{q}_k \quad (3.1.2.),$$

$$\epsilon_k \equiv (\hbar^2/2m)k^2 \quad (3.1.3.).$$

(3.1.1.) can be regarded as a Legendre transformation from a lagrangian formulation - in terms of \hat{q}, \hat{q} and their c.c. - to a hamiltonian formulation, in terms of canonical variables $\hat{p}_k = \hat{q}_k^*$ and \hat{q}_k . In effect, defining generalized momenta as

$$\hat{p}_k \equiv \partial \hat{L}_{ns} / \partial \hat{q}_k \quad (3.1.4.)$$

$$\text{one finds} \quad \hat{p}_k = \hat{q}_k^* \quad (3.1.5.),$$

hence (3.1.1.) can be written as

$$\hat{L}_{ns}(\hat{q}, \hat{q}) = \frac{1}{2} \sum_k (\hat{p}_k \hat{q}_k + \text{c.c.}) - \hat{H}_{IBG}(\hat{p}, \hat{q}) \quad (3.1.6.),$$

$$\text{where } \hat{H}_{IBG}(\hat{p}, \hat{q}) = \sum_k \epsilon_k \hat{p}_k \hat{q}_k \quad (3.1.7.).$$

(3.1.6.) effects a transformation from the variables of the non-separable domain $D_{ns} \equiv \{(\hat{q}_k, \hat{q}_k)\}$ to the variables of the N-S.P.S. $\Gamma_{ns} \equiv \{(\hat{p}_k, \hat{q}_k)\}$.

The total number of bosons is a fixed number, N ; the container is assumed to have a unit volume, and to be subjected to periodic boundary conditions.

The variables of the non-separable domains are defined in terms of the fields of the P.R. as follows:

$$\hat{q}_k \equiv a_k, \quad \hat{p}_k \equiv a_k^*, \quad \hat{q}_k = i\hbar \partial_{a_k} \quad (3.1.8.),$$

this is consistent with (3.1.5.). The number operator in the N-S.P.S., Γ_{ns} , is

$$\hat{N} = \sum_k \hat{p}_k \hat{q}_k = \sum_k a_k^* a_k \quad (3.1.9.),$$

\hat{N} and \hat{H}_{IBG} commute in the P.R., i.e.

$$\begin{aligned} [\hat{H}_{IBG}, \hat{N}]_{P.R.} &\equiv \sum_k \left(\frac{\partial \hat{H}_{IBG}}{\partial a_k} \frac{\partial \hat{N}}{\partial a_k^*} - \frac{\partial \hat{H}_{IBG}}{\partial a_k^*} \frac{\partial \hat{N}}{\partial a_k} \right) \\ &= 0 \end{aligned} \quad (3.1.10.).$$

Both lagrangian and hamiltonian formulations of the action principle are equivalent in the absence of constraints in D_{ns} or Γ_{ns} . The canonical eqs. of motion from a hamiltonian formulation of the action principle,

$$\delta \int \hat{H}_{IBG} dt = 0 \quad (3.1.11.),$$

are

$$-i\hbar\partial_t\hat{p}_k = [\hat{H}_{IBG}, \hat{p}_k] \quad (3.1.12.)$$

$$-i\hbar\partial_t\hat{q}_k = [\hat{H}_{IBG}, \hat{q}_k]$$

Similarly, the evolution eq. for an arbitrary operator, \hat{A} , in Γ_{ns} is given by

$$-i\hbar\partial_t\hat{A} = [\hat{H}_{IBG}, \hat{A}] \quad (3.1.13.)$$

It follows from (3.1.10,13) that both \hat{H}_{IBG} and \hat{N} (among other operators) are constants of motion, and simultaneously observables in the P.R., with well-defined eigenvalues

$$E_n^m = \langle n | \hat{H}_{IBG} | n \rangle, \quad n = \langle n | \hat{N} | n \rangle \quad (3.1.14.)$$

It is noted that $|n\rangle$ denotes here a generic n -particle state of arbitrary distribution, n_k , subject to the condition $\sum_k n_k = n$. Hence $|n\rangle$ corresponds to several energy eigenstates E_n^m . Note that no condition has been introduced so far restricting the number eigenvalue, n , to the exact (known) number of particles, N .

The constants of motion \hat{H}_{IBG} and \hat{N} generate two unitary transformations, \hat{U}_t and \hat{U}_g , respectively. These transformations induce a shift of the zero of the time scale and a local gauge transformation, respectively. Lagrangian \hat{L}_{ns} is invariant under both transformations (in the presence of Yang-Mills⁽⁷²⁾ compensating field for the latter transformation). Further comments on the relationship between conservation laws and lagrangian invariances is given in §4.1.

Let us now introduce a change of lagrangian variables, from (\hat{q}, \hat{q}) - defined in the non-separable domain D_{ns} - to (\hat{q}^i, \hat{q}^i) , defined in the separable domain $D_s \equiv \bigoplus_{i=1}^3 D_i$, $D_i \equiv \{(q_k^i, q_k^i)\}$. These variables are related through

$$\hat{q}_k = \sum_i \hat{q}_k^i, \quad \hat{q}_k = \sum_i \hat{q}_k^i \quad (3.1.15.)^{(*)}$$

(*) $\hat{q}_k^i \equiv i\hbar\partial_t q_k^i$

The immediate objective here is to prove that $\hat{L}_{ns}[\hat{q}(q^i), \hat{q}(\dot{q}^i)] \equiv \hat{L}_s(q^i, \dot{q}^i)$ admits a Legendre transformation of the form

$$\hat{L}_s(q^i, \dot{q}^i) = \frac{1}{2} \sum_{i,k} (p_k^i \dot{q}^i + \text{c.c.}) - \hat{H}_{IBG}(p^i, q^i) \quad (3.1.16.),$$

such that the generalized momenta, defined through

$$p_k^i \equiv \partial \hat{L}_s / \partial \dot{q}_k^i \quad (3.1.17.),$$

satisfy

$$\hat{p}_k = \sum_i p_k^i \quad (3.1.18.)$$

and

$$p_k^i = q_k^{i+} \quad (3.1.19.).$$

This ensures the existence of a hamiltonian in the S.P.S. picture.

Substituting (3.1.15.) in (3.1.1.) one obtains

$$\hat{L}_s(q^i, \dot{q}^i) = \hat{L}_s'(q^i, \dot{q}^i) - \hat{H}_R(q^i, \dot{q}^i) \quad (3.1.20.),$$

$$\text{where} \quad \hat{L}_s'(q^i, \dot{q}^i) \equiv \frac{1}{2} \sum_{i,k} (q_k^{i+} \dot{q}^i + \text{c.c.}) - \hat{H}_{IBG}'(q^i, \dot{q}^{i+}) \quad (3.1.21.),$$

$$\hat{H}_{IBG}' \equiv \sum_{i,k} \epsilon_k q_k^{i+} \dot{q}_k^i \quad (3.1.22.)$$

$$\hat{H}_R \equiv (1/2) \sum_{i,j,k}^{(i \neq j)} (q_k^{i+} \lambda_k^j + \text{c.c.}) \quad (3.1.23.),$$

$$\text{and} \quad \lambda_k^j \equiv -\dot{q}_k^j + \epsilon_k q_k^j \quad (3.1.24.)$$

$$= -\dot{q}_k^j + \partial \hat{H}_{IBG}' / \partial p_k^j \quad (3.1.24'.).$$

It seems, at first sight, that a hamiltonian does not exist in the S.P.S. picture; for, \hat{L}_s does not satisfy (3.1.17-19.). In effect, \hat{L}_s' satisfies

$$\partial \hat{L}_s' / \partial \dot{q}_k^i = q_k^{i+} \quad (3.1.25.),$$

but due to the fact that \hat{H}_R is a functional of the generalized velocities,

\hat{q}_k^i , \hat{L}_S itself cannot satisfy (3.1.17-19.); hence, $\hat{H}_{IBG} + \hat{H}_R$ cannot be regarded as a hamiltonian (independent of \hat{q}_k^i). The very presence of \hat{H}_R seems to spoil our programme.

The difficulty, however, is only apparent, and its resolution will be seen to bring about most important consequences. It happens that the action, formulated in terms of the dynamical variables of the separable domain, is *redundant*; in the sense that lagrangian \hat{L}_S involves a contribution, \hat{H}_R , in the form of dynamical constraints

$$\hat{H}_R \equiv (1/2) \sum_{i,j,k}^{(i \neq j)} (\hat{p}_k^i \hat{R}_k^j + \text{c.c.}) ,$$

where \hat{R}_k^j satisfy $\hat{R}_k^j = 0$, and these constraints are identical to the Euler-Lagrange (E-L) eqs. for the generalized coordinates obtained from the action principle.

To show this, it will be most illuminating to incorporate an external force field in order to consider the most general case. In the non separable domain the lagrangian in the presence of external force fields is

$$\hat{L}_{ns}^F = \hat{L}_{ns} + \hat{H}_F + \hat{L}_F \quad (3.1.26.) ,$$

$$\text{where } \hat{H}_F = (1/2) \sum_k (\hat{q}_k^i \hat{F}_k^i + \hat{q}_k^{i*} \hat{F}_k^{i*}) . \quad (3.1.27.) .$$

It is recalled that $\hat{p}_k = \hat{q}_k^+$, expressed in terms of lagrangian variables, \hat{L}_{ns} in (3.1.26.) is given by (3.1.1-2). \hat{L}_F is the lagrangian for the force field itself; there is no need to introduce this expression, for the interest here is on the matter field equations, not with the equations for the force field itself. Accordingly \hat{L}_F will be omitted in the future.

Now, changing variables $(q, \dot{q}) \rightarrow (q^i, \dot{q}^i)$, and regarding \hat{F}_k as the resultant force acting upon separate spaces, S_1 , i.e.

$$\hat{F}_k = \sum_i \hat{F}_k^i \quad (3.1.28.) ,$$

one obtains the following lagrangian in the separable domain picture

$$\hat{L}_S^F = \hat{L}_S^F - \hat{H}_R^F \quad (3.1.29.),$$

where

$$\hat{L}_S^F \equiv \hat{L}_S^F + \hat{H}_F^F \quad (3.1.30.)$$

$$\hat{H}_R^F \equiv \hat{H}_R - \hat{H}_F^F \quad (3.1.31.),$$

where \hat{L}_S^F and \hat{H}_R are given by (3.1.21,22) and (3.1.23,24), respectively, and

$$\hat{H}_F^F \equiv (1/2) \sum_{i,k} (p_k^i \hat{F}_k^i + F_k^i q_k^i) \quad (3.1.32.)$$

$$\hat{H}_F^F \equiv (1/2) \sum_{i,j,k}^{(i \neq j)} (p_k^i \hat{F}_k^j + \hat{F}_k^j q_k^i) \quad (3.1.33.)$$

Note that \hat{H}_R^F can be expressed as

$$\hat{H}_R^F = (1/2) \sum_{i,j,k}^{(i \neq j)} (p_k^i \hat{R}_k^j + \hat{R}_k^j q_k^i) \quad (3.1.34.)$$

where

$$\hat{R}_k^j \equiv \hat{\lambda}_k^j - \hat{F}_k^j \quad (3.1.35.).$$

The action principle in the separable domain is given by the following statement:

$$\delta_i \int \hat{L}_S^F dt = 0, \quad \text{for } i = 1, 2, 3 \quad (3.1.36.),$$

where the symbol δ_i indicates independent variation respect to q_k^i or \dot{q}_k^i , for $i = 1, 2, 3$; thus, (3.1.36.) comprises six independent conditions. The E-L equations for the generalized coordinates obtained from (3.1.36.) are

$$\sum_j (\hat{\lambda}_k^j - \hat{F}_k^j) = 0, \quad i = 1, 2, 3 \quad (3.1.37.);$$

that is, the *independent* E-L equations for q_k^1 , q_k^2 and q_k^3 turn out to be linear combinations of each other, in fact, *identical*!

This feature of the formulation of the dynamical problem in terms of variables of a separable domain is to be understood as follows: The lagrangian \hat{L}_S^F incorporates an additive contribution, $-\hat{H}_R$, introducing some *constraints*,

namely $\hat{R}_k^j = 0$. These constraints, however, convey no new information; these are, in fact, equivalent to the E-L equations which follow from the action principle in the absence of \hat{H}_R . In other words, the constraints are redundant.

The removal of the redundancy is effected by replacing, in \hat{H}_R , the generalized forces, λ_k^j , by their actual (known) values F_k^j , in which case $\hat{R}_k^j \equiv 0$ and hence $\hat{H}_R \equiv 0$. The source of the trouble thus disappears, and one is lead to the conclusion that $\hat{L}_S^F \equiv \hat{L}_S'^F$, or $\hat{L}_S \equiv \hat{L}_S'$ in the absence of external forces.

After the redundancy is removed - by setting $\hat{H}_R \equiv 0$ - one finds that \hat{H}_{IBG} is the hamiltonian in the S.P.S. picture. That is (3.1.16.) holds and \hat{H}_{IBG}' is given by

$$\hat{H}_{IBG}' = \sum_{i,k} \epsilon_k p_k^i q_k^i \quad (3.1.38.).$$

Now, in the absence of constraints in D_S or Γ_S , the action principle in the S.P.S. picture can be formulated in terms of the hamiltonian \hat{H}_{IBG}' , leading to the following canonical equations of motion

$$\left. \begin{aligned} -i\hbar \partial_t p_k^i &= \partial \hat{H}_{IBG}' / \partial q_k^i \\ i\hbar \partial_t q_k^i &= \partial \hat{H}_{IBG}' / \partial p_k^i \end{aligned} \right\} \quad (3.1.39.).$$

Defining the generalized Poisson bracket as

$$\{\hat{A}, \hat{B}\} \equiv \sum_{i,k} [(\partial \hat{A} / \partial q_k^i)(\partial \hat{B} / \partial p_k^i) - (\partial \hat{A} / \partial p_k^i)(\partial \hat{B} / \partial q_k^i)] \quad (3.1.40.),$$

or

$$\{\hat{A}, \hat{B}\} = \sum_i \{\hat{A}, \hat{B}\}_i \quad (3.1.41.),$$

where

$$\{\hat{A}, \hat{B}\}_i = \sum_k [(\partial \hat{A} / \partial q_k^i)(\partial \hat{B} / \partial p_k^i) - (\partial \hat{A} / \partial p_k^i)(\partial \hat{B} / \partial q_k^i)] \quad (3.1.42.).$$

Equation (3.1.17.) can be rewritten as

$$\left. \begin{aligned} -i\hbar \partial_t p_k^i &= \{\hat{H}_{IBG}^i, p_k^i\} \\ -i\hbar \partial_t q_k^i &= \{\hat{H}_{IBG}^i, q_k^i\} \end{aligned} \right\} \quad (3.1.43.).$$

The evolution in time of arbitrary operators in Γ_s is governed by the following equation of motion:

$$-i\hbar \partial_t \hat{A} = \{\hat{H}_{IBG}^i, \hat{A}\} \quad (3.1.44.).$$

From this equation it follows that \hat{H}_{IBG}^i is a constant of motion, and that the number operator, \hat{N}^i - given by

$$\hat{N}^i = \sum_{i,k} p_k^i q_k^i \quad (3.1.45.) -$$

is also a constant of motion if and only if

$$\{\hat{H}_{IBG}^i, \hat{N}^i\} = 0 \quad (3.1.46.).$$

This condition can be readily verified by inspection, using the general property of Poisson brackets

$$\{\hat{A}, \hat{B}\hat{C}\} = \{\hat{A}, \hat{B}\}\hat{C} + \hat{B}\{\hat{A}, \hat{C}\} \quad (3.1.47.).$$

The condition (3.1.46.) implies that \hat{N}^i is a constant of motion, however, it does *not* ensure that \hat{H}_{IBG}^i and \hat{N}^i possess a common set of linear coherent eigenstates. In order to prove this one must show that \hat{H}_{IBG}^i and \hat{N}^i commute in the L.C.S.R., i.e.

$$[\hat{H}_{IBG}^i, \hat{N}^i]_{\text{L.C.S.R.}} = 0 \quad (3.1.48.),$$

where

$$\begin{aligned} [\hat{A}, \hat{B}]_{\text{L.C.S.R.}} &= \sum_k [(\partial \hat{A} / \partial \alpha_k) (\partial \hat{B} / \partial \alpha_k^*) - \\ &\quad - (\partial \hat{A} / \partial \alpha_k^*) (\partial \hat{B} / \partial \alpha_k)] \end{aligned} \quad (3.1.49.).$$

This can be easily verified by replacing p_k^i and q_k^i in (3.1.38., 45.) by their definitory expressions in terms of α 's and working out the commutator

(3.1.48.) using

$$[\alpha_k, \alpha_k^\dagger] = \delta_{k,k}, \quad (3.1.50.),$$

or alternatively - from the knowledge that \hat{N}' is diagonal in L.C.S.R. - simply by showing that \hat{H}'_{IBG} is also diagonal in the same representation.

The facts that a hamiltonian exists, that \hat{H}'_{IBG} and \hat{N}' are constants of motion and commute in L.C.S.R., suffices to prove that the hamiltonian and gauge symmetries are rearranged. The fact that the eigenvalues of \hat{N} and \hat{N}' over particle states and linear coherent states, respectively, are the same has already been proven in Chapter 2. Hence, in order to prove dynamical equivalence it only remains to show that the traces of \hat{H}'_{IBG} and \hat{H}_{IBG} over particle states and L.C.S., respectively, are the same. This is shown very simply by writing \hat{H}_{IBG} as follows:

$$\hat{H}_{IBG} = \hat{H}'_{IBG} + \frac{1}{2} \sum_{i,j,k}^{(i \neq j)} (p_k^i \epsilon_k^j q_k^j + c.c.) \quad (3.1.51.).$$

It can be readily tested that $p_k^j q_k^i$ expressed in terms of either α 's or a 's is non-diagonal in both representations, thus

$$\text{Tr}(\hat{H}_{IBG}) = \text{Tr}(\hat{H}'_{IBG}) \quad (3.1.52.),$$

which completes the proof of dynamical equivalence.

It is interesting to note that the condition (3.1.48.) is more restrictive than (3.1.46.). It will be convenient to express the commutator in terms of the Poisson bracket to find out the nature of the former condition. Using the chain's rule the commutator in L.C.S.R. can be written as^(*)

*It can be readily proved that the commutators in the P.R. and the L.C.S.R. are the same, i.e. $[A,B]_{P.R.} = [A,B]_{L.C.S.R.}$. This is a general feature of any two linearly related canonical representations.

$$\begin{aligned}
[A, B] = & \sum_{i, k, k'} \{ [(\hat{A}/\partial q_k^i), (\partial q_k^i/\partial \alpha_k)] \cdot \\
& \cdot (\partial \hat{B}/\partial q_k^i), (\partial q_k^i/\partial \alpha_k^+) + \\
& + (\partial \hat{A}/\partial p_k^i), (\partial p_k^i/\partial \alpha_k) \cdot \\
& \cdot (\partial B/\partial p_k^i), (\partial p_k^i/\partial \alpha_k)] - \\
& - [(\partial \hat{A}/\partial q_k^i), (\partial q_k^i/\partial \alpha_k^+) \cdot \\
& \cdot (\partial \hat{B}/\partial q_k^i), (\partial q_k^i/\partial \alpha_k) + \\
& + (\partial \hat{A}/\partial p_k^i), (\partial p_k^i/\partial \alpha_k^+) \cdot \\
& \cdot (\partial B/\partial p_k^i), (\partial p_k^i/\partial \alpha_k)] \}
\end{aligned}$$

The question of ordering does not arise; for, the partial derivatives $(\partial q_k^i/\partial \alpha_k)$, $(\partial q_k^i/\partial \alpha_k^+)$, $(\partial p_k^i/\partial \alpha_k^+)$ and $(\partial p_k^i/\partial \alpha_k)$ are all c-numbers; working out these derivatives from (2.4.3.) one finds

$$\begin{aligned}
[\hat{A}, \hat{B}] = & \sum_{k, k'} \{ u_k^2 [(\partial \hat{A}/\partial q_k^1)(\partial \hat{B}/\partial p_k^1) - \\
& - (\partial \hat{A}/\partial p_k^1)(\partial \hat{B}/\partial q_k^1)] - |v_{k, k'}|^2 [(\partial \hat{A}/\partial q_k^2)(\partial \hat{B}/\partial p_k^2) - \\
& - (\partial \hat{A}/\partial p_k^2)(\partial \hat{B}/\partial q_k^2)] \} \quad (3.1.53.).
\end{aligned}$$

From (3.1.42., 48) one finds that sufficient conditions for \hat{H}'_{IBG} and \hat{N}' to be simultaneously diagonal are

$$\left. \begin{aligned} \{ \hat{H}'_{IBG}, \hat{N}'_k \}_1 &= 0 \\ \text{and } \{ \hat{H}'_{IBG}, \hat{N}'_k \}_2 &= 0 \end{aligned} \right\} \quad (3.1.54.).$$

These relations state the fact that the number distribution operator in spaces S_1 and S_2 , namely $N_k^1 = p_k^1 q_k^1$ and $N_k^2 = p_k^2 q_k^2$, are constants of motion.

One can define states of *overall equilibrium* (o.e.) (inequilibrium (o.i.)) as $\partial_t \hat{N}' = 0$ ($\neq 0$), states of *relative equilibrium* (r.e.) (inequil-

ilibrium (r.i.)) as $\partial_t N^i = 0 (\neq 0)$, and states of *local relative equilibrium* (l.r.e.) (inequilibrium (l.r.i.)) as $\partial_t N_k^i = 0 (\neq 0)$. It is clear that there can be states of l.r.i. in r.e., which imply o.e.; or states of r.i. in a state of o.e. In either case \hat{N}' is a constant of motion but \hat{N}' and \hat{H}_{IBG}' are not simultaneously diagonal. In order for the total energy and the total number to be both well defined in L.C.S.R. a state of l.r.e. is required. As far as the I.B.G. is concerned - in thermal equilibrium, say - l.r.e. is satisfied. As will be seen in Chapter 4, however, the relative number of 'objects' in spaces S_i changes with temperatures (for a certain statistical ensemble). One thus reaches the conclusion that $[\hat{H}_{IBG}', \hat{N}'] = 0$ is *not* satisfied in *thermal inequilibrium*. Further comments on the notion of relative equilibrium will be given in §3.2., but now let us consider the connection between the present approach and the standard method of diagonalization of the *particle* hamiltonian.

The strategy of the present approach is to reformulate the dynamical problem by introducing a change of lagrangian variables, $(\hat{q}, \hat{q}) \rightarrow (q^i, \dot{q}^i)$; defined over domains of different structural properties, namely non-separable and separable, respectively. The initial aim is to determine whether a hamiltonian exists in the S.P.S. picture.

The process of proving the existence of the hamiltonian \hat{H}_{IBG}' involves the removal of some redundant conditions. It is noted that the removal of the redundancies is always justified on logical grounds, without introducing further assumptions. The removal of redundancies here is an exact procedure (not an approximate one), and entails the cancellation of non-diagonal contributions, which otherwise would appear in H_{IBG}' .

The proof of existence of the hamiltonian also leads to its functional expression. \hat{H}_{IBG}' is found to be different from the particle hamiltonian, \hat{H}_{IBG} . The difference is given by non-diagonal contributions in both representations. H_{IBG}' is found diagonal in the L.C.S.R.

The fact that \hat{L}_S admits a Legendre transformation enables to define generalized momenta; hence, the S.P.S. is well-defined. The functional expression for the number operator in the S.P.S., \hat{N}' , is dictated by structural properties of the S.P.S. One finds that \hat{N}' is different from the number operator of the N-S.P.S., \hat{N} , the difference being a non-linear contribution in both representations involved. It is found that \hat{N}' is diagonal in the L.C.S.R. and, accordingly, commutes with \hat{H}'_{IBG} . This proves symmetry rearrangement. In addition, the total energy and total number of particles predicted in both descriptions are the same, provided that L.C.S. are normalized to satisfy $\langle n | \hat{N} | n \rangle = \langle C_n | \hat{N} | C_n \rangle$. This completes the proof of dynamical equivalence.

The strategy of the standard approach, on the other hand, is to introduce a transformation of *hamiltonian* variables, $(\hat{p} \equiv a^\dagger, q \equiv a) \rightarrow (\hat{p}' \equiv \alpha^\dagger, \hat{q}' \equiv \alpha)$. On the basis of the premise that the constants of motion, namely \hat{H} and \hat{N} , remain invariant^(*) (but the 'symmetry of the states' is changed).

The diagonalization of $\hat{H}(\hat{p}', \hat{q}')$ is effected in the L.C.S.R. (or more precisely, in a representation contained in the L.C.S.R.) by imposing certain conditions on the c-number fields involved in the transformation $(\hat{p}, \hat{q}) \rightarrow (\hat{p}', \hat{q}')$. As a consequence of the fact that the P.R. and the L.C.S.R. are non-equivalent representations, it necessarily follows that the *gauge* symmetry is broken in the standard approach; for, the number operator is thought to be \hat{N} whatever the variables or the representation of states are.

A number of observations need to be made at this stage, in order to appreciate the link between both approaches, and the reasons why the present method is more satisfactory.

*The substitution $\hat{H} = \hat{H}_{IBG}$ is irrelevant as to the discussion of the standard strategy.

- (1) It is noted, in the first place, that no explicit reference as to what the dynamical variables are is made in any of the existing theories of superfluidity; the identification $\hat{p}' = \alpha^+$, $\hat{q}' = \alpha$ is made implicitly.
- (2) The transformation $(\hat{p}, \hat{q}) \rightarrow (\hat{p}', \hat{q}')$ leaves the non-separable structure of the phase space unaltered.
- (3) The question of whether the hamiltonian expressions $\hat{H}(\hat{p}, \hat{q})$ and $\hat{H}(\hat{p}', \hat{q}')$ (after diagonalization) correspond to the same dynamical problem (and the same physical system) is never asked in existing treatments of the present problem. It is never enquired whether or not $\hat{H}(\hat{p}', \hat{q}')$ (after diagonalization) is *the* hamiltonian, and not just a functional of the canonical variables α^+ and α .
- (4) As far as the I.B.G. is concerned the hamiltonian in the S.P.S. picture turns out to have the same functional expression, in terms of elementary excitations and c-number fields, as the *particle* hamiltonian after diagonalization. This is solely due to the fact that the velocity independent segment of \hat{H}_R is *non-diagonal* for this particular problem. But this is casual. It will be shown in §3.2. that, for the interacting problem, \hat{H}_R involves a *diagonal* segment as well as a non diagonal part (if first and second order coherent fields are both involved in the L.C.S.R.). The strategy of diagonalization of the *particle* hamiltonian *fails* to give *the correct hamiltonian* for this problem.
- (5) Finally, it is most important to note that the involvement of variables of a *separable* domain is *not* a necessary element of the method of reformulation of the lagrangian problem proposed in this thesis. The resort to variables of a separable domain obeys to the need for counting independent configurations; that is, for statistical purposes, and *not* from dynamical requirements.

One could, of course, define new lagrangian variables as $\hat{q}_k' \equiv \alpha_k$, $\hat{q}_k' \equiv i\hbar \partial_t \alpha_k$ (i.e. defined in a non-separable domain); and regard the c-number fields as auxiliary parameters (time dependent or not). One

could then proceed to determine whether or not a hamiltonian exists according to the method proposed here. The algebra turns out to be more involved than for the choice of variables adopted in this work; but one finds eventually that a hamiltonian exists for the IBG only if *the old* diagonalization conditions are *imposed additionally*. The redundancy does *not* occur for this choice of variables.

For the interacting problem, however, the conditions of existence of hamiltonian do *not* coincide with the *old* diagonalization conditions. The new conditions involve the coefficients of some diagonal contribution as well. This variant, based on the choice of variables in non-separable domains, will not be pursued further in this thesis; for, it does not lead to the appropriate setting to discuss superfluidity from a statistical viewpoint.

§3.2. The interacting problem: A model for ^4He

The strategy adopted in this thesis, as far as dynamics is concerned, can be phrased as follows: Given a *lagrangian* formulation of an arbitrary problem, in terms of dynamical variables of a non-separable domain, to produce another *dynamically equivalent* formulation of the same problem, in terms of variables of a separable domain. Two independent and complementary aspects of this strategy should be noted.

The first aspect concerns the relationship between both sets of variables, $\{\hat{q}_k, \hat{p}_k\}$ and $\{q_k^i, \dot{q}_k^i\}$, namely $\hat{q}_k = \sum_i q_k^i$, $\hat{p}_k = \sum_i \dot{q}_k^i$; irrespective of the way in which these variables are defined in terms of the fields of two canonically related representations of quantum states. The idea, as far as this aspect of the strategy is concerned, is to prove that if a hamiltonian, $\hat{H}(\hat{p}, \hat{q})$, exists in the non-separable picture, and if the number functional in the non-separable phase space, $\hat{N}(\hat{p}, \hat{q})$, is a constant of motion; then, a hamiltonian, $\hat{H}'(p^i, \dot{q}^i)$, exists in the separable picture, and the number operator in the separable phase space is also a constant of motion.

The other aspect of the present strategy concerns the way in which the dynamical variables are defined in terms of two non-equivalent representations, linked by canonical transformation. As to this aspect the objectives are: (i) To derive a relationship between the elementary fields of both representations, such that the relations $\hat{p}_k = \hat{p}_k(p_k^i)$, $\hat{q}_k = \hat{q}_k(q_k^i)$ become two *identities*, for the appropriate definitions or \hat{p} , \hat{q} , p^i and q^i . (ii) To prove that \hat{H}' and \hat{N}' are diagonal in the transformed (coherent state) representation, provided that \hat{H} and \hat{N} are diagonal in the initial (particle) representation, and (iii) to prove that the eigenvalues of \hat{H}' and \hat{N}' in the C.S.R. are the same as the eigenvalues of \hat{H} and \hat{N} in the P.R.

It was mentioned before that the problem of the ideal gas is the only problem for which dynamical equivalence can be demonstrated, *if* the variables of the separable domain are defined in terms of the fields of the L.C.S.R. It will be shown in this section that the interacting problem does *not* admit an equivalent formulation *if* the variables of the separable domain are defined in terms of the L.C.S.R.

It will be shown that the first part of the strategy outlined above can be successfully brought to an end. It will also be shown that the number operator \hat{N}' *is* diagonal in the L.C.S.R.^(*) It will become clear, however, that the hamiltonian in the separable picture is *not* diagonal in L.C.S.R.

The conclusion that the *hamiltonian* symmetry is broken in a L.C.S.R. description does not indicate a limitation of the strategy proposed above, it just points at an inherent limitation of the L.C.S.R. to serve as a basis for the definition of the dynamical variables. It also suggests that a more elaborate, non-linear, C.S.R. should be employed to rearrange the hamiltonian symmetry (while keeping the gauge symmetry rearranged). It is

*This operator is, in fact, the same functional as for the problem of the IBC.

noted that, as to the hamiltonian symmetry, the present result parallels, to some extent, the results obtained before by Umezawa (66) and Coniglio and Marinaro (18). But the consequences as to the gauge symmetry are radically opposed. A discussion of the relationship of the approach in Refs. (18,66) and the present one is given in this section.

Two roads are open for research in this state of the affair. The first aims at a rigorous proof that the hamiltonian symmetry is rearranged. This line of research follows essentially the same technique as that of Ref. (66). The idea is to devise an iterative procedure to generate a series of non-linear C.S.R.'s of increasing complexity, starting from the L.C.S.R. as a zeroth order trial. The series of representations, hopefully, converges to 'The physical representation', in terms of which diagonalization of the separable picture hamiltonian is achieved. The interest in this thesis as to a rigorous proof is only marginal. The interest here as to this line of research is addressed to isolate the generator of the series of representation, and to gathering information in support of the *conjecture* that the hamiltonian symmetry *should be* rearranged in the physical representation proposed here. This is conjectured to occur in the *finite* volume limit, unlike in the proof by Umezawa, which requires of the passage to the *infinite* volume limit to achieve the rearrangement of hamiltonian symmetry.

The second option lacks the rigour of the first, but it is rather simpler and free from technical difficulty. This option is in the vein of current mean field theories, and consists of disregarding to the non-diagonal segment of \hat{H} in the L.C.S.R., as a first approximation. This segment can be retrieved at higher order of a hierarchy along the lines of that of Suhl and Wherthamer (61), reviewed in §1.2. This option will be investigated in this work, in some detail. The main objective being

to show that the *approximate* dynamical problem thus obtained is dynamically equivalent to the *exact* problem posed in the particle picture, except for the fact that the eigenvalues of energy are not identical, but only approximately equal.

Let us now prove that a hamiltonian exists in the separable picture. The lagrangian identifying a collection of ^4He atoms in a box of unit volume, subject to periodic boundary conditions, in terms of dynamical variables of a non-separable domain, is given by

$$\hat{L} \equiv \hat{L}_{ns}(\hat{q}, \dot{\hat{q}}) = (1/2) \sum_k (\dot{\hat{q}}_k^* \dot{\hat{q}}_k + \text{c.c.}) - \hat{H} \quad (3.2.1.),$$

where \hat{H} is a functional of \hat{q} and its c.c., and explicitly independent of time. Defining generalized momenta, as usual, by

$$\hat{p}_k \equiv \partial \hat{L}_{ns} / \partial \dot{\hat{q}}_k = \dot{\hat{q}}_k^* \quad (3.2.2.),$$

(3.2.1.) can be expressed as a Legendre transformation, i.e.

$$\hat{L}_{ns}(\hat{q}, \dot{\hat{q}}) = (1/2) \sum_k (\hat{p}_k \dot{\hat{q}}_k + \text{c.c.}) - \hat{H}(\hat{p}, \hat{q}) \quad (3.2.3.),$$

where the hamiltonian $\hat{H}(\hat{p}, \hat{q})$ is given by

$$\hat{H} = \sum_k \epsilon_k \hat{p}_k^* \hat{q}_k + (1/2) \sum_{\ell, p, q} V(\ell) \hat{p}_{p+\ell}^* \hat{p}_{q-\ell} \hat{q}_q \hat{q}_p \quad (3.2.4.).$$

The canonical variables are usually defined in terms of particle field operators as follows:

$$\hat{p}_k \equiv a_k^*, \quad \hat{q}_k \equiv a_k \quad (3.2.5.).$$

Introducing now the change of variables

$$\hat{q}_k = \sum_i q_k^i, \quad \dot{\hat{q}}_k = \sum_i \dot{q}_k^i \quad (3.2.6.)$$

into (3.2.1.), or - alternatively -

$$\hat{q}_k = \sum_i q_k^i, \quad \hat{p}_k = \sum_i p_k^i \quad (3.2.6.)$$

into (3.2.3.), an expression for $\hat{L} \equiv \hat{L}_S(q^i, p^i)$ is obtained. The situation here is slightly more complex than for the problem of the Ideal Bose Gas. The interaction segment of the particle hamiltonian can be written as

$$U \equiv \sum \overline{ppqq} \quad (3.2.7.)$$

with the help of the following notation: The symbol $\sum \dots$ denotes $(1/2) \sum_{\ell, p, q} v(\ell) \dots$ and the sub-indices of the p's and the q's are p + ℓ , q - ℓ , q and p from left to right. Substituting (3.2.6) into (3.2.7.) one obtains 81 terms, which - after some thought - can be written compactly in the following combinational form: (*)

$$\hat{U} = \hat{U}' + \hat{U}'' \quad (3.2.8.),$$

where

$$\hat{U}' \equiv \sum \overline{\left(\sum_{i,j} p^i p^j q^i q^j + \sum_{i,j} p^i p^i q^j q^j \right)} \quad (3.2.9.).$$

$$\begin{aligned} \hat{U}'' \equiv \sum \overline{\left[\sum_{i,j} (p^i p^i q^j q^j + p^i p^j q^i q^i) + \right.} \\ \left. \sum_{i,j,s} (p^i p^i q^j q^s + p^j p^s q^i q^i + p^i p^s q^i q^j) \right]} \quad (3.2.10.). \end{aligned}$$

The dash on the summation symbol indicates that the super-indices are all different. It can be verified through a straightforward but lengthy calculation that

$$\hat{U}'' = (1/2) \sum_{m,\ell,k} [p_k^m (\partial \hat{U}' / \partial p_k^\ell) + (\partial \hat{U}' / \partial q_k^\ell) q_k^m] \quad (3.2.11.).$$

The above result parallels that of the kinetic segment, using (3.1.20-24.) and (3.2.8-11.). The functional expression for the lagrangian in terms of the new variables is

*The symbol $\dots q^i q^j \dots$ denotes $\dots q^i q^j \dots + q^j q^i \dots$, for $i \neq j$.

$$\hat{L}_S(q^i, \dot{q}^i) = (1/2) \sum_{i,k} (p_k^i \dot{q}_k^i + \text{c.c.}) - \hat{H}' - \hat{H}'_R \quad (3.2.12.)$$

where $p_k^i = q_k^{i+}$ (i.e. expressed in terms of lagrangian variables), and

$$\hat{H}' = \sum_{k,i} \epsilon_k p_k^i q_k^i + \hat{U}' \quad (3.2.13.)$$

$$\hat{H}'_R = \sum_{i,j,k} (p_k^i \hat{\lambda}_{k,j}^j + \hat{\lambda}_k^{j+} q_k^i) \quad (3.2.14.)$$

The generalized forces, $\hat{\lambda}_k^{j+}$ and its c.c., are now given by

$$\hat{\lambda}_k^{j+} = -\dot{q}_k^j + \partial \hat{H}' / \partial p_k^j \quad (3.2.15.)$$

Removing the redundancy by replacing $\hat{\lambda}^{j+}$ and its c.c. by the expression for the external forces (zero, say) one obtains $\hat{H}'_R \equiv 0$. Thus, (3.1.12.) becomes a legendre transformation, satisfying

$$p_k^i \equiv \partial \hat{L}_S / \partial \dot{q}_k^i = q_k^{i+} \quad (3.2.16.)$$

The functional expression for the hamiltonian in the S.P.S. picture is

$$\begin{aligned} \hat{H}' = & \sum_{i,k} \epsilon_k p_k^i q_k^i + (1/2) \sum_{\ell, p, q} v(\ell) \left[\sum_i p_{p+\ell}^i p_{q-\ell}^i q_q^i q_p^i + \right. \\ & \left. + \sum_{i,j} (p_{p+\ell}^i p_{q-\ell}^j q_q^i q_p^j + p_{p+\ell}^i p_{q-\ell}^j q_q^j q_p^i) \right] \quad (3.2.17.)^{(*)} \end{aligned}$$

The canonical equations of motion are

$$-i\hbar \partial_t p_k^i = \{\hat{H}', p_k^i\} \quad (3.2.18.)$$

$$-i\hbar \partial_t q_k^i = \{\hat{H}', q_k^i\} \quad (3.2.19.),$$

where the Poisson bracket is given by (3.1.40.). It can be readily verified (see Appendix B) that the number operator N' , given by (3.1.45.), is a constant of motion, i.e.

$$\{\hat{H}', \hat{N}'\} = 0 \quad (3.2.20.).$$

*It can readily be tested that the last term of (3.2.17.) is non-diagonal in the L.C.S.R., here it is denoted by \hat{T}' .

The search for the physical representation, according to Umezawa's method, can be separated into two parts. An intermediate representation is devised first, such that their elementary operators, $\bar{\alpha}_k^+$ and $\bar{\alpha}_k$, are linearly related to particle operators (The intermediate representation is L.C.S.R., say, for the sake of generality.). The *particle* hamiltonian is expressed in terms of (intermediate) elementary excitation operators. A relation is introduced *ad hoc* effecting the cancellation of *low* order dangerous contributions, namely those contributions linear and quadratic in $\bar{\alpha}$'s. Finally the remaining non-linear segment of $\hat{H}(\bar{\alpha}^+, \bar{\alpha})$ is employed to devise an exponential canonical transformation linking the intermediate representation and the physical representation.

Here the strategy as to the very formulation of the dynamical problem is different. As a consequence of this the question here is that of finding a representation such that \hat{H}' (*not* \hat{H}) is diagonal in it. In the process of deriving \hat{H}' some redundant conditions had to be removed. These conditions are the counterparts of the *ad hoc* conditions of cancellation of dangerous contributions in Umezawa's method. But the two sets of conditions are by no means identical or equivalent. As a matter of fact the redundant conditions are expressed here in terms of the dynamical variables not in terms of operators of a particular representation. The cancellation then holds whatever the representation involved! On the other hand the cancellation brought about by the removal of the redundancies is an *exact* one; that is, the removal of the redundancy effects the cancellation of *all* dangerous contributions. Not only low order ones but *also high* order dangerous contributions. This amounts to an important difference respect to Umezawa's approach; for, the generator of the canonical transformation linking the intermediate representation and the physical representation is here *free from dangerous contributions*. This is not the case in Umezawa's work. For instance, a contribution of

the form $\overline{\alpha^+ \alpha^+ \alpha^+ \alpha}$ is included in Umezawa's generator. This contribution is a part of the segment $p^1 p^1 q^2 q^1$, which is a part of the redundant conditions, and excluded from the hamiltonian \hat{H}' .

The canonical transformation linking the L.C.S.R. and the physical representation is given here by

$$\sigma_p = \exp \hat{T}'(\alpha^+, \alpha), \quad \hat{T}' \text{ being the second term in (3.2.9.),}$$

and excludes all dangerous contributions. In Umezawa's work the diagonalization of \hat{H} is achieved in the infinite volume only. This is due to the presence of a remaining non-diagonal segment Q_v , which happens to vanish in the bulk limit. The occurrence of Q_v in Umezawa's work is linked to the occurrence of contributions of the form $\overline{\alpha^+ \alpha^+ \alpha^+ \alpha}$ and its c.c. in the transformation linking the intermediate representation and the physical representation. For this reason it is conjectured here that it should be possible to diagonalize \hat{H}' in the physical representation, but in the *finite* volume limit.

Another advantageous feature of the present approach is that the *gauge* symmetry is rearranged in the physical representation (in fact it is already rearranged in the intermediate representation). The reason for this is that the kinetic energy segment, \hat{K}' , should be diagonal in the physical representation if \hat{H}' is diagonal, but \hat{K}' is diagonal if and only if \hat{N}' is diagonal (in every representation). According to the standard approach, however, the gauge symmetry is broken since \hat{N} is never diagonal in a non-equivalent representation of the P.R., and the physical representation is clearly one of these.

An investigation addressed to producing a proof that the physical representation exists, and that the exact hamiltonian symmetry is rearranged in the finite volume case, is currently in progress. No conclusive evidence in this sense has been produced as yet. There is, however, strong indication that this is the case indeed. An account of

the progress in this direction is outside the scope of this thesis. The conclusions of these investigations are to be presented elsewhere.

Confronted with the fact that \hat{H}' is not diagonal in the L.C.S.R. the position adopted in the present work is: To devise a model of the exact problem, obtained by discarding the non-diagonal segment, i.e. \hat{T}' , and derive observable predictions; to be compared with those of alternative approaches based on the standard paradigm, and with experiment.

The interest here will eventually lay in formulating the dynamical problem in a, self-consistent, mean field approximation. This is carried out in the next section. It is noted that the guide lines to produce a linear model from a non-linear one are as follows: (i) identify the irreducible terms of the hamiltonian and discard them, namely those quartic contributions not reducible to a quadratic form by taking averages on a pair of operators; and (ii) reduce all reducible quartic contributions to the hamiltonian to a quadratic form by taking averages on pairs of operators. It is noted that \hat{T}' is the irreducible segment of \hat{H}' ; hence it is to be disregarded for the purpose of linearization of the dynamical problem anyway.

§3.3. Mean Field Approximation (M.F.A.) for the zeroth order problem

The conclusion that emerged in the preceding section indicates that one must go beyond the L.C.S.R. in order to be able to diagonalize the S.P.S. hamiltonian exactly. Umezawa was lead to the same conclusion, as to the impossibility of diagonalizing the particle hamiltonian in a simple linear representation of coherent states, and developed an iterative scheme addressed to obtain the physical representation, and, eventually, to prove hamiltonian symmetry rearrangement.

The majority of the works on superfluidity,^(*) however, do not follow Umezawa's programme, but are confined to a description in terms of certain, simple, linear representations of coherent states

^{*}(6,20,22,23,29,32,40,46,51,55,59,60,62,69,68,73)

(contained in the L.C.S.R.). It is generally acknowledged that the *particle* hamiltonian, \hat{H} , cannot be fully diagonalized in such representations, but most authors are content with diagonalizing the largest possible segment of \hat{H} ; endorsing the belief that the approximate predictions obtained from the truncated hamiltonian (as to the excitation spectrum, for instance), are very close to the exact predictions obtainable from the exact hamiltonian.

The present theory introduces two novel elements in the study of superfluidity, namely a lagrangian reformulation (as opposed to a particle hamiltonian formulation) and the involvement of dynamical variables of a separable domain. The involvement of these two elements in the present theory amounts to a significative shift of view point, and calls for a simple presentation - in the first place - enabling the comparison with existing theories as to the methods and results. The position adopted in the remainder of this work - in view of this - is to introduce certain approximations to the exact problem posed by \hat{H} , of the same nature as those approximations involved in existing self-consistent theories; thus, making the comparison possible. This will permit to show, in a simple fashion, the conceptual and practical advantages of the approach proposed here.

Two approximations of different nature are introduced in this section. The S.P.S. picture hamiltonian is truncated in the first place, discarding the non-diagonal segment in the L.C.S.R., i.e. \hat{T}' , in the simplest (zeroth order) approximation. The remaining segment of \hat{H} , namely H'_0 , defines the *zeroth order problem*, and admits a diagonal resolution in the L.C.S.R. A hierarchial scheme can be envisaged, along the lines of the methods of Suhl and Wherthamer (61) or Umezawa (66), to retrieve \hat{T}' at higher order of the hierarchy. This latter scheme, however, will not be persued here.

It is most important to note that \hat{T}' *must* be discarded if a description in terms of the L.C.S.R. is persued; for, \hat{T}' is intrinsically

non-diagonal in this representation, hence its presence renders the dynamical problem unsolvable in this representation.

The other approximation introduced in this section is the well-known M.F.A., implemented here on the basis of the L.C.S.R. as a trial representation. It will soon become clear that the notion of anomalous averages does *not* arise here, due to the fact that the dynamical variables are defined in terms of the creation and annihilation operators of the L.C.S.R., over which mean field averages are taken. In other words, the M.F.A. employed here is the standard version, not the generalized Random phase approximation method of Anderson. It will be seen shortly that the above approximation effects the linearization of the equations of motion for the canonical variables q_k^i and p_k^i for $i = 1, 2$ only, but leaves the corresponding (c-number) equations for variables $i = 3$ non-linear. A further approximation must be introduced for the c-number fields to accomplish the linearization of their equations of motion. This approximation is the c-number counterpart of the M.F.A. for q-number fields.

The objectives in this section are: Firstly, to derive expressions for the three branches of the excitation spectrum in the approximation outlined above. Secondly, to compare the present method and results as to the excitation spectra with the method and comparable results in existing theories in the same approximation. In order to achieve the second aim it will be necessary to develop anew the programme of existing theories on the basis of the more general L.C.S.R.

The analysis in this section is confined to a pure state description, a statistical description on the basis of a Grand canonical ensemble, and the comparison with experiment are postponed until section 4.4.

The starting point here is the zeroth order hamiltonian

$$\hat{H}'_0 = \sum_{k,i} \epsilon_k p_k^i q_k^i + (1/2) \sum_{i,j} V(\ell) \sum_{p,l} p_{p+l}^i p_{q-l}^j q_q^i q_p^j \quad (3.3.1.).$$

It is recalled that \hat{H}'_0 is diagonal in the L.C.S.R.^(*) and that dangerous contributions have already been removed. As a consequence of this the linearized equations for the canonical variables $i = 1, 2$ will turn out to be decoupled in terms of *elementary excitation* operators, though *not* necessary decoupled in terms of the *dynamical variables* p^i and q^i themselves.

The canonical equations of motion,

$$\left. \begin{aligned} -i\hbar \partial_t p_k^i &= \{\hat{H}'_0, p_k^i\} \\ -i\hbar \partial_t q_k^i &= \{\hat{H}'_0, q_k^i\} \end{aligned} \right\} \quad (3.3.2.),$$

take the form

$$-i\hbar \partial_t p_k^i = \epsilon_k p_k^i + \sum_{p,l} V(\ell) \sum_j \overbrace{p_{p+l}^i p_{k-l}^j} q_p^j \quad (3.3.3.)$$

$$i\hbar \partial_t q_k^i = \epsilon_k q_k^i + \sum_{p,l} V(\ell) p_{p+l}^j \overbrace{q_{k+l}^i q_p^j} \quad (3.3.4.).$$

The immediate aim here is to reduce the above set of six non-linear equations to a linear form. This is achieved, as usual, by (i) adding and subtracting to the R.H.S. of (3.3.3.,4.) a linear contribution, amounting to the mean field average of the non-linear terms. (ii) neglecting fluctuations about mean field values, and (iii) discarding irreducible contributions, namely those contributions whose mean field values are zero. Let us illustrate the procedure by considering the non-linear term in equation (3.3.3.) for $i = 3$.

*See Appendix C

$$\begin{aligned}
\sum_{p,l} V(l) \sum_{j=1}^3 \overbrace{p_{p+l}^3 p_{k-l}^j q_p^j} &= \sum_{p,l} V(l) [p_{p+l}^3 p_{k-l}^3 q_p^3 + \\
&+ \sum_{j=1}^2 (p_{p+l}^3 \langle p_{k-l}^j q_p^j \rangle + p_{k-l}^3 \langle p_{p+l}^j q_p^j \rangle + \\
&+ \overbrace{p_{p+l}^3 p_{k-l}^j q_p^j} - p_{p+l}^3 \langle p_{k-l}^j q_p^j \rangle - \\
&- p_{k-l}^3 \langle p_{p+l}^j q_p^j \rangle)] \quad (3.3.5.).
\end{aligned}$$

Now, it is noted that

$$\begin{aligned}
\langle p_p^1 q_q^1 \rangle &= \sum_{t,t'} u_{p,t} u_{q,t}^* \langle \alpha_t^+ \alpha_t \rangle \\
&= \sum_t |u_{p,t}|^2 \langle \alpha_t^+ \alpha_t \rangle \delta_{p,q} \quad (3.3.6.),
\end{aligned}$$

and

$$\begin{aligned}
\langle p_p^2 q_q^2 \rangle &= \sum_{t,t'} v_{p,t}^* v_{p,t} \langle \alpha_t^+ \alpha_t \rangle \\
&= \sum_t |v_{p,t}|^2 (\langle \alpha_t^+ \alpha_t \rangle + 1) \delta_{p,q} \quad (3.3.7.).
\end{aligned}$$

Hence (3.3.5.) can be rewritten as

$$\begin{aligned}
\sum_{p,l} V(l) \sum_{j=1}^3 \overbrace{p_{p+l}^3 p_{k-l}^j q_p^j} &= \sum_{p,l} V(l) [p_{p+l}^3 p_{k-l}^3 q_p^3 + \\
&+ p_k^3 \sum_l [V(0) + V(l)] \sum_{j=1}^2 N_{k-l}^j] + S + I \quad (3.3.8.),
\end{aligned}$$

where

$$N_k^j \equiv \langle p_k^j q_k^j \rangle \quad (3.3.9.),$$

S are fluctuations about mean field averages, namely

$$\begin{aligned}
S \equiv \sum_{j=1}^2 \left[\sum_{p,l} V(l) p_{p+l}^j p_{k-l}^3 p_p^j \delta_{l,0} - \sum_l V(0) p_k^3 N_{k-l}^j \right] + \\
+ \sum_{j=1}^2 \left[\sum_{p,l} V(l) p_{p+l}^3 p_{k-l}^j p_p^j \delta_{p+l,k} - \sum_l V(l) p_k^3 N_{k-l}^j \right] \quad (3.3.10.),
\end{aligned}$$

and I constitutes the irreducible contributions, namely

PAGINATION ERROR

$$I \equiv \sum_{p,l} V(l) \sum_{j=1}^2 \overbrace{p_{p+l}^3 p_{k-l}^j}^j q_p^j (1 - \delta_{l,0}) (1 - \delta_{p+l,k}) \quad (3.3.11.).$$

I is discarded at zeroth order within a hierarchy of linearized equations of motion, S is neglected provided that fluctuations about mean field averages are small compared with the averages themselves. Hence equation (3.3.3.) becomes

$$-i\hbar \partial_t p_k^3 = \bar{J}_k p_k^3 + \sum_{p,l} V(l) p_{p+l}^3 p_{k-l}^3 q_p^3 \quad (3.3.12.).$$

For equation (3.3.4.) one similarly obtains

$$i\hbar \partial_t q_k^3 = \bar{J}_k q_k^3 + \sum_{p,l} V(l) p_{p+l}^3 q_p^3 q_{k+l}^3 \quad (3.3.13.),$$

where

$$\bar{J}_k = \epsilon_k + \sum_l [V(0) + V(l)] \sum_{j=1}^2 N_{k-l}^j \quad (3.3.14.).$$

It must be recalled that the averages in (3.3.5.), and in all subsequent equations, are regarded here as averages over pure (n-elementary-excitation coherent) states, $|C_n\rangle$. Later in §4.4. after an appropriate ensemble of states has been introduced this average will be regarded as quantum and thermal averages over a Grand canonical ensemble, and $\epsilon_k = (\hbar^2/2m)k^2$ will be taken as $\epsilon_k' = \epsilon_k - \mu$, where μ is the chemical potential.

The set of two equations (3.3.12.,13.) is non-linear, after replacing p_k^3 and q_k^3 by their definitory expressions ϕ_k^* and ϕ_k , respectively, this set of equations can be recognized as Gross' equations for the "inhomogeneous condensate", except for a linear contribution $(\bar{J}_k - \epsilon_k) p_k^3$ and $(\bar{J}_k - \epsilon_k) q_k^3$, respectively, which are the mean field Hartree-Fock energy contributions, associated with the interactions between one particle in space S_3 and an average particle in spaces S_1 and S_2 . These 'other' particles, of course, were not present in Gross' treatment^(35,58).

Gross has studied the solution of the set of equations (3.3.12.,13) in detail, in several approximations, for several model potentials and for diverse boundary conditions (35). It is known, (8,9) in particular, that

the dispersion relation ω_k^3 - defined through

$$\left. \begin{aligned} p_k^3(t) &= p_k^3(t_0) \exp[i(\omega_k^3/\hbar)(t - t_0)] \\ q_k^3(t) &= q_k^3(t_0) \exp[-i(\omega_k^3/\hbar)(t - t_0)] \end{aligned} \right\} \quad (3.3.15.) -$$

is *gapless* and linear in the long wave limit. One can appreciate that by noting that the *effective* hamiltonian, H_e^3 , from which (3.3.12.,13.) follow - according to

$$\left. \begin{aligned} -i\hbar \partial_t p_k^3 &= \{H_e^3, p_k^3\} \\ -i\hbar \partial_t q_k^3 &= \{H_e^3, q_k^3\} \end{aligned} \right\} \quad (3.3.16.) -$$

is

$$H_e^3 = \sum_k \bar{J}_k p_k^3 q_k^3 + (1/2) \sum p_{p+l}^3 p_{q-l}^3 q_q^3 V(l) \quad (3.3.17.).$$

This effective hamiltonian is well known (8,9,25,51,69) to be invariant under the following infinitesimal transformation

$$\left. \begin{aligned} p_k^3 &\rightarrow p_k^3 - i(p_{k+t}^3 + p_{k-t}^3) \delta\epsilon \\ q_k^3 &\rightarrow q_k^3 + i(q_{k+t}^3 + q_{k-t}^3) \delta\epsilon \end{aligned} \right\} \quad (3.3.18.),$$

where t is an arbitrary wave vector and $\delta\epsilon$ is an arbitrary infinitesimal. The invariance of H_e^3 under transformation (3.3.18.) implies that ω_k^3 is gapless, i.e. $\lim_{k \rightarrow 0} \omega_k^3 = \omega_0^3 = 0$, according to a celebrated theorem due to Bogoljubov (8,9).

Now, in order to reduce the non-linear equations to a linear set of self-consistent equations the following approximation is introduced into (3.3.12.,13.):

$$\left. \begin{aligned} p_p^3 q_q^3 + \langle p_p^3 q_q^3 \rangle &\approx p_p^3 q_p^3 \delta_{p,q} \\ p_p^3 p_q^3 + \langle p_p^3 p_q^3 \rangle &\approx |p_p p_q| \delta_{p,-q} \end{aligned} \right\} \quad (3.3.19.),$$

the R.H.S. being regarded as time independent. Equations (3.3.12.,13.) become

$$-i\hbar \partial_t p_k^3 = J_k p_k^3 + b_k q_{-k}^3 \quad (3.3.20.)$$

$$-i\hbar \partial_t q_k^3 = J_k q_k^3 + b_k p_{-k}^3 \quad (3.3.21.).$$

where

$$\begin{aligned} J_k &= \bar{J}_k + \sum_{\ell} [V(0) + V(\ell)] N_{k-\ell}^3 \\ &= \epsilon_k + \sum_{\ell} [V(0) + V(\ell)] N_{k-\ell}' \end{aligned} \quad (3.3.22.),$$

N_k' being $\sum_i N_k^i$ and

$$\begin{aligned} b_k &= \sum_{\ell} V(\ell) |p_{-k+\ell}^3 p_{k-\ell}^3| \\ &= \sum_{\ell} V(\ell) |p_{k-\ell}^3 q_{k-\ell}^3| \\ &= \sum_{\ell} V(\ell) N_{k-\ell}^3 \end{aligned} \quad (3.3.23.).$$

The set of linear coupled equations can be decoupled as follows: Differentiating (3.3.20) with respect to time, multiplying by $(i\hbar)$ and making use of (3.3.21.,22.) one obtains

$$\begin{aligned} -\hbar^2 \partial_t^2 p_k^3 &= J_k (J_k p_k^3 + b_k q_{-k}^3) - \\ &\quad - b_k (J_k q_{-k}^3 + b_k p_k^3) \\ &= (J_k^2 - b_k^2) p_k^3 \end{aligned} \quad (3.3.24.).$$

One similarly finds for the equation for q_k^3

$$-\hbar^2 \partial_t^2 q_k^3 = (J_k^2 - b_k^2) q_k^3 \quad (3.3.25.).$$

This set of second order differential equations has the solution (3.3.15.) with

$$\omega_k^3 = \{J_k^2 - b_k^2\}^{1/2} \quad (3.3.26.)$$

as the dispersion relation in this approximation.

Let us now go back to equations (3.3.3.,4.) for $i = 1, 2$ and linearise them using (3.3.6.,7.,19.) and

$$\left. \begin{aligned} \langle p_{pq}^1 \rangle^2 &= \sum_t [u_{p,t} v_{q,t}^* \langle \alpha_t^+ \alpha_t \rangle + u_{q,t} v_{p,t}^* (\langle \alpha_t^+ \alpha_t \rangle + 1)] \\ \langle q_{pq}^1 \rangle^2 &= \sum_t [u_{p,t}^* v_{q,t} (\langle \alpha_t^+ \alpha_t \rangle + 1) + u_{q,t}^* v_{p,t} \langle \alpha_t^+ \alpha_t \rangle] \end{aligned} \right\} \quad (2.3.27.).$$

One obtains the following set of four equations

$$i\hbar \partial_t p_k^i = J_k p_k + \sum_p B_{p,k}^* q_p^j \quad (3.3.28.)$$

$$-i\hbar \partial_t q_k^i = J_k q_k^i + \sum_p B_{p,k} p_p^j \quad (3.3.29.),$$

for $i, j = 1, 2$ and $i \neq j$. J_k is given by (3.3.22.) and the pairing energy in space $S_1 \otimes S_2$ is

$$B_{p,k}^* \equiv \sum_{\ell} V(\ell) \langle p_{p+\ell}^1 p_{k-\ell}^2 \rangle \quad (3.3.30.).$$

Equations (3.3.28.,29.) are linear but coupled in the dynamical variables of spaces S_1 and S_2 . These equations are decoupled in terms of elementary excitations as will be shown later in this section, i.e. these involve either creation or annihilation operators of the L.C.S.R. for the same mode.

Now, two types of stationary state solutions of different physical nature can be expected to be possible for the dynamical variables. In principle the stationary state solutions for the dynamical variables can take the following form:

$$\left. \begin{aligned} (Case\ 1) \quad p_k^1(t) &= p_k^1(t_0) \exp[i\omega_k^1(t - t_0)/\hbar] \\ q_k^1(t) &= q_k^1(t_0) \exp[-i\omega_k^1(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.31.)$$

$$\left. \begin{aligned} p_k^2(t) &= p_k^2(t_0) \exp[i\omega_k^2(t - t_0)/\hbar] \\ q_k^2(t) &= q_k^2(t_0) \exp[-i\omega_k^2(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.32.).$$

Another theoretically possible stationary state solution, however, is

$$\text{(Case 2)} \quad \left. \begin{aligned} p_k^1(t) &= p_k^1(t_0) \exp[i\omega_k^1(t - t_0)/\hbar] \\ q_k^1(t) &= q_k^1(t_0) \exp[-i\omega_k^1(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.33.)$$

$$\left. \begin{aligned} p_k^2(t) &= p_k^2(t_0) \exp[-i\omega_k^2(t - t_0)/\hbar] \\ q_k^2(t) &= q_k^2(t_0) \exp[i\omega_k^2(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.34.).$$

In either case

$$\left. \begin{aligned} \omega_k^1 &\geq 0 \\ \omega_k^2 &\geq 0 \end{aligned} \right\} \quad (3.3.35.).$$

The two cases above exhaust all the possibilities. Case 1 corresponds to the event in which both dynamical objects, associated with variables $i = 1$ and $i = 2$, possess *positive* energy. In Case 2, however, the dynamical objects whose dynamical variables are p_k^2 and q_k^2 possess *negative* energy; that is, are *holes* of the dynamical objects $i = 2$ for the former case. The latter possibility (3.3.33., 34.), seems rather odd at first sight, however, it will be seen shortly that it is not only consistent with the present definition of variables, but is - in fact - *the only* satisfactory stationary state solution. But before considering these matters let us consider an argument ruling out the cases in which the dynamical objects $i = 1$ possess negative energy.

The argument in question is rather simple. The particle problem is one in which the dynamical objects possess *positive* energy, however, if the dynamical variables $i = 1$ have the time dependence

$$\left. \begin{aligned} \text{(Cases 3,4)} \quad p_k^1(t) &= p_k^1(t_0) \exp[-i\omega_k^1(t - t_0)/\hbar] \\ q_k^1(t) &= q_k^1(t_0) \exp[i\omega_k^1(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.36.),$$

for variables $i = 2$ depending on time either as (3.3.32.) or (3.3.34.), one would be lead to the conclusion that the particle system as a whole (i.e. the collection of ^4He atoms) has *negative* energy. This can be seen from the fact that in the limit

$$v_{k,q} \rightarrow 0, \quad u_{k,q} \rightarrow 1, \quad \phi_k \rightarrow 0 \quad (3.3.37.)$$

or

$$T \rightarrow \hat{1}, \quad \alpha_k \rightarrow a_k \quad (3.3.37'.)$$

one obtains

$$\left. \begin{aligned} p_k^1(t) \rightarrow \hat{p}_k(t) &= a_k^+(t) \\ q_k^1(t) \rightarrow \hat{q}_k(t) &= a_k(t) \\ p_k^2(t) &\rightarrow 0 \\ q_k^2(t) &\rightarrow 0 \\ p_k^3(t) &\rightarrow 0 \\ q_k^3(t) &\rightarrow 0 \end{aligned} \right\} \quad (3.3.38.);$$

and such a limit is a theoretical possibility (at least for some modes) contingent upon the solution of the integral equations characterizing the present model (see §4.4.).

One can convince oneself of the feasibility of a solution of the type (3.3.33.,34.) by noting that variables $i = 2$ - unlike variables $i = 1$ - are *defined* such that the generalized momenta (coordinates) are proportional to the annihilation (creation) operator for the L.C.S.R., in consequence the dynamical variables satisfy

$$q_k^1|0\rangle = 0 = \langle 0|p_k^1, \quad \text{for all } k \quad (3.3.39.),$$

as corresponds to dynamical objects of positive energy, and

$$p_k^2|0\rangle = 0 = \langle 0|q_k^2 \quad (3.3.40.),$$

corresponding to hole-like dynamical objects.

It is interesting to seek for a stationary state solution for the elementary excitation operators as well, in the simplest case. To be consistent with (3.3.37.,38) the stationary state time dependence of the latter operators should be

$$\left. \begin{aligned} \alpha_k^+(t) &= \alpha_k^+(t_0) \exp[i\omega_k^e(t - t_0)/\hbar] \\ \alpha_k(t) &= \alpha_k(t_0) \exp[-i\omega_k^e(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.41.),$$

where

$$\omega_k^e \geq 0 \quad (3.3.42.).$$

From the time dependences (3.3.31.,32.), (3.3.33.,34.) and (3.3.42.) it follows that the time dependence of the second order coherent fields for cases 1 and 2, respectively, are

$$\left. \begin{aligned} u_{k,q}(t) &= u_{k,q}(t_0) \exp[i(\omega_k - \omega_q)(t - t_0)/\hbar] \\ u_{k,q}^*(t) &= u_{k,q}^*(t_0) \exp[-i(\omega_k - \omega_q)(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.43.)$$

$$\left. \begin{aligned} v_{k,q}(t) &= v_{k,q}(t_0) \exp[-i(\omega_k + \omega_q)(t - t_0)/\hbar] \\ v_{k,q}^*(t) &= v_{k,q}^*(t_0) \exp[i(\omega_k + \omega_q)(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.44.)$$

and

$$\left. \begin{aligned} u_{k,q}(t) &= u_{k,q}(t_0) \exp[i(\omega_k - \omega_q)(t - t_0)/\hbar] \\ u_{k,q}^*(t) &= u_{k,q}(t_0) \exp[-i(\omega_k - \omega_q)(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.45.)$$

$$\left. \begin{aligned} v_{k,q}(t) &= v_{k,q}(t_0) \exp[i(\omega_k - \omega_q)(t - t_0)/\hbar] \\ v_{k,q}^*(t) &= v_{k,q}^*(t_0) \exp[-i(\omega_k - \omega_q)(t - t_0)/\hbar] \end{aligned} \right\} \quad (3.3.46.),$$

where

$$\omega_k^e = \omega_k^1 = \omega_k^2 \equiv \omega_k \quad (3.3.47.).$$

Let us now show that the tentative solution (3.3.31.,32.,41.,47.) is *not* possible, for it leads to an inconsistency. Substituting (3.3.31.,32.) in equation (3.3.28.) for $i = 1$ and in equation (3.3.29.) for $i = 2$, and replacing the dynamical variables by their expressions in terms of c -number fields and elementary excitation operators one obtains

$$\sum_q \omega_k u_{k,q} \alpha_q^+ = \sum_q J_k u_{k,q} \alpha_q^+ + \sum_{q,p} B_{p,k}^* v_{p,q} \alpha_q^+ \quad (3.3.48.)$$

$$\sum_q \omega_k v_{k,q} \alpha_q^+ = \sum_q J_k v_{k,q} \alpha_q^+ + \sum_{q,p} B_{p,k} v_{p,q} \alpha_q^+ \quad (3.3.49.).$$

These relations are satisfied if and only if

$$\omega_k u_{k,q} = J_k u_{k,q} + \sum_p B_{p,k}^* v_{p,q} \quad (3.3.50.)$$

$$\omega_k v_{k,q} = J_k v_{k,q} + \sum_p B_{p,k} u_{p,q} \quad (3.3.51.).$$

Now, multiplying (3.3.50.) by $v_{k,q}$ and (3.3.51.) by $u_{k,q}$ adding up the two relations and making use of the defining properties (2.3.24.-26.) one obtains the following quadratic equation

$$2(J_k - \omega_k) u_{k,q} v_{k,q} + \sum_p B_{p,k}^* (v_{k,q})^2 + \sum_p B_{p,k} (u_{k,q})^2 = 0 \quad (3.3.52.),$$

which has the following solution

$$(\sum_p B_{p,k}^*) v_{k,q} = \{-(J_k - \omega_k) \pm [(J_k - \omega_k)^2 - \sum_p |B_{p,k}|^2]^{1/2}\} u_{k,q} \quad (3.3.53.)$$

where

$$\sum_p B_{p,k}^* \sum_{p'} B_{p',k} = \sum_p |B_{p,k}|^2 \quad (3.3.54.)$$

- obtainable from (2.3.24.-26.), (3.3.27.,30.) - has been used.

The excitation spectrum ω_k corresponding to this type of solution is obtained by multiplying both (3.3.50.) and (3.3.53.) by $u_{k,q}$ and introducing the latter into the former, one obtains

$$(J_k - \omega_k)^2 - \sum_p |B_{p,k}|^2 = 0 \quad (3.3.55.)$$

or finally

$$\omega_k = J_k \pm \sum_p |B_{p,k}| \quad (3.3.56.).$$

However, if one replaces this expression into (3.3.53.) one finds

$$(\sum_p B_{p,k}^*) v_{k,q} = \mp \sum_p |B_{p,k}| u_{k,q},$$

multiplying this equation by its c.c. and summing over q one finds

$$\sum_p |B_{p,k}|^2 \sum_q |v_{k,q}|^2 = \sum |B_{k,q}|^2 \sum_q |u_{k,q}|^2$$

or

$$\sum_q (|u_{k,q}|^2 - |v_{k,q}|^2) = 0 \quad (3.3.57.);$$

in contradiction with

$$\sum_q (|u_{k,q}|^2 - |v_{k,q}|^2) = 1 \quad (3.3.58.),$$

which must be exactly satisfied. In consequence the type of solution (3.3.31.,32.,41.,47.) must be discarded.

Let us now consider the other possible solution and evaluate the excitation spectrum and show that this type of solution is compatible with (3.3.58.).

Introducing (3.3.33.,34.) into equation (3.3.28.) for $i = 1$ and equation (3.3.29.) for $i = 2$, and replacing the dynamical variables by their expressions in terms of the c-number fields and the elementary excitation operators one finds

$$\sum_q \omega_k u_{k,q} \alpha_q^+ = \sum_q J_k u_{k,q} \alpha_q^+ + \sum_{p,q} B_{p,k}^* v_{p,q} \alpha_q^+ \quad (3.3.59.)$$

$$- \sum_q \omega_k v_{k,q} \alpha_q^+ = \sum_q J_k v_{k,q} \alpha_q^+ + \sum_{p,q} B_{p,k}^* u_{p,q} \alpha_q^+ \quad (3.3.60.).$$

The different signs in equations (3.3.49.,60.) must be noted. Again, these equations are satisfied if and only if

$$\omega_k u_{k,q} = J_k u_{k,q} + \sum_p B_{p,k}^* v_{p,q} \quad (3.3.61.)$$

$$\omega_k v_{k,q} = J_k v_{k,q} + \sum_p B_{p,k} u_{p,q} \quad (3.3.62.).$$

Again, multiplying (3.3.61.) by $v_{k,q}$ and (3.3.62.) by $u_{k,q}$, making use of (2.3.24.-26.) and adding up the two relations one obtains

$$2J_k u_{k,q} v_{k,q} + \sum_p B_{p,k}^* (v_{k,q})^2 + \sum_p B_{p,k} (u_{k,q})^2 = 0 \quad (3.3.63.),$$

which is the familiar pairing equation. Note the difference respect to (3.3.52.). The roots of this quadratic equation are now

$$\left(\sum_p B_{p,k}^* \right) v_{k,q} = \{ -J_k \pm [J_k^2 - \sum_p |B_{p,k}|^2]^{1/2} \} u_{k,q} \quad (3.3.64.).$$

The excitation spectrum is obtained as before, namely multiplying (3.3.61. and 64.) by $u_{k,q}$, using (2.3.24.-26.), and substituting the former into the latter; one finds

$$\omega_k = \pm [J_k^2 - \sum_p |B_{p,k}|^2]^{1/2} \quad (3.3.65.).$$

The minus sign must be discarded to be consistent with (3.3.35.). Introducing now (3.3.65.) into (3.3.64.), multiplying the resulting relation by its c.c., and summing over q one obtains

$$\sum_p |B_{p,k}|^2 \sum_q |v_{k,q}|^2 = (J_k - \omega_k)^2 \sum_q |u_{k,q}|^2 \quad (3.3.67.).$$

Using now the identity (3.3.58.) and (3.3.65.) one obtains

$$\sum_p |B_{p,k}|^2 \left(\sum_q |u_{k,q}|^2 - 1 \right) = (J_k^2 + \omega_k^2 - 2J_k\omega_k) \sum_q |u_{k,q}|^2$$

or

$$\sum_q |u_{k,q}|^2 = (J_k + \omega_k)/2\omega_k \quad (3.3.68.).$$

Replacing this expression into (3.3.58.) one obtains

$$\sum_q |v_{k,q}|^2 = (J_k + \omega_k)/2\omega_k - 1$$

or

$$\sum_q |v_{k,q}|^2 = (J_k - \omega_k)/2\omega_k \quad (3.3.69.).$$

The somehow surprising conclusion just reached, namely the dynamical objects $i = 2$ have negative energy, is obtained as a consequence of the definition of dynamical variables. This definition, in turn, is necessary in order to obtain

$$\hat{p}_k = \sum_i p_k^i, \quad \hat{q}_k = \sum_i q_k^i \quad (3.3.70.)$$

as an identity, so that the volumes of both phase spaces, Γ_{ns} and Γ_s are the same. The average energy in a pure state description, in the M.F.A., is then

$$\begin{aligned} E_\eta &= \langle C_\eta | \hat{H}_0' | C \rangle \\ &= \sum_k \omega_k (N_k^1 - N_k^2) + \omega_k^3 N_k^3 \end{aligned} \quad (3.3.71.).$$

The ground state energy is the minimal energy subject to the renormalisation condition. This is obtained by certain distributions N_k^{i0} . It is clear that any excited state corresponds to distributions N_k^i , such that $N^i = \sum_k N_k^i$, such that $N^2 < N^{20}$, otherwise the excited state energy would be less than the ground state energy. In consequence the observed spectrum would show the negative energy branch as a positive energy branch.

Let us now reproduce the standard approach of mean field theories on the basis of the L.C.S.R. as the trial representation, and compare the method and the resulting excitation spectrum with the method and results obtained in this section.

The starting point of the standard approach are the canonical equations of motion for particle operators, obtained from the exact hamiltonian^(*). These equations are

$$-i\hbar\partial_t a_k^+ = \epsilon_k a_k^+ + \sum_{p,l} V(l) a_{p+l}^+ a_{k-l}^+ a_p \quad (3.3.72.)$$

$$i\hbar\partial_t a_k = \epsilon_k a_k + \sum_{p,l} V(l) a_{p+l}^+ a_p a_{k+l} \quad (3.3.73.)$$

The above set of equations is then linearized, by taking averages over the trial representation, the L.C.S.R. here. The resulting linear equations are

$$-i\hbar\partial_t a_k^+ = J_k a_k^+ + \sum_p \bar{B}_{p,k}^+ a_p \quad (3.3.74.)$$

$$i\hbar\partial_t a_k = J_k a_k + \sum_p \bar{B}_{p,k}^+ a_p^+ \quad (3.3.75.),$$

where

$$\begin{aligned} J_k &= \epsilon_k + \sum_l [v(0) + v(l)] \langle a_{k+l}^+ a_{k+l} \rangle \\ &= \epsilon_k + \sum_l [v(0) + v(l)] N_{k+l}^+ \end{aligned} \quad (3.3.76.)$$

and

$$\begin{aligned} \bar{B}_{p,k}^+ &= \sum_l v(l) \langle a_{p+l}^+ a_{k-l}^+ \rangle \\ &= \sum_l v(l) \langle \overset{1}{p_{p+l}} \overset{2}{p_{k-l}} \rangle + \sum_l v(l) \phi_{p+l}^* \phi_{k-l}^* \end{aligned}$$

or, after introducing approximation (3.3.19.)

$$\bar{B}_{p,k}^+ = B_{p,k} + b_k \delta_{p,-k} \quad (3.3.77.),$$

where $B_{p,k}$ and b_k are given by (3.3.30.,23.), respectively.

*The pair hamiltonian is employed in some works, but the exact Hamiltonian operator will be employed here.

The above coupled set of equations is decoupled by introducing the following change of variables

$$\left. \begin{aligned} a_k^+ &= \sum_q u_{k,q} \alpha_q^+ + \sum_q v_{k,q}^* \alpha_q + \phi_k^* \\ a_k &= \sum_q u_{k,q}^* \alpha_q + \sum_q v_{k,q} \alpha_q^+ + \phi_k \end{aligned} \right\} \quad (3.3.78.).$$

Here the ϕ 's are regarded as time dependent (for the sake of comparison) and the v 's are time independent. After some work one finds that the equations of motion for the α 's are decoupled if the c-number fields satisfy the following conditions

$$-i\hbar \partial_t \phi_k^* = J_k \phi_k^* + \sum_p \bar{B}_{p,k}^* \phi_p \quad (3.3.79.)$$

$$2J_k \left(\sum_q u_{k,q} \right) \left(\sum_q v_{k,q} \right) + \sum_p \bar{B}_{p,k}^* \left(\sum_q v_{k,q} \right)^2 + \sum_p \bar{B}_{p,k} \left(\sum_q v_{k,q} \right)^2 = 0 \quad (3.3.80.),$$

and similarly for their c.c. substituting (3.3.78.) into (3.3.74.,75.) and making use of (3.3.79.,80.) one obtains

$$\left. \begin{aligned} -i\hbar \partial_t \alpha_k^+ &= W_k \alpha_k^+ \\ i\hbar \partial_t \alpha_k &= W_k \alpha_k \end{aligned} \right\} \quad (3.3.81.),$$

where the excitation spectrum, W_k , is given by

$$W_k = \{J_k^2 - \sum_p |\bar{B}_{p,k}|^2\}^{1/2} \quad (3.3.82.).$$

The dispersion relation for the c-number parameters ϕ^* and ϕ has an identical expression as W_k . Now, these results are *different* from those obtained before in this section. (3.3.82.) contains a contribution in b_k^2 which is *not* present in (3.3.65.) and the c-number dispersion relation contains a contribution in $\sum_p |\bar{B}_{p,k}|^2$ which is not in (3.3.26.) either. It is most important to compare in detail the above procedure with that developed before in order to find the source of disagreement.

It is noted that the standard procedure leading to the derivation of W_k introduces the change of dynamical variables *after* linearization of the equations of motion for *particle* operators. This feature difficulties a direct comparison, for this purpose it will be convenient to reverse the order, and introduce the change of variables *before* linearization. An advantage of this alternative procedure is that the notion of anomalous averages does not arise.

A relevant observation here is that the method applied at the beginning of this section involves two elements, none of which is present in the standard approach, namely the reformulation of the problem on the basis of the same lagrangian in terms of two sets of dynamical variables, and the separability of the domain of definition of the new variables. The former methodological element enables to ascertain that \hat{H}' is, in rigour, *the* hamiltonian in the S.P.S. picture, different in general from the *particle* hamiltonian, but yet describing *the same* dynamical problem (but in terms of different canonical variables). The other element enables the existence of independent configurations in the S.P.S., allowing the construction of a Restricted Ensemble, which permits the emergence of an order parameter.

Now, the standard theory does not employ separable domains, but - in any event - one *must* consider the fundamental question: whether the functional obtained from \hat{H} by replacing particle operators by elementary excitation operators (of the L.C.S.R., say) is *the* hamiltonian, functional of the new dynamical variables, describing *the same* dynamical problem as $\hat{H}(a^+, a)$; or, on the contrary, whether such a functional, $\hat{H}(\alpha^+, \alpha)$, contains additional, spurious contributions, which affect the resulting expression for the (only one) excitation spectrum, giving an incorrect result.

This question cannot be answered within the context of the standard theory. To answer this question one must proceed according to the method

proposed in this thesis, namely (1) By formulating the problem on the basis of the same lagrangian; (2) Introducing the change of variables

$$(\hat{q}_k \equiv a_k, \hat{q}_k \equiv i\hbar \partial_t a_k) \rightarrow (\hat{q}'_k \equiv \alpha_k, \hat{q}'_k \equiv i\hbar \partial_t \alpha_k) ,$$

related through

$$\left. \begin{aligned} \hat{q}_k &= \int_t u_{k,t}^* \hat{q}'_t + \int_t v_{k,t} \hat{q}'_t{}^+ + k \\ \hat{q}'_k &= \int_t [u_{k,t}^* \hat{q}'_t + v_{k,t} \hat{q}'_t{}^+ + \hat{u}_{k,t} \hat{q}'_t + \hat{v}_{k,t} \hat{q}'_t{}^+] + \phi_k \end{aligned} \right\} (3.3.83.).$$

(3) To determine under what conditions *the* new hamiltonian exists, i.e. under what conditions

$$\hat{p}'_k \equiv \partial L / \partial \hat{q}'_k = \hat{q}'_k{}^+ \quad (3.3.84.)$$

is satisfied, and in the positive case (4) Determining the expression for the new hamiltonian $\hat{H}(\hat{p}', \hat{q}')$.

The method outlined above will not be developed in detail here; for, the algebraic complexity (measured by the number of additive contributions, and independent operations, leading to the conditions of existence of hamiltonian) is increased in this case by two orders of magnitude (!) compared with the similar derivation in §3.2. Also because - in the last analysis - a treatment in terms of variables of a non-separable domain is not appropriate for future statistical purposes. We limit ourselves here to stating the final results, which, on the other hand, can be forecasted, due to the fact that even though the dynamical variables in this case are not the same as before, the relations (3.3.83.) are the same.

In effect the hamiltonian $\hat{H}(\hat{p}', \hat{q}')$ is found to exist if appropriate conditions for the c-number parameters are adopted. The hamiltonian in this case turns out to be *the same* functional $\hat{H}'(\hat{p}^i, \hat{q}^i)$, but p^i and q^i are now *not* independent variables for different values of i , but functionals of p', q' (for $i = 1, 2$) and independent of these for ($i = 3$).

The conditions enabling the existence of the hamiltonian are now *not* redundant (for, there is only one pair of variables here), but must be stated *independently* of the action principle. The first pair of conditions, involving the first order coherent fields, are

$$-i\hbar\partial_t\phi_k^* = \partial\hat{H}'/\partial\phi_k \quad (3.3.85.)$$

and its c.c. The other two conditions, involving the v 's are very complicated. However, in the M.F.A. in which they will be used here, these latter conditions take a rather simple expression, namely

$$2J_k(\sum_q u_{k,q})(\sum_q v_{k,q}) + \sum_p B_{p,k}^*(\sum_q v_{k,q})^2 + \sum_p B_{p,k}(\sum_q u_{k,q})^2 = 0 \quad (3.3.86.)$$

and its c.c. Equation (3.3.85.) takes the following form in the M.F.A.:

$$-i\hbar\partial_t\phi_k^* = J_k\phi_k^* + b_k\phi_{-k} \quad (3.3.87.)$$

The difference between these conditions and (3.3.79., 80.) must be noted. It must also be noted that (3.3.87.) is identical to (3.3.20.), and that (3.3.86.) is the same as (3.3.63.).

We are now in a position to explain the cause of the disagreement between the spectrum W_k (and the dispersion relation W_k), and the expressions obtained through the method proposed in this thesis. This is: The standard method fails to compensate dangerous contributions. In addition, the contributions arising from the inherently non-diagonal segment of \hat{H} (or of \hat{H}') in the L.C.S.R., namely \hat{T}' , are not discarded either in equations (3.3.72., 73.); as a result of this the former equations (3.3.72., 73.) involve some *spurious* contributions. In order to decouple these equations (after replacing the variables \hat{p}_k and \hat{q}_k by \hat{p}_k' and \hat{q}_k' and *then* linearizing) the c-number 'diagonalization conditions' must also involve some spurious contributions, rendering them different from the correct conditions (3.3.86., 87.) which *ensure the existence of the hamiltonian* of the new

dynamical variables, \hat{p}'_k and \hat{q}'_k . The involvement of the spurious contribution leads to an erroneous expression for the excitation spectrum W_k - given by (3.3.82.) (and for the dispersion relation, also given by (3.3.82.)).

In order to be able to appreciate the truth of the above explanation it will be convenient to resort to the following artifice: The change of variables $(\hat{p}_k, \hat{q}_k) \rightarrow (\hat{p}'_k, \hat{q}'_k)$ is effected by replacing the former variables by p_k^i and q_k^i , namely

$$\hat{p}_k = \sum_i p_k^i, \quad \hat{q}_k = \sum_i q_k^i \quad (3.3.88.),$$

regarding p_k^i and q_k^i (for $i = 1, 2, 3$) not as independent variables, but as functions of \hat{p}'_k and \hat{q}'_k . This artifice will enable to compare equations (3.3.72., 73.) with equations (3.3.3., 4.), for which contributions from the dangerous segment and \hat{T}' have been left out explicitly.

Introducing (3.3.88.) into (3.3.72.) one finds

$$\begin{aligned} -i\hbar \partial_t \sum_i p_k^i &= \epsilon_k \sum_i p_k^i + \sum_{p,l} V(l) \left(\sum_{i,j} \overbrace{p_{p+l}^i p_{k-l}^j} q_p^j + \right. \\ &\quad \left. + \sum_{i,j} \overbrace{p_{p+l}^j p_{k-l}^i} q_p^i + \sum_{i,j,s} \overbrace{p_{p+l}^i p_{k-l}^j} q_p^s \right) \quad (3.3.89.). \end{aligned}$$

Now, summing equation (3.3.3.) over i , one finds

$$-i\hbar \partial_t \sum_i p_k^i = \epsilon_k \sum_i p_k^i + \sum_{p,l} V(l) \sum_{i,j} \overbrace{p_{p+l}^i p_{k-l}^j} q_p^j \quad (3.3.90).$$

From the comparison of (3.3.89., 90.) it is clear that the later two contributions of (3.3.89.) are not present in (3.3.90.).

It is clear that the latter two terms of (3.3.89.) correspond to contributions arising from \hat{T}' and the dangerous segment of \hat{H}

$$\sum_{i,j,s} \overbrace{p^i p^j} q^s q^i,$$

respectively. Equation (3.3.89.) takes the following form in the M.F.A.

$$\begin{aligned}
-i\hbar\partial_t \sum_i p_k^i &= [J_k \sum_i p_k^i + \sum_p B_{p,k}^* (q_p^1 + q_p^2) \\
&\quad + b_k q_{-k}^3] + [\sum_p b_p \delta_{p,-k} (q_p^1 + q_p^2) + \\
&\quad + \sum_p B_{p,k}^* q_p^3]
\end{aligned} \tag{3.3.91.},$$

where the spurious contributions have been associated in the second bracket. It is clear that adding up these two terms one finds

$$-i\hbar\partial_t \sum_i p_k^i = J_k \sum_k p_k^i + \sum_p B_{p,k}^* \sum_i q_p^i \tag{3.3.92.},$$

which is identical to equation (3.3.74.), but clearly incorrect for the latter two terms in (3.3.91.) should *not* be included; the one because it arises from the dangerous segment of \hat{H} , and the other because it arises from the segment of \hat{H} which can never be diagonalized in the L.C.S.R.. Now, if one uses (3.3.79.,80.) equation (3.3.92.) is decoupled, and the spectrum (3.3.82.) follows. But in that event equations (3.3.86.,87.) are *not* satisfied, and - in consequence - a hamiltonian does *not* exist! In order to obtain the *correct* spectrum one must discard the second bracket in (3.3.91.). Making use of the conditions ensuring the existence of the hamiltonian, namely (3.3.86.,87.), one finds that equation (3.3.91.) is decoupled, leading to an excitation spectrum in agreement with (3.3.36.).

The argument above shows the inadequacy of the assumption that the hamiltonian is the same functional regardless of the choice of dynamical variables. It also shows the failure of the criterion of diagonalization of the particle hamiltonian in the C.S.R. (or, equivalently, the criterion of decoupling of the canonical equations of motion). Stressing the need of formulating the dynamical problem on the basis of a lagrangian, in conjunction with the criterion of dynamical equivalence.

§4. Rearrangement of Gauge invariance, O.D.L.R.O. and statistical Mechanics in a separable phase space (S.P.S.)

§4.1. Introduction

Four different topics are considered in this chapter. The question of rearrangement of gauge invariance - discussed in the previous chapter - is investigated further in section 4.2. Explicit expressions for the generators of gauge transformations are obtained for both separable and non-separable phase spaces. The transformation laws for all the fields involved are also obtained. The Lagrange functional is explicitly shown to be invariant under *both* gauge transformations - in separable and non-separable phase spaces - in the presence of a compensating vector field (72), which follows the same transformation law in both cases. The compensating field is seen to play the rôle of an external (transverse) vector field of velocity. Euler-Lagrange equations are obtained for the dynamical variables of both formulations and for the external velocity field.

The investigations of sections 4.3. and 4.4. are fairly related. A *unique* system is considered in section 4.3. This *unreal* system is described *not* by an ensemble of states, but by a *pure state*. It is shown that O.D.L.R.O. occurs in the first two reduced matrices (r.d.m.) independently. It will become clear that this is necessary but insufficient to conclude that O.D.L.R.O. occurs in real systems, described by a statistical ensemble.

Section 4.4. is concerned with the formulation of the statistical problem on the basis of ensembles constructed from the S.P.S. A number of important results are obtained there; accordingly it will be convenient to group them in four numerals.

(1) A *non-superfluid* ensemble is constructed first. It is shown that the thermal averages of the first and second order coherent field *amplitudes*, $\langle\langle \phi \rangle\rangle$, $\langle\langle uv \rangle\rangle$, are identically *zero* over the non-superfluid ensemble; even though their corresponding *densities*, $\langle\langle |\phi|^2 \rangle\rangle$, $\langle\langle |v|^2 \rangle\rangle$, are *finite*,

in general. It is shown that O.D.L.R.O. does *not* occur at all. It is also shown that a physical system described by such an ensemble - in some temperature region - does *not* exhibit the property of superfluidity.

(2) All possible identifications of configurations in the S.P.S. with 'superfluid configurations' are considered in the second place. All options but one are discarded from physical considerations, namely because the resulting thermodynamical properties resulting from most options are in strong qualitative disagreement with experiment. The remaining semantic option identifies the *pairing* field density, $|v|^2$ with the order parameter of the superfluid phase. Both the density of elementary excitations $\langle\langle\hat{n}_k\rangle\rangle$ and the density of first order coherent field, $\langle\langle|\phi_k|^2\rangle\rangle$ turn out to correspond to the normal (non-superfluid) segment of the density distribution. The partition function of the *physical superfluid ensemble* is obtained. Some thermodynamic quantities of interest are obtained from it. A physical system described by such an ensemble is shown to exhibit the property of superfluidity.

(3) The excitation spectra for variables $i = 1, 2$ - found in §3.3. on the basis of a purestate description - are shown to split into two branches when evaluated in the physical superfluid ensemble, in thermal equilibrium. It is shown that excitations in between these two branches are possible in thermal equilibrium, leading to the observable prediction of a broad *band*. This is in good qualitative agreement with experiment (19). The lower branch of the spectrum obtained in a pure state description remains unaltered in the physical superfluid ensemble description.

(4) The integral equations characterizing the present mean field model in thermal equilibrium are obtained, for a superfluid ensemble. These equations for the superfluid ensemble do *not* resemble those obtained by several authors before (23,51). This is due to the special kind of statistical counting of configurations appropriate to the superfluid ensemble.

The conditions of existence of superfluid solution - also signaling the onset of the phase transition - are obtained. Finally, it is concluded that O.D.L.R.O. occurs in the second order r.d.m., but is ruled out in the first.

The final section considers further developments of the present theory of superfluidity. Three topics are considered there. Firstly, the possibility of constructing a purely quantum C.S.R.; for which c-numbers are replaced by q-numbers. Secondly, it is shown that first order coherence - and indeed O.D.L.R.O. in the first r.d.m. - is theoretically possible in Fermi systems, against a well-known indictment by Yang (71). The strategy and results of the present theory for the Bose superfluid are extrapolated to fermions. A speculative - and rather surprising - consequence is reached concerning the nature of the order parameter of the superconducting phase. Finally, the main elements of a new theory of magnetism are proposed, along the lines of the present theory of superfluidity. Free from the indictment of a breakdown of rotational symmetry and leading to a non-superfluid ordered phase.

§4.2. Rearrangement of gauge invariance

One of the main features of the theory of superfluidity proposed in this thesis is that gauge invariance is *not* broken, but rearranged. This aspect of the theory is investigated further in this section. It was made clear in §2.2. that the functional expression for the number operator, in terms of the dynamical variables, is determined by the structure of the phase space. This is independent of the representation of states employed to define the dynamical variables themselves. Later in section 2.4. - after defining the variables of the separable phase space in terms of the

fields of L.C.S.R. - it was shown that the number functional \hat{N}' is diagonal in L.C.S.R. The hamiltonian of the separable variable picture, \hat{H}' , was obtained in §3.2. It was shown there that \hat{N}' is a constant of motion, in the sense that $\{\hat{H}', \hat{N}'\} = 0$. As it turned out, however, \hat{H}' is not diagonal in L.C.S.R. An iterative scheme was outlined in §3.2. to obtain a more elaborate representation of states such that the *hamiltonian* symmetry is rearranged. It was also shown there that \hat{N}' is - again - a constant of motion for the zeroth order problem posed by \hat{H}'_0 , i.e. $\{\hat{H}'_0, \hat{N}'\} = 0$; and - in addition - it was shown that \hat{H}'_0 and \hat{N}' commute in L.C.S.R.

An interesting feature of the iterative scheme proposed in §3.2. to produce the *physical representation* (in Umezawa's terminology), is that it does not affect the *structure* of the phase space, but only the definition of the dynamical variables in terms of new fields (of representations of increasing complexity). In consequence the functional expressions for \hat{H}' and \hat{N}' in terms of the dynamical variables are not affected by the iterative procedure. The method of section 3.2. remains valid at any order of iteration, and $\{\hat{H}', \hat{N}'\} = 0$ - in particular - holds as an exact result. In view of this it is most important to prove that the gauge symmetry is rearranged, by showing that \hat{L}_g is *explicitly* invariant under gauge transformations in Γ_g ; without introducing particular fields of L.C.S.R. or any other representation. It is noted - on the other hand - that existing gauge theories of superfluidity (16,42 and Refs. therein) have been very successful in predicting a vast range of hydrodynamical phenomena in a direct and simple fashion (as the quantization of circulation, the existence of vortex lines and the critical value of vorticity, for instance). These theories, however, appear as *incomplete* in view of the results obtained here as to the rearrangement of the gauge invariance. In fact, all existing gauge theories start from the premise that the *full* gauge invariance - for *both* the normal fluid and the superfluid - is *broken*. Only a segment of the full lagrangian is believed to be gauge invariant. This segment is a

c-number lagrangian, L_c , functional of c-number *variables*; which are eventually identified with the order parameter of the superfluid phase, and most often than not - with the condensate. The remaining q-number segment of the full lagrangian, \hat{L}_Q , is associated with the normal fluid (and this, in turn, is often identified with the depletion). \hat{L}_Q is believed *not* to be gauge invariant. The rearrangement of the overall gauge invariance is accounted by the emission of a Goldstone boson (33b) or - more recently - through the Higgs mechanism (see Ref. (42) and Refs. therein).

The main goal of these gauge theories is to derive a set of Euler-Lagrange equations *for the superfluid*, exhibiting the correct coupling to the compensating field (72). From this equation hydrodynamic equations of continuity and current flow are obtained. These theories, however, face a strong limitation. The fields associated with the normal fluid do not appear naturally in the formalism. This is due to the fact that only the superfluid lagrangian segment is thought to be gauge invariant. In view of this limitation, and in order to be able to produce equations of continuity and current flow for the *entire* system (superfluid plus normal fluid), most authors find it necessary to identify the compensating vector field, A , with the *normal* fluid velocity field; instead of regarding it as an external field of velocity, exerted upon the *entire* system.

The viewpoint here is radically different. The full gauge symmetry is shown here to be rearranged, without having to resort to Goldstone or Higgs mechanisms. It is most important, then, to construct a *complete* gauge theory on this basis. Such a theory should correctly describe the coupling of *both* normal and superfluid segments to an external velocity field, without having to identify - for the moment - normal and superfluid variables, and without having to identify the *external* velocity field with the normal fluid's velocity either.

The objectives in this section are (i) to obtain generators of gauge transformations operating in both (separable and non-separable) phase spaces. (ii) To obtain the transformation laws for the dynamical variables of both formulations of the same problem. (iii) To demonstrate that the Lagrangian is invariant under both transformations, in the presence of an external vector field, A , transforming according to the same law in both cases. (iv) And to obtain Euler-Lagrange equations for all variables of the separable space picture and for the compensating field.

It is customary to consider the question of gauge invariance from a formulation in coordinate basis. This convention is followed here for the sake of comparison. The non-relativistic lagrangian associated with a collection of N ^4He atoms in a unitary volume, in the presence of an external field A , is given by

$$L_{ns}(\hat{q}, \hat{q}, \text{c.c.}) = \frac{1}{2} \int [\hat{q}^+(x) \hat{q}(x) + \text{c.c.}] d^3x - \int \hat{H}[\hat{p}(x), \hat{q}(x), A] d^3x + \lambda \int [\text{curl} A(x)]^2 d^3x \quad (4.2.1.),$$

where $\hat{H}(\hat{p}, \hat{q})$ is the hamiltonian density operator and the latter term in (4.2.1.) gives the energy of the external field A , regarded here as a c-number. λ is a characteristic constant with units of length. The hamiltonian is given by

$$\int \hat{H}(\hat{p}, \hat{q}) d^3x = \frac{1}{2m} \int (i\hbar \partial_x - m A) \hat{p}(x) \cdot (-i\hbar \partial_x - m A) \hat{q}(x) d^3x + \frac{1}{2} \iint \hat{p}(x) \hat{p}(y) V(|x - y|) \hat{q}(x) \hat{q}(y) d^3x d^3y \quad (4.2.2.).$$

It can be readily verified that generalized momenta - defined by $\hat{p}(x) \equiv \partial \hat{L}_{ns} / \partial \hat{q}(x)$ - is the canonical conjugate of $\hat{q}(x)$, hence the first term of (4.2.1.) can be written as

$$\frac{1}{2} \int [\hat{p}(x) \hat{q}(x) + \text{c.c.}] d^3x$$

In the particle picture generalized coordinates, momenta and velocities are

defined in terms of particle field operators as follows

$$\hat{q}(x) \equiv \hat{\Psi}(x); \hat{p}(x) \equiv \hat{\Psi}^+(x); \hat{\dot{q}}(x) \equiv i\hbar\partial_t\hat{\Psi}^+(x) \quad (4.2.3.),$$

where $\hat{\Psi}^+(x)$ and $\hat{\Psi}(x)$ are the Fourier transforms of a_k^+ and a_k , respectively. The kinematical momentum in the presence of external field A is given by

$$(i\hbar\partial_t - mA)\hat{p}(x) \text{ and its c.c. by } (-i\hbar\partial_t - mA)q(x),$$

m is here the coupling constant with units of mass, in order to render A in units of velocity. m is identified here with the mass of a ^4He atoms^(*).

Lagrangian \hat{L}_{ns} is formulated in terms of variables of a non-separable domain $D_{ns} \equiv \{\hat{q}(x'), \hat{q}(x)\}$. Transformations associated with lagrangian invariances operate upon the domain of generalized coordinates $\hat{q}(x)$ and their canonical conjugate $\hat{q}^+(x) = \hat{p}(x)$; that is, operate upon the non-separable phase space Γ_{ns} . Gauge transformations of the second kind are generated by the following exponential unitary operator:

$$U_G \equiv \exp[i \int s(x) N(x) d^3x] \quad (4.2.4.),$$

where $s(x)$ is an arbitrary c-number function of coordinates (but independent of time, for simplicity). $N(x)$ is the number distribution of particles in coordinate basis, namely

$$\hat{N}(x) = \hat{\Psi}^+(x) \hat{\Psi}(x) \quad (4.2.5.).$$

$$\text{The total number of particles is } \hat{N} = \int N(x) d^3x \quad (4.2.6.).$$

The volume of the phase space is normalized to the total number of particles, as usual, i.e.

*One could also consider both A and the coupling constant as quantum fields on their own, this very interesting possibility, however, is outside the scope of the present simple work.

$$\left. \begin{aligned} \text{Vol}(\Gamma_{\text{ns}}) &\equiv \text{Tr} \left\{ \int \hat{p}(x) \hat{q}(x) d^3x \right\} \\ &= \text{Tr} \{ \hat{N} \} = N \end{aligned} \right\} \quad (4.2.7.).$$

Now, according to the general rule of transformation theory, quantum fields transform as

$$\left. \begin{aligned} \hat{p}(x) \rightarrow \bar{\bar{p}}(x) &= U_G \hat{p}(x) U_G^{-1} = \hat{p}(x) \exp[-is(x)] \\ \hat{q}(x) \rightarrow \bar{\bar{q}}(x) &= U_G \hat{q}(x) U_G^{-1} = \hat{q}(x) \exp[is(x)] \\ \hat{\dot{q}}(x) \rightarrow \bar{\bar{\dot{q}}}(x) &= U_G \hat{\dot{q}}(x) U_G^{-1} = \hat{\dot{q}}(x) \exp[is(x)] \end{aligned} \right\} \quad (4.2.8.).$$

The later equality is obtained from (4.2.4.) by using the commutation relations

$$\left. \begin{aligned} [\Psi(x), \Psi^+(x')] &= \delta^3(x - x') \\ [\Psi(x), \Psi(x')] &= [\Psi^+(x), \Psi^+(x')] = 0 \end{aligned} \right\} \quad (4.2.9.)$$

It can be readily verified that \hat{L}_{ns} - given by (4.2.1., 2.) - is invariant under transformation (4.2.8.) if and only if the vector field $A(x)$ transforms according to

$$A(x) \rightarrow \bar{A}(x) = A(x) + (\hbar/m) \text{grad } s(x) \quad (4.2.10.).$$

Now, variables of non-separable and separable domains are related through

$$\hat{q}(x) \equiv \sum_i q^i(x); \quad \hat{p}(x) \equiv \sum_i p^i(x); \quad \hat{\dot{q}}(x) \equiv \sum_i \dot{q}^i(x) \quad (4.2.11.)^{(*)}$$

The same Lagrange operator in terms of the newly introduced variables is given by

*The super index i is not to be confounded with the imaginary unit, nor with the i th power.

$$\hat{L}_S = \frac{1}{2} \sum_i \int [p^i(x) q^i(x) + \text{c.c.}] d^3x - \int \hat{H}'(p^i, q^i) d^3x + \lambda \int [\text{curl } A(x)]^2 d^3x \quad (4.2.12.),$$

where the new hamiltonian is

$$\begin{aligned} \int \hat{H}'(p^i, q^i) d^3x &= \frac{1}{2m} \sum_i (\hbar \partial_x - mA) p^i(x) \cdot (-\hbar \partial_x - mA) q^i(x) d^3x + \\ &+ \frac{1}{2} \sum_{i,j} \iint p^i(x) p^j(x) V(|x-y|) \overbrace{q^i(x) q^j(y)} d^3x d^3y + \\ &+ \frac{1}{2} \sum_{i,j}^{(i \neq j)} \iint p^i(x) p^i(y) V(|x-y|) q^j(x) q^j(y) d^3x d^3y. \end{aligned} \quad (4.2.13.).$$

The redundant contribution to \hat{L}_S has already been removed.

Our immediate interest now is in obtaining a general gauge transformation in Γ_S . It cannot be expected that the most general generator of gauge transformations in Γ_S be expressible in terms of a single operator, operating independently in all three separate spaces. Instead, one is interested in three generators bringing about the following transformation

$$\left. \begin{aligned} p^i(x) + \bar{p}^i(x) &= p^i(x) \exp[-is(x)] \\ q^i(x) + \bar{q}^i(x) &= q^i(x) \exp[is(x)] \\ \dot{q}^i(x) + \bar{\dot{q}}^i(x) &= \dot{q}^i(x) \exp[is(x)] \end{aligned} \right\} \quad (4.2.14)$$

where $s(x)$ is *the same* arbitrary function for all three pairs of dynamical variables. An explicit expression for the generators can only be obtained from the knowledge of the definition of the dynamical variables p^i, q^i in terms of the (q or c -number) fields. But this generator is not important to know at this state. It suffices to know that the general law (4.2.14.) is a general gauge transformation in $\Gamma_S^{(*)}$.

*Even though is not *the most* general one, this is obtained for three *different* - in general - and *independent* arbitrary functions $s^i(s)$. The lagrangian, however, is *not* invariant under such a transformation (nor it needs to be, for the number of objects in s_i is not required to be conserved).

It can be very simply tested - by inspection - that transformation (4.2.14.) leaves \hat{L}_S invariant, provided that A transforms in the same way as before, namely according to (4.2.10.). This proves explicitly the rearrangement of gauge invariance.

It will be interesting to investigate now how the fields of L.C.S.R. transform according to (4.2.14.). After Fourier transforming the definition of dynamical variables in terms of the fields of L.C.S.R. one obtains

$$\left. \begin{aligned} q^1(x) &\equiv \int u^*(x,y) \theta(y) d^3y \\ q^2(x) &\equiv \int v(x,y) \theta^+(y) d^3y \\ q^3(x) &\equiv \phi(x) \end{aligned} \right\} \quad (4.2.15.),$$

where $u^*(x,y)$, $v(x,y)$, $\theta(x)$ and $\theta^+(x)$ are the Fourier transforms of the $u_{k,q}^*$, $v_{k,q}$, a_k and a_k^+ respectively. $\theta(x)$ transforms according to $\theta(x) \rightarrow \bar{\theta}(x) = \theta(x) \exp[i s(x)]$, then $u(x,y)$ transforms as

$$u(x,y) \rightarrow \bar{u}(x,y) = u(x,y) \exp[-s(x) + s(y)] \quad (4.2.16);$$

accordingly $v(x,y)$ must transform as

$$v(x,y) \rightarrow \bar{v}(x,y) = v(x,y) \exp i[s(x) + s(y)] \quad (4.2.17.),$$

and finally $\phi(x)$ transforms as

$$\phi(x) \rightarrow \bar{\phi}(x) = \phi(x) \exp[i s(x)] \quad (4.2.18.).$$

Note that

$$R \equiv \int v^*(x',y) v(x,y) d^3y = \int |v(x,y)|^2 d^3y$$

transforms according to

$$\begin{aligned} R \rightarrow \bar{R} &= \exp\{i[s(x) - s(x')]\} \int v^*(x',y) v(x,y) d^3y \\ &= \exp\{i[s(x) - s(x')]\} \int |v(x,y)|^2 d^3y \end{aligned} \quad (4.2.15.).$$

This transformation law will turn out to be the most important to bring about a curl-free velocity field for the pairing density, which will turn out to be associated with the superfluid.

To end this section let us write down the Euler-Lagrange equations for generalized coordinates and their c.c.

$$\begin{aligned} i\hbar\partial_t q^i(x) = & -\frac{\hbar^2}{2m} (\partial_x - \frac{m}{\hbar} A)^2 q^i(x) + \\ & + \sum_j V(|x-y|) p^j(y) \overbrace{q^j(x) q^i(y)} d^3y \\ & + \sum_{j \neq i} V(|x-y|) p^i(y) q^j(x) q^j(y) d^3y \end{aligned} \quad (4.2.16.)$$

$$\begin{aligned} -i\hbar\partial_t p^i(x) = & -\frac{\hbar^2}{2m} (\partial_x - \frac{m}{\hbar} A)^2 p^i(x) + \\ & + \sum_j V(|x-y|) \overbrace{p^i(x) p^j(y)} q^j(y) d^3y \\ & + \sum_{j \neq i} V(|x-y|) p^j(x) p^j(y) q^i(y) d^3y \end{aligned} \quad (4.2.17.),$$

and for the velocity field in the Coulomb gauge, $\text{div } A = 0$

$$\begin{aligned} \lambda \text{Curl Curl } A = & \frac{i\hbar}{2m} \sum_i \{ p^i(x) [\text{grad } q^i(x)] - [\text{grad } p^i(x)] q^i(x) \} - \\ & - \sum_i p^i(x) q^i(x) A \end{aligned} \quad (4.2.18.).$$

Equations (4.2.16 - 18.) give a *complete* gauge theory of the coupling of an external field of velocity to the entire fluid in the separable phase space picture. Subsequent developments of this theory should now follow the same general lines as existing theories. It should be noted, however, that normal and superfluid variables have not been specified. This will be done in §4.4. It must also be noted that velocity fields arise naturally for all three pairs of variables involved, hence there is no need for identifying A with any of them. In fact the velocity fields associated with these variables should follow the piloting effect of the external field. Whether or not some of these velocity fields follow A *coherently*.

i.e. curl-free, depends on whether the statistical average enables the gauge phase $\exp[\pm i\phi(x)]$ to be finite, or - on the contrary - to cancel out due to incoherent thermal collisions. This idea will be developed further in §4.4. But now let us consider the question of whether O.D.L.R.O. occurs in either of the first two r.d.m.

§4.3. O.D.L.R.O.

A powerful characterization to classify physical systems exhibiting coherent and superfluid behaviour on a macroscopic scale was developed in the fifties and sixties by Penrose and Onsager and Penrose⁽⁵⁷⁾, Yang (71), Frölich (27) and Glauber (31), based on the factoring properties of the reduced density matrices (r.d.m.).

During the sixties and seventies Frölich proposed and developed a programme aimed at obtaining predictions about the hydrodynamical behaviour of superfluids from certain structural, macroscopic properties of the r.d.m. - O.D.L.R.O., in particular - without a detailed solution of the many-body problem. This very economical programme has been developed further by a number of authors since. Hyland and Rowlands developed a closed set of hydrodynamical equations for the Bose superfluid(41), Taylor did the same for superconductors(64) and Haken for lasers (80).

The starting point of all these approaches is the hierarchy of master equations of motion for the r.d.m. proposed by Frölich (27), and ansatz for the structure of the first few r.d.m., usually the first two. This effectively truncates the hierarchy (usually at second order) yielding a complete set of equations. The solution of this set of equations gives *the structure* of hydrodynamic equations in remarkable agreement with experiment. This is true for the Bose superfluid, as well as for superconductors and lasers.

The above programme was based on the use of density matrices defined over a *non-separable phase space*, associated with the particle picture.

The aims in this section are (i) to show that the same scheme can be developed from a separable phase space picture, with minor change; (ii) to show that defining the dynamical variables of Γ_s in terms of L.C.S.R. the ansatz for the first two r.d.m. of Frölich, and Hyland and Rowlands is confirmed and generalized, for a *unique* system described by means of *pure states* (not a statistical mixture).

Let us recapitulate the main basic features of the approach to superfluidity based on O.D.L.R.O. (27). From Liouville's equation for the von Neumann density matrix, $\hat{\Omega}$

$$i\hbar \partial_t \hat{\Omega} = [\hat{H}, \hat{\Omega}] \quad (4.3.1.),$$

where \hat{H} is the particle hamiltonian - given by (1.2.3.)F - and the definition of the *particle* r.d.m., namely

$$\left. \begin{aligned} \Omega_1(x, x') &\equiv \text{Tr} \{ \Psi^+(x') \Psi(x) \hat{\Omega} \} \\ \Omega_2(x, y; x', y') &\equiv \text{Tr} \{ \Psi^+(x') \Psi^+(y') \Psi(x) \Psi(y) \hat{\Omega} \} \end{aligned} \right\} \quad (4.3.2.)$$

etc., the following hierarchy of master equations is obtained:

$$i\hbar \partial_t \Omega_1(x, x') = - \frac{\hbar^2}{2m} (\partial_x^2 - \partial_{x'}^2) \Omega_1(x, x') + W_1 \quad (4.3.3.)$$

$$\begin{aligned} i\hbar \partial_t \Omega_2(x, y; x', y') &= - \frac{\hbar^2}{2m} [(\partial_x^2 + \partial_{y'}^2) - (\partial_{x'}^2 + \partial_y^2)] \\ &\quad + V(|x - y|) \Omega_2(x, y; x', y') + W_2 \end{aligned} \quad (4.3.4.)$$

etc., where

$$W_1 \equiv \int [V(|x - y|) - V(|x' - y'|)] \Omega_2(x, y; x', y') d^3y \quad (4.3.5.),$$

$$\begin{aligned} W_2 &\equiv \int [V(|x - z|) + V(|y - z|) - \\ &\quad - V(|x' - z|) - V(|y' - z|)] \Omega_3(x, y, z; x', y', z) d^3z \end{aligned} \quad (4.3.6.)$$

etc.

The ansatz for the first two r.d.m. for the Bose problem are

$$\Omega_1(x;x') = \Lambda_1(x,x') + \phi^*(x') \phi(x) \quad (4.3.7.),$$

where $\Lambda_1(x;x') \rightarrow 0$ as $|x - x'| \rightarrow \infty$

$$\begin{aligned} \Omega_2(x,y;x',y') = & \phi^*(x') \phi^*(y') \phi(x) \phi(y) + \phi^*(x') \phi(x) \Lambda_1(y;y') + \\ & + \phi^*(y') \phi(y) \Lambda_1(x;x') + \phi^*(x') \phi(y) \Lambda_1(x;y') + \\ & + \phi^*(y') \phi(x) \Lambda_1(y;x') + \Lambda_1(x;x') \Lambda_1(y;y') + \\ & + \Lambda_1(x;x') \Lambda_1(y;x') + \Lambda_2(x,y;x',y') \end{aligned} \quad (4.3.8.),$$

where $\Lambda_2 \rightarrow 0$ if $d[(x,y);(x',y')] \rightarrow \infty$.

That is O.D.L.R.O. was assumed in Ω_1 , but not in Ω_2 , for which the only factorization is that originating from that in the first r.d.m., $\Omega_1^{(**)}$. For superconductors the ansatz is⁽⁶⁴⁾

$$\Omega_1(x;x') = \Lambda_1(x;x') \quad (4.3.9.)$$

$$\begin{aligned} \Omega_2(x,y;x',y') = & \phi^*(x,y') \phi(x,y) + \Lambda_1(x;x') \Lambda_1(y;y') \\ & - \Lambda_1(x;y') \Lambda_1(y;x') + \Lambda_2(x,y,x',y') \end{aligned} \quad (4.3.10.);$$

that is, O.D.L.R.O. is assumed in Ω_2 but not in Ω_1 . In fact, it was noted by Yang (71) that O.D.L.R.O. in Ω_1 is *not* possible for Fermi systems due to the fact that a contribution of the form $\phi^*(x') \phi^*(y') \phi(x) \phi(y)$ - which would occur in Ω_2 - does not have the correct antisymmetry under permutation of coordinates $x \leftrightarrow y$; for, ϕ 's are thought to be *abelian* functions^(*).

*It will be shown in §4.5. that under appropriate circumstances O.D.L.R.O. can occur in Ω_1 for Fermi systems.

**An improved ansatz was later proposed by Frölich encompassing O.D.L.R.O. in Ω_2 for the Bose problem.

Introducing the ansatz (4.3.7.,8.) into the master equation (4.3.3.-6) and going to the far from local limit, $|x - x'| \rightarrow \infty$, the equations of motion for the first order coherent fields are obtained, namely

$$-i\hbar\partial_t\phi(x) = -\frac{\hbar^2}{2m}\partial_x^2\phi(x) + \int V(|x-y|) [\phi(x)\sigma_T(y) + \phi(y)\Lambda_1(x,y)]d^3x \quad (4.3.11.),$$

and similarly for its c.c., where $\sigma_T(y)$ is the total density at the point y . Introducing equation (4.3.11.) and its c.c. in the master equation for $\Omega_1(x;x')$ in the near local limit the equation of motion for $\Lambda_1(x;x')$ is obtained. Writing ϕ 's and Λ_1 as their moduli times their phases, and separating real and imaginary parts, the equations of continuity and conservation of current are obtained. Conservation equations for flow of energy and entropy are also obtained from the definition of energy in terms of suitably defined velocities, and from the assumption that only Λ_1 (and not $\phi^*\phi$) contributes to the flow entropy (41).

The programme summarized above can be easily posed in terms of the separable phase space (S.P.S.) picture, with minor modification. The density matrix, for a start, is different in general (see next section, $\hat{\Omega}'$ instead of $\hat{\Omega}$ say). The Liouville equation in the S.P.S. is also different, namely

$$i\hbar\partial_t\hat{\Omega}' = \{\hat{H}',\hat{\Omega}'\} \quad (4.3.12.).$$

As to the definition of the r.d.m., it is most important to note that these are defined as quantum and thermal averages of the *n*-body propagator functional, $\hat{G}_n(x,y, \dots; x',y', \dots)$ in the N-S.P.S. and $G'_n(x,y, \dots; x',y', \dots)$ in the S.P.S., say. The thermal average is carried out over an ensemble constructed either in Γ_{ns} or Γ_s , whose density matrices are $\hat{\Omega}$ and $\hat{\Omega}'$, respectively. That is, the r.d.m. in the N-S.P.S. and S.P.S.

are defined as follows:

$$\Omega_n(x, y, \dots; x', y', \dots) \equiv \text{Tr}\{\hat{G}_n(x, y, \dots; x', y', \dots)\hat{\Omega}\} \quad (4.3.13.)$$

and

$$\Omega'_n(x, y, \dots; x', y', \dots) \equiv \text{Tr}\{\hat{G}'_n(x, y, \dots; x', y', \dots)\hat{\Omega}'\} \quad (4.3.14.),$$

respectively.

The n-body propagator functionals are defined, in turn, as functionals of the corresponding canonical variables, and are very dependent of the phase space's architecture. The first two propagator functionals in the N-S.P.S., for instance, are defined as

$$\left. \begin{aligned} \hat{G}_1(x; x') &\equiv \hat{p}(x') \hat{q}(x) \\ \hat{G}_2(x, y; x', y') &\equiv \hat{p}(x') \hat{p}(y') \hat{q}(x) \hat{q}(y) \end{aligned} \right\} \quad (4.3.15).$$

Definitions (4.3.2.) are recovered by defining $\hat{p}(x) \equiv \Psi^+(x)$ and $\hat{q}(x) = \Psi(x)$. The propagator functionals in the S.P.S. take a different form, dictated by the structure of Γ_S . The first propagator, for instance, is given by

$$\hat{G}_1^i(x, x') \equiv \int_1 p^i(x') q^i(x) \quad (4.3.16).$$

It is recalled that contributions of the form $p^i q^j$ do not occur in \hat{G}_1^i ; for, they make reference to *two* (distinguishable) objects. Similarly contributions of the form $p^i p^j q^k$, $p^i p^j q^k q^l$ do not occur in \hat{G}_2^i , as they refer to three and four (distinguishable) objects.

Utmost care must be exercised in defining the \hat{G}_n^i for $n \geq 2$, in order to avoid inconsistency. It might be thought that as long as these functionals are to be *defined*, and *not derived*, one is free to choose their functional expressions at will. That is *not* so; for, one is aiming at an equivalent reformulation of a given dynamical problem in terms of variables of two phase spaces. This strategy dictates a criterion *determining* the functional expressions of all the \hat{G}_n^i uniquely.

The functional expression of \hat{G}_2^i is determined from the following considerations: The interaction term, \hat{U} , in the particle hamiltonian is proportional to the 2-body propagator functional^(*) only, i.e. *all* two-body interactions and *only* two-body interactions contribute to \hat{U} , namely

$$\hat{U} = \iint V(|x - y|) \hat{G}_2(x, y; x, y) d^3x d^3y \quad (4.3.17.).$$

In consequence the (two-body) interaction segment of the S.P.S. picture hamiltonian, \hat{U} , *must* be a functional of \hat{G}_2^i *only* (a functional of *the whole* \hat{G}_2^i , and not just of a segment of it), namely

$$\hat{U} = \iint V(|x - y|) \hat{G}_2^i(x, y; x, y) d^3x d^3y \quad (4.3.18.).$$

Should this *not* be the case, the two formulations would *not* be equivalent, in so far as the pair correlation *functionals*, \hat{G}_1^i and $\hat{G}_2^{i(*)}$, *must* be constants of motion in both formulations (and have the same expectation values). From the inspection of the S.P.S. picture hamiltonian it follows, then, that \hat{G}_2^i *must* be defined as

$$\begin{aligned} \hat{G}_2^i(x, y; x', y') = & \sum_{i, j} p^i(x') p^j(y') \overbrace{q^i(x) q^j(y)} + \\ & + \sum_{i, j}^{(i \neq j)} p^i(x') p^i(y') q^j(x) q^j(y) \end{aligned} \quad (4.3.19.)$$

The last term is non-diagonal in L.C.S.R. (if the canonical variables are defined as in §2.4.), hence gives no contribution to Ω_2^i .

The above method can be generalized to obtain expressions for the n^{th} propagator functional as follows:

(i) Write down the summation of all *variations* of

$$p^i(x'_1) \dots p^j(x'_n) q^i(x_1) \dots q^j(x_n),$$

involving none, one, two and three different superindices, and sum up over all different super-indices from one to three. Note that the sub-indices

*In the local limit.

of x' and x do *not* indicate the space to which the variables, p and q , belong, but indicate two different coordinates (of distinguishable or indistinguishable objects).

(ii) Decompose this sum into two parts

$$\begin{aligned} \bar{G}_n' + \frac{1}{2} \{ & \sum_{i,j}^{(i \neq j)} \sum_{m=1}^n [p^i(x_m') (\partial \bar{G}_n' / \partial p^j(x_m')) + \\ & + (\partial \bar{G}_n' / \partial q^j(x_m)) q^j(x_m)] \} \end{aligned}$$

(ii) Discard the second term, and $\bar{G}_n' \equiv \hat{G}_n'$ is the n^{th} order propagator functional.

It is clear that the above definitions of r.d.m. make no reference to a particular representation of states. If the dynamical variables are defined in terms of L.C.S.R. as in §2.4. the following expressions are obtained for the first two r.d.m.

$$\Omega_1'(x; x') = \sum_{k, k'} \Omega_1'(k, k') \exp[i(kx - k'x')] \quad (4.3.20.)$$

$$\begin{aligned} \Omega_2(x, y; x', y') = \sum_{\substack{k, k' \\ q, q'}} \Omega_2'(k', q'; k, q) \exp\{i[(kx + qy) - \\ - (k'x' + q'y')]\} \end{aligned} \quad (4.3.21.),$$

where

$$\Omega_1'(k; k') = \text{Tr}\{[\hat{\Lambda}_1(k, k') + \phi_k^* \phi_k] \Omega'\} \quad (4.3.22.),$$

$$\hat{\Lambda}_1(k; k') \equiv \hat{\Lambda}_1^T(k; k') + \Lambda_1^0(k; k') \quad (4.3.23.),$$

$$\hat{\Lambda}_1^T(k; k') = \hat{\Lambda}_1^T(k; k') = \sum_{t, t'} (u_{k, t}^* u_{k', t} + v_{k, t} v_{k', t}^*) \alpha_t^+ \alpha_{t'} \quad (4.3.24.),$$

$$\Lambda_1^0(k; k') = \sum_t v_{k', t}^* v_{k, t} \quad (4.3.25.);$$

$$\begin{aligned}
\Omega_2^1(u_k, q; k', q') = & \text{Tr}\{[\phi_k^*, \phi_q^*, \phi_k \phi_q + \phi_{k', q}^*, \phi_{k, q} + \\
& + \phi_k^*, \phi_k \hat{\Lambda}_1(q; q') + \phi_q^*, \phi_q \hat{\Lambda}_1(k; k') + \\
& + \phi_k^*, \phi_q \hat{\Lambda}_1(k; q') + \phi_q^*, \phi_k \hat{\Lambda}_1(q; k') + \\
& + \phi_{k', q}^*, K_{k, q} + \phi_{k, q} K_{k', q}^* + \\
& + \hat{\Lambda}_2(k, q; k', q')]\hat{\Omega}^1\}
\end{aligned} \quad (4.3.26.),$$

where

$$\phi_{k, q} \equiv \sum_t u_{k, t}^* v_{q, t} \quad (4.3.27.),$$

$$K_{k, q} \equiv 2 \sum_t u_{k, t}^* v_{q, t} \alpha_t^+ \alpha_t \quad (4.3.28.)$$

and

$$\begin{aligned}
\hat{\Lambda}_2(k, q; k', q') = & \sum_{\substack{t, t' \\ s, s'}} [u_{k', s}^* u_{q', t}^* u_{k, s}^* u_{q, s}^* \alpha_s^+ \alpha_t^+ \alpha_s \alpha_t + \\
& + v_{k', s}^* v_{q', t}^* v_{k, s}^* v_{q, t}^* \alpha_s^+ \alpha_t^+ \alpha_s \alpha_t + \\
& + u_{k', s}^* v_{q', t}^* u_{k, s}^* v_{q, t}^* \alpha_s^+ \alpha_t^+ \alpha_s \alpha_t + \\
& + u_{k', s}^* v_{q', t}^* v_{k, s}^* u_{q, t}^* \alpha_s^+ \alpha_t^+ \alpha_s \alpha_t + \\
& + v_{k', s}^* u_{q', t}^* u_{k, s}^* v_{q, t}^* \alpha_t^+ \alpha_s^+ \alpha_s \alpha_t + \\
& + v_{k', s}^* u_{q', t}^* v_{k, s}^* u_{q, t}^* \alpha_t^+ \alpha_s^+ \alpha_s \alpha_t]
\end{aligned} \quad (4.3.29.).$$

If only quantum averages were involved in the definition of the r.d.m. - as is the case for a *unique* system, described by a pure state (as opposite to a mixture of states) - it is clear from the inspection of (4.3.22., 26.) that O.D.L.R.O. would take place in both r.d.m.'s, Ω_1^1 and Ω_2^1 , independently. The expression for Ω_1^1 (in a pure state description) validates Fröhlich's

ansatz. The expression for Ω_2 also validates Frölich's ansatz for the second order r.d.m., including independent O.D.L.R.O. in Ω_2 . It is interesting to note that a contribution of the form $\phi_k^* \phi_q^* \phi_{k,q} + \phi_{k',q}^* \phi_k \phi_k$ does not occur in Ω_2^1 , as could be expected from a structural decomposition of Ω_2^1 . This contribution is proportional to some of the redundant terms and its presence leads to inconsistencies. It is interesting to note that this contribution - *not* included in Frölich's ansatz! - corresponds to the diagonal segment of \hat{H}_R (see §3.2,3.3).

The irreducible part of Ω_2^1 , namely $\hat{\Lambda}_2$, takes the following form in the mean field approximation:

$$\begin{aligned} \hat{\Lambda}_2(k,q;k',q') = & \hat{\Lambda}_1^T(k;k') \langle \hat{\Lambda}_1^T(q;q') \rangle + \\ & + \hat{\Lambda}_1^T(k;q') \langle \hat{\Lambda}_1^T(q;k') \rangle + \hat{\Lambda}_2^F(k,q;k',q') \quad (4.3.30.). \end{aligned}$$

The first two terms are the mean field values of $\hat{\Lambda}_2$ and the last term $\hat{\Lambda}_2^F$ represents fluctuations about mean values. It is noted that the expression above is independent of Λ_1^0 .

The discussion so far, as to the occurrence of O.D.L.R.O., has been confined to unique systems described by pure states. Real systems, however, *must* be regarded as a mixture of states (an ensemble) associated with a collection of identical replicas of the same system (of the same or different, but macroscopic, size). In consequence the expressions for the r.d.m.'s must be obtained as thermal averages over a suitable statistical ensemble. The occurrence of O.D.L.R.O. in this case is *not* ensured by the factoring of the r.d.m.'s in a pure state description. O.D.L.R.O. in Ω_1^1 and/or Ω_2^1 will occur if the thermal averages of $\phi_k^* \phi_k$ and/or $\phi_{k',q}^* \phi_{k,q}$ respectively, are non-zero for $k' \neq k$, $q' \neq q$. This will occur if and only if the ensemble averages of ϕ_k and/or $\phi_{k,q}$ are finite; in other words, if the statistical weights of the phases of ϕ and/or ϕ do *not* add up randomly, but coherently. O.D.L.R.O. will take place, then, if and only if two sub-

systems differing only by the phases of ϕ and/or Φ are thermodynamically identical, i.e. if $|\phi|^2$ and/or $|\Phi|^2$ are order parameters.

Should that be the case and O.D.L.R.O. take place in either Ω_1^i or Ω_2^i , it is clear that the system will be a superfluid; for, a fraction of the *ensemble average* density will be fully ordered. If O.D.L.R.O. turns out to occur in either Ω_1^i or Ω_2^i and the system is subject to an external field of velocity $A = A_T + A_L$, where A_T and A_L are transverse and longitudinal components, i.e. $A_L \propto \text{grad } s(x)$, the values of $\phi^*(x')\phi(x)$ and/or $\int v^*(|x' - y|) v(|x - y|) d^3y$ (i.e. the Fourier transform of ϕ_k^*, ϕ_k and/or $\sum_q v_{k',q}^* v_{k,q}$) will turn out to be multiplied by a phase factor of the form $\exp[i(s(x) - s(x'))]$. This means that a longitudinal field of velocity will be imposed on $\phi(x)$ or $\phi(x - y)$. Due to the fact that the average phases of these fields are finite, a macroscopic curl-free velocity field will turn out to be associated to the factoring amplitudes of Ω_1^i and Ω_2^i .

Finally, it is interesting to point out that the definitory expressions for Ω_1^i and Ω_2^i enable to derive the first master equation of motion for Ω_1^i from Liouville's equation (4.3.12.), i.e.

$$i\hbar \partial_t \Omega_1^i = - \frac{\hbar^2}{2m} (\partial_x^2 - \partial_{x'}^2) \Omega_1^i + W_1^i$$

where

$$W_1^i \equiv \int [V(|x - y|) - V(|x' - y|)] \Omega_2^i(x, y; x', y) d^3y \quad (4.3.31.).$$

In view of the way in which higher order r.d.m.'s are defined, one can expect that the entire hierarchy of master equations in the S.P.S. have the same form as Fröhlich's hierarchy in the N-S.P.S. with the only difference that Ω_n are replaced by Ω_n^i . In fact, should that not be the case the two formulations would *not* be dynamically equivalent.

§4.4. Statistical counting in the S.P.S.

The discussion on the problem of ^4He has been confined so far to dynamical considerations on the basis of a pure state description. The main concern has been with the question of whether it is possible or not to formulate the same (microscopic) dynamical problem on the basis of two sets of dynamical variables, defined in domains of different structure (separable and non-separable), expressed in terms of the fields of two non-equivalent representations. None of these considerations, however, enables to ascertain whether a realistic *macroscopic* model-system undergoes a phase transition to or from a *superfluid* phase from or to a *normal* (non-superfluid) phase.

In order to be able to draw any conclusion at this respect one must consider the statistical mechanical problem of a collection of macroscopically small subsystems in thermal equilibrium with a large reservoir at temperature T . This section is devoted to investigate this matter.

The first aim in this section is to construct *two* different, but *statistically comparable*, ensembles on the basis of the counting of configurations in the S.P.S. It will be shown, initially, that the most general Grand canonical ensemble (G.C.E.) constructed on the basis of configurations defined in the S.P.S. always admits a restricted ensemble (R.E.). Such an ensemble, without further constraints, is referred to here as *non-superfluid ensemble*. The other ensemble constructed here is obtained from the non-superfluid ensemble by introducing a statistical constraint. This is a condition stating that some set of the various sets of independent configurations in the S.P.S. - is *statistically equivalent*. The resulting ensemble being referred to here as the *superfluid ensemble*. These two ensembles - superfluid and non-superfluid - are statistically comparable in so far as they differ *only* as to the imposition or not of the statistical constraint. One can ascertain,

then, which of the two statistical descriptions is energetically favourable, by *comparing* the two free energies as functions of temperature.

It will become clear that several different variants of superfluid ensembles are theoretically possible, depending on what the statistically equivalent configurations are chosen to be from the three sets of independent configurations in the S.P.S. (or factors of them). After considering all these possible 'semantic options' it will be concluded that the only interpretation in qualitative agreement with experiment, as to the excitation spectrum and the temperature dependence of the specific heat at low T , is that for which different distributions of *pairing fields*, $|V_{k,q}|^2$, are statistically equivalent.

It will be shown that a macroscopic system described statistically by a superfluid (non-superfluid) ensemble does (not) exhibit the property of superfluidity, in the sense than an (no) additive part of the total ensemble average density is fully ordered; and, in consequence, flows without (with) dissipation of energy.

The main prediction to be obtained in this section concerns the excitation spectrum. Experimental observation shows a low lying gapless branch and *also* an upper band at about 20°K . It will be shown here that the excitation spectra associated with the fields p_k^i and q_k^i for $i = 1, 2$ splits up into $2N$ closely packed branches for the superfluid ensemble in thermal equilibrium, in qualitative agreement with the experiment (19). The low lying branch, ω_k^3 , is shown to remain unaltered in both superfluid and non-superfluid ensembles, taking the same expression as in the pure state description.

The integral equations characterizing the mean field model of section 3.3. in thermal equilibrium are obtained for the superfluid ensemble.

Finally, the condition determining the onset of the superfluid phase and, eventually, the critical temperature is obtained. It is concluded

that O.D.L.R.O. takes place in the superfluid phase in the second order reduced density matrix, but is ruled out in the first.

The type of ensemble one is able to construct in order to describe the, macroscopic, statistical behaviour of a given dynamical system is conditioned by the structure of the phase space in which the dynamical variables are defined, and on which the statistical counting of configurations is carried out. The G.C.E. constructed for a dynamical system whose variables are defined in a *non-seperable* phase space, for instance, does not admit a restricted ensemble (R.E.), unless an *a priori* partition is introduced into the phase space.

The Grand partition function for a G.C.E. associated to a dynamical system whose constants of motion, \hat{H} and \hat{N} , say, are functionals of N.S.P.S. variables is given, as usual, by

$$Z_G = \sum_{\hat{G}_k} \text{Tr}\{\hat{\Omega}\} \quad (4.4.1.),$$

where

$$\hat{\Omega} = \exp[-\beta(\hat{H} - \mu\hat{N})] \quad (4.4.2.)$$

is the density matrix in thermal equilibrium at temperature $T = (K_B\beta)^{-1}$, K_B being the Boltzman constant and μ the chemical potential.

The G.C.E. ensemble for the same dynamical problem formulated in terms of variables of a *seperable phase space*, on the other hand, always admits a R.E. In effect, the Grand partition function in this case is given by

$$Z_r = \sum_{\hat{G}_k^1} \sum_{\hat{G}_k^2} \sum_{\hat{G}_k^3} \dots \sum_{\hat{G}_k^d} \text{Tr}\{\hat{\Omega}'\} \quad (4.4.3.),$$

where the density matrix $\hat{\Omega}'$ is now given by

$$\hat{\Omega}' = \exp[-\beta(\hat{H}' - \mu' \hat{N}')] \quad (4.4.4.).$$

The summations in (4.4.1.,3.) run over all possible (non-equivalent) configurations, namely

$$C_k \equiv \text{Tr}\{\hat{p}_k \hat{q}_k\} \quad (4.4.5.)$$

for the non-separable phase space, Γ_{ns} , and

$$C_k^i \equiv \text{Tr}\{p_k^i q_k^i\} \quad (4.4.6.)$$

for the S.P.S., Γ_s . The summation over configurations in Γ_s is a product of summations, this is due to the fact that the C_k^i 's are independent configurations. (4.4.3.) is the general expression for the partition function of a restricted ensemble. In the present work $d = 3$.

The fact that the average number of particles in both ensembles (4.4.1.,3.) is the same, i.e.

$$N = \partial \langle \hat{H} - \mu \hat{N} \rangle / \partial \mu \quad (4.4.7.)$$

$$N' = \partial \langle \hat{H}' - \mu' \hat{N}' \rangle / \partial \mu' \quad (4.4.8.)$$

$$N = N' \quad (4.4.9.),$$

follows from the fact that the volumes of both phase spaces Γ_{ns} and Γ_s are the same.

The strategy underlying the present formulation of the statistical problem differs considerably from the standard strategy (4,5,6,15,18,20, 23,29,31,32,34,45,46,51,55,60,65,67,68). The present paradigmatic view, however, being in close connection with Hohenberg and Martin's strategy (38), to which the present scheme provides a generalization. Some brief remarks on this departure from the standard view are appropriate at this stage.

It was pointed out before that the main element of existing standard theories of superfluidity is *dynamical*. The main interest has been in devising appropriate representations of states describing the superfluid phase's dynamics; and deriving predictions as to the excitation spectrum in agreement with experimental observation. The statistical problem, however, has been relegated - to some extent - to a secondary position, in the sense that it was believed that this latter problem does not require of additional novel conceptual elements for its appropriate formulation. Hohenberg and Martin challenged this view. These authors suggested that a superfluid should be characterised - in general - exclusively within the statistical context, by means of certain necessary and sufficient conditions satisfied by certain ensembles (defining a sub-set of the restricted ensembles). These authors, however, did not rule out the possibility that - in particular cases - certain elements originating in the dynamical scene provided sufficient (but not necessary) conditions for superfluidity, as the occurrence of Bose-Einstein condensation.

The characterisation proposed by Hohenberg and Martin is rather simple and conveys a direct prediction of superfluidity, but - on the other hand - it does not provide a mechanism by means of which superfluid behaviour comes about, and is too dependent on the occurrence of Bose-Einstein condensation. The central idea is that the statistical ensemble describing a superfluid should incorporate independent configurations (which they associated with configurations of the condensate and depletion modes). Superfluidity comes about if the entropy associated with a fraction of the ensemble is fully ordered, the relative order being measured by an order parameter. The fundamental property of superfluid ensembles was then associated with the thermodynamic indistinguishability of two statistical *stadia* differing only by the distribution of the superfluid density segment (the condensate population).

The above idea is taken here as the main element of the strategy towards a general theory of superfluidity, but the reliance of the condensate is eliminated. The notion of separable phase space provides the basis for discriminating independent configuration for all modes, rendering a partition of the wave vector axis (condensate-depletion) unnecessary. The consequences of the involvement of the S.P.S. as far as dynamics is concerned were outlined in Chapter Three. The most significant are: the rearrangement of symmetry, the occurrence of three branches of the spectrum and the negativeness of the energy v. momentum relation for the dynamical objects described by one of the separate parts of the phase space.

The main implications of the use of a S.P.S., however, lay on the statistical context. It enables to construct two comparable statistical ensembles, differing only by the fact that one is superfluid and the other is not. The way in which these ensembles are constructed does *not* provide a *mechanism* explaining *how* the - otherwise non-superfluid - system of particles becomes a superfluid, but gives a *criterion of existence* of superfluid solution, determining - in principle - the critical temperature. It is in this respect that the present approach differs from existing theories.

Now, the interest in this work is not with the resolution of the exact dynamical problem but of a model problem in the M.F.A. The model is obtained by neglecting the segment \hat{T}' from \hat{H}' which is non-diagonal in the (new, as well as the old) L.C.S.R. The M.F.A. reduces the zeroth order hamiltonian \hat{H}_0' to a bilinear form. In this approximation the density matrix (4.4.4.) is given by

$$\hat{\Omega}' \approx \exp[-\beta(\sum_{i,k} \omega_k^i p_k^i q_k^i)] \quad (4.4.19.)^{(*)},$$

(*) Equation numerals (4.4.10.-18.), both included, were omitted in error.

where ω_k^i are given by (3.3.26., 36.), except for the fact that ϵ_k is being replaced by $\epsilon_k' \equiv \epsilon_k - \mu' \epsilon_k^{(*)}$. The fact that $\hat{H}' - \mu' \hat{N}'$ reduces to an additive expression in the separate spaces S_i , without inter-space coupling, entails that

$$\text{Tr}\{\hat{\Omega}'\} = \prod_i \Omega^i \quad (4.4.20.),$$

where

$$\Omega^i = \exp(-\beta \sum_k \omega_k^i c_k^i) \quad (4.4.21.)$$

in the present M.F.A. In consequence the partition function Z_T can be expressed as a product of three factoring partition functions, i.e.

$$Z_T = \prod_i Z^i \quad (4.4.22.),$$

where

$$Z^i = \prod_k \sum_{c_k^i} \exp(-\beta \omega_k^i c_k^i) \quad (4.4.23.).$$

One finds as a consequence of (4.4.22., 23.) that the G.C.E. for the dynamical system in this approximation is separable into three additive, independent parts. This entails that all intensive thermodynamical quantities are the sum of the corresponding contributions in the three separate parts of the ensemble, i.e. the free energy is

$$\begin{aligned} F &= -\beta^{-1} \ln Z \quad (Z = Z_G \text{ or } Z_T) \\ &= -\beta^{-1} \sum_i \ln Z^i \\ &= -\beta^{-1} \sum_i F^i \end{aligned} \quad (4.4.24.).$$

The internal energy is obtained from

(*) The dispersion relation for $i = 2$ is taken as $\omega_k^2 \equiv -\omega_k \leq 0$.

$$\begin{aligned}
U &= -\partial \ln Z / \partial \beta \\
&= - \sum_i \partial \ln Z^i / \partial \beta \\
&= \sum_i U^i
\end{aligned} \tag{4.4.25.},$$

similarly the entropy is given by

$$\begin{aligned}
S &= T^{-1}(U - F) \\
&= T^{-1} \sum_i (U^i - F^i) \\
&= \sum_i S^i
\end{aligned} \tag{4.4.26.}$$

and the specific heat by

$$\begin{aligned}
C_V &= \partial U / \partial T \\
&= \sum_i \partial U^i / \partial T \\
&= \sum_i C_V^i
\end{aligned} \tag{4.4.27.},$$

etc.

Now, it is clear that configurations C_k^i can take non-integer values, in principle. These configurations are now given by

$$C_k^1 = \sum_q |u_{k,q}|^2 \eta_q \tag{4.4.28.}$$

$$C_k^2 = \sum_q |v_{k,q}|^2 (\eta_q + 1) \tag{4.4.29.}$$

$$C_k^3 = |\phi_k|^2 \tag{4.4.30.},$$

where

$$\eta_q = \langle \alpha_k^+ \alpha_k \rangle \tag{4.4.31.},$$

in view of the fact that the c-number fields are not second quantized fields the C_k^i 's can take any, non-negative, real value. In consequence the summations in (4.4.23.) are really integrals, which diverge if the

dispersion relations have a zero, as is indeed the case of ω_k^3 . A *postulate of quantization of c-number configurations*, $|\phi_k|^2$ and $|v_{k,q}|^2$, is introduced at this stage in order to avert the infrared catastrophe, which otherwise would occur. The condition of quantization will be adopted in this work as a postulate. The need to impose this condition *additionally* suggests that the type of representation employed here, involving c-number fields, might not be the best suited for statistical purposes. An attractive variation of the present representation of coherent states, wherein c-numbers are replaced by second quantized q-number fields, is briefly considered in the final section of this chapter.

The partition function (4.4.22.,23.) as it stands, without further conditions, is associated with the non-superfluid ensemble. The partition function is denoted by Z_{ns} in this case. A closed expression for this function can be obtained by carrying out the summations in (4.4.23.) over all possible configurations, i.e.

$$\begin{aligned} Z_{ns}^i &= \prod_k \sum_{C_k^i=0}^{\infty} \exp(-\beta \omega_k^i C_k^i) \\ &= \prod_k [\exp(-\beta \omega_k^i) - 1]^{-1} \end{aligned} \quad (4.4.32.).$$

The partition function of a superfluid ensemble, on the other hand, is obtained from (4.4.22.,23.) if any one set of configurations $\{C_k^i\}$, or factors of configurations, are statistically equivalent. Several options are possible. Let us consider an option which will eventually prove *not* to be appropriate for the problem of ^4He , but which will illustrate the notion of statistical equivalence and the nature of the superfluid ensemble. Let us assume that all configurations C_k^3 are statistically equivalent. This semantic option will be shown to amount to interpreting $\sum_k |\phi_k|^2$ as the order parameter of the superfluid phase.

Any two different configurations $C_k^3(1)$ and $C_k^3(2)$ may correspond to

two different dynamical states, but according to the condition of statistical equivalence any two sub-systems (of different size) differing only by the population in N^3 are indistinguishable as far as their thermodynamic properties are concerned. In other words, any two sub-systems (also called a cells) characterized by the same configurations C_k^1 and C_k^2 , but by different configuration C_k^3 , are in the same thermodynamic *stadium*. Let us denote the partition function in this case by $Z_S(3) = \prod_i Z_S^i(3)$. One obviously has

$$Z_S^i(3) = Z_{ns}^i \quad \text{for } i = 1, 2 \quad (4.4.33.),$$

but in order to obtain $Z_S^3(3)$ in this case one must take into account only one configuration value C_k^3 , this can be any one value (0,N) consistent with the normalization condition. One thus has

$$Z_S^3(3) = \exp(-\beta \omega_k^3 |\bar{\phi}_k|^2) \quad (4.4.34.),$$

i.e.

$$Z_S^3(3) \neq Z_{ns}^3 \quad (4.4.35.).$$

One can prove that the ensemble whose partition function is $Z_S(3)$ (Z_{ns}) describes the thermodynamic behaviour of a superfluid (non-superfluid) by showing that the entropy of at least one (no) part of the ensemble is zero. It will be interesting to show this from $S_S^3(3) = [U_S^3(3) - F_S^3(3)]T^{-1} = 0$ ($S_{ns}^i = T^{-1} [U_{ns}^i - F_{ns}^i] \neq 0$, for all i).

The free energies obtained from Z_{ns} and $Z_S(3)$ are

$$F_{ns}^i = \beta^{-1} \sum_k \ln[\exp(-\beta \omega_k^i) - 1], \quad \text{for all } i \quad (4.4.36.),$$

$$F_S^i(3) = F_{ns}^i, \quad \text{for } i = 1, 2 \quad (4.4.37.),$$

$$F_S^3(3) = \sum_k \omega_k^3 C_k^3, \quad \text{for } i = 3 \quad (4.4.38.),$$

respectively. The internal energies are

$$U_{ns}^i = \sum_k \omega_k^i (\exp \beta \omega_k^i - 1)^{-1}, \quad \text{for all } i \quad (4.4.39.)$$

$$U_s^i(3) = U_{ns}^i, \quad \text{for } i = 1, 2 \quad (4.4.40.),$$

$$U_s^i(3) = \sum_k \omega_k^i c_k^3 \quad (4.4.41.).$$

The average distribution of objects in space S_i is

$$\langle N_k^i \rangle_{ns} = \frac{1}{Z_{ns}^i} \sum_{N_k^i} \text{Tr} \{ N_k^i \exp(-\beta \omega_k^i N_k^i) \} / Z_{ns}^i \quad (4.4.42.)$$

$$= -\beta^{-1} \partial \ln Z_{ns}^i / \partial \omega_k^i$$

$$= (\exp \beta \omega_k^i - 1)^{-1}, \quad \text{for all } i \quad (4.4.43.),$$

and

$$\langle N_k^i \rangle_s(3) = \langle N_k^i \rangle_{ns}, \quad \text{for } i = 1, 2 \quad (4.4.44.),$$

$$\langle N_k^i \rangle_s(3) = |\bar{\phi}_k|^2, \quad \text{for } i = 3 \quad (4.4.45.).$$

Finally the entropies are given by

$$S_{ns}^i = T^{-1} \sum_k \{ \omega_k^i \langle N_k^i \rangle_{ns} - \beta^{-1} \ln [\exp(-\beta \omega_k^i) - 1]^{-1} \}, \quad \text{for all } i \quad (4.4.46.),$$

or simply by

$$S_{ns}^i = K_B \sum_k [\langle N_k^i \rangle_{ns} \ln \langle N_k^i \rangle_{ns} + (\langle N_k^i \rangle_{ns} + 1) \ln (\langle N_k^i \rangle_{ns} + 1)] \quad (4.4.47.),$$

and

$$S_s^i(3) = S_{ns}^i, \quad \text{for } i = 1, 2 \quad (4.4.48.),$$

$$S_s^i(3) = 0, \quad \text{for } i = 3 \quad (4.4.49.).$$

The last result proves that a finite additive part of the ensemble is *fully ordered*. $Z_s(3)$ describes the behaviour of a superfluid as long as

$\sum_k |\phi_k|^2 \neq 0$. From (4.4.42.,47.), on the other hand, it follows that $S_{ns}^i \neq 0$ for all i , unless $\sum_k \langle N_k^i \rangle_{ns} = 0$ for some i . In consequence, Z_{ns} describes the thermodynamic behaviour of a non-superfluid.

Let us now show that the ensemble averages of the c-number field amplitudes, $\langle \phi_k \rangle = \langle q_k^3 \rangle$ and $\langle \phi_k^* \rangle = \langle p_k^3 \rangle$, are zero in the non-superfluid ensemble and non-zero in the superfluid ensemble. These averages are obtained in general from

$$\langle \phi_k \rangle = \frac{1}{Z} \sum_k \text{Tr} \{ \phi_k \exp(-\beta \omega_k^3 |\phi_k|^2) \} / Z^3 \quad (4.4.50.)$$

or using a familiar artifice in statistical mechanics

$$\langle \phi_k \rangle = -\beta \partial \ln Z^3 / \partial \omega_k^3 \phi_k^* \quad (4.4.51.).$$

Now, taking the derivative of $\ln Z_{ns}^3$ one finds

$$\langle \phi_k \rangle_{ns} = 0 \quad (4.4.52.);$$

for, Z_{ns}^3 is independent of ϕ^* . Now, for the superfluid ensemble average one finds from (4.4.34.,51.) that

$$\langle \phi_k \rangle_s(3) = \bar{\phi}_k \quad (4.4.53.).$$

This result can be obtained in a more direct manner from (4.4.50.).

As a consequence of (4.4.53.) one finds that

$$\text{Tr} \{ \phi_k^*, \phi_k \hat{\Omega}' \} / Z_s(3) = \phi_k^*, \phi_k \quad (4.4.54.),$$

i.e. O.D.L.R.O. occurs in the first order reduced density matrix, for this particular case of superfluid ensemble.

The superfluid ensemble considered so far seems very attractive at first sight, many authors before have, in fact, conjectured that the first order coherent field should be at least part of the order parameter (18, 20,35,46,59,65). It is noted, in passing, that $\sum_q |\phi_q|^2$ is indeed the

order parameter for the superfluid phase described by the superfluid ensemble whose partition function is $Z_s^3(3)$. The problem with this interpretation is that it leads to predictions in strong qualitative disagreement with experiment.

First of all, the objects in the part of the ensemble whose partition function is $Z_s^3(3)$ cannot be excited *individually*, due to the global property which amounts to their (collective) order. This objects could only be excited *collectively*. This, however, would require a formidable amount of energy, certainly not the amount of energy that thermal neutrons, or x-rays, can convey. In consequence the gapless branch of the spectrum ω_k^3 would not be observed in thermal neutron scattering experiments. On the other hand, it is well-known that the temperature dependence of the specific heat capacity at low temperatures follows the Debye-law, proportional to T^3 . This temperature dependence is obtainable from Z_{ns}^3 , as is well known (e.g. Ref. (47)), it is noted that ω_k^3 is linear for small values of k (see Gross (1966)). However, from $Z_s^3(3)$ one obtains

$$(C_V)_s^3(3) = \partial U_s^3(3) / \partial T = 0 \quad (4.4.55.);$$

for, $U_s^3(3)$ is independent of temperature. This result is, of course, in agreement with $S_s^3(3) \equiv 0$. Thus, if $\sum_k |\phi_k|^2$ is the order parameter, or part of it, the T^3 dependence of C_V is lost. In view of these remarks the interpretation of the superfluid phase's order parameter considered above must be ruled out and with it O.D.L.R.O. in $\Omega_1'(x, x')$.

Let us consider now the other possible interpretations of statistically equivalent configurations. The case of the sets $\{C_k^1\}$ and $\{C_k^2\}$ being statistically equivalent^(*) is not very appealing. The idea

*Note that C_k^1 and C_k^2 have similar expressions in terms of $|v_{k,q}|^2$ and n_q , hence should one be statistically equivalent the other should also be so.

of the various distributions of elementary excitations being statistically equivalent is not unconceivable, but is just very odd. This interpretation, on the other hand, would lead to the conclusion that the only observable branch of the spectrum would be the low lying gapless branch ω_k^3 . Now, recent experiments (19) have discovered an upper band in addition to the gapless branch. The presence of this band has been explained phenomenologically as follows (see Ref. (19) and Refs. within): It is conjectured that the broad band is the excitation spectrum associated with the scattering of clusters of two or more excitations whose single excitation energy spectrum is the gapless branch. The broadening of the upper spectrum is understood as the characteristic broadening of multi-excitation scattering. This explanation is phenomenological in the sense that the starting point is an asymptotic formula for the dynamic structure factor of multi-excitation scattering, which must be adjusted to give the observed position and shape of the band by fitting two parameters.

According to this latter interpretation the upper energy spectrum is *not* a band, i.e. a closely packed set of well defined branches, but a broadened line. It is clear that the above interpretation of statistically equivalent configurations C_k^1 and C_k^2 cannot be ruled out from the fact that it does not reproduce the upper broadened spectrum. However, after considering the third remaining interpretation of statistically equivalent configuration it will become clear that this latter view *is* the appropriate interpretation for the problem of superfluid ^4He .

The third interpretation regards a factor of C_k^1 and of C_k^2 as statistically equivalent, i.e. any two configurations $C_k^1(1)$ and $C_k^1(2)$, or $C_k^2(1)$ and $C_k^2(2)$ for that matter, are statistically equivalent (non-equivalent) if and only if the distribution of elementary excitations, n_q , is the same (different), regardless of the distribution of pairing fields, $|V_{k,q}|^2$ and $|U_{k,q}|^2$, all of which are statistically equivalent.

In other words, any two cells of the ensemble characterized by configurations $C_k^1(1)$, $C_k^2(1)$, C_k^3 and $C_k^1(2)$, $C_k^2(2)$, C_k^3 , differing only by the distribution of pairs, $|v_{k,q}|^2$ and $|u_{k,q}|^2$, are in the same thermodynamic state that is, cannot be distinguished by their macroscopic properties.

The partition function corresponding to this version of a superfluid ensemble is denoted by $Z_s = \prod_i Z_s^i$. The partition function in this case is determined by the summation over different configurations of elementary excitations (the only non-equivalent configurations in this interpretation), i.e.

$$Z_s^1 = \prod_k \left[\prod_q \sum_{n_q=0}^{\infty} \exp(-\beta \omega_k |u_{k,q}|^2 n_q) \right] \quad (4.4.56.)$$

$$= \prod_k \left\{ \prod_q [\exp(-\beta \omega_k |u_{k,q}|^2) - 1]^{-1} \right\} \quad (4.4.57.),$$

$$Z_s^2 = \prod_k \left[\prod_q \sum_{n_q=0}^{\infty} \exp(\beta \omega_k |v_{k,q}|^2 n_q) \right] \cdot \left[\prod_q \exp(\beta \omega_k |v_{k,q}|^2) \right] \quad (4.4.58.)$$

$$= \prod_k \left\{ \prod_q [\exp(\beta \omega_k |v_{k,q}|^2) - 1]^{-1} \cdot \left[\prod_q \exp(\beta \omega_k |v_{k,q}|^2) \right] \right\} \quad (4.4.59.),$$

and

$$Z_s^3 = Z_{ns}^3 \quad (4.4.60.).$$

It is most important to observe that Z_s^1 and Z_s^2 turned out to be products of partition functions in this case, i.e.

$$Z_s^1 = \prod_q Z_s^1(q) \quad (4.4.61.)$$

and

$$Z_s^2 = \prod_q Z_s^2(q) z_s(q) \quad (4.4.62.),$$

where

$$Z_S^1(q) \equiv \prod_k \{ \exp[-\beta \bar{\omega}_k^1(q)] - 1 \}^{-1} \quad (4.4.63.),$$

$$Z_S^2(q) \equiv \prod_k \{ \exp[-\beta \bar{\omega}_k^2(q)] - 1 \}^{-1} \quad (4.4.64.)$$

and

$$z_s(q) \equiv \prod_k \exp[-\beta \bar{\omega}_k^2(q)] \quad (4.4.65.).$$

$\bar{\omega}_k^1(q)$ and $\bar{\omega}_k^2(q)$ are *effective* excitation spectra, given by

$$\bar{\omega}_k^1(q) = \omega_k |u_{k,q}|^2 \quad (4.4.66.)$$

$$\bar{\omega}_k^2(q) = \omega_k |v_{k,q}|^2 \quad (4.4.67.).$$

From the fact that Z_S^1 and Z_S^2 factorize into N and N^2 factors, respectively, it follows that the separate parts of the ensemble, associated with these partitions functions, and denoted by E_S^1 and E_S^2 , are the *additive* superposition of N and $2N$ parts, respectively^(*), i.e. in a symbolic notation

$$E_S^1 = \sum_q E_S^1(q), \quad E_S^2 = \sum_q E_S^2(q) + e_s(q) \quad (4.4.68.),$$

where $Z_S^1(q)$, $Z_S^2(q)$ and $z_s(q)$ are the partition functions of the separate parts of the ensemble $E_S^1(q)$, $E_S^2(q)$ and $e_s(q)$, respectively.

Now, for the same value of k , $|u_{k,q}|^2$ and $|v_{k,q}|^2$ take - in general - different values for different q . In consequence the effective spectra can take, in principle, N different values each. The part of the ensemble $\sum_q E_S^1(q) + E_S^2(q)$ is, thus, the ensemble corresponding to a dynamical system whose energy spectrum is a *band comprising $2N$ branches*, the density of branches depending upon the distribution of pairing fields $|u_{k,q}|^2$ and $|v_{k,q}|^2$. This direct prediction of an upper band is in qualitative agreement with experiment, and is obtained here independently of any consideration as to the low lying gapless branch. The band is seen here to be *not* a

*Note that q can take N discrete values.

broadened line, characteristic of the scattering of clusters of single excitations, but a true band consisting of closely packed lines, associated with the scattering of *single* excitations, independent of the excitations associated with the low lying gapless branch.^(*)

The prediction of an upper band arises here from the conjunction of four elements: (i) The involvement of pairing of *non-zero* overall momentum. (ii) The separability of the phase space. (iii) The definition of the dynamical variables (and, hence, of the configurations in the S.P.S.) such that c-number fields are factors of the dynamical variables (and, hence, of the configurations) and (iv) The special way of counting configurations, avoiding the multiple counting of statistically equivalent configurations.

It is the latter element of the present theory that effects the splitting of the excitation spectrum, which in a pure state description is a single branch. The involvement of this latter element is also that conveying the superfluid properties. It is noted that a single branch is predicted from the non-superfluid ensemble description. It will be argued later in this section that the average number of pairs is zero above the transition, in consequence, the width of the band predicted in the superfluid phase should reduce with increasing temperature and disappear at the transition. But now let us consider two cases of interest. Firstly, the case in which the dynamical variables of the separable phase space are defined in terms of a L.C.S.R. involving pairing of *zero-overall momentum only*. Secondly, the case of standard existing theories in which the phase space is *non-separable* and the c-number fields are *not* factors of the dynamical variables, but auxiliary parameters.

In the former case the dynamical variables are defined as

(*) Dr. W.A.B. has addressed the author's attention to the fact that neutron scattering experiments do in fact show broadened lines; also predicted from the pair theory of the dynamic structure factor $S(k, \omega)$.

$$\bar{p}_k^{-1} \equiv u_k \alpha_k^*, \quad \bar{q}_k^{-1} \equiv u_k \alpha_k \quad (4.4.69.),$$

$$\bar{p}_k^{-2} \equiv v_k^* \alpha_{-k}, \quad \bar{q}_k^{-2} \equiv v_k \alpha_{-k}^* \quad (4.4.70.),$$

$$\bar{p}_k^{-3} \equiv p_k^3 \equiv \phi_k^*, \quad \bar{q}_k^{-3} \equiv q_k^3 \equiv \phi_k \quad (4.4.71.).$$

The excitation spectrum ω_k takes the expression

$$\omega_k = \{\bar{J}_k^2 - |B_k|^2\}^{1/2} \quad (4.4.72.),$$

where

$$\bar{J}_k = \epsilon_k^1 + \sum_l [V(o) + V(l)] \sum_i \langle \bar{p}_{k+l}^{-i} \bar{q}_{k+l}^{-i} \rangle \quad (4.4.73.)$$

and

$$B_k^* = \sum_l V(l) \langle \bar{p}_{k+l}^{-1} \bar{p}_{-k-l}^{-2} \rangle \quad (4.4.74.).$$

ω_k^3 remains the same as before. The c-number fields u_k and v_k now satisfy

$$u_k^2 = (\bar{J}_k + \omega_k)/2\omega_k \quad (4.4.75.)$$

$$|v_k|^2 = (J_k - \omega_k)/2\omega_k \quad (4.4.76.).$$

The partition functions Z_S^1 and Z_S^2 take the following form, for the present interpretation of the pairing field density $\sum_k |v_k|^2$ as the order parameter,

$$\bar{Z}_S^1 = \prod_k [\exp(-\beta \omega_k u_k^2) - 1]^{-1} \quad (4.4.77.),$$

$$\begin{aligned} \bar{Z}_S^2 = \prod_k [\exp(\beta \omega_k |v_k|^2) - 1]^{-1} \cdot \\ \cdot [\exp(\beta \omega_k |v_k|^2)] \end{aligned} \quad (4.4.78.).$$

It is clear, then, that the upper-branch of the spectrum in a pure state description, namely ω_k , now splits into two effective branches in thermal equilibrium, namely

$$\bar{\omega}_k^1 = \omega_k u_k^2 \quad (4.4.79.)$$

and

$$\omega_k^2 = \omega_k |v_k|^2 \quad (4.4.80.),$$

or according to (4.4.75.,76.)

$$\omega_k^1 = (1/2) (J_k + \omega_k) \quad (4.4.81.)$$

$$\omega_k^2 = -(1/2) (J_k - \omega_k) \quad (4.4.82.).$$

The fact that the dynamical objects $i = 2$ possess a negative energy spectrum was briefly discussed in Chapter Three. Further research is required to ascertain whether this is observable, and if so, by what means.

Now, in the *standard* theory the phase space is non-separable and the canonical variables are defined as

$$\hat{p}_k^i \equiv \alpha_k^+ \text{ and } \hat{q}_k^i \equiv \alpha_k \quad (4.4.83.).$$

The mean field hamiltonian takes the form

$$H = \sum_k W_k \alpha_k^+ \alpha_k + \text{zero point energy} \quad (4.4.84.),$$

in consequence the only partition function that can be constructed in this N.S.P.S. corresponds to a non-superfluid ensemble, in the present connotation, i.e.

$$\begin{aligned} Z &= \prod_k \sum_{n_k=0}^{\infty} \text{Tr}\{\exp(-\beta W_k n_k)\} \\ &= \prod_k [\exp(-\beta W_k) - 1]^{-1} \end{aligned} \quad (4.4.85.).$$

That is, the effective excitation spectrum predicted from this non-superfluid ensemble is only one branch, the same excitation spectrum as in a pure state description. Finally, it is noted that this spectrum, W_k , is currently interpreted as the gapless low lying branch, while here it is seen to correspond to the upper band.

Let us now go back to the 'pairing version' of the superfluid ensemble and show that a part of this ensemble is *fully* ordered, another part is

partially ordered and the remaining part is normally disordered (i.e. fully ordered only at absolute zero temperature). The entire ensemble, denoted by E_S , can now be regarded as the additive super-position of three parts, E_S^1 , E_S^2 and E_S^3 , say, whose partition functions are $\prod_q [Z_S^1(q)Z_S^2(q)]$, $\prod_q z_S(q)$ and $Z_S^3 = Z_{ns}^3$, respectively. Let us show first that the ensemble E_S^2 is fully ordered.

The internal energy and the free energy are

$$U_S^2 = -\sum_{q,k} \omega_k |v_{k,q}|^2 = F_S^2 \quad (4.4.86.),$$

in consequence the entropy of this part of the ensemble is

$$S_S^2 \equiv 0 \quad (4.4.87.).$$

The number distribution of objects in this part of the ensemble is

$$N_S^2 = \sum_k (N_k)_S^2 = \beta^{-1} \sum_{q,k} \partial \ln z_S(q) / \partial \omega_k = \sum_k |v_{k,q}|^2 \quad (4.4.88.),$$

in consequence the physical system described by this ensemble,

$E_S = E_S^1 + E_S^2 + E_S^3$, will exhibit the property of superfluidity provided that $|v_{k,q}|^2 \neq 0$.

Now, it is noted that the dynamical objects in this part of the ensemble can only exchange energy collectively with other objects in other parts of the ensemble, or the thermal bath, but cannot be scattered individually, in consequence the spectrum associated with this part of the ensemble is not observed by neutron scattering experiments.

The part of the ensemble denoted by E_S^3 is the same as the part of the non-superfluid ensemble, whose partition function is Z_{ns}^3 . This part of the ensemble is known to be fully ordered only at zero temperature where the number of objects

$$N_S^3 = \sum_k (N_k)_S^3 = \sum_k (\exp \beta \omega_k^3 - 1)^{-1} = 0.$$

Let us evaluate now the remaining distribution of number of objects in E_S^1

$$N_s^1 = \sum_k (N_k)_s^1 = -\beta^{-1} \sum_{q,k} (\partial \ln Z_s^1(q) Z_s^2(q) / \partial \omega_k^1) \sum_{q,k} (|u_{k,q}|^2 \langle \eta_q \rangle_s^1 + |v_{k,q}|^2 \langle \eta_q \rangle_s^2) \quad (4.4.89.),$$

where

$$\langle \eta_q \rangle_s^1 = [\exp(\beta \omega_k |u_{k,q}|^2) - 1]^{-1} \quad (4.4.90.)$$

and

$$\langle \eta_q \rangle_s^2 = [\exp(\beta \omega_k |v_{k,q}|^2) - 1]^{-1} \quad (4.4.91.)$$

are the average distribution of elementary excitations in the ensemble whose partition functions are $Z_s^1(q)$ and $Z_s^2(q)$, respectively.

The free energy and the internal energy in E_s^1 are

$$F_s^1 = -\beta^{-1} \sum_{k,q} \{ \ln[\exp(-\beta \omega_k |u_{k,q}|^2) - 1]^{-1} + \ln[\exp(\beta \omega_k |v_{k,q}|^2) - 1]^{-1} \} \quad (4.4.92.),$$

and

$$U_s^1 = \sum_{k,q} \omega_k |u_{k,q}|^2 \langle \eta_q \rangle_s^1 - \omega_k |v_{k,q}|^2 \langle \eta_q \rangle_s^2 \quad (4.4.93.)$$

respectively. Finally the entropy is given by⁽⁴⁸⁾

$$S_s^1 = -k_B \sum_q \sum_{i=1}^2 [\langle \eta_q \rangle_s^i \ln \langle \eta_q \rangle_s^i - (\langle \eta_q \rangle_s^i + 1) \ln (\langle \eta_q \rangle_s^i + 1)] \quad (4.4.93.)$$

This can be tested by noting that

$$F_s^1 / \langle \eta_q \rangle_q^i = 0, \quad \text{for } i = 1, 2 \quad (4.4.94.)$$

entails (4.4.90.,91.). From the inspection of (4.4.89.,93.) it is clear that only a fractional part of the ensemble E_s^1 is capable of disordering, i.e. the specific entropy (i.e. entropy divided by the average number of objects) is smaller in E_s^1 than in a comparable non-superfluid ensemble. The behaviour of this part of the ensemble, nevertheless, is that of a viscous fluid, but with anomalously low viscosity, i.e. N_s^1 can be large and yet S_s^1 can be rather small, if the average number of elementary excitations is small.

The specific heat capacity obtained from this ensemble is proportioned to T^3 at low temperature, this is the contribution $(C_V)_S^3 = (C_V)_{ns}^3$. $(C_V)_S^2$ is identically zero and the contribution $(C_V)_S^1$ shows roughly an exponential behaviour due to the gap in the various branches of the spectrum.⁽⁴⁷⁾ A detailed evaluation of C_V is outside the scope of this work; for it requires a detailed knowledge of the various branches of the excitation spectrum, and in order to obtain such expressions a complicated set of integral equations must be solved first by numerical methods. Presently we shall be content with obtaining this set of equations but no attempt of solving it will be pursued in this thesis. An investigation as to the numerical solution of these equations for simple model potentials, and the resulting excitation spectra and the thermodynamic quantities of interest, is currently in progress, the results of this investigation will be given elsewhere. But before deriving the integral equations characterizing the present mean field model in thermal equilibrium let us work out the ensemble averages of the pairing field amplitudes $\langle u_{k,q} \rangle$ and $\langle v_{k,q} \rangle$.

From (4.4.22.,23.,28.,29.) it follows that

$$\langle u_{k,q} \rangle = -\beta^{-1} (\partial \ln Z / \partial \omega_k u_{k,q}^*) \quad (4.4.95.)$$

$$\langle v_{k,q} \rangle = \beta^{-1} (\partial \ln Z / \partial \omega_k v_{k,q}^*) \quad (4.4.96.).$$

For the non-superfluid ensemble one obtains

$$\langle u_{k,q} \rangle_{ns} = \langle v_{k,q} \rangle_{ns} \equiv 0 \quad (4.4.97.),$$

and similarly for the averages of their c.c. This result follows from the fact that Z_{ns} is independent of $u_{k,q}$ and $v_{k,q}$. For the non-superfluid ensemble, on the other hand, one obtains

$$\begin{aligned}
\langle u_{k,q} \rangle_s &= \sum_{C_k^1} \sum_{C_k^2} \sum_{C_k^3} \text{Tr}(u_{k,q} \hat{\Omega}') / Z_s \\
&= u_{k,q} \sum_{C_k^1} \sum_{C_k^2} \sum_{C_k^3} \text{Tr}(\hat{\Omega}') / Z_s \\
&= u_{k,q} \quad (4.4.98.),
\end{aligned}$$

where the second equality follows from the fact that the various configurations of $|u_{k,q}|^2$ are statistically equivalent. For $\langle v_{k,q} \rangle_s$ one similarly obtains

$$\langle v_{k,q} \rangle_s = v_{k,q} \quad (4.4.99.).$$

These results can be obtained from (4.4.95.,96.), i.e.

$$\langle u_{k,q} \rangle = -\beta^{-1} \partial \ln Z_s^1 / \partial \omega_k u_{k,q}^* = u_{k,q} \quad (4.4.100.).$$

For the average of $v_{k,q}$, however, one must be careful not to count twice, i.e.

$$\begin{aligned}
\langle v_{k,q} \rangle_s &= \sum_{C_k^1} \sum_{C_k^2} \sum_{C_k^3} \text{Tr}(v_{k,q} \hat{\Omega}') / Z_s \\
&= \beta \partial \ln [\prod_q Z_s^2(q)] / \partial \omega_k v_{k,q}^* \\
\text{or} \quad &= \beta \partial \ln [\prod_q z_s(q)] / \partial \omega_k v_{k,q}^* \\
&= v_{k,q} \quad (4.4.101.),
\end{aligned}$$

in agreement with (4.4.99.). Note, however, that

$$\beta^{-1} \partial \ln Z_s^2 / \partial \omega_k v_{k,q}^* = 2v_{k,q} \quad (4.4.102.),$$

this indicates that the artifice (4.4.95.,96.) must be employed with care to avoid double counting.

As a consequence of (4.4.100.,101.) it follows that O.D.L.R.O. in Ω_2^1 does take place, but not in Ω_1^1 , as follows from the fact that

$$\langle \phi_k \rangle_s = \langle \phi_k^* \rangle_s \equiv 0. \quad (4.4.102.),$$

which can be readily tested.

It emerged here that the average amplitude of pairs over the pairing version of the superfluid ensemble is non-zero, while the average amplitude of first order coherent fields is zero. This conclusion was also reached by Evans and Imry before, but through a different argument. These authors argued that the average $\langle \phi_k \rangle$ (or $\langle \phi_k^* \rangle$) must *necessarily* be zero; for, the ensemble average equals the time average over a very long period of time (infinite in theory) - according to the ergodic hypothesis (admittedly valid in the present case). But, due to the fact that random collisions change randomly the phase of the *particles* (the phases of a_k^+ and a_k in Evans and Imry's work, or the phases of ϕ_k^+ and ϕ_k in the present argument), the time average is necessarily zero. In consequence the ensemble average can hardly be finite. This argument, however, assumes that random collisions *do* change the phases of the field amplitudes (either a_k^+ and a_k , or ϕ_k^+ and ϕ_k) at random. One is quite justified in assuming this in the context of the standard theory, where the notion of statistical equivalence is not introduced. From the present point of view, however, this assumption does not hold. In fact, *individual* dynamical objects in the ordered part of the ensemble *cannot* change their phases independently; for, if they did they would disorder, against the global property with states - a priori - their full order. These objects could change their phase collectively; however, it is very unlikely that an individual dynamical object in the non-ordered part of the ensemble, or an incoming neutron for that matter, changes the entire phase of the totality of the ordered objects. They do not have enough energy to do that. It is still possible, however, to change the overall phase of the *macroscopic* field amplitude by applying a macroscopic external field of transverse velocity, but this is quite another matter. In summary should config-

urations $|\phi_k|^2$ be statistically equivalent, which is a valid theoretical possibility, the macroscopic phases of the macroscopic field amplitudes ϕ_k^* and ϕ_k are *not* changed randomly by random collisions, circumventing in this way Evans and Imry's indictment.

Here, however, it is found that $\langle \phi_k \rangle$ and $\langle \phi_k^* \rangle$ should be zero, but for different reasons, namely due to the fact that if these averages are not zero the gapless branch of the spectrum would not be observed and the T^3 dependence of the specific heat would be lost, against experimental observation.

The same argument given above can be adopted to advocate the non-zero average value of $v_{k,q}$ and $u_{k,q}$, without having to assume that the change of phase of one of the particles of wave vector q , say, is followed by a corresponding change of phase of the partner particle of the pair (of wave vector k). In fact, the phase of individual objects of the pair does not change at all by collisions with other individual objects.

It was shown in §4.2. that a change of gauge of external field of velocity effects a change of phase of the Fourier transform at $v_{k,q}$, i.e.

$$v(x,y) \rightarrow v(x,y)\exp[iS(x) + iS(y)] \quad (4.4.103.),$$

this phase will turn out to be a macroscopic observable. Later in §4.3. it was shown that a segment of the first order reduced density matrix takes the form

$$\int v(x,y) v^*(x',y) d^3y = \int |v(x,y)|^2 d^3y \quad (4.4.104.)$$

this contribution was shown to transform under the gauge transformation as

$$\begin{aligned} \int v(x,y) v^*(x',y) d^3y &\rightarrow \exp[iS(x) - iS(x')] \int v^*(x',y) v(x,y) d^3y = \\ &= \exp[iS(x) - iS(x')] \int |v(x,y)|^2 d^3y \quad (4.4.105.). \end{aligned}$$

In consequence, even though, O.D.L.R.O. does *not* take place in Ω_1' in the absence of an external field of velocity, a *diagonal* part exhibits a factorizable *phase* in the presence of an external field of velocity. If the domain of integration in (4.4.105.) is finite (not infinite) the R.H.S. of (4.4.105.) is a function of x . In the far from local limit, i.e. $|x - x'|$ very large compared with the range of the potential, the first order reduced density matrix factorizes as

$$\Omega_1(x, x') = \{ |v(x)| \exp iS(x) \} \{ v(x) \exp[-iS(x')] \} \quad (4.4.106.),$$

from which a one-point velocity field can be obtained, as usual (e.g. Frölich (1973)), as

$$V_s = (\hbar/m) \text{grad} S(x) \quad (4.4.107.).$$

This velocity field is a *macroscopic* observable in the superfluid ensemble, is a *fine grained* quantity, as $|V(x)|^2$ itself, and - in addition - it is *curl-free*, i.e.

$$\text{Curl } V_s \equiv 0 \quad (4.4.108.).$$

This is currently regarded as the hydrodynamic condition of superfluidity. Here it is seen to have its origin in (i) the notion of statistical equivalence, which entails that the phase of $v_{k,q}$ is a macroscopic observable, and which can vary over *macroscopic distances*, and (ii) the fact that the gauge symmetry is rearranged. Should either of these two conditions not be satisfied (4.4.108.) would not follow.

Let us now derive the integral equations characterizing the present mean field model in thermal equilibrium. These sets of equations encompass an equation for the Hartree-Fock energy, J_k , for the pairing fields, $B_{p,k}$, and its c.c. and for the pairing fields, b_k . This set of equations is completed by the normalization condition. From the definition of J_k , namely

$$J_k = \epsilon_k' + \sum_{\ell} [v(0) + v(\ell)] \sum_{\mathbf{i}} \langle p_{k+\ell}^{\mathbf{i}} p_{k+\ell}^{\mathbf{i}} \rangle \quad (4.4.109.)$$

one has

$$\begin{aligned} J_k = \epsilon_k' + \sum_{\ell} [v(0) + v(\ell-k)] \sum_q \{ & |u_{\ell,q}|^2 (\exp \beta \omega_{\ell} |u_{\ell,q}|^2 - 1)^{-1} + \\ & + |v_{\ell,q}|^2 [(\exp -\beta \omega_{\ell} |v_{\ell,q}|^2 - 1)^{-1} + 1] + \\ & + (\exp \beta \omega_{\ell}^3 - 1)^{-1} \} \end{aligned} \quad (4.4.110.),$$

where

$$\sum_q |u_{k,q}|^2 = (J_k + \omega_k) / 2\omega_k \quad (4.4.111.)$$

$$\sum_q |v_{k,q}|^2 = (J_k - \omega_k) / 2\omega_k \quad (4.4.112.).$$

The normalization condition is

$$\begin{aligned} N = \sum_{k,q} \{ & |u_{k,q}|^2 (\exp -\beta \omega_k |u_{k,q}|^2 - 1)^{-1} + \\ & + |v_{k,q}|^2 (\exp -\beta \omega_k |v_{k,q}|^2 - 1)^{-1} + \\ & + (\exp \beta \omega_k^3 - 1)^{-1} \} \end{aligned} \quad (4.4.113.).$$

The equation for the pairing energy b_k is

$$b_k = \sum_{\ell} v(\ell-k) (\exp \beta \omega_{\ell}^3 - 1)^{-1} \quad (4.4.114.),$$

the other pairing energy is defined as

$$\begin{aligned} \sum_p \bar{B}_{p,k} &= \sum_{\ell,p} v(\ell) \langle \overbrace{p_{p+\ell}^1 p_{k-\ell}^2} \rangle \\ &= \sum_{q,\ell,p} v(\ell) [u_{p+\ell,q} v_{k-\ell,q}^* \langle \bar{\eta}_q \rangle_s + \\ &+ u_{k-\ell,q} v_{p+\ell,q}^* (\langle \bar{\eta}_q \rangle_s + 1)] \end{aligned} \quad (4.4.115.),$$

where

$$\begin{aligned} \langle \bar{\eta}_q \rangle_s &\equiv (\exp \beta \omega_{p+\ell} |u_{p+\ell,q}|^2 - 1)^{-1} + \exp -\beta \omega_{k-\ell} |v_{k-\ell,q}|^2 - 1)^{-1} \\ \langle \bar{\eta}_q \rangle_s &\equiv (\exp \beta \omega_{k-\ell} |u_{k-\ell,q}|^2 - 1)^{-1} + \exp -\beta \omega_{p+\ell} |v_{p+\ell,q}|^2 - 1)^{-1} \end{aligned} \quad (4.4.116.)$$

where the excitation spectra ω_k and ω_k^3 are given by

$$\omega_k = \{J_k^2 - \sum_p |B_{p,k}|^2\}^{1/2} \quad (4.4.117.)$$

$$\omega_k^3 = \{J_k^2 - b_k^2\}^{1/2} \quad (4.4.118.).$$

The resulting set of equations in the present model is much more complicated than for the standard theory. This is mainly due to (i) the fact that the u's and v's cannot be eliminated, i.e. replaced in terms of J_k and $\sum_p |B_{p,k}|^2$. This is in view of the fact that a summation over q is involved in (4.4.111,112.). (ii) The fact that the spectrum associated with the pairing energy is now a set of 2N branches. The set of equations is not amenable to analytic solution, and even a numerical solution of this set of equations is computer time consuming. Some further approximations have been employed in the search for numerical reducing the computing time to a reasonable level. A detailed account of the progress in this sense is out of the scope of this work, which aimed at laying the foundation for the subsequent complete resolution of the problem. However, the main simplifications considered in this further work are worth mentioning here. Instead of considering the whole set of 2N branches one can consider the two *average* branches, i.e.

$$\omega_k^1(\text{av.}) = \sum_q \omega_k |u_{k,q}|^2 = (1/2)(J_k + \omega_k) \quad (4.4.119.)$$

$$\omega_k^2(\text{av.}) = -\sum_q \omega_k |v_{k,q}|^2 = -(1/2)(J_k - \omega_k) \quad (4.4.120.),$$

which coincide with the two branches of the spectrum in thermal equilibrium in the case in which the dynamical variables p_k^i and q_k^i , for $i = 1, 2$, are defined in terms of the fields of the pair representation of *zero overall momentum*. With the help of this simplification (4.4.110.,113.) reduce to

$$J_k = \epsilon_k^2 + \sum_{\ell} [v(\ell) + v(\ell-k)] \{ (1/2) [(J_{\ell}/\omega_{\ell}) + 1] [\exp \beta \omega_{\ell}^1(\text{av}) - 1]^{-1} + \\ + (1/2) [(J_{\ell}/\omega_{\ell}) - 1] [\exp \beta \omega_{\ell}^2(\text{av}) - 1]^{-1} + 1) \\ + (\exp \beta \omega_{\ell}^3 - 1)^{-1} \} \quad (4.4.121.)$$

$$N = \sum_k \{ (1/2) [(J_k/\omega_k) + 1] [\exp \beta \omega_k^1(\text{av.}) - 1]^{-1} + \\ + (1/2) [(J_k/\omega_k) - 1] [\exp \beta \omega_k^2(\text{av.}) - 1]^{-1} + 1) \\ + (\exp \beta \omega_k^3 - 1)^{-1} \} \quad (4.4.122.)$$

A further simplification is obtained by imposing the condition

$$u_{p,q} v_{k,q'}^* = u_{p,q} v_{k,q'}^* \delta_{p,-k} \delta_{q,q'} \quad (4.4.123.),$$

in which case $\sum_p B_{p,k}^*$ reduces to (after taking the modulus)

$$|B_k| \cong \sum_{\ell} v(\ell-k) \sum_q |v_{\ell,q}| |u_{\ell,q}| (2\langle \eta_{\ell} \rangle_s + 1)$$

where

$$\langle \eta_{\ell} \rangle_s = [\exp \beta \omega_{\ell}^1(\text{av.}) - 1]^{-1} + \\ + [\exp \beta \omega_{\ell}^2(\text{av.}) - 1]^{-1} \quad (4.4.124.),$$

and $|B_k| \equiv |B_{-k,k}|$. Making use of (4.4.111.,112.) one finds that

$$|B_k| \cong \sum_{\ell} v(\ell-k) (1/2) [(J_{\ell}^2/\omega_{\ell}^2) - 1]^{1/2} (2\langle \eta_{\ell} \rangle_s + 1)$$

or from the fact that the spectrum is

$$\omega_k = \{J_k^2 - |B_k|^2\}^{1/2} \quad (4.4.125.)$$

in this approximation, one finally obtains

$$|B_k| = (1/2) \sum_{\ell} v(\ell-k) (|B_{\ell}|/\omega_{\ell}) (1 + 2\langle \eta_{\ell} \rangle_s) \quad (4.4.126.).$$

The resulting approximate set of equations (4.4.114.,121.,122.,124-126.) is

still rather involved, but at least the v 's and u 's have been fully replaced by the unknowns J_k and $|B_k|$. A further elaboration of this model may take into account the various branches between $\omega_k^1(\text{av.})$ and $\omega_k^2(\text{av.})$ by regarding the set of discrete lines as a continuum. In this event the possibilities of solution for $|B_k|$ are largely increased.

The final aspect to be considered in this section is the criterion of existence of superfluid solution. The description provided by a superfluid ensemble will prevail at a given temperature provided that the free energy derived from the superfluid ensemble is smaller than from the non-superfluid ensemble, i.e. if and only if

$$F_{ns} - F_s \geq 0 \quad (4.4.127.).$$

The equal sign determines, in principle, the transition temperature. Note that the average number of pairs $\sum_{k,q} |v_{k,q}|^2$ needs not be zero in the non-superfluid phase, but the average of the amplitudes $v_{k,q}$ must be zero. However, from the known experimental fact that the upper band lowers in the superfluid phase with increasing temperature, and eventually coincides with the gapless branch at the transition and above, one can guess that $\sum_q |v_{k,q}|^2$ may be zero in the normal phase described by the non-superfluid ensemble.

From (4.4.127.) one obtains the following condition

$$\ln(Z_{ns}/Z_s) \leq 0$$

or

$$Z_{ns}^1 Z_{ns}^2 \leq Z_s^1 Z_s^2 \quad (4.4.128.).$$

In the latter approximation this condition is

$$\prod_k [\exp(-\beta\omega_k) - 1]^{-2} \leq \prod_k \{\exp[-\beta\omega_k^1(\text{av.})] - 1\}^{-1} \cdot \{\exp[-\beta\omega_k^2(\text{av.})] - 1\}^{-1} \quad (4.4.129.)$$

which can be solved for β once J_k and ω_k are known.

§4.5. Further developments

This section is concerned with a brief examination of some questions which can provide a refinement as to the representation employed in this work, and an extension of the present theory as to its application in other fields.

Three topics will be briefly considered here. The first concerns the feasibility of defining a purely quantum representation of coherent states, whereby c-numbers are replaced by q-number fields. The use of such a representation, in order to define the dynamical variables of the S.P.S., looks very attractive, in principle; for, it would enable to dispose of the postulate of quantization introduced, *a priori*, in the preceding section. It will become clear, however, that the definition of such a purely quantum representation is not without problems, the most restrictive of which will be shown to be that the expressions for the elementary operators of the new representation in terms of particle operators is an infinite series in increasing powers of particle operators, if the second order coherents (c-number) fields are replaced by second quantized fields.

The second topic considered in this final section is the theoretical feasibility of defining the L.C.S.R. (involving first order coherence) for *Fermi* fields. An edictment due to Yang (71) rules out the possibility of O.D.L.R.O. in the first reduced density matrix; for, this was shown to be inconsistent with the characteristic antisymmetry of n-body distribution functions, for fermions, under permutation of coordinates. It will be shown here, however, that if the L.C.S.R. for Fermi systems is *appropriately* defined O.D.L.R.O. occurs in Ω_1^t (in a pure state description at least) and no contradiction arises.

The third aspect considered here is the general applicability of the present programme to arbitrary systems. This will be argued in view of the fact that the present theory does not rely on particular premises

holding for ${}^4\text{He}$ only, but is based on notions of general applicability, as dynamical equivalence, separability of the phase space and statistically equivalent configurations. Two examples are briefly considered to illustrate this idea, on rather speculative grounds. An outline of a theory of superconductivity is proposed along the lines of the present theory, in the first place. As far as dynamics are concerned it is argued that the problem of a superconductor can be formulated on the basis of a L.C.S.R. description such that the symmetries are rearranged, not broken as in the standard theory. As to the statistical problem a rather surprising conclusion is anticipated: the order parameter should be associated with the first order coherent fields (!) (entailing the occurrence of O.D.L.R.O. in α_1) if a prediction of the excitation spectrum in qualitative agreement with experiment is to be drawn. This interpretation is significantly different from the usual one in standard theories which identify the order parameter with the pairing fields.

The second example considered here is that of a collection of N localised spins, at fixed sites of a crystal lattice, interacting according to the Heisenberg model. A first coherent representation is defined for this problem. The questions of *microscopic* symmetry rearrangement and *macroscopic* symmetry breakdown are discussed. The difference between superfluid and non-superfluid (partly) ordered phases is also briefly discussed. Finally, some interesting applications to other problems, requiring further research, are also mentioned.

An investigation as to the theoretical possibility of defining a purely coherent representation of states, whereby c-numbers are replaced by second quantized fields seems attractive; for, it would enable all the dynamical variables of the S.P.S. to be q-number fields, and all configurations of the S.P.S. to be quantized from the outset. This is more in line with the usual formulation of the many-body problem. This extension, however, is by no means straightforward. In fact some deep difficulties arise,

which prevent a simple extension. The main difficulties are considered here.

Consider a *first order coherent transformation* of the form

$$T_1 = \exp \hat{\Theta}_1 \quad (4.5.1.),$$

where the exponent is given by

$$\hat{\Theta}_1 = \sum_k (a_k^+ \phi_k - \phi_k^+ a_k) \quad (4.5.2.).$$

a_k^+ and a_k are, as usual, Bose-particle creation and annihilation operators, and ϕ_k^+ and ϕ_k are the corresponding elementary excitation operators of a *certain*, unspecified, representation of states. Let us assume that these latter operators satisfy Bose-like commutation relations, i.e.

$$\left. \begin{aligned} \phi_k \phi_{k'}^+ - \phi_{k'}^+ \phi_k &= e_k^{1/2} e_{k'}^{1/2} \delta_{k,k'} \\ \phi_k \phi_{k'} - \phi_{k'} \phi_k &= 0 \\ \phi_k^+ \phi_{k'}^+ - \phi_{k'}^+ \phi_k^+ &= 0 \end{aligned} \right\} \quad (4.5.3.),$$

where e_k is a real number.

The elementary excitation operators of the new, purely quantum, first order coherent representation are

$$\left. \begin{aligned} \alpha_k^+ &= T_1 a_k^+ T_1^{-1} \\ \alpha_k &= T_1 a_k T_1^{-1} \end{aligned} \right\} \quad (4.5.4.),$$

or from the result of Appendix A

$$\alpha_k^+ = a_k^+ + \sum_{n=1}^{\infty} C_n / n! \quad (4.5.5.),$$

where C_n are the successive commutators defined as

$$\left. \begin{aligned} C_1 &\equiv [\hat{\theta}, a_k^+] \\ C_2 &\equiv [\hat{\theta}, C_1] \\ &\vdots \\ C_n &\equiv [\hat{\theta}, C_{n-1}] \end{aligned} \right\} \quad (4.5.6.)$$

The expression (4.5.5.) can be evaluated from definition (4.5.6.) using (4.5.2.) and the commutation relations for the a 's and the ϕ 's. One finds

$$\left. \begin{aligned} C_{2n+1} &= -(-e_k)^n \phi_k^+, \quad n = 0, 1, 2, \dots \\ C_{2n} &= (-e_k)^n a_k^+, \quad n = 1, 2, 3, \dots \end{aligned} \right\} \quad (4.5.7.)$$

thus

$$\left. \begin{aligned} \alpha_k^+ &= a_k^+ \cos(e_k^{1/2}) - (\phi_k^+ / e_k^{1/2}) \sin(e_k^{1/2}) \\ \alpha_k &= a_k \cos(e_k^{1/2}) - (\phi_k / e_k^{1/2}) \sin(e_k^{1/2}) \end{aligned} \right\} \quad (4.5.9.)$$

These expressions reduce to the familiar expressions

$$\left. \begin{aligned} \alpha_k^+ &= a_k^+ - \phi_k^+ \\ \alpha_k &= a_k - \phi_k \end{aligned} \right\} \quad (4.5.9.)$$

in the limit $e_k^{1/2} \rightarrow 0$, in which case ϕ_k^+ and ϕ_k become abelian c-numbers ϕ_k^+ & ϕ_k .

The commutation relations for the new elementary excitation operators are

$$\begin{aligned} [\alpha_k, \alpha_{k'}^+] &= [\cos(e_k^{1/2}) \cos(e_{k'}^{1/2}) + \\ &\quad \sin(e_k^{1/2}) \sin(e_{k'}^{1/2})] \delta_{k,k'} \\ &= \delta_{k,k'} \end{aligned} \quad (4.5.10.),$$

that is, the α 's are also Bose operators.^(*) It has been assumed that

(*) As also follows from (4.5.4.)

$$[a_k, \phi_k^+] = [a_k, \phi_k,] = [a_k^+, \phi_k,] = [a_k^+, \phi_k^+] = 0.$$

Now, the question is: To what representation of states do ϕ_k^+ and ϕ_k belong? If one allows $e_k = 1$ one can regard the ϕ 's as operators of the particle representation, though formally defined over different domains as the a 's (i.e. by introducing an *a priori* differentiation between the coordinates (or wave vectors) of two groups of otherwise indistinguishable particles). Should this be the case, then, by operating with the second relation in (4.5.8.) on the vacuum of the particles one would find

$$\alpha_k |0\rangle = 0 \quad (4.5.11.).$$

But, on the other hand, the following relation is also satisfied

$$\alpha_k |C_0\rangle = 0 \quad (4.5.12.),$$

where

$$|C_0\rangle = T_1 |0\rangle \quad (4.5.13.).$$

In consequence either the vacuum of the new representation is not unique, i.e. $|0\rangle \neq |C_0\rangle$, in which case is *not* a *good* vacuum state, or the two representations $\{|C_n\rangle\}$ and $\{|n\rangle\}$ are *identical*, i.e. $|C_0\rangle = |0\rangle$ which implies that $T_1 \equiv I$. Clearly the resulting representation is not appropriate for our present purposes in either case.

On the other hand the ϕ 's cannot be elementary operators of the new C.S.R.; for, one cannot formulate a definition by employing the very notion to be defined. In any case, should this be allowed, one would conclude

$$a_k |C_0\rangle = 0 \quad (4.5.14.)$$

by operating with the second relation in (4.5.8.) upon $|C_0\rangle$ which together with

$$a_k|0\rangle = 0 \quad (4.5.15.),$$

would lead to the conclusion that both representations are identical. Note that the vacuum of the particle representation is unique by definition.

The only remaining possibility is for the ϕ 's to be the elementary operators of a third representation (non-equivalent to the other two). A more elaborate analysis would show that the ϕ 's cannot be related to the a 's or the α 's by canonical transformation, so this purely quantum coherent representation would be of no help for the present programme; for, in order to prove that the volume of both phase spaces are the same, the two representations of states *must* be related through a canonical transformation.

Leaving this difficulty aside, for the moment, let us show that the difficulty with a *second* order coherent representation is even worse. Consider the transformation

$$T_2 = \exp \hat{\theta}_2 \quad (4.5.16.),$$

where

$$\hat{\theta}_2 \equiv \sum_{k,q} (g_k g_q a_k^+ a_q^+ - g_k^+ g_q^+ a_k a_q) \quad (4.5.17.),$$

where the g 's are also Bose-like operators, satisfying similar commutation relations to those of the ϕ 's. Now, the successive commutators, C_n , do *not* form a cyclic series in this case, but a series in increasing powers of particle operators,

$$\begin{aligned} C_1 &= - \sum_q g_k^+ g_q^+ a_q, \\ C_2 &= \sum_{k,q} (g_k g_q g_k^+ g_q^+ a_k^+ + \\ &\quad \sum_q [g_k g_q, g_k^+ g_q^+] a_k^+ a_q^+) \end{aligned} \quad (4.5.18.).$$

C_3 would give a contribution proportional to the particle operators to the fifth power, and C_n a contribution proportional to the a 's to the $(n+2)$ th power.

Therefore the relation $\alpha_k = \alpha_k(a)$ is an infinite series in increasing powers of particle operators. This is what happens for the partly-c-number C.S.R. for third and higher orders. Thus for a purely quantum C.S.R., a second order representation is already untractable.

Let us consider now the question of how to define an *appropriate* L.C.S.R. for Fermi fields, such that *first* order coherence *is* involved, and yet *no* contradiction arises. Let us reproduce, first of all, Yang's argument against O.D.L.R.O. in Ω_1 for Fermi systems. Should O.D.L.R.O. occur in Ω_1 , i.e.

$$\Omega_1(x;x') = \phi_1^*(x')\phi_1(x) + \Lambda_1(x,x') \quad (4.5.19.).$$

The second order reduced density matrix would take the following expression

$$\begin{aligned} \Omega_2(x,y;x',y') = & \phi_1^*(x')\phi_1^*(y')\phi_1(x)\phi_1(y) + \\ & \phi_1^*(x')\phi_1(x)\Lambda_1(y;y') - \phi_1^*(x')\phi_1(y)\Lambda_1(x;y') + \\ & + \phi_1^*(y')\phi_1(y)\Lambda_1(x;x') - \phi_1^*(y')\phi_1(x)\Lambda_1(y;x') + \\ & + \Lambda_1(x;x')\Lambda_1(y;y') - \Lambda_1(x;y')\Lambda_1(y;x') + \\ & + \Lambda_2(x,y;x',y') + \phi_2^*(x',y')\phi_2(x,y) \end{aligned} \quad (4.5.20.),$$

where ϕ_2 is present if intrinsic O.D.L.R.O. occurs in Ω_2 , independently of O.D.L.R.O. in Ω_1 .

Now, Ω_2 must be antisymmetric under permutation of coordinates $x \nleftrightarrow y$ or $x' \nleftrightarrow y'$, i.e.

$$\begin{aligned} \Omega_2(x,y;x',y') &= -\Omega_2(y,x;x',y') = \\ &= -\Omega_2(x,y;y',x') = \\ &= \Omega_2(y,x;y',x') \end{aligned} \quad (4.5.21.).$$

Both Λ_2 and ϕ_2 are, presumably, antisymmetric under permutations of coordinates. Thus, the last eight contributions to Ω_2 are manifestly antisymmetric; but the first contribution is *not*. No provision is taken within the context of Yang's argument *ensuring* the antisymmetry of $\phi_1^*(x')\phi_1^*(y')\phi_1(x)\phi_1(y)$; for, these c-number fields are *regarded* as *abelian*, and to regard them differently would be difficult to justify in this context. However, it is clear that the resolution of the difficulty is brought about by *regarding the first-order coherent fields as antisymmetric*. This property can be built in rather simply through an appropriate definition of the L.C.S.R. for Fermi operators.

Consider the canonical transformation

$$T_F = \exp \hat{\theta}_F \quad (4.5.22.),$$

where

$$\hat{\theta}_F = \sum_{k,q} (f_k c_k^+ - f_k^* c_k + g_{k,q} c_k^+ c_q^+ - g_{k,q}^* c_k c_q) \quad (4.5.23.)$$

c_k^+ and c_k are Fermi particle operators, satisfying

$$\left. \begin{aligned} [c_k, c_{k'}^+] &= \delta_{k,k'} \\ [c_k, c_{k'}] &= 0 \\ [c_k^+, c_{k'}^+] &= 0 \end{aligned} \right\} \quad (4.5.24.),$$

and f_k and $g_{k,q}$ are c-number fields satisfying

$$\left. \begin{aligned} f_k f_{k'}^+ + f_{k'}^* f_k &= 0 \\ f_k f_{k'} + f_{k'} f_k &= 0 \\ f_k^* f_{k'}^+ + f_{k'}^* f_k &= 0 \end{aligned} \right\} \quad (4.5.25.)$$

$$g_{k,q} = -g_{q,k} \quad (4.5.26.)$$

The resulting expressions for the elementary operators $\beta_k^+ = T_F c_k^+ T_F^{-1}$ and $\beta_k = T_F c_k T_F^{-1}$ in terms of particle operators c_k^+ and c_k can be obtained in the usual way, after some work one finds that the inverse reaction takes the form

$$\left. \begin{aligned} c_k^+ &= u_k \beta_k^+ + \sum_q v_{k,q}^* \beta_q + \phi_k^* \\ c_k &= u_k \beta_k + \sum_q v_{k,q} \beta_q^* + \phi_k \end{aligned} \right\} \quad (4.5.27.)$$

or even more generally

$$\left. \begin{aligned} c_k^+ &= \sum_q (u_{k,q} \beta_q^+ + v_{k,q}^* \beta_q) + \phi_k^* \\ c_k &= \sum_q (u_{k,q}^* \beta_q + v_{k,q} \beta_q^*) + \phi_k \end{aligned} \right\} \quad (4.5.28.),$$

if a contribution $i \sum_{k,q} h_{k,q} c_k^+ c_k$ is included in $\hat{\theta}_F$. The u 's and v 's can be shown to satisfy the following identity:

$$\sum_q |u_{k,q}|^2 + |v_{k,q}|^2 = 1 \quad (4.5.29.),$$

and

$$\left. \begin{aligned} u_{k,q} &= u_{q,k} \\ v_{k,q} &= -v_{q,k} \end{aligned} \right\} \quad (4.5.30.).$$

The ϕ 's now satisfy

$$\left. \begin{aligned} \phi_k \phi_k^* + \phi_k^* \phi_k &= 0 \\ \phi_k \phi_k^* + \phi_k^* \phi_k &= 0 \\ \phi_k^* \phi_k^* + \phi_k^* \phi_k &= 0 \end{aligned} \right\} \quad (4.5.31.).$$

It can be easily tested that (4.5.29.,31.) imply that the β 's satisfy Fermi anticommutation relations

$$[\beta_k, \beta_{k'}^+]_+ = \delta_{k,k'} \quad (4.5.32.).$$

This representation can be used to define the dynamical variables of the S.P.S. The expressions for the reduced density matrix (in a pure state description) in terms of the dynamical variables is the same as in §4.3.; but, due to the fact that the field operators satisfy different inner product relations, the actual expressions for the Fermi case differ in signs respect to the expressions for the Bose case. The first two reduced density matrices in this case are

$$\Omega_1(x; x') = \sum_{k, k'} \Omega_1(k; k') \exp i(kx - k'x') \quad (4.5.33.),$$

$$\Omega_1(k; k') = \phi_k^* \phi_{k'} + \Lambda_1(k, k') \quad (4.5.34.),$$

$$\begin{aligned} \Omega_2(x, y; x', y') = \sum_{\substack{k, k' \\ q, q'}} \Omega_2(k, q; k', q') \exp i[(kx + qy) - \\ - (k'x' + q'y')] \end{aligned} \quad (4.5.35.),$$

$$\begin{aligned} \Omega_2(k, q; k', q') = & \phi_k^* \phi_q^* \phi_{k'} \phi_{q'} + \\ & + \phi_k^* \phi_{k'} \Lambda_1(q; q') - \phi_k^* \phi_{q'} \Lambda_1(k; q') + \\ & + \phi_q^* \phi_{q'} \Lambda_1(k; k') - \phi_q^* \phi_{k'} \Lambda_1(k; k') + \\ & + \Lambda_1(k; k') \Lambda_1(q; q') - \Lambda_1(k; q') \Lambda_1(q; k') + \\ & + \Lambda_2(k, q; k', q') + \phi_{k', q'}^* \phi_{k, q} + \\ & + \phi_{k', q'}^* K_{k, q} + K_{k', q'}^* \phi_{k, q} \end{aligned} \quad (4.5.36.),$$

where Λ_1 , Λ_2 , ϕ and K are defined as before in §4.3., but now $v_{k, q}$ is antisymmetric respect to permutation of variables, which implies that

$$\begin{aligned}
 \phi_{k,q} &= -\phi_{q,k} \\
 K_{k,q} &= -K_{q,k} \\
 \Lambda_2(k,q;k',q') &= -\Lambda_2(q,k;k',q') = \\
 &= -\Lambda_2(k,q;q',k') = \\
 &= \Lambda_2(q,k;q',k')
 \end{aligned}
 \tag{4.5.37.}$$

and the first order coherent fields satisfy (4.5.31.). In consequence Ω_2 is manifestly antisymmetric under permutation of coordinates, and yet O.D.L.R.O. takes place in Ω_1 .

The implications of the theoretical feasibility of first order coherence in Fermi systems are far reaching, and enables to see the problem of superconductivity and superfluidity in ^3He on a new light. It will be interesting to extrapolate the results obtained here for the problem of ^4He to the case of superconductors.

The structure of the effective phonon mediated electron interaction is the same as the inter-Helium-atom interaction. In consequence the results of section 3.2. apply to the case of a superconductor. As to the results of section 3.3. the only difference expected as to the excitation spectra is a change of sign. For superconductors one should obtain

$$\omega_k^i = \{J_k^2 + \sum_p |B_{p,k}|^2\}^{1/2} \equiv \omega_k, \quad \text{for } i = 1, 2 \tag{4.5.38.}$$

and

$$\omega_k^3 = \{J_k^2 + b_k^2\}^{1/2} \tag{4.5.39.}$$

This is due to the different commutation relations satisfied by the α 's and the β 's.

Now, a surprising consequence arises in the statistical context. Should one regard the pairing field as the order parameter (as in the case

of the Bose problem) the spectra ω_k would split into a number of separate branches, which are *not* observed experimentally. It thus seems as if the order parameter *cannot* be identified with the *pairing fields*! The only remaining option is to identify the order parameter with the *first* order coherent fields. In such a case the upper two branches remain identical, as in a pure state description. And the lower branch *does not appear* in photon scattering experiments, leading to a prediction in qualitative agreement with experiment.

The present analysis is, of course, rather speculative and further research is required to be able to support this conclusion on a more reliable basis. An investigation in this direction is currently in progress.

Let us now consider another problem of a different nature, namely the problem of magnetism. Some systems of spins, interacting via Heisenberg exchange interactions, exhibit a transition to a magnetic phase, ferromagnetic, antiferromagnetic or helimagnetic, depending on the nature of the interactions and the geometrical array of the localized spins at the sites of a periodic crystal.

At a *macroscopic* scale the onset of the low temperature phase is marked by a *breakdown of the rotational symmetry*. In the sense that, as far as the magnetic properties are concerned, the system is rotationally invariant under the full group of continuous rotations in the paramagnetic phase. In the magnetic phase, however, a finite fraction of the spins become aligned, bringing about a finite macroscopic value for the magnetisation. In consequence the macroscopic system is invariant only under rotations around the axis of magnetization. This happens as a consequence of the fact that the order parameter of the magnetic phase is a vector, namely the magnetization. The above macroscopic characterization, however, is not the only possible one. In fact one can characterize a macroscopic system in thermal equilibrium by the number of independent variables required

to specify the thermodynamic state of the system, and use the name 'number of symmetries' to designate the latter. In this case one should conclude that the number of macroscopic symmetries is larger in the ordered phase than in the paramagnetic case; for, an additional variable needs to be determined, namely the magnetization, in order to specify the state of the system completely. But the conflict here is just a matter of linguistics, not of physics.

The real conflict arises when the breakdown of rotational symmetry is thought to occur not only at a *macroscopic* (statistical) level, but also at a *microscopic* (dynamical) level. A large number of authors support the idea that the breakdown of rotational symmetry of a macroscopic level is a *manifestation of a breakdown of a microscopic symmetry*. In the sense that the number of constants of motion are different for two formulations of the same problem in terms of two sets of states, believed to give the best dynamical descriptions in the paramagnetic and ferromagnetic phases, say. This is a belief analogous to that supporting the standard theories of superfluidity and superconductivity.

It is usually overshadowed that while there is no reason to rule out a macroscopic breakdown of symmetry, there is a fundamental requirement that the overall microscopic symmetry should *not* be broken, but rearranged. Note that this requirement does not rule out the emission of Goldstone or Higgs bosons. Hence in the absence of empirical evidence as to the real occurrence of a dynamical breakdown of symmetry accompanied by the emission of a particle carrying the remaining symmetry for the magnetic problem, one should look for a theoretical treatment whereby the overall symmetry is rearranged. The theory proposed in this thesis comes handy in this respect.

Most existing first principle treatments of the problem of a collection of spins parallel current theories of superfluidity to some extent. As to the question of the microscopic antecedent of the macroscopic breakdown of symmetry, for instance, and as to the treatment of the statistical problem of the low temperature phase.

It is often stated (53) that the breakdown of rotational symmetry - in the ferromagnetic phase, say, is a consequence of a breakdown of dynamical symmetry at a *microscopic* level. It is commonly thought that 'the dynamical descriptions' of the paramagnetic and ferromagnetic phases are *not* equivalent, in the sense that the 'ferromagnetic representation of states', unlike the 'paramagnetic representation of spin states', incorporates a preferred direction. In consequence, an infinitesimal transformation amounting to an arbitrary rotation (i) leaves the hamiltonian invariant, (ii) transforms a paramagnetic state into another of the same energy, but (iii) transforms a ferromagnetic state into another of different energy (unless the rotation is about the preferred z-axis of the latter representation). This, microscopic, paradigm is the same as that prevailing in standard theories of superfluidity and superconductivity and amounts to the ascertainment that the overall number of constants of motion (which are good quantum numbers) is less in the ferromagnetic representation description (in a pure state) than in the paramagnetic description.

In order to illustrate the similarities of the treatment of the statistical mechanical problem of, say, ferromagnetic and superfluid phases it will be interesting to consider the statistical problem of a collection of spin-waves. The spin-waves are the low lying excitations of a dynamical system of localised spins interacting via exchange-dipole interactions (83). It is customary, in dealing with this particular problem, to introduce a transformation to project the well-known isospin representation into a Bose representation, according

to the Holstein-Primakoff transformation rule (84). This approximate method amounts to formulating the dynamical problem of a collection of N spins as the problem of an unspecified number of 'spin deviations' (from the ground state configuration). The approximate description of spins in terms of bosons holds if the number of spin deviations is smaller than the total spin, this is certainly the case at low temperatures, but the notion of spin-waves loses meaning at higher temperatures, much below the transition temperature.

A striking similarity with the problems of superfluidity and superconductivity arises when the dynamical problem of a collection of spins is formulated in terms of the Holstein-Primakoff representation. The approximate spin hamiltonian in terms of Bose operators, a_k^+ and a_k , creating and destroying, respectively, a unit of spin deviation is (after discarding non-linear contributions)

$$\hat{H} = \sum_k (W_k a_k^+ a_k + B_k a_k^+ a_{-k}^+ + B_k^* a_k a_{-k}) \quad (4.5.40.).$$

This hamiltonian is 'brought to a diagonal form' by introducing a 'change of variables' $(a_k^+, a_k) \rightarrow (\alpha_k^+, \alpha_k)$ to the fields of the *pair representation*!

$$\left. \begin{aligned} a_k^+ &= u_k \alpha_k^+ + v_k^* \alpha_{-k} \\ a_k &= u_k \alpha_k + v_k \alpha_{-k}^+ \end{aligned} \right\} \quad (4.5.41.),$$

where

$$u_k^2 - |v_k|^2 = 1 \quad (4.5.42.).$$

The diagonalization of \hat{H} is obtained by selecting v_k and v_k^* appropriately. The excitation spectrum obtained (in a pure state description) is in qualitative agreement with the experiment. It is interesting to note that the observed excitation spectrum of spin-waves is nearly a quadratic band, showing a gap.

The thermodynamic properties of a collection of spin-waves in thermal equilibrium at low temperature are obtained from the partition

function (83)

$$Z = \sum_{\eta_k} \text{Tr}(\exp(-\beta \hat{H})) \quad (4.5.43.),$$

where the summation is carried out over all possible distributions of elementary excitations, $\eta_k \equiv \text{Tr}\{\alpha_k^\dagger \alpha_k\}$, *not* over the possible distributions of spin-deviations, $N_k \equiv \text{Tr}\{a_k^\dagger a_k\}$. This procedure is entirely analogous to that followed in the standard theories of superfluidity (68) and superconductivity (3, 34 and Refs. therein).

It is most important to note that the entire ensemble describing a collection of spin deviations is *different*, more general in fact, than the ensemble whose partition function is (4.5.43.). The partition function for the former ensemble involves also a summation over configurations associated with the order parameter, namely the magnetization. It has been shown in §4.4. how important it is to perform the summation over *all* configurations, not only those associated with the non-ordered part of the ensemble.

The above observations as to the alleged microscopic breakdown of symmetry, and the partial treatment of the statistical problem suggests that a new light could be brought to understanding the present problem from the standpoint of the theory proposed in this thesis. The interest on this problem in this work is only marginal. The final part of this section investigates the possible formulation of the spin problem in terms of variables of a separable phase space, and introduces a C.S.R. for spins, in terms of which the new dynamical variables are defined, such that a dynamically equivalent formulation is possible. The discussion here is rather informal and aims only at laying the tentative foundation for future research.

Consider the Heisenberg hamiltonian

$$\hat{H} = - \sum_{i,j} J_{i,j} \hat{S}_i \cdot \hat{S}_j \quad (4.5.44.),$$

where \hat{S}_i is the vector spin operator at the location r_i in a crystal lattice. $J_{i,j}$ are two body interactions depending on $|r_i - r_j|$ only.

Let us define the dynamical variables as

$$\hat{p}_i \equiv (\hat{p}_{xi}, \hat{p}_{yi}, \hat{p}_{zi}) \equiv (\hat{S}_{xi}, \hat{S}_{yi}, \hat{S}_{zi}) \quad (4.5.45.)$$

$$\hat{q}_i \equiv \begin{pmatrix} q_{xi} \\ q_{yi} \\ q_{zi} \end{pmatrix} \equiv \begin{pmatrix} \hat{S}_{xi} \\ \hat{S}_{yi} \\ \hat{S}_{zi} \end{pmatrix} \quad (4.5.46.)$$

$$\hat{q}_i \equiv i\hbar \delta_t \hat{q}_i \quad (4.5.47.).$$

The hamiltonian $\hat{H}(\hat{p}, \hat{q})$ can now be written as

$$H = - \sum_{i,j} J_{i,j} \hat{p}_i \cdot \hat{q}_j \quad (4.5.48.),$$

and the Lagrangian as

$$\hat{L}_{ns} = (1/2) \sum_i (\hat{p}_i \hat{q}_i + \text{c.c.}) - \hat{H}(\hat{p}, \hat{q}) \quad (4.5.49.).$$

Note that

$$\hat{p}_i \equiv \hat{q}_i^* = \partial \hat{L}_{ns} / \partial \hat{q}_i \quad (4.5.50.).$$

Now, defining new dynamical variables defined in separable domains

$$\hat{p}_i \equiv \sum_m \hat{p}_i^m, \quad \hat{q}_i \equiv \sum_m \hat{q}_i^m, \quad \hat{q}_i \equiv \sum_m \hat{q}_i^m \quad (4.5.51.),$$

where $m = 1, 2$, the lagrangian becomes

$$L_s = (1/2) \sum_{i,m} (\hat{p}_i^m \hat{q}_i^m + \text{c.c.}) - \hat{H}' - \hat{H}_R \quad (4.5.52.),$$

where

$$\hat{H}'(\hat{p}^m, \hat{q}^m) = - \sum_{i,j} J_{i,j} \sum_m \hat{p}_j^m \hat{q}_i^m \quad (4.5.53.)$$

$$\hat{H}_R = (1/2) \sum_{i,m,n}^{(m \neq n)} (\hat{p}_i^m \hat{\lambda}_i^n + \text{c.c.}) \quad (4.5.54.),$$

where

$$\hat{\lambda}_i^n = - \hat{q}_i^n + \partial \hat{H}' / \partial \hat{p}_i^n \quad (4.5.55.).$$

This shows that \hat{H}' is the new hamiltonian and \hat{H}_R is a redundant condition.

The volumes of the phase spaces $\Gamma_{ns} \equiv \{(\hat{p}_i, \hat{q}_i)\}$ and $\Gamma_s = \bigoplus_{m=1} S_m$, $S_s \equiv \{(\hat{p}_i^m, \hat{q}_i^m)\}$ are

$$\text{Vol}(\Gamma_{ns}) = \sum_i \text{Tr}\{\hat{p}_i \cdot \hat{q}_i\} \quad (4.5.56.)$$

and

$$\text{Vol}(\Gamma_s) = \sum_{i,m} \text{Tr}\{\hat{p}_i^m \cdot \hat{q}_i^m\} \quad (4.5.57.),$$

respectively.

Now, the dynamical variables of the N.S.P.S. are defined over the standard isospin representation, namely the representation defined by the elementary operators \hat{S}_{xi} , \hat{S}_{yi} and \hat{S}_{zi} and the set of simultaneous eigenstates of $\hat{S}^2 = \sum_i \hat{S}_i \hat{S}_i$, $\hat{S}_z = \sum_i \hat{S}_{zi}$ and $\hat{H}(\hat{p}, \hat{q})$. Let us denote such a set of states as $\{|p_n\rangle\}$. This is of course for an arbitrary choice of axis. Note that

$$\text{Vol}(\Gamma_{ns}) = \text{Tr}\{S^2\} \quad (4.5.58.).$$

In order to define the variables of the S.P.S., Γ_s , one must employ a representation of states involving two additional fields. Such a representation should have in addition a preferred direction for the z-axis.

A first order coherent state representation for a collection of spins 1/2 have been recently introduced (63) to treat the Ising model. An extended version of this representation could be used to define the dynamical variables of the S.P.S. and to prove dynamical equivalence.

This attractive looking transformation is given by

$$T_M = \prod_i \exp \theta_M \quad (4.5.59.)$$

$$\theta_{Mi} = \xi_i (\hat{S}_{xi} + i\hat{S}_{yi}) - \xi_i^* (\hat{S}_{xi} - i\hat{S}_{yi}) \quad (4.5.60.),$$

where ξ_i and ξ_i^* are complex c-numbers. An investigation as to the application of the programme of this thesis to the problem of magnetic systems is currently in progress. The aims are to prove the dynamical equivalence of the formulations of the problem of a collection of spins in the separable and non separable pictures, such that the dynamical variables are defined in terms of the fields $\hat{R}_{xi} = T_M \hat{S}_{xi} T_M^{-1}$, $\hat{R}_{yi} = T_M \hat{S}_{yi} T_M^{-1}$, $\hat{R}_{zi} = T_M \hat{S}_{zi} T_M^{-1}$ and ξ_i and ξ_i^* . A second aim is to construct two comparable ensembles, one of which is partly ordered at finite temperature. This latter ensemble should describe the properties of the low temperature magnetic phase. The magnetic phase will not be a superfluid phase in so far as the dynamical variables (and hence the configurations in the phase space) are not defined in real space but in the spin space. The spins, in fact, are fixed to the rigid lattice so there is no flow of spins.

It is too early, of course, to advance any conclusion as to the real advantages of producing alternative treatments for the general problem of phase transitions on the basis of the programme proposed in this theory. But if one takes into consideration the present state of the less elaborate theories of super-responsive and condensed behaviour, as the theory of excitonic matter and pion condensation, for instance, the hope of a unified theory looks attractive enough as to consider it seriously. On the other hand, if one takes into consideration the fact that the best known theories are invariably based upon the old paradigm of a broken microscopic symmetry, as the theories of superconductivity and the theory of lasers, for instance, the crossed examination of these theories becomes

a matter of urgency.

The present programme suggests a number of lines of further research. Within the realm of the microscopic theory of spin-glasses a treatment in which the (magnetic) second order coherent fields are the order parameters looks very attractive, and a theory of ^3He incorporating the notions of first and second order coherence (in the particle sense) and/or first order coherence (in the magnetic sense) look very interesting to explain the numerous phase transitions exhibited by this system at low temperature.

On the other hand, the availability of a theory of superfluidity freed from the incumbence of Bose-Einstein condensation as a necessary ingredient, seems suited to study the behaviour of physical systems of complex structure (neither of Bose nor of Fermi nature) displaying 'coherent phenomena', as excitonic matter, pionic matter or confined quarks⁽¹⁷⁾.

§5. Summary and Conclusions

§5.1. Summary

A theory of superfluidity is proposed from dynamical and statistical first principles. The underlying strategy is that superfluidity - from a theoretical standpoint - should come about *purely* from statistical considerations, being impossible to characterize a superfluid system only from considerations as to its dynamical behaviour, or the representation of states in terms of which the dynamical variables are defined.

As far as statistical mechanisms are concerned the main element of the present theory is a characterisation of superfluid and non-superfluid ensembles. This characterisation enables to prove that macroscopic systems, in thermal equilibrium at finite temperature, described by the former ensemble does posses the property of superfluidity and the latter does not. The only difference between these two ensembles is that certain configurations of the former ensemble are *statistically equivalent*. The comparison of the free energies obtained from these two ensembles provides a criterion of occurrence of a phase transition and determines, in principle, the critical temperature. The notion of statistical equivalence of configurations contributing fractionally to the density conveys the property of superfluidity from a theoretical standpoint.

The construction of a superfluid ensemble, and of a comparable non-superfluid ensemble, requires of the possibility of constructing a *restricted ensemble*, involving at least two independent configurations in the phase space. A central notion in this work is that of *separable phase space*. It was shown that any ensemble constructed on the basis of the counting of configurations in a separable phase space is a restricted ensemble. A S.P.S. involving three separate parts was constructed, it was shown that the overall volume of the S.P.S. is the sum of the volumes of its separate parts. The notion of separable

phase space adopted in this thesis incorporates the notion of coordinates of distinguishable objects, this suffices to obtain the general expression for the one-object propagator operator in the S.P.S., purely from the structural properties of the S.P.S. The interpretation of certain configurations in particular as the superfluid configurations, among the various possibilities, is left here until the latest possible stage, unlike in standard theories for which the 'semantic input' occurs at the very beginning. The main difference between the present theory and the standard theories of superfluidity, as far as statistics is concerned, is that the configurations associated with the superfluid are taken into account here for the derivation of the partition function. This enables to *prove* that the superfluid ensemble possesses the property of superfluidity, and, by comparison with the corresponding non-superfluid ensemble, conveys a criterion of existence of superfluidity. The statistical ensemble in standard theories, on the other hand, does *not* take into consideration the various (c-number) configurations. The partition function is constructed as the statistically weighted summation of configurations of elementary excitations. In other words the ensemble considered in standard theories is only *a part of the entire ensemble*, namely the part associated with the non-superfluid segment of the ensemble. As such if the *entire* ensemble corresponds to that a superfluid it does so *a priori*, i.e. no *proof* can be advanced as to the superfluid behaviour of the system or otherwise.

The main innovation of the present theory on the dynamical front is the notion of *dynamical equivalence* of two *lagrangian* formulations of the same dynamical problem. This notion encompasses the ideas of symmetry rearrangement and expectation value invariance. The former condition requires the group of lagrangian invariances to be the same, regardless of the structure of the domain of definition of the dynamical variables (separable or non-separable) and also irrespective of the representation

of states in terms of which the dynamical variables are defined. The latter condition requires the expectation values for the constants of motion to be the same, the identity of the volumes of the phase spaces in particular. The notion of dynamical equivalence is central in this theory, and its demonstration constitutes the tautology supporting the present formulation. The use of such a strategy is the main difference respect to existing theories of superfluidity, which are based upon the assumption that the constants of motion are the same, regardless of what the dynamical variables are, or how these are defined in terms of the fields of certain representation of quantum states. The satisfaction of the properties defining dynamical equivalence makes it impossible to discriminate any dynamical difference between two formulations, while for the standard theory two formulations in terms of two non-equivalent representations are *non-equivalent*, and distinguishable by their different number of symmetries.

The proof of dynamical equivalence of two formulations in terms of variables of separable and non-separable domains is carried out in two stages. The first stage aims at proving that given a lagrangian in terms of dynamical variables of a non-separable domain, such that an explicitly time independent hamiltonian exists, and such that both the hamiltonian and the number functional are constants of motion, there is a set of dynamical variables of a separable domain, linearly related to the variables of the non-separable domain, such that *the same* lagrangian in terms of the separable domain variables admits an explicitly time independent hamiltonian, and such that the new hamiltonian and number functional defined over the S.P.S. are also constants of motion.

In order to produce the first part of the proof one needs to consider only two abstract sets of dynamical variables, without having to define them in terms of the fields of two canonically related representations of states. It was found that the first part of the proof of dynamical

equivalence can be carried out for both the ideal Bose gas and the interacting problem. It was shown that the dynamical problem in the separable domain picture is posed redundantly. The hamiltonian of the S.P.S. picture is obtained after removing the redundant condition. It is found that the hamiltonians of the N.S.P.S. as S.P.S. pictures are *different* functionals. Similarly it is found that the number functionals in the N.S.P.S. and S.P.S. pictures are also different functionals. Finally, it is shown that, if the hamiltonian and number functional in the non-seperable domain picture are both constants of motion, the hamiltonian and number functionals in the separable domain picture are also constants of motion. This is shown by using the Poisson brackets as dynamical brackets in both cases.

The second stage of the proof of dynamical equivalence requires of the definition of both sets of dynamical variables in terms of the fields of two related representations of states. It is noted that in order to define the variables of the seperable phase space one must employ a representation involving three independent pairs of fields. Furthermore both representations of states must be related such that, after defining both separable and non-seperable domain variables in terms of the fields of both representations, the linear relationship between the two sets of variables becomes an identity.

The non-seperable domain variables are defined from the fields of the Bose particle representation. A general linear representation of coherent states was defined in Chapter 2, the variables of the seperable domain were defined in terms of such L.C.S.R. The L.C.S. are normalised such that the average number of particles in the particle representation is the same as the average number of particles in the L.C.S.R. This entails that the volume of the N.S.P.S. is the same as the volume of the S.P.S. It was shown in Chapter 2 that the number operators in the N.S.P.S. and S.P.S. are diagonal in the P.R. and the L.C.S.R., respectively.

This together with the fact that both functionals are constants of motion entails that the gauge symmetry is rearranged. In addition the identity of the volumes of the phase spaces implies dynamical equivalence as to the number conservation.

Dynamical equivalence as to energy conservation can only be proved in rigour for the ideal Bose gas, if the dynamical variables of the separable phase space are defined in terms of the L.C.S.R. In this case it is shown that the hamiltonians in the N.S.P.S. and S.P.S. pictures are diagonal in the P.R. and the L.C.S.R., respectively. This together with the fact that both functionals are constants of motion and yield the same average values in their corresponding representations entails dynamical equivalence.

For the interacting problem the exact hamiltonian of the S.P.S. picture is not diagonal in the L.C.S.R. In order to prove the rearrangement of the hamiltonian symmetry one must employ a more elaborate, non-linear, representation of coherent states; the physical representation of Umezawa, say. It was conjectured in Chapter 3 that one should be able to demonstrate the hamiltonian symmetry rearrangement in the *finite* volume limit. This is conjectured in view of the fact that all the dangerous contributions to the S.P.S. hamiltonian have been cancelled in the process of removing the redundancy. In consequence the hamiltonian segment generating the series, (hopefully) converging to the physical representation, is free from dangerous contributions, unlike in Umezawa's treatment.

The problem of interacting ⁴He was considered in Chapter 3 in a mean field approximation. This approximation consists of discarding the non-diagonal segment of the S.P.S. hamiltonian in the L.C.S.R., and neglecting fluctuations about (pure state) average values of the three independent number of objects of the present theory. Three branches of the spectrum were obtained. The lowest branch is gapless and the upper

two branches coincide and show a gap. The occurrence of several branches of the excitation spectrum in a pure state description is an inherent feature of the formulation of the dynamical problem in terms of dynamical variables of a S.P.S. The fact that the lowest branch of the spectrum is gapless follows from the fact that the affective hamiltonian associated with the first order coherent field is invariant under Bogoljubov's phonon-like transformation. The fact that the upper two branches show a gap follows from the gapless nature of the lowest branch, and a general relationship between the three expressions for the spectrum.

It was shown that the standard criterion of diagonalisation of the particle hamiltonian in the C.S.R., adopted in all standard mean field theories, leads to error if first order coherence is included. The source of the error comes from the failure to cancel high order dangerous contributions, and the inherently non-diagonal segment of the particle hamiltonian in the C.S.R. The gapless branch, on the other hand, does not appear in existing mean field theories, due to the fact that the c-number fields (particularly the first order coherent fields) are regarded as time independent variational parameters, instead of truly dynamical fields, as is the present theory. It becomes clear from the present analysis that the gap in the excitation spectrum obtained by many authors before is *not* in error, but indicates that the excitation spectrum obtained corresponds to an upper branch.

The rearrangement of the gauge invariance was explicitly shown in Chapter 4. Transformation laws were obtained for all the fields involved, and the Euler-Lagrange equations of a complete theory of the coupling with an external field of velocity were obtained. Expressions for the first two reduced density matrices were obtained in a pure state description. It was shown that O.D.L.R.O. occurs in both reduced density matrices, confirming Fröhlich's ansatz.

The statistical problem was considered in §4.4. An additional postulate of quantization of c-number configurations was introduced.

A non-superfluid ensemble was defined. It was shown that such an ensemble describes the thermodynamic behaviour of a non-superfluid. Several semantic options were considered as to the interpretation of the statistically equivalent configurations. It was shown that all the theoretically possible superfluid ensembles describe the thermodynamic properties of a superfluid. The possibility of the first order coherent fields being regarded as the order parameter was ruled out on physical grounds. The only realistic option remaining was that of the pairing fields being associated with the order parameter.

It was shown that if the distribution of pairs are all statistically equivalent the coincident two upper branches, in a pure state description, split up into a band comprising $2N$ branches in a mixed state description, this being in excellent qualitative agreement with experiment.

It was shown that, for the above interpretation, O.D.L.R.O. occurs in the second order reduced density matrix, but not in the first. It was also shown that, in the presence of an external field of velocity, the superfluid segment flows with longitudinal (curl free) velocity. The exact integral equations characterising the mean field model in thermal equilibrium (and also an approximate set) were obtained. The criterion of occurrence of a phase transition to a superfluid phase was proposed. This can be applied after the set of integral equations is solved numerically. This solution will also provide the expressions for the excitation spectra as a function of wave vector, and will eventually determine whether Bose-Einstein condensation occurs or not. It is noted that the existence of B.E.C. is contingent to the solution of the integral equations. B.E.C. can take the form of a singularity in the distributions of first order coherent fields, in the distribution of elementary excitations or in the distribution of second order coherent fields. Only in the latter case the condensate should be associated with the superfluid.

Finally it is shown that Fermi systems can exhibit O.D.L.R.O. in the first reduced density matrix without contradiction. It was conjectured that the present theory can be applied to a variety of systems as superconductors and magnetic systems, for instance.

§5.2. Conclusions

The main conclusions obtained in this thesis are listed next in order of appearance.

1. The fields to be identified with the order parameter must be dynamical variables, or factors of dynamical variables, defined in the phase space.
 - 1.1. Variational parameters are not suited to play the role of order parameters.
 2. A restricted ensemble is required to characterise a superfluid ensemble.
 - 2.1. The phase space must be separable in order to be able to construct a restricted ensemble, without introducing an a priori partition in the phase space.
 - 2.2. Γ_S , as defined by (2.2.2.,3.)A, is a separable phase space.
 - 2.3. The number functional in the S.P.S. is $\hat{N}^i = \sum_{k,i} p_k^i q_k^i$.
 - 2.4. The partition function of an ensemble constructed from the S.P.S. takes the form $Z_r = \sum_{\hat{C}_k^1} \dots \sum_{C_k^n} \text{Tr}\{\hat{\Omega}\}$, where C_k^1, \dots, C_k^n are independent configurations and $\hat{\Omega}$ is the statistical operator.
3. A dynamical problem is identified by the group of lagrangian invariances and the expectation values of the constants of motion.
4. The relationship between elementary excitations of two representations related through the canonical transformation $T = \exp \int (\sigma_k a_k^+ + \gamma_{k,p} a_k^+ a_p^+ - \text{c.c.})$ is linear. The inclusion of third or higher powers of a^+ in the exponent leads to an infinite series in powers of particle operators.

- 4.1. The P.R. and the L.C.S.R. are non-equivalent representations of the same commutation relations, i.e. $[a_k, a_{k'}^+] = [\alpha_k, \alpha_{k'}^+] = \delta_{k,k'}$, & $[\hat{N}, \hat{\eta}] \neq 0$.
- 4.2. The quantum averages of a_k , $a_k a_q$, \hat{N} and \hat{H} in the L.C.S.R. are given by (2.3.35., 36., 38. and 41.), respectively.
- 4.3. The conditions $\langle n | \hat{N} | n \rangle = \langle C_n | \hat{N} | C_n \rangle$ and $\langle n | \hat{N} | n \rangle = \langle C_n | \hat{\eta} | C_n \rangle$ cannot be satisfied simultaneously, unless $T \equiv 1$.
5. The linear relation between variables of the N.S.P.S. and S.P.S., given by (2.4.4.), is an identity if the dynamical variables of the S.P.S. are defined as in (2.4.3.).
- 5.1. The number operator \hat{N}' is diagonal in the L.C.S.R.
- 5.2. $\langle n | \hat{N} | n \rangle = \langle C_n | \hat{N} | C_n \rangle$ implies $\langle n | \hat{N} | n \rangle = \langle C_n | \hat{N}' | C_n \rangle$.
6. The dynamical variables of the separate parts of the S.P.S. are not Bose fields, but the dynamical variables for the entire phase space are.
7. The formulation of the dynamical problem in the S.P.S. picture is redundant.
- 7.1. The redundancy is removed by replacing the generalised forces by the known values of the external forces.
- 7.2. The functional expressions for the hamiltonians in the N.S.P.S. and S.P.S. pictures are different.
- 7.3. The difference is given by the dangerous contributions.
8. The S.P.S. hamiltonian for the ideal Bose gas is diagonal in the L.C.S.R.
- 8.1. This hamiltonian is a constant of motion as well as the number operator in the S.P.S.
- 8.2. The expectation values of the hamiltonians of the N.S.P.S. and S.P.S. pictures over the P.R. and the L.C.S.R., respectively, are the same, i.e. $\langle n | \hat{H} | n \rangle = \langle C_n | \hat{H}' | C_n \rangle$.

- 8.3. The formulations for the problem of the ideal Bose gas in the separable and non-separable pictures, defined in terms of the L.C.S.R. and the P.R., are dynamically equivalent.
- 8.4. The equations of motion for the problem of the ideal Bose gas are given by (3.1.43.).
9. The commutators in the P.R. and the L.C.S.R. are the same.
- 9.1. Commutators and Poisson brackets are related through (3.1.53.).
10. For the interacting problem the S.P.S. picture hamiltonian is not diagonal in the L.C.S.R.
- 10.1. The perturbation series generated by the non diagonal segment, \hat{T} , is free from dangerous contributions.
- 10.2. A dangerous contribution is diagonal, namely $\phi\phi_{uv}^* \alpha^+ \alpha$ and its c.c. This contribution fails to be cancelled by the criterion of diagonalisation, leading to an error.
- 10.3. The zeroth order hamiltonian is a constant of motion, and its expectation value in the L.C.S.R. is approximately the same as the expectation value of the particle hamiltonian in the P.R.
- 10.4. The Poisson bracket of the zeroth order hamiltonian and the number operator in the S.P.S. is zero, i.e. \hat{N}' is a constant of motion.
- 10.5. The zeroth order problem in the S.P.S. is (approximately) dynamically equivalent to the particle problem.
- 10.6. The equations of motion for the interacting zeroth order problem are given by (3.3.3.,4.).
11. The standard linearisation procedure linearises the equations of motion for the fields $i = 1, 2$ but fails to linearise the equations of motion for the field $i = 3$.
- 11.1. The equations of motion for $i = 3$ are Gross' equations plus a linear mean field contribution from the pairing fields.
- 11.2. The effective hamiltonian for the fields $i = 3$ is invariant under Bogoljbov's phonon-like transformation, ensuring that the

- dispersion relation ω_k^3 is gapless and linear in the long wave limit.
- 11.3. The dispersion relation for ω_k^3 is given by (3.3.26.).
 - 11.4. The pairing fields are time dependent.
 - 11.5. The excitation spectra for the fields $i = 1, 2$ are given by (3.3.65.).
 - 11.6. The equations of motion for the fields $i = 1, 2$ are decoupled in the α 's.
 12. A gauge transformation in the S.P.S. is given by (4.2.14.).
 - 12.1. The lagrangian (4.2.12.) is invariant under the gauge transformation (4.2.14.), if the vector field transforms as (4.2.10.), i.e. in the same way as for a gauge transformation in the N.S.P.S.
 - 12.2. The Euler-Lagrange equations of a complete theory of the coupling of the entire system with an external field of velocity are given by (4.2.16.-18.).
 13. The Liouville equation in the S.P.S. is given by (4.3.12.).
 - 13.1. The first two reduced density matrices of the S.P.S., in a pure state description are given by (4.3.20.-29.).
 - 13.2. The first two equations of the hierarchy of Frölich master equations are invariant under change of phase space $\Gamma_{ns} \rightarrow \Gamma_s$.
 - 13.3. The first two reduced density matrices factorise in a pure state description.
 - 13.4. Contributions of the form $\phi_k^*, \phi_q^*, \phi_{k,q}$ and $\phi_{k',q}, \phi_k \phi_q$ do not occur in Ω_2^1 .
 14. The partition function for a non-superfluid ensemble is given by (4.4.3.).
 - 14.1. The macroscopic behaviour of a system described by this partition function is that of a non-superfluid.
 - 14.2. If c-number configurations are allowed to take real values the partition function diverges.
 - 14.3. The statistical operator in the M.F.A. is given by (4.4.19.).
 - 14.4. The partition function in the M.F.A. is the product of three partition functions defined in the separate spaces of Γ_s .

- 14.5. The thermodynamic quantities are the sum of their corresponding magnitudes in the separate parts of the ensemble.
- 14.6. The free energy, internal energy and average number distribution from the non-superfluid ensemble are given by (4.4.36.), (4.4.39.) and (4.4.42.), respectively.
- 14.7. The entropy for the non-superfluid ensemble is given by (4.4.47.).
- 15. The configurations C_k^3 cannot be statistically equivalent.
- 15.1. O.D.L.R.O. does not occur in Ω_1^1 .
- 15.2. The only interpretation of the superfluid configurations in qualitative agreement with experiment is that for which the various distributions of pairs are statistically equivalent.
- 15.3. O.D.L.R.O. occurs in Ω_2^1 .
- 15.4. The partition function for the pairing interpretation of the superfluid ensemble is given by (4.4.56.-60.).
- 15.5. A physical system described by a superfluid ensemble exhibits the property of superfluidity.
- 15.6. The excitation spectrum for the fields $i = 3$ in thermal equilibrium is the same as in a pure state description.
- 15.7. The two upper branches - which coincide in a pure state description, except for their sign, split up into two bands comprising $2N$ branches.
- 15.8. The normalisation condition for the pairing superfluid ensemble are given by (4.4.113.).
- 15.9. The integral equations characterising the mean field model in thermal equilibrium are given by (4.4.110.-118.).
- 15.10. The condition of existence of superfluid solution is given by (4.4.127.,129.).
- 15.11. In the presence of an external field of velocity the superfluid segment of the density will sustain a longitudinal velocity.

16. Fermi systems can show O.D.L.R.O. in the first order reduced density matrix.
- 16.1. The present theory should be applicable to arbitrary systems undergoing a phase transition.

Appendix A

Derivation of the relations between particle operators and elementary excitation operators

Consider the unitary transformation

$$T = \exp \theta \quad (\text{A.1.}),$$

where

$$\theta = \sum_{q,p}' (\sigma_p a_p^+ - \sigma_p a_p + \gamma_{p,q} a_p^+ a_q^+ - \gamma_{p,q}^* a_p a_q + i \xi_{p,q} a_q^+ a_p) \quad (\text{A.2.}).$$

The dash on the summation symbol indicates the omission of double counting.

σ_p , $\gamma_{p,q}$ and their c.c. are c-numbers, satisfying the following defining conditions

$$\left. \begin{aligned} |\sigma_p| &= |\sigma_{-p}|, \quad \xi_{p,q} = \xi_{q,p}, \quad \xi_{p,p} = 0 \\ \gamma_{p,q} &= \gamma_{q,p} = \gamma_{-p,-q} \\ \gamma_{p,q} \gamma_{p',q'}^* &= |\gamma_{p,q}|^2, \quad \text{if } p' = p, q' = q \\ &= 0, \quad \text{otherwise} \end{aligned} \right\} \quad (\text{A.3.}).$$

The elementary excitation operators of the linear coherent state representation are defined as follows

$$\left. \begin{aligned} \alpha_k^+ &= T a_k^+ T^{-1} = a_k^+ + [T, a_k^+] T^{-1} \\ \alpha_k &= T a_k T^{-1} = a_k + [T, a_k] T^{-1} \end{aligned} \right\} \quad (\text{A.4.}).$$

The aim in this appendix is to obtain explicit expressions for (A.4.).

Expanding T in powers of θ one finds

$$T = \sum_{n=0}^{\infty} (1/n!) \theta^n \quad (\text{A.5.}),$$

one then finds that

$$[T, a_k^+] = \sum_{n=1}^{\infty} (1/n!) \sum_{m_0=0}^{n-1} \theta^{m_0} C_1 \theta^{(n-m_0-1)} \quad (A.6.),$$

where

$$C_1 \equiv [\theta, a_k^+] \quad (A.7.).$$

Shifting C_1 one place to the left for every term of the summation over m_0 (except for $m_0 = 0$, of course), by using

$$\dots \theta^x C_1 \theta^y \dots = \dots \theta^{(x-1)} C_1 \theta^{(y+1)} \dots + \dots \theta^{(x-1)} C_2 \theta^y \dots \quad (A.8.),$$

where

$$C_2 \equiv [\theta, C_1] = [\theta, [\theta, C_1]] \quad (A.9.),$$

one finds

$$\begin{aligned} [T, a_k^+] = & \sum_{n=1}^{\infty} (1/n!) \sum_{m_0=0}^{n-1} \sum_{m_1=0}^{m_0-1} [\theta^{m_1} C_1 \theta^{(n-m_1-1)} + \\ & + \theta^{m_1} C_2 \theta^{(n-m_1-2)}] \end{aligned} \quad (A.10.).$$

Shifting now C_1 and C_2 one place to the left one obtains

$$\begin{aligned} [T, a_k^+] = & \sum_{n=1}^{\infty} (1/n!) \sum_{m_0=0}^{n-1} \sum_{m_1=0}^{m_0-1} \sum_{m_2=0}^{m_1-1} [\theta^{m_2} C_1 \theta^{(n-m_2-1)} + \\ & + \theta^{m_2} C_2 \theta^{(n-m_2-2)} + \theta^{m_2} C_3 \theta^{(n-m_2-3)}] \end{aligned} \quad (A.11.),$$

where

$$C_3 = [\theta, C_2] \quad (A.12.).$$

Proceeding in the same way until all the C_j 's are placed on the extreme left one finds the following expression

$$[T, a_k^+] = \sum_{n=1}^{\infty} (1/n!) \sum_{j=1}^n F(n, j) C_j \theta^{(n-j)} \quad (A.13.).$$

Now, it is to be noted that the successive shifts of C_1 (C_j) produce

terms involving $C_2 (C_{j+1})$ situated in all possible relative positions. In consequence $F(n, j)$ is just but the number of combinations of n elements taken $(n-j)$ by j ; that is

$$F(n, j) = \binom{n}{j} = [n! / j!(n-j)!] \quad (\text{A.14.}).$$

Thus

$$[T, a_k^+] = \sum_{n=1}^{\infty} \sum_{j=1}^n (C_j / j!) [\theta^{(n-j)} / (n-j)!].$$

Changing variables, i.e. $n' \equiv n-j$, one finally obtains

$$\begin{aligned} [T, a_k^+] &= \sum_{n'=0}^{\infty} \sum_{j=1}^{\infty} (C_j / j!) (\theta^{n'} / n'!) \\ &= \sum_{j=1}^{\infty} [C_j (k) / j!] T \end{aligned} \quad (\text{A.15.}),$$

where

$$C_j(k) \equiv [\theta, \dots j \text{ times } \dots [\theta, a_k^+] \dots] \quad (\text{A.16.}).$$

Introducing this result in (A.4.) one obtains

$$a_k^+ = a_k^+ + \sum_{j=1}^{\infty} (C_j / j!) \quad (\text{A.17.}).$$

Now, for the present expression for θ one finds

$$C_1(k) = -(\sigma_k^* + \sum_p \gamma_{p,k}^* a_p^*) + i \sum_p \xi_{p,k} a_p^+ \quad (\text{A.18.})$$

$$C_2(k) = i \sum_p \xi_{p,k} C_1(p) - \sum_p \gamma_{p,k}^* C_1^+(p) \quad (\text{A.19.}),$$

where (A.3.) has been employed. From (A.18., 19.) one finds that the C_j 's satisfy a cyclic property, namely

$$C_{2n+1}(k) = \chi_k^{2n} C_1(k); \quad n=0, 1, 2, \dots \quad (\text{A.20.})$$

$$C_{2n}(k) = X_k^{2n-2} C_2(k); n = 1, 2 \dots \quad (\text{A.21.})$$

where

$$X_k \equiv \sum_p |X_{p,k}|, \quad |X_{p,k}|^2 \equiv |\gamma_{p,k}|^2 - (\xi_{p,k})^2 \quad (\text{A.21'.})$$

Hence

$$\begin{aligned} \alpha_k^+ &= a_k^+ + \sum_{n=0}^{\infty} C_{2n+1}/2n+1)! + \\ &+ \sum_{n=1}^{\infty} C_{2n}/2n! = \\ &= a_k^+ + [C_1(k)/X_k] \sum_{n=0}^{\infty} X_k^{2n+1}/2n+1)! + \\ &+ [C_2(k)/X_k^2] \left[\sum_{n=0}^{\infty} (X_k^{2n}/2n!) - 1 \right] = \\ &= a_k^+ + [C_1(k)/X_k] \sinh(X_k) + \\ &+ [C_2(k)/X_k^2] [\cosh(X_k) - 1] \end{aligned} \quad (\text{A.22.})$$

From (A.18,19.) and making use of (A.3.) one finds

$$\begin{aligned} C_2(k) &= (\sigma_k \sum_t \gamma_{t,k} - i\sigma_k^* \sum_t \xi_{t,k}) + \\ &+ X_k^2 a_k^+ \end{aligned} \quad (\text{A.23.})$$

Using this result and (A.18.) in (A.22.) one finally obtains

$$\alpha_k^+ = \sum_q u_{k,q} a_q^+ - \sum_q v_{k,q}^* a_q + \rho_q^* \quad (\text{A.24.}),$$

where

$$u_{k,q} \equiv \cosh(X_k) \delta_{k,q} + i(\xi_{k,q}/X_k) \sinh(X_k) \quad (\text{A.25.})$$

$$v_{k,q} \equiv (\gamma_{k,q}/X_k) \sinh(X_k) \quad (\text{A.26.})$$

and

$$\begin{aligned} \rho_k^* &\equiv (\sigma_k \sum_t \gamma_{t,k}^* - i \sigma_k^* \sum_t \xi_{t,k}) \cdot \\ &\quad \cdot [\cosh(X_k) - 1]/X_k^2 - \\ &\quad - (\sigma_k^*/X_k) \sinh(X_k) \end{aligned} \quad (\text{A.27.}).$$

Similarly for α_k one finds

$$\alpha_k = \sum_q u_{k,q}^* a_q - \sum_q v_{k,q} a_q^+ + \rho_q \quad (\text{A.28.}).$$

It is noted that from definition it follows that

$$\begin{aligned} \sum_q (|u_{k,q}|^2 - |v_{k,q}|^2) &= \cosh^2(X_k) + \\ &+ [\sum_q (\xi_{k,q}^2 - |\gamma_{k,q}|^2)/X_k^2] \sinh^2(X_k) = \\ &= 1 \end{aligned} \quad (\text{A.29.}).$$

Now multiplying (A.24.) by $u_{q,k}$ and summing over k , (A.28.) by $v_{k,q}^*$ and summing over k and adding up these two one finds

$$a_q^+ = \sum_k u_{k,q}^+ a_k + \sum_k v_{k,q}^* \alpha_k + \phi_q^* \quad (\text{A.30.})$$

and similarly for a_q

$$a_q = \sum_k u_{k,q}^* \alpha_k + \sum_k v_{k,q} a_k^+ + \phi_q \quad (\text{A.31.}),$$

where

$$\phi_q^* = \sum_k u_{k,q} \rho_k^* + \sum_k v_{k,q}^* \rho_k \quad (\text{A.32.}).$$

Now, upon the adoption of definition (A.1.,2.) and the same definition for the variables $i = 1,2,3$ adopted before we obtain the following identity

$$\hat{p}_k = \sum_i p_k^i, \quad \hat{q}_k = \sum_i q_k^i \quad (\text{A.33.}).$$

Appendix B

$$\text{Proof of } \{H'_0, N'\} = 0 \quad (\text{B.1.})$$

The zeroth order hamiltonian and the number operator in the S.P.S. are given by

$$\hat{H}'_0 = \sum_{i,k} \epsilon_k p_k^i q_k^i + \sum_{i,j} \sum_{\bar{}} p^i p^j q^i q^j \quad (\text{B.2.})$$

and

$$\hat{N}' = \sum_{i,k} p_k^i q_k^i \quad (\text{B.3.}).$$

The kinetic energy contribution $\hat{K}' = \sum_{i,k} \epsilon_k p_k^i q_k^i$ can easily be shown to satisfy

$$\{\hat{K}', \hat{N}'\} = 0 \quad (\text{B.4.}),$$

i.e.

$$\begin{aligned} \{\hat{K}', \hat{N}'\} &= \sum_{\substack{k,k' \\ i,i'}} \epsilon_k [\{p_k^i q_k^i, p_{k'}^{i'} q_{k'}^{i'}\} + \\ &\quad + p_{k'}^{i'} \{p_k^i q_k^i, q_{k'}^{i'}\}] \\ &= \sum_{k,i} \epsilon_k (p_k^i q_k^i - p_k^i q_k^i) = 0. \end{aligned}$$

A similar proof for the interacting part is more elaborate, but straightforward.

$$\begin{aligned} (1/2) \sum_{p,\ell,q,k} v(\ell) \sum_{i,j,i'} \{p_{p+\ell}^i p_{q-\ell}^j q_q^i q_p^j, p_k^{i'} q_k^{i'}\} &= \\ = (1/2) \sum_{p,\ell,q,k} v(\ell) \sum_{i,j,i'} [\{p_{p+\ell}^i p_{q-\ell}^j q_q^i q_p^j, p_k^{i'}\} q_k^{i'} &+ \\ + p_k^{i'} \{p_{p+\ell}^i p_{q-\ell}^j q_q^i q_p^j, q_k^{i'}\}] \end{aligned}$$

$$\begin{aligned}
&= (1/2) \sum_{p, \ell, q, k} v(\ell) \sum_{i, j, i'} \left(\overbrace{p_{p+\ell}^i p_{q-\ell}^j q_q^i q_k^{i'}}^{\delta_{k, p+\ell} \delta_{j, i'}} + \right. \\
&\quad + \overbrace{p_{p+\ell}^i p_{q-\ell}^j q_p^j q_k^{i'}}^{\delta_{k, q} \delta_{i, i'}} - \\
&\quad - \overbrace{p_k^{i'} p_{p+\ell}^i q_q^i q_p^j}^{\delta_{k, q-\ell} \delta_{j, i'}} - \\
&\quad \left. - \overbrace{p_k^{i'} p_{q-\ell}^j q_q^i q_p^j}^{\delta_{k, p+\ell} \delta_{i, i'}} \right) \\
&= (1/2) \sum_{p, \ell, q} v(\ell) \sum_{i, j} \left(\overbrace{p_{p+\ell}^i p_{q-\ell}^j q_q^i q_p^j}^{\delta_{p, q} \delta_{\ell, -\ell}} + \right. \\
&\quad + \overbrace{p_{p+\ell}^i p_{q-\ell}^j q_p^j q_q^i}^{\delta_{p, q} \delta_{\ell, -\ell}} - \\
&\quad - \overbrace{p_{q-\ell}^j p_{p+\ell}^i q_q^i q_p^j}^{\delta_{p, q} \delta_{\ell, -\ell}} - \\
&\quad \left. - \overbrace{p_{p+\ell}^i p_{q-\ell}^j q_q^i q_p^j}^{\delta_{p, q} \delta_{\ell, -\ell}} \right)
\end{aligned}$$

Now, the first and last contributions cancel out because $\overbrace{p_{p+\ell}^i p_{q-\ell}^j q_q^i q_p^j}^{\delta_{p, q} \delta_{\ell, -\ell}} = \overbrace{p_{p+\ell}^i p_{q-\ell}^j q_p^j q_q^i}^{\delta_{p, q} \delta_{\ell, -\ell}}$. Changing variables for the third term, i.e. $p \leftrightarrow q$ $\ell \rightarrow -\ell$ one finds that the second and third terms also cancel out, thus (B.1.) is satisfied.

Appendix C

The zeroth order hamiltonian is diagonal in the L.C.S.R. In order to prove that H'_0 is diagonal in the L.C.S.R. the defining properties (A.3.) of the c-number fields will be exploited.

The kinetic energy contribution is clearly diagonal in the L.C.S.R., i.e.

$$\hat{K}' = \sum_k \epsilon_k [|\phi_k|^2 \sum_q (|u_{k,q}|^2 + |v_{k,q}|^2) \alpha_q^+ \alpha_q + \sum_q |v_{k,q}|^2] \quad (C.1.)$$

is manifestly diagonal.

The proof that the interaction term is also diagonal is more elaborate, but straightforward. The interaction term is

$$U' = \sum_{i,j} \sum p^i p^j q^i q^j \quad (C.2.).$$

The contribution $i = j = 3$ is a c-number, hence diagonal in the L.C.S.R.

The contributions $i = 3, j \neq i$ or $j = 3, i \neq j$ have the following form

$$\begin{aligned} \sum_{j=1}^2 \sum (\phi_{p+l}^* \phi_{p-q-l}^j q_q^j + \phi_{p+l}^* \phi_{q-l}^j p_p^j + \\ + \phi_{q-l}^* \phi_{p+l}^j q_q^j + \phi_{q-l}^* \phi_{q-l}^j p_p^j) \end{aligned} \quad (C.3.),$$

but from the defining properties of the pairing fields, ensuring momentum conservation, it follows that

$$p_p^j q_q^j = p_p^j q_p^j \delta_{p,q} \quad \text{for } j = 1, 2., \text{ i.e.}$$

$$\begin{aligned} p_p^1 q_q^1 &= \sum_{p',q'} u_{p,p'} u_{q,q'}^* \alpha_{p'}^+ \alpha_{q'} = \sum_{p',q'} |u_{p,p'}|^2 \alpha_{p'}^+ \alpha_{p'} \delta_{p',q'} \\ &= \sum_{p'} |u_{p,p'}|^2 \alpha_p^+ \alpha_p \end{aligned}$$

which is manifestly diagonal.

Now, for $i, j \neq 3$ one has contributions of the form

$$\begin{aligned}
& \sum_{a,b,c,d} (u_{p+l,a} u_{q-l,b} u_{q,c}^* u_{p,d}^* \alpha_a^+ \alpha_b^+ \alpha_c^+ \alpha_d^+ + \\
& + v_{p+l,a}^* v_{q-l,b}^* v_{q,c} v_{p,d} \alpha_a^+ \alpha_b^+ \alpha_c^+ \alpha_d^+ + \\
& + u_{p+l,a} v_{q-l,b}^* u_{q,c}^* v_{p,d} \alpha_a^+ \alpha_b^+ \alpha_c^+ \alpha_d^+ + \\
& + u_{p+l,a} v_{q-l,b}^* v_{q,c} u_{p,d}^* \alpha_a^+ \alpha_b^+ \alpha_c^+ \alpha_d^+ + \\
& + v_{p+l,a}^* u_{q-l,b} v_{q,c} u_{p,d}^* \alpha_a^+ \alpha_b^+ \alpha_c^+ \alpha_d^+ + \\
& + v_{p+l,a}^* u_{q-l,b}^* u_{q,c} v_{p,d} \alpha_a^+ \alpha_b^+ \alpha_c^+ \alpha_d^+) \quad (C.4.).
\end{aligned}$$

Now, due to the defining properties of the c-number fields the first contribution is non-zero if and only if $a = c$, $b = d$ or $a = d$, $b = c$ so this contribution is diagonal in the L.C.S.R. The second contribution is non-zero if and only if $a = c$, $b = d$ or $a = d$, $b = c$. Again, the second contribution is also diagonal. The third contribution is non-zero if and only if $a = b$, $c = d$ or $a = c$, $b = d$, thus this contribution is also manifestly diagonal. It can readily be tested that the remaining contributions are also diagonal. So H'_0 is diagonal in the L.C.S.R.

The fact that \hat{T}' is not diagonal in the L.C.S.R. can be readily tested by inspection, i.e.

$$\begin{aligned}
\hat{T}' &= \sum_{i,j} \sum' p_i^i p_j^j q^i q^j = \\
&= \sum_{a,b,c,d} [u_{p+l,a} u_{q-l,b} \alpha_a^+ \alpha_b^+ (\phi_q \phi_p + v_{q,c} v_{p,d} \alpha_c^+ \alpha_d^+) + \\
&+ v_{p+l,a}^* v_{q-l,b}^* \alpha_a \alpha_b (\phi_q \phi_p + u_{q,c}^* u_{p,d}^* \alpha_c^+ \alpha_d^+) + \\
&+ \phi_{p+l}^* \phi_{q-l}^* (u_{q,a}^* u_{p,b}^* \alpha_a \alpha_b + v_{q,a} v_{p,b} \alpha_a^+ \alpha_b^+)] \quad , \quad (C.5.),
\end{aligned}$$

which is manifestly non-diagonal.

REFERENCES

1. P. W. ANDERSON, Phys. Rev., 112, 1900 (1958).
2. P. W. ANDERSON, Rev. Mod. Phys., 38, 298 (1966).
3. H. ARAKI and E. J. WOODS, J. Math. Phys., 4, 637 (1963).
4. J. BARDEEN, L. N. COOPER and J. R. SCHRIEFFER, Phys. Rev., 108, 1175 (1957).
5. S. T. BELIAEV, Sov. Phys. J.E.T.P., 7, 289, 299 (1958).
6. N. N. BOGOLJUBOV, J. Phys. (U.S.S.R.), 11, 23 (1947).
7. N. N. BOGOLJUBOV, N. Cimento, 7, 784 (1958).
8. N. N. BOGOLJUBOV, Dubna Report, D-781 (1961) unpublished.
9. N. N. BOGOLJUBOV, Physica, 26, 51 (1960).
10. R. BONIFACIO and P. SCHWENDIMANN, Phys. Rev., A4, 302 (1971).
11. G. V. BROW and M. H. COOPERSMITH, Phys. Rev., 178, 327 (1979).
12. K. A. BRUECKER and K. SAWADA, Phys. Rev., 106, 1117, 1128 (1957).
13. P. CARRUTHERS and N. M. NIETO, Am. J. Phys., 33, 537 (1965).
14. R. C. CASELLA, J. Phys. Chem. Solids, 24, 19 (1963).
15. A. CASHER and M. REVZEN, Am. J. Phys., 35, 1154 (1967).
16. J. CHELA-FLORES, J. Low Temp. Phys., 21, 307 (1975),
28, 213 (1977).
17. J. CHELA-FLORES, Phys. Rev. D, 18, 2632 (1978).
J. CHELA-FLORES and F. de LISA, N. Cimento A, 58, 67 (1980).
18. A. CONIGLIO and M. MARINARO, N. Cimento B, 48, 262 (1967),
48, 262 (1967).
A. CONIGLIO, F. MANCINI and M. MANTURI, N. Cimento B, 63, 227 (1969).
19. R. A. COWLEY and A. D. B. WOODS, Phys. Rev. Lett., 21, 787 (1968).
Rep. Prog. Phys., 36, 1135 (1973).
20. F. W. CUMMINGS and J. R. JOHNSTON, Phys. Rev., 151, 105 (1966),
164, 270(E) (1967).
21. (a) F. W. CUMMINGS, G. J. HYLAND and G. ROWLANDS, Phys. Kond. Matter,
12, 90 (1970).

36. P. C. HOENBERG, Ph.D. Thesis (unpublished).
37. P. C. HOENBERG, Phys. Rev., 158, 383 (1967).
38. P. C. HOENBERG and P. C. MARTIN, Ann. Phys., 34, 291 (1965).
39. K. HUANG and C. N. YANG, Phys. Rev., 105, 767 (1957).
K. HUANG, T. D. LEE and C. N. YANG, Phys. Rev., 106, 1135 (1957).
40. N. M. HUGENHOLTZ and D. PINES, Phys. Rev., 116, 489 (1959).
41. G. J. HYLAND and G. ROWLANDS, Phys. Lett. 30A, 222 (1969); 33A, 197
(1970); 36A, 233 (1971); 48A, 255 (1974),
 Phys. Kond. Matter, 12, 90 (1970),
 Physica, 54, 542 (1971),
 J. Low. Temp. Phys., 7, 271 (1972).
42. M. ICHIYANAGI, J. Phys. Soc. Japan, 48, 793 (1980).
43. F. IWAMOTO, Prog. Theor. Phys., 44, 1121 (1970).
44. H. W. JACKSON, Phys. Rev., 10A, 278 (1974).
45. J. R. JOHNSTON, Am. J. Phys., 38, 516 (1970).
46. D. H. KOBE, Ann. Phys., 47, 15 (1968).
D. H. KOBE and G. GOBLE, Phys. Rev., 10A, 851 (1974).
47. (a) L. D. LANDAU, J. Phys. (U.S.S.R.), 5, 71 (1941),
 (b) 8, 1 (1944), 11, 91 (1947),
 Phys. Rev., 75, 884 (1949).
48. L. D. LANDAU and E. M. LIFSHITZ, "Statistical Physics" Third Ed.
Pergamon Press (1980), p.161.
49. J. S. LANGER, Phys. Rev., 167, 183 (1968).
50. L. LAPLAE, R. N. SEN and H. UMEZAWA, Progr. Theor. Phys., Suppl.
(extra number), 637 (1965).
51. M. LUBAN, Phys. Rev., 128, 965 (1962).
52. F. LONDON, In "Superfluids" (London 1954) Vol. II.
53. R. D. MATTUCK and B. JOHANSSON, Advan. Phys., 17, 509 (1968).
54. H. A. MOOK, R. SCHERN and M. K. WILKINSON, Phys. Rev., 8A, 2268 (1972)
H. A. MOOK, Phys. Rev. Lett., 32, 1167 (1974).
55. R. H. PARMENTER, Phys. Rev., 170, 194 (1968).

56. W. E. PARRY, *Physica*, 27, 1045 (1961).
 W. E. PARRY and D. Ter HAAR, *Ann. Phys.*, 19, 496 (1962).
 W. E. PARRY and R. E. TURNER, *Phys. Rev.*, 128, 929 (1962).
57. O. PENROSE, *Phil. Mag.*, 42, 1373 (1951).
 O. PENROSE and L. ONSAGER, *Phys. Rev.*, 104, 576 (1956).
58. L. P. PITAEVSKII, *Zh. Eksp. Teor. Fiz.*, 40, 646 (1961). English
 Transl. *Sov. Phys. JETP*, 13, 451 (1961).
59. A. K. RAJAGOPAL and I. RAMARAO, *Phys. Rev.*, 16B, 3148 (1977).
60. H. STOLZ, *Physica*, 86A, 111 (1977).
 See also:
 P. DORRE, H. HAUG and D. B. TRAN THOAI,
 K. WEISS and H. HAUG,
61. H. SUHL and N. R. WERTHAMER, *Phys. Rev.*, 122, 359 (1961); 125, 1402 (1962).
62. F. TAKANO, *Phys. Rev.*, 123, 699 (1961).
63. S. TAKENO, *J. Phys. Soc. Japan*, 48, 1075 (1980).
64. A. W. B. TAYLOR, *J. Phys.*, 21C, 52 (1970).
65. L. A. TURSKI, *Physica (utr.)*, 57, 432 (1972).
66. H. UMEZAWA, *Acta Physica Hung.*, 19, 9 (1965),
 N. Cimento, 40A, 450 (1965).
67. J. G. VALATIN, *N. Cimento*, 7, 843 (1958).
68. J. G. VALATIN and BUTLER, *N. Cimento*, 10, 37 (1958).
69. H. WAGNER, *Z. Physik*, 195, 273 (1966).
70. G. WENTZEL, *Phys. Rev.*, 108, 1593 (1957); 120, 1572 (1960).
71. C. N. YANG, *Rev. Mod. Phys.*, 34, 694 (1962).
72. C. N. YANG and R. L. MILLS, *Phys. Rev.*, 96, 191 (1954).
73. D. N. ZUBAREV, *Sov. Phys. Uspekhi*, 3, 320 (1960).

Compendia References.

For a comprehensive list of references on microscopic theories of superfluidity the following compendia are available.

74. "Statistical physics, phase transitions and superfluidity".
 Brandeis Univ. (1966), Chretien, Gross and Deser (Eds.), Gordon
 and Breach Sc. Pub. N.Y., Vol. I, II.

75. Proceedings of the XIIth, XIIIth (Vol I) and XIVth (Vol I) International Conference on low temperature physics. Editors E. Kanda (Academic press of Japan (1971)); K. D. Timmerhaus (Plenum Press, N.Y. (1974)) and M. Krusius (North Holland, Amsterdam, Oxford (1975)), respectively.
76. J. WILKS, "The properties of Liquid and Solid Helium", W. Marshall and D. H. Wilkinson (Eds.), Clarendon Press, Oxford (1967).
77. "Superconductivity", R. D. Parks (Ed.), Marcel Dekker, Inc., N.Y. (1969) Vols. I, II.
78. G. RICKAYZEN, "Theory of Superconductivity". Interscience Monographs and Texts in Physics and Astronomy, Vol. XIV, R. E. Marshak Ed., John Wiley & Sons. (1965).
79. D. PINES and P. NOZIERES, "The Theory of Quantum Liquids", Vol. I, Benjamin Inc. (1966).
80. N. N. BOGOLJUBOV, V. V. TOMACHEV and D. V. SHIRKOV, "A new method in the theory of superconductivity", consultants Bureau, Inc. N.Y. (1959).
81. P. G. DE GENNES, "Superconductivity of metals and alloys", D. Pines (ed.), Benjamin, Inc., N.Y. (1966).
82. R. BROUT, In "Phase transitions", Benjamin Press (N.Y.) (1965).
83. L. R. WALKER, In "Magnetism", Rado and Suhl (Eds.), Vol. I, Chapter 8, Academic Press (1963).
84. T. HOLSTEIN and H. PRIMAKOFF, Phys. Rev., 58, 1098 (1940).