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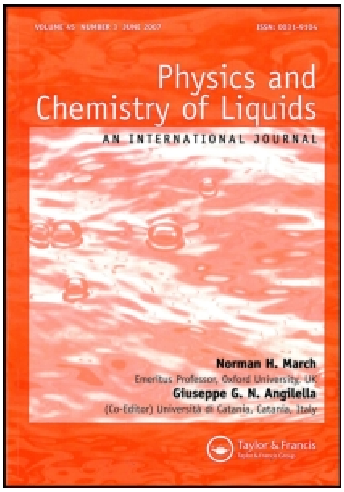

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The Nature of Condensation in Momentum Space for an Interacting Bose Liquid

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THE NATURE OF CONDENSATION IN MOMENTUM SPACE FOR AN INTERACTING BOSE LIQUID

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Earlier it has been shown that the properties of superfluid helium four have an intimate connection with a non-vanishing coherent pairing as well as the generalized Bose Einstein condensation. Here, the nature of condensation for an interacting Bose system is re-examined. It is shown that, under conditions of constant temperature and pressure, minimization of the Gibbs free energy leads to a generalized condensation of the type first proposed by Girardeau. Extrapolation of these ideas to quasiparticle models of interacting Bose systems such as helium-II leads to the conclusion that the condensation in momentum space should also be regarded as generalized in the same sense. A bonus of this approach is the disappearance of macroscopic fluctuations in the density encountered in the usual theory of the condensed ideal Bose system.

KEY WORDS: Bose condensation, Superfluid Helium four, density fluctuations.

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I INTRODUCTION

Experimental and theoretical studies[1] of the last few years on superfluid helium four have stimulated substantial new interests in the structure and properties of this quantum fluid. Liquid helium four undergoes a phase transition at $T_\lambda = 2.18$ K accompanied by a characteristic change[2] in physical properties. In spite of a wealth[2] of experimental results a complete theory of superfluid Bose system is still missing. Indeed, little is known rigorously and approximations are introduced depending sometimes more on mathematical convenience rather than physical insight. For instance, theoretical and experimental estimates of the condensate fraction (the fraction of atoms condensed into the zero-momentum state) of liquid helium four depend strongly upon the methods used. The predictions[3] range between fifty and zero percentage. Even the presently trusted theoretical[4] results are in clear disagreement with experiments[5].

The purpose of this paper is to re-examine the nature of condensation in momentum space for interacting Bose systems and attention has been drawn to an alternative kind of condensation of a type first thought of by Girardeau[6] and which was termed by him a generalized condensation.

The paper proceeds as follows. In Section II below, the nature of the ideal Bose–Einstein condensation is considered and the density fluctuations due to the presence of the condensate contribution are shown to be large. Section III deals with the generalized Bose–Einstein condensation applied to the interacting Bose system and it is shown that within the model the density fluctuations are vanishingly small. Section IV is concerned with the generalized condensation in the context of the pair theory of Bose superfluids, where it was found that the excitation energy becomes manifestly gapless and initially linear in **k**. Finally Section V concluded with a summary and brief discussion.

II THE IDEAL BOSE–EINSTEIN CONDENSATION (BEC)

The pioneering work on the microscopic nature of particle statistics of Bose[7] and its extension by Einstein[8] revealed that a non-interacting Bose system undergoes a phase transition at a low enough temperature in which a single particle zero momentum state ($\mathbf{k} = 0$) will be macroscopically occupied. This phenomenon is called the simple Bose–Einstein condensation (BEC). Subsequently, London[9] pointed out that there are similarities between the condensation in momentum space which occurs in the ideal boson gas and the λ-transition in liquid helium four. Although the belief seems rather widespread that the appearance of a simple BEC is of crucial physical significance in superfluid phase, this belief is by no means universal. Little is known experimentally about the connection between Bose-Einstein condensation and superfluidity. Landau[10] and Feynman[11] never invoked the concept of the BEC and the striking success of the BCS[12] model to describe the superconducting phase of charged fermions encouraged others[13] to propose an analogous model for Bose systems.

Hohenberg and Platzman[14] have suggested that the inelastic scattering of neutrons at large momentum transfer can be used to measure directly the momentum distribution of individual atoms, i.e.

$$n_{\mathbf{k}} = \langle a_{\mathbf{k}}^{+} a_{\mathbf{k}} \rangle, \tag{2.1}$$

(where $a_{\mathbf{k}}^{+}(a_{\mathbf{k}})$ is the creation (destruction) operator and the bracket denotes the thermal average of operators in the grand canonical ensemble of statistical mechanics) as a function of **k** in superfluid helium four and thereby observe directly the simple BEC which could appear as a sharp peak at the maximum of the line shape for the van Hove[15] dynamic liquid structure factor, $S(\mathbf{q}, \omega)$, at large momentum value. Based on this assumption, later on, experiments[5] were performed to observe directly if a condensate fraction n_0/N exists in superfluid helium four. Unfortunately, because of the experimental complications one cannot measure $S(\mathbf{q}, \omega)$ for sufficiently large $\mathbf{q}$ (momentum transfer) so as to expect the condensate peak not be broadened by final state effects. In spite of the instrumental broadening and other effects, the experimental data predicted[5] a few percentage of the simple BEC. The experimental data have been re-analyzed and some[4] argued in detail that the numerical inaccuracies exist in data and results are consistent with the complete absence of any simple BEC but others[16] concluded that simple condensate most probably exists in helium-II in spite

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of errors in data. There has been a continuing effort[1] both experimentally and theoretically to extract the value of condensate fraction in superfluid helium-II but a direct demonstration is yet to be seen. In this respect further experimental work on $S(\mathbf{q}, \omega)$ for high $\mathbf{q}$ values seems highly desirable.

In the usual theory of the ideal Bose gas one argues[2] that below a certain temperature, T_c, defined by

$$T_c = \frac{2\pi h^2}{mk_B}(\rho/\xi(3/2))^{2/3} \tag{2.2}$$

(here $\rho = N/V$ is the number density, while $\xi(x)$ is the Riemann zeta function), one needs to look at the $\mathbf{k} = 0$ term carefully so as to realize the proper condensate contribution, i.e. there will exist a macroscopic occupation of the $\mathbf{k} = 0$ level and one needs to isolate it carefully.

The number expectation value is given by

$$N = \sum_{\mathbf{k}} n_{\mathbf{k}} = \sum_{\mathbf{k}} 1/[\exp(\beta\varepsilon_{\mathbf{k}}) - 1], \tag{2.3}$$

where $\varepsilon_{\mathbf{k}} = (h^2k^2/2m - \mu)$.

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Since the Bose gas is spatially isotropic, one may replace (the factor depending upon vector) in the summation over $\mathbf{k}$ in Eq.(2.3) by its angular average over all orientations of $\mathbf{k}$. Since all factors in the summands depend on $|\mathbf{k}|$ only.

If $n_{\mathbf{k}}$ is to be a continuous function of $\mathbf{k}$ and the summation may be converted to an integration, i.e.

$$V^{-1}\sum_{\mathbf{k}} = (2\pi^2)^{-1}\int_0^{\infty} |\mathbf{k}|^2\, d|\mathbf{k}|. \tag{2.4}$$

For the ideal Bose gas because of the simple BEC, one cannot use Eq. (2.4) as it will miss out the $|\mathbf{k}| = 0$ contribution. However, one treats the Bose system properly, if one writes

$$N = \sum{}' 1/[\exp(\beta\varepsilon_{\mathbf{k}}) - 1] \tag{2.5}$$

and the prime on the above summation signifies the exclusion of the $\mathbf{k} = 0$ summand from the sum, i.e. one adds the condensate contribution as

$$n_{|\mathbf{k}|} = 1/[\exp(\beta\varepsilon_{|\mathbf{k}|}) - 1] + n_0\frac{2\pi^2}{|\mathbf{k}|^2}\delta(|\mathbf{k}^-|) \tag{2.6}$$

and then uses Eq. (2.4).

If n_0 is the average number of atoms in the ground state than for $T \leq T_c$, the temperature dependence of the condensate[2,9] is given by

$$n_0 = N[1 - (T/T_c)^{3/2}], \tag{2.7}$$

i.e. n_0 is of order N whereas for $T > T_c$, n_0 is only of $0(1)$. Thus from Eq.(2.7) one finds that the ideal Bose system undergoes 100% condensation at the absolute zero temperature. Many properties including the one just mentioned for ideal Bose gases are not seen in superfluid helium four. For $T \leq T_c$, the chemical potential, μ, is fixed for the boson case in such a way that $\varepsilon_0 \sim 0(N^{-1/2})$ becomes macroscopically small[17]. For this to be so one requires that the chemical potential to be of order N^{-1}, i.e.

$$n_0 = 1/[\exp(-\beta\mu) - 1] \approx 1/\beta\mu, \tag{2.8}$$

i.e.

$$\mu = -1/\beta n_0. \tag{2.9}$$

The number n_0 is then obtained by subtracting the total number of bosons in levels $\mathbf{k} > 0$ from the total number, N, of bosons present.

If this is the type of condensation that could exist in an ideal Bose system then it is trivial to show that the fluctuation in the density

$$\frac{\langle(\rho - \langle\rho\rangle)^2\rangle}{\langle\rho\rangle^2} = \frac{\langle(N - \langle N\rangle)^2\rangle}{\langle N\rangle^2} \tag{2.10}$$

will be of $0(1)$. This is a consequence of the condensate contribution to $\langle(N - \langle N\rangle)^2\rangle$, i.e.

$$\langle(n_0 - \langle n_0\rangle)^2\rangle = \langle n_0^2\rangle - \langle n_0\rangle^2 = \langle n_0\rangle^2 + \langle n_0\rangle. \tag{2.11}$$

Since the application of the elevated temperature form of Wick's theorem shows that

$$\langle a_0^+ a_0 a_0^+ a_0\rangle = 2\langle a_0^+ a_0\rangle^2 + \langle a_0^+ a_0\rangle \tag{2.12}$$

for an ideal Bose system.

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III THE GENERALIZED CONDENSATION

In earlier work[18], the "super" properties of helium-II have been connected with the Hartree-Fock-Gor'kov phase[13] in addition to the possibility of self-consistent existence of generalized condensate contribution. If one takes the condensate contribution properly into account, it can easily be shown that both the coherence pairing and the generalized Bose-Einstein condensation will vanish at the same critical temperature, T_λ (for details see Ref. 18).

Frequently, in models of interacting Bose systems one works with Landau's quasiparticle approximation[19], thus ending up with boson quasiparticles of well-defined energies (but of course, a novel dispersion spectrum[20]). Such models often display a simple BEC which come about in a precisely analogous fashion[2] to the case of the ideal gas. But these models used an improper treatment to replace the real potential by a repulsive interaction and reproduced either Bogoliubov's spectrum[21] or a gap in the energy spectrum which has proved to be unphysical[13].

It has long been known[22] that the scattering length of the helium four interparticle potential is negative. Girardeau[6] has shown that for such a situation the lowest energy state is not the one in which the zero-momentum state contains a macroscopic occupation of particles, i.e. the simple BEC is not possible. He argues that when the interparticle interactions are included properly a small volume of momentum space (which may contain a few states near the ground state, i.e. $\mathbf{k} \leq \mathbf{k}_c$ rather than a single momentum state $\mathbf{k} = 0$) is occupied predominantly. The work[23] of Sawada and Vasudevan and others support the above idea of generalized or smeared condensation.

Here the argument pertains to systems at constant temperature and pressure (and particle number) as these are the conditions most commonly met within the laboratory. General and well-known thermodynamic arguments dictate that the Gibbs free energy

$$G = \bar{E} - TS + pV \tag{3.1}$$

will be a minimum for the equilibrium system. Assuming the system scales in the normal way, one deduces that

$$G = \mu N \tag{3.2}$$

so that the equilibrium condition of minimum G can be thought of as minimizing the chemical potential, μ (subject of course to constant temperature, pressure and particle number).

Returning to the case of generalized condensation, one now postulates[6] that because of the interaction in the condensed phase, the chemical potential is of order $N^{-\alpha}$ where $0 < \alpha \leq \frac{2}{3}$. Hence the states up to $\mathbf{k}_c$ (see Ref. 18) will have a population of order $N^{2/3}$ only, which is large yet amounts to only an infinitesimal fraction of N. As in the case of the ideal BEC the contributions of the higher states decrease monotonically with increasing values of $\mathbf{k}$. Thus

$$\mu = -\gamma/N^{\alpha} \tag{3.3}$$

where γ is a constant. Then we have (cf. (2.9))

$$\sum_{\mathbf{k}<\mathbf{k}_c} n_{\mathbf{k}} = -1/\beta\mu = N^{\alpha}/(\beta\gamma), \tag{3.4}$$

i.e. the $\mathbf{k} = 0$ level does not contain a macroscopic number of particles as in the simple condensation. Levels adjacent to the $\mathbf{k} = 0$ state will have $\varepsilon_{\mathbf{k}<\mathbf{k}_c} \sim N^{-2/3}$, so that for these levels

$$\sum_{\mathbf{k}<\mathbf{k}_c} n_{\mathbf{k}} = N_0 \approx 1/[\beta(N^{-2/3} + \gamma N^{-\alpha})] \tag{3.5}$$

which will be of the same order of magnitude as n_0 as long as $0 < \alpha \leq \frac{2}{3}$. Thus one has now conceived of a possibility of accommodating the same number of particles as in the normal treatment of the simple BEC, but the chemical potential will now be much lower than for simple condensation (i.e. $\gamma N^{-\alpha} \ll 0(N^{-1})$). Consequently, one can conclude that the generalized BEC is favoured as opposed to simple condensation in the interacting Bose system from free energy considerations. Furthermore, it is trivial to show, by simple application of Wick's theorem, that the density fluctuations in this model of the condensed phase of an interacting Bose system will be $0(N^{\alpha-1})$, i.e. vanishingly small for large systems.

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IV GENERALIZED CONDENSATION AND THE PAIR MODEL OF BOSE SUPERFLUIDS

The pair theory of the Bose superfluid as detailed in Ref. 13 is a generalization of the usual Hartree-Fock description of the normal phase to include in addition the possibility of the self-consistent existence of a coherence pairing.

The integral equations for Bose pair theory were developed in Ref. 13 and from the work of the author[18], one realizes that such models display a generalized BEC as this minimises the Gibbs free energy. (For a fuller discussion, the reader is referred to Rashid[18].)

Isolating the contribution from the smeared condensate (states $\mathbf{k} < \mathbf{k}_c$) using the relationship

$$N_0 = \sum_{\mathbf{k}<\mathbf{k}_c} n_{\mathbf{k}} = \sum_{\mathbf{k}<\mathbf{k}_c} \frac{\tilde{\varepsilon}_{\mathbf{k}}}{2E_{\mathbf{k}}} \tag{4.1}$$

The total number of particles, N, self-consistent self-energy, ξ_k, coherence energy, Δ_k, are obtained (for details see Ref. 13) from the solutions of coupled non-linear integral equations, viz.

$$N = \sum_{\mathbf{k}} n_{\mathbf{k}} = N_0 + \sum_{\mathbf{k}}{}' \left[\frac{\tilde{\varepsilon}_{\mathbf{k}}}{2E_{\mathbf{k}}} \coth\left(\frac{\beta E_{\mathbf{k}}}{2}\right) - \frac{1}{2}\right] \tag{4.2}$$

$$\xi_{\mathbf{k}} = \xi_0 + \sum_{\mathbf{k}'}{}' V_{\mathbf{k}-\mathbf{k}'} n_{\mathbf{k}'}; \; V_{\mathbf{k}} N_0 = \xi_0 \tag{4.3}$$

$$\Delta_{\mathbf{k}} = -V_{\mathbf{k}} N_0 \operatorname{sign}(\Delta_0) - \sum_{\mathbf{k}'}{}' V_{\mathbf{k}-\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \coth\left(\frac{\beta E_{\mathbf{k}'}}{2}\right), \tag{4.4}$$

where

$$\tilde{\varepsilon}_{\mathbf{k}} = \frac{k^2}{2m} + \xi_{\mathbf{k}} - \xi_0 - |\Delta_0| \tag{4.5}$$

and the excitation energy

$$E_{\mathbf{k}} = \sqrt{\left(\frac{k^2}{2m} + \xi_{\mathbf{k}} - \xi_0 - |\Delta_0|\right)^2 - |\Delta_{\mathbf{k}}|^2} \tag{4.6}$$

The prime on the summation symbols denote the exclusion of the $\mathbf{k}$ up to $\mathbf{k}_c$ vectors summand from the sum. The terms N_0, ξ_0, ε_0 $(= NV_0 + \xi_0 - \mu = +|\Delta_0|)$ are due to any condensate contribution within the region $\mathbf{k} < \mathbf{k}_c$. From Eq. (4.6) one can see that the excitation spectrum is manifestly gapless and initially linear in $\mathbf{k}$ since one can see[13] $\xi_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$ are even functions of $\mathbf{k}$. Also $V_{\mathbf{k}}$ in the above is to be understood as a pseudopotential and not as the bare potential.

It has been demonstrated[13] earlier that a system interacting via a repulsive potential has no coherence and as such will not be superfluid in pair model. On the other hand, if the free energy is minimized by having a non-vanishing pair coherence $\Delta_{\mathbf{k}}$, then Eq. (4.4) will have a non-trivial solution.

If now a solution to equations of the model is considered with all $\Delta_{\mathbf{k}} = 0$ then

$$E_{\mathbf{k}} = \tilde{\varepsilon}_k \tag{4.7}$$

and

$$n_{\mathbf{k}} = 1/[\exp(\beta\tilde{\varepsilon}_{\mathbf{k}}) - 1] \tag{4.8}$$

This is the Bose analogue of a Hartree–Fock (Fermi) gas. At a certain critical temperature, T_c (see Eq. (2.2)) the BEC (simple or generalized depends upon the form of the interaction) will start in the system and one has the following possibilities:

(i) The system lacks the necessary properties to afford a non-vanishing solution to Eq. (4.4) even at $T = 0$ K. The system will not be superfluid in the present model even though it contains the simple or generalized BEC.

(ii) The system has realistic potential, i.e. has repulsive as well as a sufficiently attractive interaction for a non-trivial solution to Eq. (4.4) to exist at low enough temperatures. It is also conceivable that the pair interactions could be such that the system will allow a non-trivial solution to Eq. (4.4) but that all the particles will be depleted from the $\mathbf{k} = 0$ or $\mathbf{k} < \mathbf{k}_c$. This system will still be superfluid in the pair model even though the momentum condensation is absent.

However, in the present model, one is concerned with the case when both the coherence and the generalized condensation simultaneously occur. Moreover, it has been shown[13,18] that as long as the pair coherence is present in the system, the experimental trends are reproduced by the present theory.

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V SUMMARY AND CONCLUSIONS

Here we have mainly discussed the problem of the Bose–Einstein condensation in interacting Bose systems. For this purpose Girardeau's ansatz[6] has been used and as a result we gain some insights into the nature of momentum condensation in superfluid helium four.

For an interacting Bose system, the lifetime effect of quasiparticles is important and clearly, therefore, the condensation in these models can also be thought of as being generalized in the sense of Girardeau as this minimizes the Gibbs free energy. This means that the particles with lowest energy are smeared into a small volume in momentum space around $\mathbf{k} = 0$. The fluctuations in such models also becomes macroscopically small thus removing a major point of criticism of such models. Finally, one should emphasize that this is independent of the nature of the interaction assumed in the quasiparticle model.

The problem of what actually happens in a strongly interacting Bose system is, of course, much more complicated. Going beyond the quasiparticle approximations, one expects that the spectral functions of the single particle propagators be broadened to a width which depends on the interaction strength. Then it is clear that no single k-vector can be preferred energy-wise over the neighbours as the single particle energies are not well defined. The condensation peak (thought of as a plot of $n_{\mathbf{k}}$ against $\mathbf{k}$)

would be still further broadened by the scattering mechanisms until its width is of order of the interaction strength, i.e. $0(1)$. In this case, of course, the fluctuations may be expected to be $0(N^{-1})$. The present calculations and experimental data[1], however, indicate that the problem of momentum condensation in superfluid helium four at least merits further investigation.

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