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Bose-Einstein condensation in an interacting Bose liquid

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An exact expression for the single-particle reduced density matrix of a translationally invariant system of bosons is obtained, as an average of a functional of the density and current operators. An approximation scheme, based on small fluctuations in density and current, is used in its lowest order, to approximate the single-particle reduced density matrix and the condensate density by a functional of the structure factor, which is a measurable quantity. This is done for the ground state and for finite temperatures. The resulting expressions for the condensate density are discussed. For the ideal gas the result is correct below the condensation temperature. For the case of an interacting liquid, Bose-Einstein condensation exists, in the ground states for two- and three-dimensional systems, and for finite temperatures it does exist only in three dimensions. The present experimental knowledge of the structure factor enables only a crude estimate of the condensed fraction which is found to be 0.1–0.2.

I. INTRODUCTION

The idea that the λ phase transition occurring in liquid He^4 at the λ temperature is a Bose-Einstein condensation modified by the interaction between particles, was first suggested by London.[1] The condensate density had been calculated, and it played a dominant role in certain approximations that stress the single-particle aspect.[3-5] These approximations seem, however, to be unsatisfactory at liquid-He densities. On the other hand, in other approximations that give a fairly good agreement with experiment for the ground-state and excitation spectrum of the system, such as the Feynman,[6] the Pityevski,[7] and the Feynman-Cohen[8] theories, the condensate does not play any role at all, and no way of calculating it is suggested. The reason for this is that the above theories stress the idea of collective excitations, while the condensate is easily expressible only in single-particle language.

The aim of this paper is twofold: to express the single-particle reduced density matrix, and hence the condensate density, in terms of collective coordinates, and to express the above quantities in terms of measurable quantities. In Sec. II, a formal identity is derived, expressing the single-particle reduced density matrix as an average of a function of the density and current operators. An approximation scheme, based on the idea of expanding the physical quantities of interest in terms of density and current fluctuations, and which was previously used in deriving the excitation spectrum,[9] is used in Sec. III in its lowest order to obtain an approximation of the ground-state single-particle reduced density matrix and condensate density as functionals of the ground-state structure factor. In Sec. IV, the same is done for finite but low temperatures, and the results are discussed.

II. FORMAL IDENTITY

It is known that all the information about occupation numbers of the single-particle states can be derived from the single-particle reduced density matrix

$$f(\vec{r}) = \langle \psi^\dagger(\vec{r}')\psi(\vec{r}'+\vec{r})\rangle , \tag{1}$$

where $\langle\cdots\rangle$ denotes either ground-state or thermal average, according to whether we are interested in ground-state or finite-temperature properties. Next, we express $f(\vec{r})$ in terms of current and density operators in order to be able to use some convenient approximations derived for the operators and for the ground state.[9-11] For simplicity we choose $\vec{r} = (x, 0, 0)$,[12] so that

$$\langle \psi^\dagger(\vec{r}')\psi(\vec{r}'+\vec{r})\rangle = \left\langle \sum_{n=0}^{\infty} \frac{x^n}{n!} \psi^\dagger(\vec{r}') \frac{\partial^n}{\partial x'^n} \psi(\vec{r}') \right\rangle . \tag{2}$$

We define

$$\Lambda_n(\vec{r}') = \psi^\dagger(\vec{r}') \frac{\partial^n}{\partial x'^n} \psi(\vec{r}') . \tag{3}$$

Differentiation of Eq. (3) with respect to x' gives

$$\frac{\partial}{\partial x'} \Lambda_n(\vec{r}') = \frac{\partial}{\partial x'} \psi^\dagger(\vec{r}') \frac{\partial^n}{\partial x'^n} \psi(\vec{r}') + \psi^\dagger(\vec{r}') \frac{\partial^{n+1}}{\partial x'^{n+1}} \psi(\vec{r}') . \tag{4}$$

Rearranging this, and using the relation $\psi(\vec{r})[1/\rho(\vec{r})]\psi^\dagger(\vec{r}) = I$,[13] where $\rho(\vec{r})$ is the density operator, one obtains

$$\Lambda_{n+1}(\vec{r}') = \left[\frac{\partial}{\partial x'} - \left(\frac{\partial}{\partial x'} \psi^\dagger(\vec{r}')\right)\psi(\vec{r}') \frac{1}{\rho(\vec{r}')}\right] \Lambda_n(\vec{r}') . \tag{5}$$

Using the relation

$$\Lambda_0(\vec{r}') = \rho(\vec{r}'), \tag{6}$$

one obtains

$$f(\vec{r}) = \left\langle \exp\left\{ x \left[\frac{\partial}{\partial x'} - \left(\frac{\partial}{\partial x'} \psi^\dagger(\vec{r}') \right) \times \psi(\vec{r}') \frac{1}{\rho(\vec{r}')} \right] \right\} \rho(\vec{r}') \right\rangle. \tag{7}$$

Using the notation of Ref. 9, one defines

$$\Gamma^\dagger(\vec{r}) = J(\vec{r}) + \tfrac{1}{2} i \nabla \rho(\vec{r}), \tag{8}$$

where $J(\vec{r})$ is the current-density operator. Equation (7) thus becomes

$$f(\vec{r}) = \left\langle \exp\left[x \left(\frac{\partial}{\partial x'} + i \Gamma^{x\dagger}(\vec{r}') \frac{1}{\rho(\vec{r}')} \right) \right] \rho(\vec{r}') \right\rangle, \tag{9}$$

where $\Gamma^{x\dagger}(\vec{r}')$ denotes the x component of the vector $\Gamma^\dagger(\vec{r}')$. Equation (9) represents $f(\vec{r})$ exactly in terms of an average of a function of current and density operators.

III. GROUND-STATE APPROXIMATION

We now employ an approximation scheme that was previously used to obtain the excitation spectrum of an interacting Bose liquid by approximating $f(\vec{r})$ by a functional of the structure factor. In order to clarify matters, we briefly discuss the first step of this scheme. The system under consideration is a system of N bosons interacting via a two-body potential and contained in a huge box of volume V and periodic boundary conditions. The operators

$$\Gamma_q^\dagger = \frac{1}{N^{1/2}} \int \Gamma^\dagger(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} d^3r \tag{10}$$

and

$$\rho_q = \frac{1}{N^{1/2}} \int \rho(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} d^3r \tag{11}$$

form a complete set of operators in the sense that any operator that commutes with all of them must be a c number.

Consider the algebra obeyed by these operators:

$$[\rho_q, \rho_p] = 0, \tag{12}$$

$$[\Gamma_q^{i\dagger}, \rho_p] = -N^{-1/2} p_i \rho_{q+p}, \tag{13}$$

$$[\Gamma_q^{i\dagger}, \Gamma_p^{j\dagger}] = N^{-1/2}(q_j \Gamma_{q+p}^{i\dagger} - p_i \Gamma_{q+p}^{j\dagger}), \tag{14}$$

where the indices i and j denote Cartesian components of a vector. Consider also the relation

$$\Gamma_q = \Gamma_{-q}^\dagger - q\rho_{-q}. \tag{15}$$

The assumption that the fluctuations of density and current are small enables one to replace the commutation relations in Eqs. (12)–(14) by approximate ones,

$$[\rho_q, \rho_p] = 0, \tag{12'}$$

$$[\Gamma_q^{i\dagger}, \rho_p] = -P_i \delta_{q,-p}, \tag{13'}$$

$$[\Gamma_q^{i\dagger}, \Gamma_p^{j\dagger}] = 0. \tag{14'}$$

Hence, in this approximation one can write for $q \neq 0$

$$\Gamma_q^{i\dagger} = q_i \eta_q^\dagger, \tag{16}$$

$$\rho_q = -(\eta_q^\dagger + \eta_{-q}), \tag{17}$$

where the η's obey Bose commutation relations

$$[\eta_q, \eta_p] = [\eta_q^\dagger, \eta_p^\dagger] = 0, \quad [\eta_q, \eta_p^\dagger] = \delta_{qp}. \tag{18}$$

Obviously, the η and $\eta^\dagger$ are not to be confused with particle destruction and creation operators. If the Hamiltonian is expanded, in the same spirit, to second order in the density fluctuations, and Eqs. (16) and (17) are used, it is easily seen that the ground state is the vacuum of excitations given by the condition

$$\alpha_q |0\rangle = 0 \tag{19}$$

for all q. Here the α_q are defined by the relations

$$\eta_q^\dagger = u_q \alpha_q^\dagger + v_q \alpha_{-q} \tag{20}$$

and

$$u_q^2 - v_q^2 = 1, \tag{21}$$

which, together with the requirement that u_q and v_q be real and that they depend only on the absolute value of q, implies that the α's also obey the Bose commutation relations. It is easily verified[9] that

$$u_q = \tfrac{1}{2}(\sqrt{S_q} + 1/\sqrt{S_q}), \tag{22}$$

$$v_q = \tfrac{1}{2}(\sqrt{S_q} - 1/\sqrt{S_q}), \tag{23}$$

where S_q is the ground-state structure factor. I now introduce a further approximation, also used in deriving the Feynman spectrum: I replace $1/\rho(\vec{r})$ by $1/\bar{\rho}$, where $\bar{\rho}$ is the average density. The approximate expression for $f(\vec{r})$ now becomes, according to the identity proved in the Appendix,

$$f(\vec{r}) = \left\langle \exp\left(\frac{i}{\bar{\rho}} \int_{x'}^{x'+x} \frac{\sqrt{N}}{V} \sum_q q_x \eta_q^\dagger e^{iq_x u} du\, e^{i(q_y y + q_z z)} \right) \rho(\vec{r} + \vec{r}') \right\rangle$$

$$= \left\langle \exp\left(\frac{1}{\bar{\rho}} \frac{\sqrt{N}}{V} \sum_q (e^{i\vec{q}\cdot(\vec{r}+\vec{r}')} - e^{i\vec{q}\cdot\vec{r}'}) \eta_q^\dagger \right) \rho(\vec{r} + \vec{r}') \right\rangle. \tag{24}$$

Expressing η and $\eta^\dagger$ in terms of α and $\alpha^\dagger$, one obtains for the ground-state single-particle reduced density matrix

$$f(\vec{r}) = \langle 0 | \exp\left(\frac{1}{\bar{\rho}} \frac{\sqrt{N}}{V} \sum_q u_q \alpha_q^\dagger (e^{i\vec{q}\cdot(\vec{r}+\vec{r}')} - e^{i\vec{q}\cdot\vec{r}'}) + v_q \alpha_q (e^{-i\vec{q}\cdot(\vec{r}+\vec{r}')} - e^{-i\vec{q}\cdot\vec{r}'})\right)$$

$$\times \left(\bar{\rho} - \frac{\sqrt{N}}{V} \sum_{p\neq 0} (u_p + v_p) e^{i\vec{p}\cdot(\vec{r}+\vec{r}')} (\alpha_p^\dagger + \alpha_{-p})\right) | 0 \rangle . \tag{25}$$

Using the fact that all the terms in the sum over q in (25) commute, we find

$$f(\vec{r}) = \left[\prod_{q\neq 0} \exp\left(\frac{1}{2\bar{\rho}^2} \frac{N}{V^2} u_q v_q (2 - 2\cos\vec{q}\cdot\vec{r})\right)\right] \left(\bar{\rho} - \frac{\sqrt{N}}{V} \sum_{p\neq 0} (u_p + v_p) e^{i\vec{p}\cdot(\vec{r}+\vec{r}')}\right)$$

$$\times \langle 0 | \left[\exp\left(\frac{1}{\bar{\rho}} \frac{\sqrt{N}}{V} v_p \alpha_p (e^{-i\vec{p}\cdot(\vec{r}+\vec{r}')} - e^{(-i\vec{p}\cdot\vec{r}')})\right), \alpha_p^\dagger\right] | 0 \rangle . \tag{26}$$

Using this result, as well as Eqs. (22) and (23), we get

$$f(\vec{r}) = \bar{\rho} \left[\exp\left(\frac{1}{N} \sum_{q\neq 0} \frac{S_q^2 - 1}{4S_q} (1 - \cos\vec{q}\cdot\vec{r})\right)\right]$$

$$\times \left(1 - \frac{1}{2N} \sum_{p\neq 0} (S_p - 1)(1 - e^{-i\vec{p}\cdot\vec{r}})\right) . \tag{27}$$

Taking this last equation at $r \to \infty$, we get the following result for the density of the condensate n_0

$$n_0 = \bar{\rho} \left[\exp\left(\frac{1}{N} \sum_{q\neq 0} \frac{S_q^2 - 1}{4S_q}\right)\right] \left(1 - \frac{1}{2N} \sum_{p\neq 0} (S_p - 1)\right) . \tag{28}$$

IV. LOW-TEMPERATURE APPROXIMATION

We now turn to the case of a finite temperature and assume that the Hamiltonian of the system may be written as

$$H = \sum_{q\neq 0} \omega_q \alpha_q^\dagger \alpha_q . \tag{29}$$

Obviously, the Hamiltonian (29), describing a system of noninteracting excitations, may be used only at very low temperatures. When evaluating $f(\vec{r})$ for finite temperatures, we must replace the ground-state averages in Eq. (25) by thermal averages.

The following useful relations may easily be proved[14]:

$$\langle e^{\gamma a^\dagger + \delta a} \rangle = \exp\left(\tfrac{1}{2}\gamma\delta \frac{1 + e^{-\beta\omega}}{1 - e^{-\beta\omega}}\right), \tag{30}$$

$$\langle e^{\gamma a^\dagger + \delta a} a^\dagger \rangle = \exp\left(\tfrac{1}{2}\gamma\delta \frac{1 + e^{-\beta\omega}}{1 - e^{-\beta\omega}}\right) \frac{1}{1 - e^{-\beta\omega}} , \tag{31}$$

$$\langle e^{\gamma a^\dagger + \delta a} a \rangle = \exp\left(\tfrac{1}{2}\gamma\delta \frac{1 + e^{-\beta\omega}}{1 - e^{-\beta\omega}}\right) \frac{e^{-\beta\omega}}{1 - e^{-\beta\omega}} , \tag{32}$$

where in Eqs. (30)–(32), $\langle \cdots \rangle$ denotes the thermal average with respect to the Hamiltonian

$$h = \omega a^\dagger a \tag{33}$$

and $[a, a^\dagger] = 1$. Using Eqs. (27)–(29), one obtains for finite temperature

$$f(\vec{r}) = \bar{\rho} \left\{\exp\left[\frac{1}{N} \sum_{q\neq 0} \frac{S_q^2 - 1}{4S_q} (1 - \cos\vec{q}\cdot\vec{r}) \left(1 + \frac{2}{e^{\beta\omega_q} - 1}\right)\right] \left(1 - \frac{1}{N} \sum_{p\neq 0} \frac{(S_p - 1)(1 - e^{-i\vec{p}\cdot\vec{r}})}{2(1 - e^{-\beta\omega_p})} + \frac{(S_p + 1)(1 - e^{-i\vec{p}\cdot\vec{r}})}{2(e^{\beta\omega_p} - 1)}\right)\right\} . \tag{34}$$

The condensate density is now given by

$$n_0 = \bar{\rho} \left\{\exp\left[\frac{1}{N} \sum_{q\neq 0} \frac{S_q^2 - 1}{4S_q} \left(1 + \frac{2}{e^{\beta\omega_q} - 1}\right)\right] \left(1 - \frac{1}{N} \sum_{p\neq 0} \frac{(S_p - 1)}{2(1 - e^{-\beta\omega_p})} + \frac{S_p + 1}{2(e^{\beta\omega_p} - 1)}\right)\right\} . \tag{35}$$

A few points should be noted regarding Eqs. (28) and (35). First, S_q appearing in both expressions is the ground-state structure factor. This is due to the assumption that at very low temperatures the Hamiltonian has the same expansion to second order in density fluctuations as when the ground state is considered; i.e., we assume no temperature-dependent renormalization. Hence, the u_q and v_q needed to diagonalize the Hamiltonian are the same as for the ground state. Using Eq. (28) for the ideal gas, where S_q is known to be 1 for $q \neq 0$, one obtains the correct result for the zero-temperature n_0, namely, $n_0 = \bar{\rho}$. Moreover, on close inspection of Eq. (35), we see that we obtain the correct result for all temperatures below the condensation temperature. Studying Eqs. (28)–(35)

for the interacting liquid and assuming S_q to be linear in $|q|$ for small $|q|$, we obtain the Bose-Einstein condensate (BEC) in the ground state only for the three-dimensional and two-dimensional cases. At finite temperatures one obtains, using the Feynman spectrum for small q, BEC only in three dimensions.[15,16] It is also interesting to note that when $(1/N)\sum_{q\neq 0}[(S_q^2-1)/4S_q]$ is small, the relation between n_0 and the S_q's obtained by expanding the exponential to first order in $(1/N)\times\sum_{q\neq 0}[(S_q^2-1)/4S_q]$ agrees with the results previously obtained by various model calculations and lowest-order approximations.[3,4,17] We believe (28) to be valid beyond the region of applicability of the previously mentioned model calculations, as is the case of the Feynman spectrum with respect to the model spectra. Corrections to the above approximation involving the Feynman-Cohen approximation will be dealt with in future work. These corrections will serve also to obtain a better understanding of the region of validity of Eqs. (28) and (35). Although the existing data for S_q enables us to get only a crude estimate of n_0/ρ, which in the ground state is found to be 0.1–0.2, the result is much closer to the approximate result of Ref. 2 than the result one would obtain by expanding the exponential to first order in $(1/N)\sum_{q\neq 0}\times[(S_q^2-1)/4S_q]$, which is 0.4–0.5.

It is interesting to compare the results of this paper with the results of other theories developed for the analysis of real He^4. Two approaches were used to obtain n_0/ρ. The essence of the first approach is to approximate the ground state by a Jastrow wave function, and to calculate the single-particle reduced density matrix directly. The last step is carried out by noting the formal resemblance of this problem and the problem of the statistical mechanics of a classical liquid in the canonical ensemble.[2,18–21] The results for n_0/ρ in the ground state range from 0.08 to 0.25. The second approach, initiated by Hohenberg and Platzman[22] and developed by others,[23] suggests a direct way of measuring n_0, using neutron diffraction at high momenta. Recent experiments[24] give a value of 0.024 ± 0.01 for n_0/ρ. The reason for the discrepancy between the results of the two approaches might be, as already pointed out,[23] that the experiments mentioned were carried out at $T=1.2\,^{\circ}\mathrm{K}$ and not at $T=0\,^{\circ}\mathrm{K}$.

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APPENDIX

In this appendix we prove that

$$\exp\left[\alpha\left(\frac{\partial}{\partial x}+O(x)\right)\right] = Ax\left[\exp\left(\int_x^{x+\alpha} O(x')\,dx'\right)\right]\exp\left(\alpha\frac{\partial}{\partial x}\right), \tag{A1}$$

where $O(x)$ is an operator depending on the parameter x (such as a field or density operator), α is a c number, and Ax means anti-x ordering. Let $|n,(x,0)\rangle$ be a state depending on the parameter x, and let us define

$$|n(x,\alpha)\rangle = \exp\left[\alpha\left(\frac{\partial}{\partial x}+O(x)\right)\right]|n(x,0)\rangle, \tag{A2}$$

so that

$$\frac{\partial}{\partial\alpha}|n(x,\alpha)\rangle = \left(\frac{\partial}{\partial x}+O(x)\right)|n(x,\alpha)\rangle. \tag{A3}$$

Defining

$$|\phi(x,\alpha)\rangle = \exp\left(-\alpha\frac{\partial}{\partial x}\right)|n(x,\alpha)\rangle \tag{A4}$$

we obtain

$$\frac{\partial}{\partial\alpha}|\phi(x,\alpha)\rangle = \exp\left(-\alpha\frac{\partial}{\partial x}\right)O(x)\exp\left(\alpha\frac{\partial}{\partial x}\right)|\phi(x,\alpha)\rangle = O(x-\alpha)|\phi(x,\alpha)\rangle, \tag{A5}$$

because $\exp(\alpha\,\partial/\partial x)$ translates x to $x+\alpha$.

The solution of Eq. (A5) is

$$|\phi(x,\alpha)\rangle = \nabla\exp\left(\int_0^{\alpha} O(x-\alpha')\,d\alpha'\right)|\phi(x,0)\rangle, \tag{A6}$$

where ∇ denotes α ordering. Finally, after using the definition of $|\phi\rangle$ and changing the variable of integration, we get

$$|n(x,\alpha)\rangle = Ax\left[\exp\left(\int_x^{x+\alpha} O(x')\,dx'\right)\right]\exp\left(\alpha\frac{\partial}{\partial x}\right)|n(x,0)\rangle, \tag{A7}$$

so that (A1) is established.

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