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Systematic Approach to the Bose Liquid

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An approximation scheme for a Bose liquid is presented, based on small fluctuations in density and currents. The method of obtaining the elementary excitations and their interactions in any order of the approximation is outlined. Also it is shown that the first-order calculations are in agreement with the calculations of Feynman, Bogoliubov, and Pitayevski. Second-order calculations agree with the improved results of Feynman and Cohen.

I. INTRODUCTION

In this paper, a systematic approximation scheme for the interacting Bose liquid is derived. The method used is based on the assumption of small fluctuations of the density operator $\rho(r)$ and the current operator $J(r)$ from their averages. It differs, however, in several important aspects from Pitayevski's coarse-grained theory, which is based on a similar idea.[1] In Sec. II the Hamiltonian is expressed in terms of the current and density operators, and the commutation relations of the Fourier transforms of these operators are derived. Section III uses the assumption of small fluctuations of ρ and J from their average values in order to approximate the commutation relations, as well as the Hamiltonian. This first-order calculation yields the results of three apparently different theories: the Bogoliubov microscopic theory,[2] the Feynman variational theory,[3] and the Pitayevski theory. In Sec. IV the commutation relations and Hamiltonian are treated in a higher-order approximation. The procedure for obtaining the elementary excitations is discussed; it is easily shown that the wave functions obtained, in this order, are the Feynman-Cohen wave functions.[4,5] Higher-order expansions are discussed in Sec. V. The method for systematically deriving, the quasiparticle interactions without using phenomenological models is outlined, though actual calculations of this kind are postponed for later publication. Some general results holding for any order of the expansion are also explicitly derived in Sec. V.

II. HAMILTONIAN AND COMMUTATION RELATIONS

The Hamiltonian for a system of N identical bosons contained in a box of volume Ω and interacting via a two-body potential $v(r)$ is given by Eq. (1) ($\hbar = m = 1$):

$$H = \frac{1}{2}\int \nabla\psi^{\dagger}\cdot\nabla\psi d^3r + \frac{1}{2}\int \psi^{\dagger}(r)\psi^{\dagger}(r')\,v(r-r') \times\psi(r)\psi(r')\,d^3r d^3r' , \qquad (1)$$

where $\psi^{\dagger}(r)$ and $\psi(r)$ are creation and destruction operators, respectively, of a particle at point r

and obey the usual Bose commutation relations:

$$[\psi(r), \psi(r')] = [\psi^\dagger(r), \psi^\dagger(r')] = 0\ ,$$
$$[\psi(r), \psi^\dagger(r')] = \delta(r - r')\ . \quad (2)$$

For our purposes it is more convenient to write H in a less conventional form,[6-8] in terms of $J(r)$ and $\rho(r)$, the current and density operators, respectively:

$$H = \tfrac{1}{2}\int \Gamma^\dagger(r)\cdot \frac{1}{\rho(r)}\Gamma(r)d^3r + \tfrac{1}{2}\int \rho(r)v(r-r')\rho(r')\,d^3r d^3r' - \tfrac{1}{2}v(0)N\ , \quad (3)$$

$$\Gamma^\dagger(r) = J(r) + i\tfrac{1}{2}\nabla\rho(r)\ . \quad (4)$$

It will prove convenient to employ the Fourier variables

$$\Gamma_q^\dagger = \frac{1}{N^{1/2}}\int \Gamma^\dagger(r)e^{-iq\cdot r}d^3r\ , \quad (5)$$

$$\rho_q = \frac{1}{N^{1/2}}\int \rho(r)e^{-iq\cdot r}d^3r\ . \quad (6)$$

Expressing $\Gamma_q^\dagger$ and ρ_q in terms of the creation and destruction operators of a particle in the momentum states, we obtain

$$\Gamma_q^\dagger = N^{-1/2}\textstyle\sum_k k a_k^\dagger a_{k+q}\ , \quad (5')$$

$$\rho_q = N^{-1/2}\textstyle\sum_k a_k^\dagger a_{k+q}\ . \quad (6')$$

Using expressions (5′) and (6′), we have the commutation relations

$$[\rho_q, \rho_p] = 0\ , \quad (7)$$

$$[\Gamma_q^{i\dagger}, \rho_p] = -N^{-1/2}p_i\rho_{q+p}\ , \quad (8)$$

$$[\Gamma_q^{i\dagger}, \Gamma_p^{j\dagger}] = N^{-1/2}[q_j\Gamma_{q+p}^{i\dagger} - p_i\Gamma_{q+p}^{j\dagger}]\ , \quad (9)$$

where the indices i and j denote Cartesian components of a vector. A further useful relation is

$$\Gamma_q = \Gamma_{-q}^\dagger - q\rho_{-q}\ . \quad (10)$$

III. FIRST-ORDER APPROXIMATION

In this section we propose approximations to the commutation relations [Eqs. (7) – (9)], which are based on the assumption of small fluctuations of the quantities $\Gamma^{i\dagger}(r)$ and $\rho(r)$ from their averages. We first note that for a stationary fluid the average of $\Gamma^\dagger(r)$ is zero. The simplest approximations to the commutation relations are given by

$$[\rho_q, \rho_p] = 0\ , \quad (7')$$

$$[\Gamma_q^{i\dagger}, \rho_p] = -p_i\delta_{q,-p}\ , \quad (8')$$

$$[\Gamma_q^{i\dagger}, \Gamma_p^{j\dagger}] = 0\ . \quad (9')$$

The operators $\Gamma_q^{i\dagger}$ and ρ_p, for $q, p \neq 0$, can be written in this approximation as

$$\Gamma_q^{i\dagger} = q_i\eta_q^\dagger\ , \quad (11)$$

$$\rho_p = \gamma_p\ , \quad (12)$$

where the operators $\mathcal{g}_p$, $\eta_q^\dagger$ obey the commutation relations

$$[\gamma_q, \gamma_p] = 0, \quad [\eta_q^\dagger, \eta_p^\dagger] = 0, \quad [\eta_q^\dagger, \gamma_0] = \delta_{q,-p}\ . \quad (13)$$

We also use the definitions

$$\gamma_0 = \eta_0^\dagger = 0\ . \quad (14)$$

On substituting (11) and (12) into (10), we obtain

$$\gamma_{-q} = -(\eta_{-q}^\dagger + \eta_q)\ . \quad (15)$$

Now it is easily seen that the commutation relations (13) hold if the operators η_q, $\eta_q^\dagger$ obey the usual boson commutation relations:

$$[\eta_q, \eta_p] = [\eta_q^\dagger, \eta_p^\dagger] = 0\ , \quad (16)$$

$$[\eta_q, \eta_p^\dagger] = \delta_{qp}\ . \quad (17)$$

Now we focus our attention on the Hamiltonian. If again we apply the assumption of small density fluctuations, i.e.,

$$\rho(r) = \bar\rho + \delta\rho \quad \frac{|\delta\rho|}{\bar\rho} < 1, \quad (18)$$

where $\bar\rho$ is the average density, we can expand the Hamiltonian in the Taylor series:

$$H = \tfrac{1}{2}\sum_{n=0}^{\infty}(-1)^n\int \Gamma^\dagger(r)\cdot\left(\frac{\delta\rho}{\bar\rho}\right)^n\Gamma(r)d^3r + \tfrac{1}{2}\int \rho(r)v(r-r')\rho(r')d^3r d^3r'\ . \quad (19)$$

Retaining only the first term in the kinetic-energy expansion, we obtain, apart from the constant terms,

$$H = \tfrac{1}{2}\textstyle\sum_q \Gamma_q^\dagger\cdot\Gamma_q + \tfrac{1}{2}\sum_q \bar\rho\, v(q)\rho_q\rho_{-q}\ , \quad (20)$$

where $v(q)$ is the Fourier transform of the two-body potential $v(r)$.[9] On using (11), (12), and (15), we find that (19) transforms into

$$H = \tfrac{1}{2}\textstyle\sum_q H_q\ , \quad (21)$$

$$H_q = \tfrac{1}{2}q^2[\eta_q^\dagger\eta_q + \eta_{-q}^\dagger\eta_{-q}] + \bar\rho\, v(q)(\eta_q^\dagger + \eta_{-q})(\eta_{-q}^\dagger + \eta_q)\ . \quad (22)$$

This Hamiltonian is exactly the one that appears in the Bogoliubov[2] theory, with the condensate density N_0 replaced by the total density. H_q is diagonalized easily by the well-known Bogoliubov transformation

$$\eta_q^\dagger = u_q\alpha_q^\dagger + v_q\alpha_{-q}\ . \quad (23)$$

The u's and v's are chosen so as to ensure that the operators α and $\alpha^\dagger$ obey the Bose commutation relations and that the Hamiltonian is diagonalized in the α scheme. Under these conditions we obtain

$$u_q^2 = \tfrac{1}{2}\{1 + [\tfrac{1}{2}q^2 + \bar{\rho}\,v(q)]/[\tfrac{1}{4}q^4 + q^2\bar{\rho}\,v(q)]^{1/2}\},$$
$$v_q^2 = \tfrac{1}{2}\{-1 + [\tfrac{1}{2}q^2 + \bar{\rho}\,v(q)]/[\tfrac{1}{4}q^4 + q^2\bar{\rho}\,v(q)]^{1/2}\}. \tag{24}$$

Apart from the constant terms, the Hamiltonian can be written as

$$H = \textstyle\sum_q [\tfrac{1}{4}q^4 + q^2\bar{\rho}\,v(q)]^{1/2}\alpha_q^\dagger\alpha_q \equiv \sum \omega_q\alpha_q^\dagger\alpha_q . \tag{25}$$

If we compute the Fourier transform of the pair correlation function S_q, we obtain

$$S_q = q^2/2\omega_q . \tag{26}$$

This is exactly the Feynman result for the excitation spectrum.[3] The same result is also obtained by Pitayevski.[1] His treatment is based, however, on coarse-grained operators,[10] i.e., he uses the hydrodynamical Hamiltonian describing a continuous fluid. His result for the energy spectrum as a function of q is also different:

$$\omega_q^{\mathrm{Pit}} = q[\bar{\rho}\,v(q)]^{1/2} . \tag{27}$$

The wave functions of the first excited states are given by

$$\psi_q = \alpha_q^\dagger\,|0\rangle = (\alpha_q^\dagger + \alpha_{-q})|0\rangle . \tag{28}$$

Now it is easily seen that, apart from a normalization factor, we have

$$\psi_q = \gamma_q|0\rangle . \tag{29}$$

IV. SECOND-ORDER APPROXIMATION

In order to obtain a better physical picture we must treat the commutation relations (5′)–(7′), as well as the Hamiltonian (18), more accurately. The commutation relations can be improved by inserting on the right-hand side the approximate expression for the operators ρ_{q+p} and Γ^i_{q+p}:

$$[\rho_q, \rho_p] = 0 , \tag{7″}$$

$$[\Gamma_q^{i\dagger}, \rho_p] = -p_i\delta_{q,-p} - N^{-1/2}p_i\gamma_{q+p} , \tag{8″}$$

$$[\Gamma_q^{i\dagger}, \Gamma_p^{j\dagger}] = N^{-1/2}[q_j(q+p)_i - p_i(q+p)_j]\eta^\dagger_{q+p}$$
$$= N^{-1/2}[q_jq_i - p_ip_j]\eta^\dagger_{q+p} . \tag{9″}$$

Instead of the simple results (11) and (12), we now obtain

$$\Gamma_q^{i\dagger} = q_i\eta_q^\dagger - \frac{q_i}{N^{1/2}}\sum_{L\neq 0,q}\left(\frac{q\cdot(q-L)}{(q-L)^2} + \frac{L\cdot q}{q^2}\right)\eta_L^\dagger\gamma_{q-L}$$
$$+ \frac{1}{N^{1/2}}\sum_{L\neq 0,q} L_i\eta_L^\dagger\gamma_{q-L} , \tag{30}$$

$$\rho_p = \gamma_p + \frac{1}{N^{1/2}}\sum_{k\neq p,0}(p\cdot k/k^2)\gamma_k\gamma_{p-k} . \tag{31}$$

As a result of the assumption of small fluctuations in the quantities $\rho(r)$ and $\Gamma^{i\dagger}(r)$, we considered the operators $\rho_q/N^{1/2}$ and $\Gamma_q^{i\dagger}/N^{1/2}$ to be very small compared to 1 and neglected them on the right-hand side of Eqs. (8′) and (9′). An obvious result of (11) and (12) is that $\eta_q/N^{1/2}$ and $\eta_q^\dagger/N^{1/2}$ are also very small compared to 1. Hence, Eqs. (30) and (31) constitute a solution of Eqs. (7″)–(9″) up to first order in these operators. The uniqueness of the solution in this order will be discussed elsewhere. In order to obtain the improved elementary excitation spectrum, we have to use a higher-order expansion of the Hamiltonian, insert expressions (30) and (31), perform a Bogoliubov transformation, arrange the operators in normal order, and require that the bilinear part of the Hamiltonian be diagonal. This complicated calculation will be treated in a subsequent publication. We may, however, obtain some general results without going into the detailed calculations. The wave function describing an excitation of momentum q will be given by

$$\psi_q = \alpha_q^\dagger|0\rangle , \tag{32}$$

where $\alpha_q^\dagger$ is the operator creating the excitation. Using the same reasoning as in Eqs. (28) and (29), we obtain, even now,

$$\psi_q = \gamma_q|0\rangle . \tag{33}$$

Iterating Eq. (30) and identifying the vacuum with the ground state, we have

$$\psi_q = \left(\rho_q - N^{-1/2}\sum_{k\neq q,0}(q\cdot k/k^2)\rho_k\rho_{p-k}\right)\psi_G . \tag{34}$$

This expression is the one derived by Feynman and Cohen for the first excited wave function of the liquid.[4,5]

V. HIGHER ORDERS

The method of obtaining systematically higher-order corrections to the wave functions and excitation spectrum must already be clear to the reader. The expression obtained for the nth approximation for the operators $\Gamma_q^{i\dagger}$ and ρ_p is to be inserted in the right-hand side of Eqs. (7)–(9). Solving for the operators on the left-hand side we obtain the $(n+1)$th approximation for these operators. Taking more terms in the density expansion of the Hamiltonian (19) and obtaining the elementary excitations, the interactions of these excitations may be derived without resorting to phenomenological models. Since the elementary excitations are to be found by the same procedure as that described in Sec. IV, the wave functions describing them will be given in any order of approximation by the same expression:

$$\psi_q = \gamma_q|0\rangle . \tag{35}$$

γ_q is related to the creation and destruction operators of the excitations, $\alpha_q^\dagger$ and α_q, respectively, by the following equations:

$$\gamma_q = -(u_q + v_q)\,\alpha_q^\dagger + \alpha_{-q}) , \tag{36}$$

$$\gamma_q|0\rangle = -(u_q + v_q)\,\alpha_q^\dagger|0\rangle . \tag{37}$$

Hence, $$(u_q + v_q)^2 = \langle 0|\gamma_q\gamma_{-q}|0\rangle . \tag{38}$$

For brevity we denote the ground-state expectation value of $\gamma_q\gamma_{-q}$ by F_q. The equations determining the u's and v's will be

$$(u_q + v_q)^2 = F_q , \tag{39}$$

$$u_q^2 - v_q^2 = 1 . \tag{40}$$

The solutions are

$$u_q^2 = (F_q + 1)^2/4F_q , \tag{41}$$

$$v_q^2 = (F_q - 1)^2/4F_q . \tag{42}$$

Hence, the u's and v's can be determined from the ground-state properties of the system.

VI. SUMMARY

A systematic approximation scheme based on the assumption of small density and current fluctuations was presented. The operators ρ_q and $\Gamma_p^\dagger$ appearing in the Hamiltonian were expanded, using the above assumption, in terms of simple operators. The possibility of obtaining the excitation wave functions and spectrum to any desired order, either by using known ground-state expectation values or by using the procedure described in Sec. IV, is outlined. Hence, this method allows one to obtain the interquasiparticle interactions. To demonstrate the applicability of the method, it was shown that the first-order calculation yields the well-known Feynman results as well as the results of Bogoliubov and Pitayevski. It was further shown that second-order calculations yield the improved result of Feynman and Cohen.

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Theory of Gas Lasers and Its Application to an Experiment

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The semiclassical theory of gas lasers has been reformulated by adding rate terms to the density-matrix component differential equations. The solution to these equations, in the form of a Fourier series, is applicable at high laser intensities. A calculation of the effect of phase-changing collisions is also included so that the results can be compared to experimental data taken with a He-Ne laser operating at a wavelength of 1.15 μm.

I. INTRODUCTION

Lamb's semiclassical theory of the gas laser[1] accurately predicts many laser properties, such as the power output and the frequency as a function of cavity length. However, as Lamb points out, the applicability of his third-order results is limited to low laser powers. Bennett's hole-burning theory[2] is more heuristic and gives results equivalent to those of Ref. 1 at low intensities. At-