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Field-theoretic approach to many-boson systems

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It is now well established that current and density may be used as coordinates in describing a nonrelativistic many-body system. The current and density operators form a closed algebra as they obey a set of equal-time commutation relations. A particular choice of the algebra containing only the longitudinal component of the current describes a fluid in a simple way. For Bose systems, we show that there exists *a special choice* of this longitudinal current which is an irreducible representation of the algebra, but expressed in two different ways leading to the formulations of Bogoliubov and Zubarev (BZ) and that of Sunakawa and his coworkers (S). This demonstration proves the formal equivalence of the two formulations. The BZ formalism leads to a non-Hermitian Hamiltonian for which use of a certain mathematical technique recently proposed by us yields completely divergence-free results for Bose systems. A temperature-dependent matrix Green's-function theory is developed and the self-energy matrix calculated. From this, we also deduce the structure factor in a straightforward way. These results are applied here to compute numerically the excitation spectrum of the superfluid liquid helium using the experimental structure factor as the only input into the computation. Comparison of this with other calculations and with experiment is discussed in detail in this paper. The problem of a charged Bose gas is considered as a testing ground for all theories of Bose fluids since certain exact results are known for this system. We have applied our method using the BZ Hamiltonian to this problem and we are in complete agreement with the exact results. It thus appears that the current-algebra approach can be quite successfully applied in elucidating properties of interacting Bose systems.

I. INTRODUCTION

Until recently, field-theoretic approaches to many-boson systems have mostly been confined to theories based on the weak-coupling limit.[1] This theory incorporates the exact result known for a noninteracting Bose gas, namely, the macroscopic occupation of the zero-momentum state. Stated in another way, it has built in it the off-diagonal long-range order in the one-particle density matrix. It can be argued on general grounds that in any theory of interacting bosons there must be some particles in the zero-momentum state, which should be calculable. This limit is thus defined by the condition that nearly all the particles (N_0) are in the zero-momentum state at $T=0$ °K and so the operators a_0 and $a_0^\dagger$ corresponding to the destruction and creation of this excitation are replaced by c numbers, $\sqrt{N_0}$. A Bogoliubov[1] transformation is then applied to compensate for "dangerous" diagrams[2] that appear as a consequence, but these problems with the resulting Hamiltonian are well known.[3,4] For instance, each term in a perturbation expansion for the energy of excitation is divergent if the fluctuations in the zero momentum state are neglected. N_0 can, in principle, be determined self-consistently in this theory. Several interesting model boson systems have been examined in this way, some of which may be mentioned here. Brueckner[4] was able to obtain an exact convergent result in the high-density limit for the ground-state energy of a charged Bose gas by summing one- and two-ring diagrams. Lee, Huang, and Yang[5] were able to develop a low-density expansion for a hard-sphere boson gas, but problems arise when the method is applied to physical systems of interest such as superfluid liquid helium. For liquid helium, the number of particles in the zero-momentum condensate is probably less than 10%. Gersch *et al.*[6] using the experimental neutron-energy widths and the impulse approximation predict an upper bound of 3% while other estimates[7] are about 6%. It thus appears that the Bogoliubov approximation may not apply for this case. For a more complete review of this method see Ref. 8.

Bogoliubov and Zubarev[9] (BZ) gave an alternate field-theoretic approach in 1955 which was largely overlooked. They introduced a collective-variable approach in which the Fourier transform of the density ρ_k is used as a variable and expressed the Hamiltonian in terms of ρ_k and $\partial/\partial\rho_k$. (The transformation from the particle coordinate representation to these variables is noncanonical.) It is then quantized in terms of Bose operators resulting in an explicitly non-Hermitian Hamiltonian. A mathematical framework needed to deal with this Hamiltonian has recently been put forward by Rajagopal and Grest[10] (henceforth referred to as I). Expressions for the ground- and first excited-state energies, the liquid-structure factor, and two-roton scattering amplitudes were calculated in perturbation theory and found to be totally divergence-free right from the start. Sunakawa *et al.*[11] (S) have introduced a velocity operator canonically conjugate to ρ_k, and have obtained an infinite-series Hermitian Hamiltonian. To describe the superfluid state of He II at absolute zero, they restricted this velocity to be irrotational, i.e., $\vec{\nabla}\times\vec{v}(\vec{x})=0$. With this restriction, Berdahl[12] has noted that this approach is completely equivalent to the phase variable approach of Nishiyama.[13] The velocity operator is proportional to the gradient of the phase operator. Chan and Valatin[14] have shown that the BZ Hamiltonian and that of Nishiyama are related by a nonunitary canonical transformation. The perturbation theories in this scheme also have divergencies which can all be cancelled out by a careful analysis of the appropriate higher interaction terms as was shown by Grest and Rajagopal.[15] The results in Rayleigh-Schrödinger (RS) perturbation theory for both the BZ and S Hamiltonians have been shown to be completely equivalent,[10] when the calculation is correctly done. Results for the ground- and first excited-state energies are also equivalent[16] to those obtained by a variational-perturbation procedure based on the method of correlated basis functions (CBF),[17] which are non-field-theoretic in nature. One can compute the number of particles in the zero momentum state in this theory even though no assumption concerning it is made. As Zubarev's original derivation of this was unclear, we will give a derivation of it here. Berdahl[14] has also given a derivation of this using the phase and density variables.

In view of the equivalence of the results based on perturbation theory using the BZ and S Hamiltonians, it is of interest to examine these Hamiltonians more carefully to establish if there is any basic underlying reason for this. We will prove in this paper that the derivation of the BZ and S Hamiltonians stem from an alternative approach to nonrelativistic quantum mechanics—that of current algebra. Dashen and Sharp[18] have shown that one can give a *complete* description of a system of bosons or fermions by introducing density $\rho(\vec{x})$ and current $\vec{J}(\vec{x})$ as basic variables. These variables obey well-established equal-time commutation relations and the Hamiltonian is expressed in terms of these variables.[18-22] Following Landau,[23] a velocity operator can be introduced, and the only remaining problem is the proper realization of the commutation relations. We will show that by appropriate choice of the velocity operator consistent with the commutation rules, one can obtain the BZ or Sunakawa Hamiltonian as special cases of the general formulation. The corresponding current $\vec{J}(\vec{x})$, being an irreducible representation of the algebra, will be shown to be completely equivalent for the two choices of the velocity operator, thus indicating that the equivalence of results in perturbation theory found in I was not accidental.

The BZ Hamiltonian does not conserve quasiparticle number and consequently a matrix Green's-function formalism must be employed.[3] Straley[24] has earlier developed a zero-temperature Green's function theory but did not explicitly take the non-Hermiticity of the Hamiltonian into consideration. In this paper, we will develop the temperature-dependent matrix Green's-function theory for the BZ Hamiltonian. The self-energy matrix is calculated through second order in $(1/\sqrt{N})$. From this Green's function the excitation spectrum and ground-state liquid-structure factor can be calculated. As Straley[24] has previously shown, the spectrum does not display a gap, in contrast to several calculations[25] which displayed the existence of a gap in the spectrum.

Over the years, the most interesting and yet unsolved problem in many-boson systems, has been the excitation spectrum of superfluid liquid helium. Since Landau[23] proposed the phonon-roton spectrum, only a few theoretical calculations have been attempted. The first attempt was by Bijl[26] who derived a quantum theory of the excitations that exhibited both the phonon and roton aspects. Feynman[27] and later Feynman and Cohen[28] (FC) used physically plausible wave functions and derived the energy of excitation by a variational calculation. FC were forced to make many approximations for the three- and four-particle correlation functions and thus the results were no longer a variational bound. Using the experimental liquid-structure factor of Goldstein and Reekie,[29] extrapolated to zero and normalized, FC obtained a roton minimum of 11.5 °K. Later recalculation of the integrals by Burke *et al.*[30] showed that the FC results were probably not as good as was first thought. Using the structure factor obtained from neutron scattering by Henshaw,[31] extrapolated to zero for $k<0.8$ Å^{-1} by a variety of methods, they showed that the FC formula gave bad results for low-k values and only fair results in the roton region. The poor results can probably be related to the many approximations FC were forced to make in order to obtain numerical results.

A somewhat different approach was developed by Kuper,[32] who evaluated the phonon-phonon interaction using the RS perturbation formalism. The major difficulty was the practical limitations of a hand calculation; as such the energy was evaluated only at one point. Jackson and Feenberg[33]

(JF) have developed a second-order Brillouin-Wigner (BW) perturbation theory using the method of CBF. The three-particle correlation function was approximated by the convolution approximation and the Goldstein-Reekie structure factor was used to obtain numerical results. The roton minimum was about 12 °K with good agreement in the low-k region. Lee[34] has reevaluated the JF result using the theoretical structure factor of Massey[35] but obtained a roton minimum at 1.7 Å^{-1} instead of at the experimental value 1.9 Å^{-1}, probably owing to errors in the structure factor used. Campbell and Feenberg[36] have also calculated the structure factor but to the best of our knowledge, it has not been used to calculate the energy spectrum for all values of k. Several authors have attempted to improve upon the JF result,[37,38] but the numerical computations have been limited mainly to the low-k region. Except for a few calculations which are based on model He-He interatomic potentials,[11] to the best of our knowledge, there have been until now no other calculations of the excitation spectrum in liquid helium.

With all of these previous calculations of the energy spectrum there have been several difficulties. The structure factor $S(k)$ used by FC and JF was not known for low-k values and some arbitrary method had to be used to extrapolate the results to zero.[39] Recently, x-ray scattering data[40,41] at very low temperatures (less than 1 °K) have become available. The problem of extrapolating $S(k)$ arbitrarily to zero as $k \to 0$ has thus been eliminated. In the light of this new data, we thought it important to recalculate the excitation spectrum. Cowley and Woods[42] believe that $S(k)$ from x-ray data is more reliable than from neutron scattering. We will show that the BZ energy formula can be expressed as a function of the structure factor and all dependence of the unknown Fourier transform of the interatomic potential can thus be eliminated. Using the Achter-Meyer[40] (AM) data as the only input, we were able to derive the excitation spectrum. We obtain good agreement with experiment in the low-k region and a roton minimum of 12.3 °K for $k \sim 1.9$ Å^{-1}. For comparison, we have reevaluated the energy using the JF formula, and found a roton minimum of 12.9 °K for $k \simeq 1.9$ Å^{-1}. The results obtained here are in close numerical agreement with those based on a modified BW perturbation theory and the S Hamiltonian.[15] There are several remaining problems, which we will discuss later, one of these being the proper normalization of $S(k)$.

A second problem which has been of great theoretical interest is a many-boson system interacting through a Coulomb interaction. While the charged Bose gas does not describe any physical system, it has been useful over the years as a test case for approximations. The long-range interaction and the Bose statistics give rise to two types of infinities in the perturbation theory based on the Bogoliubov[1] scheme. Brueckner[4] obtained a convergent result for the ground-state energy in a perturbation expansion in the high-density limit after summing the one- and two-ring diagrams. Lee[43] has shown the CBF results in the uniform limit to be completely equivalent. Ma and Woo[44] investigated the excited-state properties using standard field-theoretic techniques and evaluated the excitation spectrum. Bhattacharyya and Woo[45] used the CBF theory and obtained equivalent results for the excitation spectrum and also calculated the liquid-structure factor. Since the potential is well known, we will discuss this model in the light of the BZ formalism. The energy spectrum has previously been shown to be explicitly equivalent to the CBF results but differences arise for the liquid-structure factor $S(k)$. We have evaluated $S(k)$ for a charged Bose gas in the high-density limit and found it differs from the previous results.[45] The reasons for this difference will be discussed later. Lee and Ree[46] have also considered improving the liquid-structure factor for a charged Bose gas by solving the hypernetted chain equation. Foldy[47] has previously calculated the number of particles in the zero-momentum condensate and his result will also be discussed here.

In Sec. II, we will discuss current and density as variables and show that the BZ and S Hamiltonians are a direct consequence of two realizations of the velocity operator. In Sec. III, we discuss the temperature-dependent matrix Green's function and derive the self-energy matrix through second order in $(1/\sqrt{N})$. In Sec. IV, we discuss the elementary excitation spectrum of liquid helium. We will present our results along with a reevaluation of the JF result using the recent experimental structure factor of Achter and Meyer. We will also discuss probable errors in our work and previous works. In Sec. V, we will examine the charged Bose gas in the light of the BZ Hamiltonian. Section VI will contain a discussion of our work as well as problems to be considered in the future.

II. CURRENTS AS COORDINATES

Consider a system of N identical spinless bosons interacting through a two-body potential $V(|\vec{x}-\vec{x}'|)$ enclosed in a volume Ω. The Hamiltonian in second quantized form is

$$H=\frac{\hbar^2}{2m}\int d^3x\,\vec{\nabla}\psi^\dagger(\vec{x})\cdot\vec{\nabla}\psi(\vec{x})$$
$$+\tfrac{1}{2}\int\int d^3x\,d^3x'\,\psi^\dagger(\vec{x})\psi^\dagger(\vec{x}')$$
$$\times V(|\vec{x}-\vec{x}'|)\psi(\vec{x}')\psi(\vec{x})\,, \tag{1}$$

where the field operators $\psi(\vec{x})$ and $\psi^\dagger(\vec{x})$ obey the usual equal-time commutation relations. Dashen and Sharp[18] have shown that one can give a *complete* description of the system in terms of the variables, number density $\rho(\vec{x})$, and current $\vec{J}(\vec{x})$. These operators are

$$\rho(\vec{x})=\psi^\dagger(\vec{x})\psi(\vec{x})\,,$$
$$\vec{J}(\vec{x})=\frac{\hbar}{2mi}\{\psi^\dagger(\vec{x})[\vec{\nabla}\psi(\vec{x})]-[\vec{\nabla}\psi^\dagger(\vec{x})]\psi(\vec{x})\}\,. \tag{2}$$

The commutation relations satisfied by these are

$$[\rho(\vec{x}),\rho(\vec{x}')]_-=0\,,$$
$$[\rho(\vec{x}),J_k(\vec{x}')]_-=-i\frac{\hbar}{m}\frac{\partial}{\partial x^k}[\delta^{(3)}(\vec{x}-\vec{x}')\rho(\vec{x})]\,, \tag{3}$$
$$[J_i(\vec{x}),J_j(\vec{x}')]_-=-i\frac{\hbar}{m}\frac{\partial}{\partial x^j}[\delta^{(3)}(\vec{x}-\vec{x}')J_i(\vec{x})]$$
$$+i\frac{\hbar}{m}\frac{\partial}{\partial x^i}[\delta^{(3)}(\vec{x}-\vec{x}')J_j(\vec{x})]\,.$$

The Hamiltonian can then be expressed[11,18]

$$H=\frac{\hbar^2}{8m}\int d^3x\left(\vec{\nabla}\rho(\vec{x})-\frac{2mi}{\hbar}\vec{J}(\vec{x})\right)\frac{1}{\rho(\vec{x})}\left(\vec{\nabla}\rho(\vec{x})+\frac{2mi}{\hbar}\vec{J}(\vec{x})\right)$$
$$+\tfrac{1}{2}\int\int d^3x\,d^3x'\,\rho(\vec{x})V(|\vec{x}-\vec{x}'|)\rho(\vec{x}')-\tfrac{1}{2}NV(0)\,, \tag{4}$$

where $N=\int d^3x\,\rho(\vec{x})$ and $V(0)$ is the interaction potential at $\vec{x}=\vec{x}'$.

The problem now reduces to a realization of the commutation relations by suitably choosing an irreducible representation for $\vec{J}(\vec{x})$. Kobe and Coomer[21] have shown that inconsistencies arise if one chooses to employ a Fock-space formulation and suggested some larger space may have to be used. This may contain states that are functionals of the density. Grodnick and Sharp[19] showed that the commutation relations (3) are satisfied by choosing operators that act in the function space $\Psi\{\rho(\vec{x})\}$,

$$\rho(\vec{x})\Psi\{\rho(\vec{x})\}=\rho(\vec{x})\Psi\{\rho(\vec{x})\}\,,$$
$$\vec{J}(\vec{x})\Psi\{\rho(\vec{x})\}=\frac{\hbar}{m}\left(\rho(\vec{x})\frac{1}{i}\vec{\nabla}\frac{\delta}{\delta\rho(\vec{x})}-\frac{1}{2i}\vec{\nabla}\rho(\vec{x})\right. \tag{5}$$
$$\left.+\vec{F}\{\rho(\vec{x})\}\right)\Psi\{\rho(\vec{x})\}\,,$$

where $\vec{F}\{\rho(\vec{x})\}$ is any functional of $\rho(\vec{x})$. The functional $\vec{F}\{\rho(\vec{x})\}$ distinguishes a Bose from a Fermi system. Grodnick and Sharp also showed that one could choose $\vec{F}=0$ for a boson system. The Hamiltonian then reduces to

$$H=\frac{\hbar^2}{2m}\int d^3x\left(\vec{\nabla}\rho(\vec{x})-\rho(\vec{x})\vec{\nabla}\frac{\delta}{\delta\rho(\vec{x})}\right)\left(\vec{\nabla}\frac{\delta}{\delta\rho(\vec{x})}\right)$$
$$+\tfrac{1}{2}\int\int d^3x\,d^3x'\,\rho(\vec{x})V(|\vec{x}-\vec{x}'|)\rho(\vec{x}')-\tfrac{1}{2}NV(0)\,. \tag{6}$$

Note that H no longer depends on the ill-defined operator, $\rho(\vec{x})^{-1}$. Introducing the Fourier components,

$$\rho(\vec{x})=N/\Omega+\rho'(\vec{x})\,,$$
$$\rho'(\vec{x})=\frac{\sqrt{N}}{\Omega}\sum_{\vec{k}\neq 0}\rho_k e^{-i\vec{k}\cdot\vec{x}}\,,$$
$$\frac{\delta}{\delta\rho(x)}=\frac{1}{\sqrt{N}}\sum_{\vec{k}\neq 0}\frac{\partial}{\partial\rho_k}e^{i\vec{k}\cdot\vec{x}}\,, \tag{7}$$
$$\rho_{k\neq 0}=\frac{1}{\sqrt{N}}\int d^3x\,\rho'(\vec{x})e^{i\vec{k}\cdot\vec{x}}$$
$$=\frac{1}{\sqrt{N}}\sum_{j=1}^{N}e^{i\vec{k}\cdot\vec{x}_j}\,,\quad \rho_{k=0}=\sqrt{N}\,,$$

the Hamiltonian can be rewritten as

$$H=\sum_{\vec{k}\neq 0}\left[\frac{\hbar^2k^2}{2m}\left(-\frac{\partial^2}{\partial\rho_k\partial\rho_{-k}}+\rho_k\frac{\partial}{\partial\rho_k}\right)+\frac{1}{2}\frac{N}{\Omega}V(k)\rho_k\rho_{-k}\right]$$
$$+\frac{1}{\sqrt{N}}\sum_{\vec{k}_1\vec{k}_2\vec{k}_3}\delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,\vec{0}}\frac{\hbar^2}{2m}(\vec{k}_1\cdot\vec{k}_2)\rho_{k_3}\frac{\partial^2}{\partial\rho_{k_1}\partial\rho_{k_2}}+\frac{N(N-1)}{2\Omega}V(k=0)-\frac{N}{2\Omega}\sum_k V(k)\,.$$

$V(k)$ is the Fourier transform of the interatomic potential,

$$V(k)=\int d^3x\,V(\vec{x})e^{-i\vec{k}\cdot\vec{x}}\,.$$

Introduce

$$\vec{R}_k=\hbar\vec{k}\left(\frac{\partial}{\partial\rho_k}-\tfrac{1}{2}\rho_{-k}\right) \tag{9}$$

and write H in terms of it:

$$
\begin{aligned}
H_{\mathrm{BZ}} = {} & \sum_{k\neq 0}\left[\frac{1}{2m}\vec{\mathrm{R}}_k\cdot\vec{\mathrm{R}}_{-k}+\left(\frac{\hbar^2k^2}{8m}+\frac{N}{2\Omega}V(k)\right)\rho_k\rho_{-k}\right] \\
& +\frac{1}{\sqrt{N}}\sum_{\vec{\mathrm{k}}_1\vec{\mathrm{k}}_2\vec{\mathrm{k}}_3}\delta_{\vec{\mathrm{k}}_1+\vec{\mathrm{k}}_2+\vec{\mathrm{k}}_3,\vec{0}}\frac{\rho_{-k_3}}{2m}\left[\vec{\mathrm{R}}_{k_1}\cdot\vec{\mathrm{R}}_{k_2}+\tfrac{1}{4}\hbar^2\vec{\mathrm{k}}_1\cdot\vec{\mathrm{k}}_2\rho_{-k_2}\rho_{-k_1}+\tfrac{1}{2}\hbar(\vec{\mathrm{k}}_2\cdot\vec{\mathrm{R}}_{k_1}\rho_{-k_2}+\rho_{-k_1}\vec{\mathrm{k}}_1\cdot\vec{\mathrm{R}}_{k_2})\right] \\
& +\frac{N(N-1)}{2\Omega}V(k=0)-\frac{N}{2\Omega}\sum_{\vec{\mathrm{k}}\neq 0}V(k)-\sum_{\vec{\mathrm{k}}\neq 0}\frac{\hbar^2k^2}{4m}\,.
\end{aligned}
\qquad (10)
$$

H_{BZ} is explicitly non-Hermitian since $\vec{\mathrm{R}}_k^\dagger=-\vec{\mathrm{R}}_{-k}$. This is the same Hamiltonian derived by BZ from different considerations. Grodnick and Sharp[19] define an inner product on the space of functionals of ρ_k which makes H_{BZ} Hermitian. Such an inner product was first defined by Chan and Valatin.[14] In the spirit of BZ, we would, however, prefer to leave the Hamiltonian non-Hermitian and use the mathematical formalism developed earlier[10] to take care of this new situation. In this way, the problem of defining a metric is automatically taken care of. We can define Bose operators to quantize ρ_k and $\vec{\mathrm{R}}_k$. This is slightly different from BZ, who quantized ρ_k and $\partial/\partial\rho_k$, but the final results are the same. Let

$$
\begin{aligned}
\rho_k &= \sqrt{\lambda_k}\,(b_k+b_{-k}^\dagger)\,, \\
\vec{\mathrm{R}}_k &= \frac{\hbar\vec{\mathrm{k}}}{2\sqrt{\lambda_k}}\,(b_{-k}-b_k^\dagger)\,,
\end{aligned}
\qquad (11)
$$

where b_k and $b_k^\dagger$ obey the usual Bose commutation relations and $b_k^\dagger$ is the *formal* adjoint of b_k. Choose λ_k to diagonalize the first term in (10),

$$
\lambda_k=\left(1+\frac{4m}{\hbar^2k^2}\frac{N}{\Omega}V(k)\right)^{-1/2}, \qquad (12)
$$

$$
H_{\mathrm{BZ}}=H_0+H_{\mathrm{I}}\,,
$$

$$
H_0=E_0^B+\sum_{k\neq 0}E_B(k)b_k^\dagger b_k\,, \qquad (13)
$$

$$
\begin{aligned}
H_{\mathrm{I}}=\sum_{\vec{\mathrm{k}}_1\vec{\mathrm{k}}_2\vec{\mathrm{k}}_3}\delta_{\vec{\mathrm{k}}_1+\vec{\mathrm{k}}_2+\vec{\mathrm{k}}_3,\vec{0}}\big[& \gamma_a^{(3)}(k_1,k_2,k_3)b_{k_1}b_{k_2}b_{k_3} \\
& +\gamma_b^{(3)}(k_1,k_2,k_3)b_{k_1}^\dagger b_{k_2}^\dagger b_{k_3}^\dagger+\gamma_c^{(3)}(k_1,k_2,k_3)b_{k_1}^\dagger b_{-k_2}b_{-k_3} \\
& +\gamma_d^{(3)}(k_1,k_2,k_3)b_{-k_3}^\dagger b_{-k_2}^\dagger b_{k_1}\big]\,,
\end{aligned}
$$

where

$$
\begin{aligned}
E_B(k) &= \frac{\hbar^2k^2}{2m\lambda_k}\,, \\
E_0^B &= \frac{N(N-1)}{2\Omega}V(k=0)-\frac{1}{4}\sum_{k\neq 0}E_B(k)\left(1-\frac{1}{\lambda_k}\right)^2\lambda_k\,,
\end{aligned}
\qquad (14)
$$

and the γ's are defined as in I.

The lowest-order approximation of the ground-state wave function defined by $b_k\varphi_0=0$ is satisfied by

$$
\varphi_0=\exp\left[\frac{1}{4}\sum_{k\neq 0}\left(1-\frac{1}{\lambda_k}\right)\rho_k\rho_k\right], \qquad (15)
$$

which is exactly the result derived by BZ. We have thus shown that the BZ Hamiltonian can be derived by choosing a representation for the current operator $\vec{\mathrm{J}}(\vec{\mathrm{x}})$. The non-Hermitian Hamiltonian is in fact no problem to handle and the results for the energy and other physical quantities are totally free from any divergences.[10]

Using the current algebra approach, Sunakawa *et al.*[11] have obtained an explicitly Hermitian Hamiltonian, but which contains an infinite series of interaction terms. It is of interest to reconsider its derivation in the light of the new formalism and relate the results to those obtained above for the BZ Hamiltonian, in view of many of the equivalences found elsewhere.[10] Following Landau,[23] it is possible to define a velocity $\vec{\mathrm{v}}(\vec{\mathrm{x}})$,

$$
\vec{\mathrm{J}}(\vec{\mathrm{x}})=\tfrac{1}{2}[\rho(\vec{\mathrm{x}})\vec{\mathrm{v}}(\vec{\mathrm{x}})+\vec{\mathrm{v}}(\vec{\mathrm{x}})\rho(\vec{\mathrm{x}})]\,. \qquad (16)
$$

The commutation relations that $\rho(\vec{\mathrm{x}})$ and $\vec{\mathrm{v}}(\vec{\mathrm{x}})$ must now satisfy are given by[11,48]

$$
\begin{aligned}
&[v_j(\vec{\mathrm{x}}),\rho(\vec{\mathrm{x}}')]_-=-\frac{i\hbar}{m}\frac{\partial}{\partial x^j}\delta^{(3)}(\vec{\mathrm{x}}-\vec{\mathrm{x}}')\,, \\
&\rho(\vec{\mathrm{x}}')[v_i(\vec{\mathrm{x}}),v_j(\vec{\mathrm{x}}')]_-=\frac{i\hbar}{m}\delta^{(3)}(\vec{\mathrm{x}}-\vec{\mathrm{x}}')[\vec{\nabla}\times\vec{\mathrm{v}}(\vec{\mathrm{x}})]_k \\
&\qquad (i,j,k)\ \text{cyclic}\,.
\end{aligned}
\qquad (17)
$$

These follow as a consequence of the commutation relations (3). Adopt $\rho(\vec{\mathrm{x}})$ and $\vec{\mathrm{v}}(\vec{\mathrm{x}})$ as a set of collective variables. The Hamiltonian (4) can be written in terms of the Fourier components of ρ_k and $\vec{\mathrm{v}}_k$[11,48] if one expands $\rho(\vec{\mathrm{x}})^{-1}=[N/\Omega+\rho'(\vec{\mathrm{x}})]^{-1}$ in powers of $\Omega\rho'(\vec{\mathrm{x}})/N$. Thus, one must assume that the fluctuations in $\rho'(\vec{\mathrm{x}})$ do not ever become as large as $-N/\Omega$:

$$
\begin{aligned}
\vec{\mathrm{v}}_k &= \frac{\sqrt{N}m}{\Omega}\int d^3x\,\vec{\mathrm{v}}(\vec{\mathrm{x}})e^{-i\vec{\mathrm{k}}\cdot\vec{\mathrm{x}}}\,, \\
\vec{\mathrm{v}}(\vec{\mathrm{x}}) &= \frac{1}{m\sqrt{N}}\sum_{\vec{\mathrm{k}}\neq 0}\vec{\mathrm{v}}_k e^{i\vec{\mathrm{k}}\cdot\vec{\mathrm{x}}}\,;
\end{aligned}
\qquad (18)
$$

$$H_s = E_0^B + \sum_{\vec{k}\neq 0}\left[\frac{1}{2m}\vec{v}_k\cdot\vec{v}_k + \left(\frac{\hbar^2 k^2}{8m} + \frac{N}{2\Omega}V(k)\right)\rho_k\rho_{-k}\right] + \frac{1}{\sqrt{N}}\sum_{\vec{k}_1\vec{k}_2\vec{k}_3}\delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,\vec{0}}\left(\frac{1}{2m}\vec{v}_{-k_1}\cdot\rho_{k_3}\cdot\vec{v}_{-k_2} + \frac{\hbar^2}{8m}(\vec{k}_1\cdot\vec{k}_2)\rho_{k_1}\rho_{k_2}\rho_{k_3}\right)$$

$$+\frac{\hbar^2}{8m}\sum_{\rho=0}^{\infty}\left(\frac{1}{\sqrt{N}}\right)^{p+2}(-1)^{p+1}\sum_{\vec{k}_1\vec{k}_2\cdots\vec{k}_{p+4}}\delta_{\vec{k}_1+\vec{k}_2+\cdots+\vec{k}_{p+4},\vec{0}}\vec{k}_1\cdot\vec{k}_{p+4}\rho_{k_1}\rho_{k_2}\cdots\rho_{k_{p+4}}. \tag{19}$$

Note that H_s is an infinite series, Hermitian Hamiltonian. As we are interested in the superfluid state at $T=0$ °K, we will restrict our discussion to irrotational velocity fields,

$$\vec{\nabla}\times\vec{v}(\vec{x}) = 0 .$$

With this restriction on $\vec{v}(\vec{x})$, Berdahl[12] has shown that the phase variable approach of Nishiyama[13] is equivalent to the Sunakawa approach. Comparing Eq. (19) with the infinite series written by Berdahl, it may be noted that $\vec{v}(\vec{x})$ is proportional to the gradient of the phase[13]. In this subspace, the commutation relations for ρ_k and $\vec{v}_k$ are given by

$$\begin{aligned}&[\rho_k,\rho_{k'}]_- = [\vec{v}_k,\vec{v}_{k'}]_- = 0 ,\\ &[\vec{v}_k,\rho_{k'}]_- = \hbar\vec{k}\delta_{k,k'} .\end{aligned} \tag{20}$$

This makes $\vec{v}_k$ canonically conjugate to ρ_k. We can now introduce creation and annihilation operators for the excitations:

$$\begin{aligned}&\rho_k = \sqrt{\lambda_k}(B_k + B^*_{-k}) ,\\ &\vec{v}_k = (\hbar\vec{k}/2\sqrt{\lambda_k})(B_{-k} - B^*_k) ,\end{aligned} \tag{21}$$

where B_k and B^*_k obey the usual Bose commutation relations and B^*_k is the Hermitian conjugate of B_k. The Hamiltonian can be expressed in terms of B_k and B^*_k but will not be written here. See Refs. 11 and 48 for further details of this derivation.

We would now like to consider expressions (10) and (19) in more detail. As the Hamiltonians were both derived from (4), we ask the question if there is a relation between $\vec{R}_k$ and $\vec{v}_k$, which would make $H_{\rm BZ}$ identically equal to H_s. Since both $\vec{R}_k$ and $\vec{v}_k$ obey the same commutation relations with ρ_k and among themselves, we look for a linear relation between $\vec{R}_k$ of BZ theory and $\vec{v}_k$ of Sunakawa theory but the dependence on ρ_k could be more complex. One can show after a little algebra that indeed

$$\vec{v}_k = \vec{R}_k + \frac{\hbar}{2}\sum_{p=1}^{\infty}(-1)^p\left(\frac{1}{\sqrt{N}}\right)^p \times \sum_{\vec{k}_1\cdots\vec{k}_{p+1}}\delta_{\vec{k}+\vec{k}_1+\cdots+\vec{k}_{p+1},\vec{0}}\vec{k}_{p+1}(\rho_{k_1}\rho_{k_2}\cdots\rho_{k_{p+1}}) . \tag{22}$$

The series can be summed to obtain

$$\vec{v}_k = \vec{R}_k + \tfrac{1}{2}\hbar\vec{k}\rho_{-k} - \frac{\sqrt{N}\hbar}{2i\Omega}\int d^3x\,[\rho^{-1}(\vec{x})\vec{\nabla}\rho(\vec{x})]e^{-i\vec{k}\cdot\vec{x}} . \tag{23}$$

In coordinate space

$$\vec{v}(\vec{x}) = \frac{\hbar}{mi}\vec{\nabla}\frac{\delta}{\delta\rho(\vec{x})} - \frac{\hbar}{2mi}\rho^{-1}(\vec{x})\vec{\nabla}\rho(\vec{x}) . \tag{24}$$

Using this in (16) we obtain

$$\vec{J}(\vec{x}) = \frac{\hbar}{mi}\left(\rho(\vec{x})\vec{\nabla}\frac{\delta}{\delta\rho(\vec{x})} - \tfrac{1}{2}\vec{\nabla}\rho(\vec{x})\right) \tag{25}$$

which is the same result as (5). Thus the velocity operator $\vec{v}(\vec{x})$ used by Sunakawa gives the same expression for $\vec{J}(\vec{x})$ employed in the BZ formulation. The two Hamiltonians are just the result of two different manipulations of the operator $\vec{J}(\vec{x})$, but consistent with the basic commutation relations. Tsu-Shen Chang[22] has also obtained an infinite-series Hamiltonian by a similar procedure. He chose to expand $\rho(x)^{-1}$ first and used the form for $\vec{J}(\vec{x})$ given by Eq. (5). This is clearly just another manipulation of the same Hamiltonian and provides no new information. Since the Sunakawa Hamiltonian was derived on the explicit assumption of an irrotational fluid, we clearly see that $H_{\rm BZ}$ also describes a superfluid.

The relationship between the $b_k, b_k^\dagger$, and B_k, B_k^* operators sought in the Appendix of Ref. 10 is now apparent after symmetrizing the terms in the multiple sum in Eq. (22) and using the δ function to simplify it further. Thus,

$$(B_k + B^*_{-k}) = (b_k + b^\dagger_{-k}) = \rho_k/\sqrt{\lambda_k} ,$$

$$(B_{-k} - B^*_k) = (b_{-k} - b^\dagger_k) + \sqrt{\lambda_k}\sum_{p=1}^{\infty}(-1)^{p+1}\left(\frac{1}{\sqrt{N}}\right)^p\frac{1}{p+1} \times \sum_{\vec{k}_1\cdots\vec{k}_{p+1}}\delta_{\vec{k}+\vec{k}_1+\cdots+\vec{k}_{p+1},\vec{0}}(\rho_{k_1}\rho_{k_2}\cdots\rho_{k_{p+1}}) .$$

Yee[20] has discussed the extension of the current algebra approach to describe the *rotational flow*. By introducing an additional current, the new excitations can easily be accommodated. To $\vec{J}(\vec{x})$ of (10), one could add

$$\vec{K}(\vec{x}) = \tfrac{1}{2}[\sigma(\vec{x})\vec{\nabla}\mu(\vec{x}) + \vec{\nabla}\mu(\vec{x})\sigma(\vec{x})] , \tag{27}$$

where $\sigma(\vec{x})$ and $\mu(\vec{x})$ satisfy commutation relations given in Ref. 20. Yee has expressed the Hamiltonian in terms of this new current, but a practical quantization scheme for these new variables is not presently available. This is one area in which much new work is needed.

In summary, in this section we have made an explicit connection between H_{BZ} and H_{S} by way of current algebra. While the current operator is the same for both Hamiltonians, the manipulations were different. Introducing $\vec{\mathrm{J}}(\vec{\mathrm{x}})$, Eq. (10), directly into the Hamiltonian (4) eliminates the $\rho^{-1}(\vec{\mathrm{x}})$ term and thus the Hamiltonian has a finite number of terms. If on the other hand one expands $\rho^{-1}(\vec{\mathrm{x}})$ in a power series and chooses to quantize the velocity operator instead, one is left with an infinite-series Hamiltonian H_{S}. Explicit calculations of the energy and other physical quantities in perturbation expansions give completely equivalent results, but H_{BZ} is considerably easier to handle.[10,15]

III. GREEN'S-FUNCTION THEORY BASED ON H_{BZ}

In order to develop a finite-temperature theory, the statistical operator P_{op}, associated with H_{BZ}, was defined in I,

$$P_{\mathrm{op}} = \sum_n |\Psi_n\rangle e^{-\beta E_n}\langle\tilde{\Phi}_n|, \quad \beta = 1/kT . \tag{28}$$

The eigenfunctions of H_{BZ} and $H_{\mathrm{BZ}}^\dagger$ are assumed to be "simple," i.e., obey the equations

$$\begin{aligned} H_{\mathrm{BZ}}|\Psi_n\rangle &= E_n|\Psi_n\rangle , \\ \langle\tilde{\Phi}_n|H_{\mathrm{BZ}} &= \langle\tilde{\Phi}_n|\tilde{E}_n^* . \end{aligned} \tag{29}$$

The range of $(H_{\mathrm{BZ}} - E)$ is assumed to be closed, and therefore the right eigenvalue of H_{BZ}, E_n, is equal to the left eigenvalue of $H_{\mathrm{BZ}}, \tilde{E}_n^*$. The corresponding right and left eigenfunctions $|\Psi_1\rangle, |\Psi_2\rangle, \ldots,$ and $\langle\tilde{\Phi}_1|, \langle\tilde{\Phi}_2|, \ldots$ of H_{BZ} together form a biorthogonal, complete set. It has been shown in I that $E_n = \tilde{E}_n$, where $\tilde{E}_n$ is the right eigenvalue of $H_{\mathrm{BZ}}^\dagger$. For more details, see I.

The thermodynamic averages of physical quantities may now be defined:

$$\langle\chi\rangle = \mathrm{Tr}P_{\mathrm{op}}\chi/\mathrm{Tr}P_{\mathrm{op}} , \tag{30}$$

where

$$\mathrm{Tr}A = \sum_n \langle\tilde{\Phi}_n|A|\Psi_n\rangle .$$

The biorthogonal set of states must be used consistently, as in the definition of the trace.

Since the BZ Hamiltonian does not conserve quasiparticle number, a matrix Green's function must be employed.[3] The "Heisenberg representation" of b_k and $b_k^\dagger$ are given in I. For operators acting only in the space of $\{|\Psi\rangle, \langle\tilde{\Phi}|\}$, we have

$$i\hbar\frac{d}{dt}\Theta = [\Theta, H_{\mathrm{BZ}}]_- . \tag{31}$$

Henceforth, we will work only with operators acting on the space of $\{|\Psi\rangle, \langle\tilde{\Phi}|\}$ in a consistent way. The final results in the development involving the states $\{|\Phi\rangle, \langle\tilde{\Psi}|\}$ are entirely equivalent as discussed in I. The one-boson matrix Green's function may be defined as

$$i\hbar\underline{\mathrm{G}}(k,t) = \frac{\mathrm{Tr}[P_{\mathrm{op}}(\underline{\Phi}_k(t)\underline{\Phi}_k^\dagger(0))_+]}{\mathrm{Tr}\{P_{\mathrm{op}}\}} , \tag{32}$$

where $\underline{\Phi}_k$ is a column matrix,

$$\underline{\Phi}_k(t) = \begin{pmatrix} b_k(t) \\ b_{-k}^\dagger(t) \end{pmatrix} . \tag{33}$$

Dyson's equation becomes a single matrix equation. In momentum space,

$$\underline{\mathrm{G}}(k,\omega) = \underline{\mathrm{G}}^0(k,\omega) + \underline{\mathrm{G}}^0(k,\omega)\underline{\Sigma}(k,\omega)\underline{\mathrm{G}}(k,\omega) . \tag{34}$$

Green's function for the "unperturbed" system $\underline{\mathrm{G}}^0(k,\omega)$ is *diagonal* and

$$\begin{aligned} G_{11}^0(k,\omega+i\eta) &= [\hbar\omega - E_B(k) + i\eta]^{-1} , \\ G_{22}^0(k,\omega+i\eta) &= G_{11}^0(k,-\omega-i\eta) . \end{aligned} \tag{35}$$

The self-energy matrix $\underline{\Sigma}$ can be derived by a linked-cluster diagrammatic expansion as was done by Straley for $T = 0$ °K even though he observed that the non-Hermiticity of H_{BZ} implies that the usual "time reversal" and "crossing" symmetry do not hold. We have given here a theory valid for nonzero temperatures. We employ an equation-of-motion method to evaluate the self-energy matrix. The equation of motion for $\underline{\mathrm{G}}(k,t)$ gives rise to terms involving new Green's functions containing three operators in view of the structure of H_{BZ}. We then derive equations of motion for these and simplify them by use of the familiar factorization method. This procedure leads to order $(1/N)$,

$$\begin{aligned} \Sigma_{11}(k,\omega+i\eta) = &-18\sum_{\vec{k}_2}\frac{\gamma_a^{(3)}(k,k_2,-k-k_2)\gamma_b^{(3)}(k,k_2,-k-k_2)[1+2n_B(k_2)]}{\hbar\omega + E_B(k_2) + E_B(k+k_2) + i\eta} \\ &+2\sum_{\vec{k}_2}\frac{\gamma_c^{(3)}(k,k_2,-k-k_2)\gamma_d^{(3)}(k,k_2,-k-k_2)[1+2n_B(k_2)]}{\hbar\omega - E_B(k_2) - E_B(k+k_2) + i\eta} \\ &-4\sum_{\vec{k}_2}\frac{\gamma_c^{(3)}(k_2,k,-k-k_2)\gamma_d^{(3)}(k_2,k,-k-k_2)[n_B(k_2) - n_B(k+k_2)]}{\hbar\omega + E_B(k+k_2) - E_B(k_2) + i\eta} , \end{aligned} \tag{36a}$$

$$\Sigma_{21}(k,\omega+i\eta)=-6\sum_{\vec{k}_2}\gamma_a^{(3)}(k,k_2,-k-k_2)\gamma_d^{(3)}(k,k_2,-k-k_2)[1+2n_B(k_2)]$$

$$\times\left(\frac{1}{\hbar\omega+E_B(k_2)+E_B(k+k_2)+i\eta}+\frac{1}{-\hbar\omega+E_B(k_2)+E_B(k+k_2)-i\eta}\right)$$

$$-4\sum_{\vec{k}_2}\frac{\gamma_c^{(3)}(k_2,k,-k-k_2)\gamma_c^{(3)}(-k-k_2,k,k_2)}{-\hbar\omega+E_B(k+k_2)-E_B(k_2)-i\eta}[n_B(k_2)-n_B(k+k_2)], \tag{36b}$$

$$\Sigma_{12}(k,\omega+i\eta)=-6\sum_{\vec{k}_2}\gamma_b^{(3)}(k,k_2,-k-k_2)\gamma_c^{(3)}(k,k_2,-k-k_2)[1+2n_B(k_2)]$$

$$\times\left(\frac{1}{\hbar\omega+E_B(k_2)+E_B(k+k_2)+i\eta}+\frac{1}{-\hbar\omega+E_B(k_2)+E_B(k+k_2)-i\eta}\right)$$

$$-4\sum_{\vec{k}_2}\frac{\gamma_d^{(3)}(k_2,k,-k-k_2)\gamma_d^{(3)}(-k-k_2,k,k_2)[n_B(k_2)-n_B(k+k_2)]}{\hbar\omega+E_B(k+k_2)-E_B(k_2)+i\eta}, \tag{36c}$$

$$\Sigma_{22}(k,\omega+i\eta)=\Sigma_{11}(k,-\omega-i\eta). \tag{36d}$$

Here $n_B(k)=\{\exp[\beta E_B(k)]-1\}^{-1}$. It should be observed that this finite-temperature theory is not valid for all temperatures. As the Hamiltonian describes only an irrotational fluid, the finite-temperature extension given here is only valid when the superfluid density is much greater than the normal fluid density, i.e., $T<0.5$ °K. The rotational states of the fluid are important for higher temperatures and this Hamiltonian does not incorporate these processes.

The excitation spectrum is given by the poles of $\underline{G}$ which occur for ω for which

$$\det|[G^0_{\alpha\beta}(k,\omega)]^{-1}-\Sigma_{\alpha\beta}(k,\omega)|=0, \tag{37}$$

that is

$$-\{\hbar\omega-\tfrac{1}{2}[\Sigma_{11}(k,\omega)-\Sigma_{22}(k,\omega)]\}^2$$
$$+\{E_B(k)+\tfrac{1}{2}[\Sigma_{11}(k,\omega)+\Sigma_{22}(k,\omega)]\}^2$$
$$-\Sigma_{12}(k,\omega)\Sigma_{21}(k,\omega)=0. \tag{38}$$

For $T=0$ °K, Straley has shown that in the long-wavelength limit, $\Sigma_{\alpha\beta}(k,\omega)\sim k$ and therefore the spectrum will not display a gap. To order $(1/N)$, the excitation spectrum at $T=0$ °K is

$$E(k)=E_B(k)+\epsilon_2(k)+O(1/N^2), \tag{39}$$

$$\epsilon_2(k)=2P\sum_{\vec{k}_2}\frac{\gamma_c^{(3)}(k,k_2,-k-k_2)\gamma_d^{(3)}(k,k_2,-k-k_2)}{E(k)-E_B(k_2)-E_B(k+k_2)}-18\sum_{\vec{k}_2}\frac{\gamma_a^{(3)}(k,k_2,-k-k_2)\gamma_b^{(3)}(k,k_2,-k-k_2)}{E(k)+E_B(k_2)+E_B(k+k_2)}. \tag{40}$$

This is the same expression derived earlier in I using only $G_{11}(k,t)$. The ground-state liquid-structure factor $S(k)$ at $T=0$ °K can also be derived in terms of this matrix Green's function, because

$$S(k)=\langle\rho_k(0^+)\rho_k^\dagger(0)\rangle=\lambda_k\langle(b_k+b^\dagger_{-k})(b_k^\dagger+b_{-k})\rangle=\lambda_k\lim_{T\to0}\lim_{t\to0^+}\sum_{\alpha\beta=1}^{2}G_{\alpha\beta}(k,t). \tag{41}$$

It is well known that

$$\lim_{t\to0^+}\underline{G}(k,t)=-\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\,\mathrm{Im}(\underline{G}(k,\omega))[1+n(\omega)], \tag{42}$$

and thus

$$S(k)=-\lambda_k\lim_{T\to0}\left(\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\,\mathrm{Im}(G^0_{\alpha\alpha}(k,\omega))[1+n(\omega)]+\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\,\mathrm{Im}(G^0_{\alpha\beta}(k,\omega)\Sigma_{\beta\gamma}(k,\omega)\,G_{\gamma\alpha}(k,\omega))[1+n(\omega)]\right). \tag{43}$$

Where one must sum over repeated indices, and $n(\omega)=1/(e^{\beta\omega}-1)$. In principle (42) can be evaluated using (34) directly. But we are here interested in computing $S(k)$ to order $1/N$ only. This involves only the diagonal elements of $\underline{G}$ in (43) and we obtain after some algebra,

$$S(k)=\lambda_k+36\lambda_k\sum_{\vec{k}_2}\frac{\gamma_a^{(3)}(k,k_2,-k-k_2)\gamma_b^{(3)}(k,k_2,-k-k_2)}{[E_B(k)+E_B(k_2)+E_B(k+k_2)][E(k)+E_B(k_2)+E_B(k+k_2)]}$$

$$+6\lambda_k\sum_{\vec{k}_2}\frac{\gamma_a^{(3)}(k,k_2,-k-k_2)\gamma_d^{(3)}(k,k_2,-k-k_2)+\gamma_b^{(3)}(k,k_2,-k-k_2)\gamma_c^{(3)}(k,k_2,-k-k_2)}{E(k)+E_B(k)}$$

$$\times\left(\frac{1}{E_B(k)+E_B(k_2)+E_B(k+k_2)}+\frac{1}{E(k)+E_B(k_2)+E_B(k+k_2)}\right), \tag{44}$$

$$S(k)\equiv\lambda_k+S_1(k).$$

It should be noted that Eqs. (40) and (44) reduce to the Rayleigh-Schrödinger result when $E(k)=E_B(k)$ on the right-hand side. These equations will be used later to evaluate the excitation spectrum for liquid He II.

A third quantity of interest which was not derived in I is the momentum distribution function in the ground state. This would verify the presence of off-diagonal long-range order in the one-particle density matrix. Owing to the presence of interaction, all particles are not expected to be in the zero-momentum condensate at $T=0$ °K in contrast with the noninteracting system. The momentum distribution function was first derived by Bogoliubov[1] using his field-theoretic method, which had explicitly built in the zero-momentum condensate. Zubarev[49] derived the same result using the BZ formalism with N_0 replaced by N, but his derivation was obscure. We have therefore given here a derivation of this result. The lowest-order wave function using the BZ analysis is given by Eq. (15). The one-particle density matrix defined in terms of the wave function is

$$n(\vec{r}_1-\vec{r}_1')=\frac{N\int\int\Psi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\Psi(\vec{r}_1',\vec{r}_2,\ldots,\vec{r}_N)d^3r_2\cdots d^3r_N}{\int\int|\Psi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)|^2d^3r_1d^3r_2\cdots d^3r_N}. \tag{45}$$

The occupation number for the state with momentum $\vec{k}$ is obtained from

$$n(k)=\int n(r)e^{-i\vec{k}\cdot\vec{r}}d^3r. \tag{46}$$

Using φ_0 from (15), we can obtain $n(k)$ to lowest order in a $(1/N)$ expansion. ρ_k is defined in (7) as a function of $(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$ and the normalization integral is easily evaluated,

$$\int\cdots\int|\varphi_0|^2d^3r_1\cdots d^3r_N=\Omega^N\exp\left(\frac{1}{2}\sum_{k\neq0}f_k\right), \tag{47}$$

where $f_k=(1-1/\lambda_k)$. To evaluate the remaining integral in (45), write ρ_k in the form

$$\rho_k=\frac{e^{i\vec{k}\cdot\vec{r}_1}}{\sqrt{N}}+\frac{1}{\sqrt{N}}\sum_{j=2}^{N}e^{i\vec{k}\cdot\vec{r}_j}$$

and make the transformation $\vec{r}_i\,(i\neq1)\rightarrow\vec{r}_i+\frac{1}{2}(\vec{r}_1+\vec{r}_1')$ in this integral. Defining $\vec{r}=(\vec{r}_1-\vec{r}_1')$ and after noting $n(\vec{r}=0)=N/\Omega$, we obtain

$$n(\vec{r})=\frac{N}{\Omega}+\frac{N}{\Omega^N}\int\cdots\int d^3r_2\cdots d^3r_N\left[\exp\left(\frac{1}{N}\sum_{\vec{k}\neq0}f_k\sum_{i>j=2}^{N}e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}\right)\right]$$

$$\times\left[\exp\left(\frac{1}{N}\sum_{\vec{k}\neq0}f_k\cos[\tfrac{1}{2}(\vec{k}\cdot\vec{r})]\sum_{j=2}^{N}e^{i\vec{k}\cdot\vec{r}_j}\right)-\exp\left(\frac{1}{N}\sum_{\vec{k}\neq0}f_k\sum_{j=2}^{N}e^{i\vec{k}\cdot\vec{r}_j}\right)\right]. \tag{48}$$

To lowest order in $1/N$, one notes that all terms in the expansion of the exponential in the first factor and only the term

$$\frac{1}{2!}\frac{1}{N^2}\sum_{\vec{k}_1\vec{k}_2\neq0}f_{k_1}f_{k_2}(\cos\tfrac{1}{2}\vec{k}_1\cdot\vec{r}\,\cos\tfrac{1}{2}\vec{k}_2\cdot\vec{r}-1)\sum_{j_1,j_2=2}^{N}e^{i(\vec{k}_1\cdot\vec{r}_{j_1}+\vec{k}_2\cdot\vec{r}_{j_2})}$$

in the second factor contribute. After some algebra one obtains

$$n(\vec{r}) = \frac{N}{\Omega} + \frac{1}{2\Omega} \sum_{\vec{k} \neq 0} f_k^2 (1 + f_k + f_k^2 + \cdots)$$

$$\times (\cos^2 \tfrac{1}{2}\vec{k}\cdot\vec{r} - 1) + O(1/N)$$

$$= \frac{N}{\Omega} - \frac{1}{4\Omega} \sum_{\vec{k} \neq 0} \left(1 - \frac{1}{\lambda_k}\right)^2 \lambda_k (1 - \cos \vec{k}\cdot\vec{r})$$

$$+ O(1/N). \qquad (49)$$

The occupation number $n(k)$ [Eq. (31)] in the momentum space is thus

$$n(k) = \left[N - 1/4 \sum_{p \neq 0} \left(1 - \frac{1}{\lambda_p}\right)^2 \lambda_p \right] \delta_{\vec{k},\vec{0}}$$

$$+ \tfrac{1}{4} \left(1 - \frac{1}{\lambda_k}\right)^2 \lambda_k + O(1/N). \qquad (50)$$

The probability distribution function for the single-particle momentum $\vec{k}$ is thus

$$W(k) = \frac{N_0}{N} \delta^{(3)}(\vec{k}) + \frac{1}{4(2\pi)^3} \frac{\Omega}{N} \left(1 - \frac{1}{\lambda_k}\right)^2 \lambda_k + O(1/N^2), \qquad (51)$$

where

$$\frac{N_0}{N} = 1 - \frac{1}{4N} \sum_{k \neq 0} \left(1 - \frac{1}{\lambda_k}\right)^2 \lambda_k + O(1/N^2). \qquad (52)$$

This result agrees with the result of Zubarev.[49]

IV. SUPERFLUID LIQUID HELIUM II

The excitation spectrum, the liquid-structure factor, and occupation number which were calculated in Sec. III can be evaluated for liquid helium if the interatomic potential is known. While there are many empirical formulas for $V(r)$, all contain a hard core, which means that their Fourier transforms do not exist. One could use a soft-core potential but then there would be at least two free parameters, the height of the soft core and its range. The resulting expressions for $E(k)$ and $S(k)$ would clearly depend on these parameters critically and any comparison to experimental results would not be unequivocal. Instead, we would prefer to use one experimental quantity, say $S(k)$, as the only input into the expressions for $E(k)$ and N_0/N. This can be done by eliminating λ_k from (40) in favor of $S(k)$ given by Eq. (44):

$$E(k) = E_F(k) + [E_B(k)/\lambda_k] S_1(k) + \epsilon_2(k) + O(1/N^2), \qquad (53)$$

where

$$E_F(k) = \hbar^2 k^2 / 2mS(k). \qquad (54)$$

In the remaining integrals $S_1(k)$ and $\epsilon_2(k)$ let $\lambda_k \to S(k)$. The error incurred then would clearly be of $O(1/N^2)$. Thus to the order we are considering, we can calculate $E(k)$ in terms of the experimental structure factor $S(k)$. A similar procedure has also been suggested by Nishiyama.[13] One feature of our calculation is the appearance of $E(k)$ in the expressions for the excitation spectrum (40) and the structure factor (44). To evaluate the remaining integrals, change the integration variable $\vec{k}_2 \to \vec{k}_2 - \frac{1}{2}\vec{k}$. The resulting integrand will contain no singularities for all $E(k)$ less than $E_F(k)$ and $2E_F(k_0)$, $k_0 = 1.9$ Å^{-1}, which is satisfied for the phonon-roton spectrum of interest. We[10] have already shown that $E(k) = E_F(k) + O(k^3)$ for $k \to 0$, as it should.

$S(k)$ has been measured experimentally by both x-ray and neutron scattering techniques. It should be noted that $S(k)$ is quite difficult to measure accurately and problems arise in normalizing it. FC have shown that $S(k)$ should satisfy the normalization condition

$$-2\pi^2 \rho_0 = \int_0^\infty k^2 [S(k) - 1]\, dk. \qquad (55)$$

For liquid helium at normal vapor pressure, using the known density ρ_0, the left-hand side is equal to -0.43 Å^{-3}. FC and JF used an $S(k)$ for which the right-hand side gave $+0.44$ Å^{-3}. There are at least three probable reasons for obtaining this result: (i) the data used in the evaluation was taken at 2.06°K, (ii) some arbitrary extrapolation had to be made for $k < 0.9$ Å^{-1} as $S(k)$ must go to zero as $k \to 0$ for $T = 0$°K, and lastly (iii) $S(k)$ was measured only up to 6 Å^{-1}. By using the more recent data of Achter and Meyer,[40] we can eliminate the first two. This data was taken at $T = 0.79$°K. The difference between it and the $T = 0$°K result should only be in the region $k < 0.4$ Å^{-1}. In this region, we extrapolated the result at $k = 0.4$ Å^{-1} linearly to zero. This gives the correct sound velocity. This data, however, only went up to 4.5 Å^{-1}; for larger values we let $S(k)$ be equal to its asymptotic value of unity. To check whether the contributions for values of $k > 4.5$ Å^{-1} are important in the evaluation of the integrals in (53), we used a model[11] $S(k)$ which oscillated about its asymptotic value for large k. It was found that the combination of integrands in (53) when integrated did not depend on the asymptotic form of $S(k)$ but each integral in (53) did. Thus the major errors incurred in the calculation of $E(k)$ are related to the experimental uncertainty in $S(k)$ only and is probably of the order of 5%. The evaluation of the integral in (55) using this $S(k)$ gave us a value of -1.3 Å^{-3}. But this integral is found to be very sensitive to the exact structure of $S(k)$ for all k, in contrast to the evaluation of (53).

Thus using $S(k)$ from the recent x-ray scattering experiments of AM, we evaluated $E(k)$ at normal vapor pressure. The results are given in Fig. 1. For comparison, we have also calculated $E(k)$ from the JF formula using this $S(k)$. Note that our result is better in the low-k region and also has a lower roton minimum, $\Delta_0^{BZ} \approx 12.3\,^\circ\mathrm{K}$ compared to $\Delta_0^{JF} \approx 12.7\,^\circ\mathrm{K}$. The region from 0.4 to 0.8 $\mathrm{\AA}^{-1}$, in which both our result and the JF result are lower than the experimental results of Cowley and Woods,[42] is of interest. Hallock[41] has recently measured $S(k)$ at very low temperatures from $k = 0$ to 1.1 $\mathrm{\AA}^{-1}$. In this region, Hallock's data are lower than those of AM. The difference is not explained but is large enough to make our results for the energy agree better with experiment in this region as $E_F(k)$ would then increase. Hallock did not measure $S(k)$ for all k, so his data are not useful in evaluating $E(k)$ for any k. The probable sources of error in our theory are the uncertainty in $S(k)$ and contributions from terms of order $(1/N^2)$ which probably become important for larger values of k. While the agreement with experiment is only fair, it seems to be the best such theoretical calculation involving experimental $S(k)$. The other types of numerical evaluation of $E(k)$ are based on model potentials with at least two free parameters.

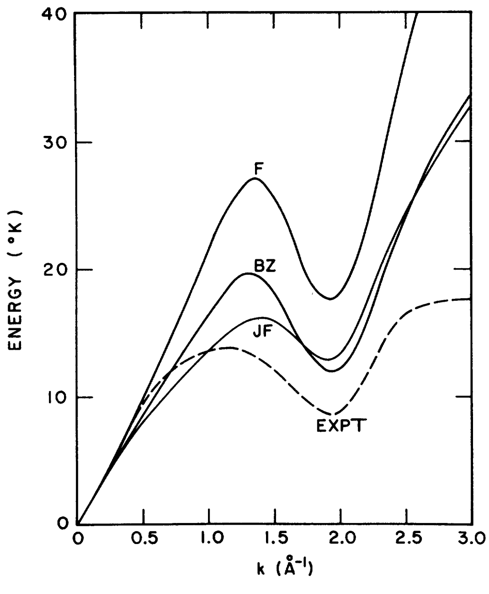

FIG. 1. Excitation spectrum of liquid He II. The curve F is $E_F(k)$ using the Achter-Meyer structure factor; the curve BZ is calculated from the BW perturbation expansion (53). For comparison, JF is the Jackson and Feenberg (Ref. 33) second-order BW perturbation expansion reevaluated using the AM structure factor. The dashed lines are the experimental results of Cowley and Woods (Ref. 42).

One could also evaluate N_0/N by a similar method by replacing λ_k with $S(k)$ in (52). We have done this, but we find N_0/N to be negative (-0.3). We believe this to be a result of the sensitivity of the integral to the exact structure of λ_k for all k. We are at this time unable to draw any further conclusions about this result. This seems to be similar to the difficulty encountered by FC, JF, and the present authors in computing (55).

V. CHARGED BOSE GAS

From our discussion of liquid helium, it is clear that the difficulties arising from a lack of knowledge of the Fourier transform of the potential $V(k)$ are a major stumbling block in deriving numerical answers from the theory. In this section, we would like to apply the BZ formalism to the case of a charged Bose gas, for which $V(k)$ is well known. To the best of our knowledge, the collective-variable approaches of BZ or S have not been applied to this problem, except for the calculation of ground-state energy by Berdahl.[12]

The Fourier transform of the Coulomb potential is

$$\begin{aligned} V(k) &= 4\pi e^2/k^2, \quad k \neq 0 \\ V(k=0) &= 0\,. \end{aligned} \tag{56}$$

$V(k=0)$ is a result of a neutralizing positive-charge background. Following Ref. 45, we introduce convenient dimensionless quantities:

$$\omega_{pl} = \left(\frac{4\pi\rho e^2\hbar^2}{m}\right)^{1/2}, \quad \vec{t} = \left(\frac{2m\omega_{pl}}{\hbar^2}\right)^{-1/2}\vec{k}\,, \qquad \lambda_t = \frac{t^2}{(1+t^4)^{1/2}}, \quad E_B(t) = \frac{t^2\omega_{pl}}{\lambda_t}\,. \tag{57}$$

Using (57) in the expression for the ground-state energy given in Ref. 10, employing RS perturbation theory, we get the exact result obtained by Brueckner[4] in the high-density limit. It may be pointed out that there are no infinities such as those encountered by Brueckner in our formulation. Lee[43] showed that the method of CBF in the uniform limit gave exactly the same result as that of Brueckner for the ground-state energy. Berdahl and Lee[16] showed that for boson systems, the ground-state energy in RS perturbation theory based on BZ is the same as that obtained by the use of CBF method in the uniform limit.

Ma and Woo[44] have shown that the single-particle excitation spectrum has a cutoff momentum. In the lowest order of approximation, this cutoff is at $t = 2$. The second-order correction to the excitation spectrum was first calculated by them using standard field-theoretic techniques in the high-density limit. They found that the cutoff momentum is now at $t=\sqrt{2}$. Bhattacharyya and Woo[45] found equivalent results with those obtained by the method of CBF. We[10] have shown these results agree exactly with a RS perturbation expansion in the BZ formalism for arbitrary $V(k)$. In this region, the integrand contains no singularity and BW perturbation theory is not needed as in the case of liquid helium. The results for the charged Bose gas are given in Refs. 44 and 45 and need not be repeated here, in view of the equivalences mentioned above.

Bhattarcharyya and Woo attempted to calculate the first-order correction to $S(k)$ but did not have an explicit formula for it such as Eq. (44) or the RS form given in I. By forcing the JF formula for the first excited state energy to be equal to the CBF result with a Jastow-type correlating function, they were able to deduce an $S(k)$. We believe this method to be of dubious value as there are additional corrections of the same order to the JF result[3] and there is no *a priori* reason to believe the two results to be equivalent. In the high-density limit, $S(k)$ can be expanded in powers of $(r_s^{3/4})$ and we obtain from the RS formula given in I [or equivalently let $E(k)\rightarrow E_B(k)$ on the right-hand side of Eq. (44)],

$$S(k)=\lambda_k+r_s^{3/4}S_1(k)+O(r_s^{3/2})\,. \qquad (58)$$

We have calculated $S_1(k)$ and the results are shown in Fig. 2. We find $S(k)$ to be slightly larger than that found by Bhattarharyya and Woo,[45] in the entire region of k considered by them. Berdahl[50] informs us that he has independently made a calculation of $S_1(k)$ and this agrees with ours. This result has also been confirmed by Family and Gould[51] who used the generalized dielectric formulation.

Foldy[47] was the first to consider the problem of the charged Bose gas. He employed the results obtained by Bogoliubov[1] for a weakly interacting Bose gas to deduce the properties of this system in the high-density limit. In the lowest order, he could evaluate the integrals explicitly that appear for the ground-state energy and the number of particles in the zero-momentum condensate.

Remembering that λ_k in the Bogoliubov theory involves N_0, in (52), Foldy[47] obtained in the lowest order

$$N_0/N=1/(1+0.211r_s^{3/4})$$

$$\simeq 1-0.211r_s^{3/4}+O(r_s^{3/2})\,. \qquad (59)$$

In our theory N appears in place of N_0 and we obtain

$$N_0/N=1-0.211r_s^{3/4}+O(r_s^{3/2}) \qquad (59')$$

and we do not expect the higher-order terms ($r_s^{3/2}$ and higher) to coincide with theories involving N_0.

With our present calculation of $S(k)$, the properties of the charged Bose gas at high densities for $T=0°$ K are thus completely enumerated. In view of the various proofs of equivalences of the results based on different approaches to the problem for arbitrary $V(k)$, the usefulness of the charged Bose gas as a testing ground may have come to an end.

VI. CONCLUDING REMARKS

This paper is a complement to our recent work[10] in several ways. A mathematical method to handle the non-Hermitian Hamiltonian of BZ was developed and the results of a RS perturbation theory of the ground- and excited-state energies, structure factor, and scattering amplitude for two-roton scattering were all shown to be equivalent to another collective-variable theory due to Sunakawa and his co-workers. In the Appendix of I, an attempt was made to relate the two theories directly in view of such a close correspondence of the results. Most importantly in Ref. 15 we showed that our theory for the BZ Hamiltonian is devoid of all divergences such as those present in the S formalism, even though they all are cancelled when the calculation is carried out to an appropriate order in the expansion parameter. In Sec. II of the present paper, by employing the theory of many-body systems with currents as coordinates[18, 19] we establish a complete equivalence of the BZ and S collective-variable formulation of the interacting many-boson system. This demonstration is an answer to the question raised in the Appendix of our recent paper.[10] It does not seem to be well

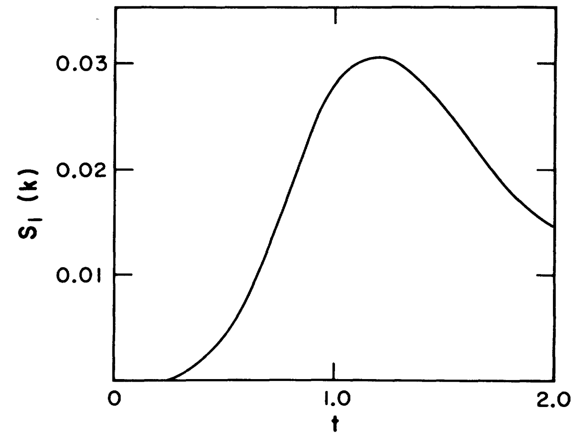

FIG. 2. Second-order contribution to the ground-state liquid-structure factor, $\vec{t}=(2m\omega_{pl}/\hbar^2)^{-1/2}\vec{k}$.

recognized that the collective-variable theory *is not inconsistent* with the notion of the presence of particles in the zero-momentum state, which is expected on general grounds based on the ideas of off-diagonal long-range order in the single-particle density matrix of the boson systems. This was shown by Zubarev[49] but his derivation seemed obscure to us and so we offer our own version of it in Sec. III. Even though the theory does not assume the presence of particles in the zero-momentum state, it is gratifying to find this feature in this formalism. We have also developed a matrix Green's-function theory which generalizes that given in I. We observe that the energy of excitation to order $1/N$ is the same as that derived in I. Also, we could deduce from this matrix Green's function the structure factor, a feature which allows us to compute the excitation spectrum in a consistent way. The second most important feature of any theory of superfluid liquid helium is a fair description of its phonon-roton spectrum which is determined experimentally. In view of the importance of this aspect of the theory, we have given in Sec. IV a fairly detailed account of the various experimental works and their relation to our calculation and other calculations. Our calculation indicates that perhaps a theory of the excitation spectrum which incorporates the experimental structure factor in computing the excitation spectrum as was originally suggested by Feynman[27] can only be improved if the experiments on the structure factor at low temperatures ($T = 0^\circ$ K) can be done accurately for very low ($k < 0.5$ Å^{-1}) to fairly high ($k = 8-10$ Å^{-1}) momenta. We hope to have made this point emphatically in Sec. IV with our discussion of both the theoretical and the experimental results.

We believe that the collective-variable theory (presented in I and here) provides a fairly complete description of the low-temperature ($T < 0.5^\circ$ K) properties of superfluid liquid helium. We are presently examining the extension of this theory to incorporate the microscopic rotational flow in the description of the system which would become important on improving the theory for the entire range of temperatures below and past the transition temperature. Only a formal attempt in this direction has been made by Yee[20] recently.

We have also examined in this paper the model of charged boson gas (Sec. V). We feel that the BZ approach gives a satisfactory description of this system also. We may therefore conclude that the BZ formulation along with the mathematical framework given in I has all the essential features of a complete theory of interacting Bose systems.

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