transmitted through the surface when rings interact with ionic charge previously stored at the surface. We observed several anomalies, especially

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¹S. Cunsolo, G. Dall'oglio, B. Maraviglia, and M. V. Ricci, Phys. Rev. Letters <u>21</u>, 74 (1968); S. Cunsolo and B. Maraviglia, in *Proceedings of the XIth International Conference on Low Temperature Physics*, edited by J. F. Allen, D. M. Finlayson, and D. M. McCall (St. Andrews Press, St. Andrews, Scotland, 1968), p. 265.

²C. M. Surko and F. Reif, Phys. Rev. Letters <u>20</u>, 582 (1968); F. Reif and C. M. Surko, in Ref. 1, pp. 312 and 300; C. M. Surko, thesis (University of California, Berkeley, 1968) (unpublished); C. M. Surko and F. Reif, Phys. Rev. <u>175</u>, 229 (1968); G. W. Rayfield, Phys. Rev. Letters <u>23</u>, 687 (1969), footnote 3.

when the stored charge is of sign opposite to that carried by the rings. We are exploring this situation further.

³S. Cunsolo, B. Maraviglia, and M. V. Ricci, Phys. Letters <u>26A</u>, 605 (1968); S. Cunsolo and B. Maraviglia, Phys. Rev. 187, 292 (1969).

⁴W. Schoepe and G. W. Rayfield, Phys. Letters <u>34A</u>, 133 (1971).

⁵R. Williams, R. S. Crandall, and A. H. Willis, Phys. Rev. Letters 26, 7 (1971).

⁶H. Lamb, *Hydrodynamics* (Dover, New York, 1945).

⁷For the space-charge-limited case, see B. E. Springett. Phys. Rev. A <u>5</u>, 2302 (1972). Our currents are small enough for Eq. (4) to be valid.

⁸B. E. Springett, J. Jortner, and M. H. Cohen, Phys. Rev. <u>159</u>, 183 (1967).

⁹M. W. Cole, Phys. Rev. B 2, 4239 (1970).

PHYSICAL REVIEW A

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Bogoliubov-Zubarev Description of a Weakly Interacting Bose Gas*

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Bogoliubov-Zubarev's exact transformation, specific to a weakly interacting Bose gas having a condensate, yields a Hamiltonian describing a gas of interacting excitations. The non-Hermiticity of the Hamiltonian arises from the nonorthogonality of the physical states; it has some significant consequences. The excitation spectrum is gapless in every approximation; the lowest-order correction is evaluated numerically and shown to be small. It is concluded that the approach presents a prospective method for a quantitative description of the weakly interacting Bose gas.

I. WEAKLY INTERACTING BOSE GAS

This paper deals with the low-lying states of a gas of weakly interacting Bose particles. Liquid helium differs from this problem in that those particles are strongly interacting at short distances. The excitation spectra of the two systems should be qualitatively similar in that (i) they are phononlike for long wavelengths, 1,2 (ii) they exhaust the f sum rule in that limit, 2,3 and (iii) they entirely determine the low-temperature specific heat^{4,5} and normal-fluid density.⁶ Apart from quantitative details, the only aspect of the helium spectrum which is due to the "hard core" is the roton feature.⁷ Thus, despite the absence of a corresponding experimental system, the weakly interacting Bose gas is an important subject for study as a model of a superfluid system. It is notable that few of the first-principles microscopic methods that have been proposed for this problem have yielded realistic results. ⁸

Fifteen years ago Bogoliubov and Zubarev (BZ)⁹ proposed a novel approach to this problem. Their paper has been given little notice; it is my intention to point out the virtues of the method and to suggest that it may allow a realistic calculation of the excitation spectrum of a weakly interacting Bose system.

In Sec. II BZ's method is outlined and commented upon. The non-Hermiticity of the BZ Hamiltonian is shown to be a necessary feature of a representation which treats phonon states as being independent. The role of the condensate in the BZ transformation is elucidated, showing that the method is specific to a superfluid system.

In Sec. III the appropriate Green's-function formalism is introduced, and it is shown that the resultant perturbation expansion gives a gapless spectrum in every approximation. The lowest-order corrections are evaluated and shown to be small.

In Sec. IV connection is made with other ap-

proaches that have been proposed for this problem.

II. OUTLINE OF METHOD OF BZ

We start with the observations that the operator $\rho_{\vec{k}} = \sum_i e^{i\vec{k}\cdot\vec{x}_i}$ is of fundamental importance in the theory of interacting boson systems, ¹⁰ and that the wave functions of a noninteracting boson system have a certain structure: They are simple polynomials in the $\rho_{\vec{k}}$. For any set of N vectors $\{\vec{k}_i\}$ there is a state whose wave function is

$$\phi(\vec{\mathbf{x}}_1, \vec{\mathbf{x}}_2, \dots, \vec{\mathbf{x}}_N; \vec{\mathbf{k}}_1, \vec{\mathbf{k}}_2, \dots, \vec{\mathbf{k}}_N) = | {}^*e^{i\vec{\mathbf{k}}_i \cdot \vec{\mathbf{x}}_j} | {}^*\Omega^{-N/2} (N!)^{-1}, \quad (1)$$

where $| \cdot | \cdot |$ denotes the permanent¹¹ of the $N \times N$ matrix $\{e^{i\vec{k}_i \cdot \vec{x}_j}\}$. In particular, the wave function for the ground state is

$$\phi_0(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N; 0, 0, \ldots, 0) = \Omega^{-N/2};$$

for the lowest-energy state having momentum \vec{k} , $\phi_{\vec{k}}(\{\vec{x}_i\}) = \rho_{\vec{k}} \phi_0$; and for the state having two such excitations, $\phi_{\vec{k},\vec{p}} = [\rho_{\vec{k}} \rho_{\vec{p}} - \rho_{\vec{k}+\vec{p}}] \phi_0$. It is readily shown that every wave function is a polynomial in the $\rho_{\vec{v}}$.

Let us then attempt to use the $\rho_{\vec{k}}$ as a set of coordinates. If the wave function is written $\Phi(\rho_{\vec{k}})$, the Hamiltonian for the noninteracting system (the kinetic-energy operator) becomes

$$T = \frac{-\bar{n}^{2}}{2m} \sum_{i} \nabla_{i}^{2} = \sum_{\vec{k}} \epsilon_{k} \left(\rho_{\vec{k}} \frac{\partial}{\partial \rho_{\vec{k}}} - N \frac{\partial^{2}}{\partial \rho_{\vec{k}} \partial \rho_{-\vec{k}}} \right) + \sum_{\vec{k} + \vec{p} \neq 0} \frac{\bar{n}^{2}}{2m} \left(\vec{k} \cdot \vec{p} \right) \rho_{\vec{k} + \vec{p}} \frac{\partial^{2}}{\partial \rho_{\vec{k}} \partial \rho_{\vec{p}}} , \quad (2)$$

where

 $\epsilon_k = \frac{1}{2} \hbar^2 k^2 / m$.

If the variables ρ_{i} are assumed independent, we can introduce an occupation-number representation for the wave functions and interpret $\rho_{\vec{t}}$ and $\partial/\partial \rho_{\vec{t}}$ as being the creation and destruction operators (respectively) in this representation. Since the Hamiltonian [Eq. (2)] is nonsymmetric in the creation and destruction operators, it is non-Hermiti-This difficulty is related to that found by Dyan. son in his discussion of the spin-wave problem¹²: the "physical states" formed as simple products of the $\sum_{i} e^{i\vec{k}\cdot\vec{x}_{j}}$ are not orthogonal; the assumption that the ρ_{z} are independent variables corresponding to independent oscillations of the system gives rise to the "ideal states," whose behavior is determined by a non-Hermitian Hamiltonian operator.

Simple examples of the relationship of the two representations are given by the states of the noninteracting system.

In the $\{x_i\}$ representation,

$$\tilde{\phi}_{\vec{k},\vec{p}} = \sum_{m} e^{i\vec{k}\cdot\vec{x}} \sum_{m} \sum_{n} e^{i\vec{p}\cdot\vec{x}}$$

is not orthogonal to $\phi_{\vec{k},\vec{p}} = \sum_n e^{i(\vec{k}+\vec{p})\cdot\vec{z}}n$; the orthogonalized function $\phi_{\vec{k},\vec{p}} = \phi_{\vec{k},\vec{p}} - \phi_{\vec{k}+\vec{p}}$ is an eigenstate of T. In the $\{\rho_{\vec{k}}\}$ representation, $\phi_{\vec{k},\vec{p}} = \rho_{\vec{k}}\rho_{\vec{p}}$ is orthogonal to $\rho_{\vec{k}+\vec{p}}$, but the eigenstate of the asymmetric Hamiltonian is $\phi_{\vec{k},\vec{p}} = \phi_{\vec{k},\vec{p}} - \rho_{\vec{k}+\vec{p}}$ as before, even though $\rho_{\vec{k}}$ is itself an eigenstate of T. The price paid for the orthogonal basis $\{\rho_{\vec{k}}\}$ is that the eigenstates are no longer orthogonal.

The Hamiltonian for the interacting system is

$$H = T + U , \qquad (3)$$
 where

$$U = (2\Omega)^{-1} \sum_{\vec{k}} \rho_{\vec{k}} V_k \rho_{-\vec{k}} - \sum_{\vec{k}} \frac{1}{2} n V_0 , \qquad (4)$$

in which V_k is the Fourier transform of the interparticle potential. The operator U mixes the eigenstates of the kinetic-energy operator but it remains true that the wave functions can be written as a function in the ρ_z representation.

BZ proceed by assuming that the last term of the kinetic-energy operator (2) can be regarded as a small perturbation. The remainder of the Hamiltonian can be diagonalized by assuming that the wave functions can be written in the form

$$\Psi = \exp[\frac{1}{4} N^{-1} \sum_{k} \rho_{\vec{k}} \rho_{-\vec{k}}] \Phi(\rho_{\vec{k}}) .$$
 (5)

If Φ is an eigenfunction of *H* [defined by Eq. (3)], then Ψ is an eigenfunction of

$$H' = \sum_{\vec{k} \neq 0} \left[\frac{1}{2} N^{-1} \left(n V_{\vec{k}} + \frac{\hbar^2 k^2}{4m} \right) \rho_{\vec{k}} \rho_{-\vec{k}} - N \epsilon_k \frac{\partial^2}{\partial \rho_{\vec{k}}^* \partial \rho_{-\vec{k}}} \right]$$

+
$$\sum_{\substack{\vec{p} \neq k \neq 0 \\ \vec{p} \neq k \neq 0}} \frac{\hbar^2}{2m} \left(\vec{k} \cdot \vec{p} \right) \rho_{\vec{k} + \vec{p}} \left(\frac{\partial}{\partial \rho_{\vec{p}}} + \frac{1}{2} N^{-1} \rho_{-\vec{p}} \right)$$

×
$$\left(\frac{\partial}{\partial \rho_{\vec{k}}} + \frac{1}{2} N^{-1} \rho_{-\vec{k}} \right) - \frac{1}{2} \sum_{\vec{k}} \left(\epsilon_k + n V_k \right) + \frac{1}{2} n N V_0 . \quad (6)$$

The first two terms are of harmonic-oscillator type; let us introduce the second-quantized operators

 $N^{1/2} 2\lambda_k b_{\vec{k}} = \rho_{-\vec{k}} + 2N\lambda_k^2 \frac{\partial}{\partial \rho_{\vec{k}}}$

and

$$N^{1/2} 2\lambda_k b_{\vec{k}}^{\dagger} = \rho_{\vec{k}} - 2N\lambda_k^2 \frac{\partial}{\partial \rho_{-\vec{k}}} ,$$

where

$$\lambda_k^4 = \epsilon_k / (2nV_k + \epsilon_k)$$

With this substitution, Eq. (6) becomes

$$H_{\rm BZ} = E_0 + H_0 + H_1 , \qquad (8)$$

where

$$E_0 = \frac{1}{2}nN V_0 + \frac{1}{2} \sum_{k} (E_k - \epsilon_k - nV_k)$$
, (9)

$$H_0 = \sum_{\vec{k} \neq 0} E_k b_{\vec{k}}^{\dagger} b_{\vec{k}} , \qquad (10)$$

and

$$H_{1} = N^{-1/2} \sum_{\substack{\vec{k}, \vec{p} \\ \vec{k} \neq \vec{p} \neq 0}} \frac{1}{2} \Gamma_{k, p} (b^{\dagger}_{-p-k} + b_{k+p})$$

(7)

(12)

$$\times (f_k b_{-k} + g_k b_k^{\dagger}) (f_p b_{-p} + g_p b_p^{\dagger}), \quad (11)$$

with

$$E_{k} = (2nV_{k} \epsilon_{k} + \epsilon_{k}^{2})^{1/2} , \qquad (12)$$

$$f_{k} = \lambda_{k}^{2} + 1 , \quad g_{k} = \lambda_{k}^{2} - 1 , \qquad (13)$$

and

$$\Gamma_{k,p} = \frac{\hbar^2}{4m} \vec{k} \cdot \vec{p} \frac{\lambda_{\vec{k} \cdot \vec{p}}}{\lambda_k \lambda_p} .$$
 (14)

Equation (12) displays a spectrum of almost independent excitations. In particular, if $\lambda_k = 1$, the three-phonon processes (H_1) contain the operator $(b^{\dagger}_{\vec{k}-\vec{p}} + b_{\vec{k}+\vec{p}}) b_{\vec{k}} b_{\vec{p}}$ only, and hence will not affect the ground state or singly excited states. If these three-phonon processes may be neglected, the Hamiltonian for Ψ becomes the first sum in Eq. (6), and Ψ may be shown to be

$$\Psi = \exp\left(-N^{-1}\sum_{\vec{k}\neq 0}\frac{E_k}{4\epsilon_k}\rho_{\vec{k}}\rho_{-\vec{k}}\right) \quad ; \tag{15}$$

the untransformed wave function Φ becomes

$$\Phi = \exp\left[\frac{1}{4}N^{-1}\sum_{\vec{k}\neq 0}\left(1-\frac{E_k}{\epsilon_k}\right)\rho_{\vec{k}}\rho_{-\vec{k}}\right] \quad . \tag{16}$$

Functions of this sort have been proposed for helium by Bijl¹³ and Jastrow.¹⁴ Reatto and Chester¹⁵ have discussed the importance of the E_k/ϵ_k singularity in the long-wavelength limit in destroying the condensate in one and two dimensions.

The excitation spectrum (12) is of the same form derived earlier by Bogoliubov¹⁶; however, in that case the condensate density n_0 appeared where we now have the total particle density n. In the present case the excitation spectrum will not display the strong dependence on the degree of depletion that other approaches suggest.

The validity of this approach is limited to cases where the system possesses a condensate by the following considerations: The states given by Eq. (1) are necessarily polynomials in ρ_{r} of order less than N. The potential V, however, mixes polynomials of order M with polynomials of order M+2: Polynomials of order greater than N in the ρ_{t} will occur in the ground-state function. These polynomials cannot readily be interpreted as states of the form of Eq. (1); but since the set of states given by Eq. (1) form a complete set (i.e., all the states of a noninteracting *N*-boson system), they should suffice to describe the interacting ground state. This apparent paradox is resolved by a reinterpretation theorem: A term of power M > N in the ρ_{z} can always be rewritten as a polynomial of order $\leq N$ in the $\rho_{\vec{i}}$. The proof lies fundamentally in the completeness of the set of states for the noninteracting system. Thus the assumption that the ρ_{z} may be regarded as independent variables breaks down where intermediate states of the form of Eq. (1) with all $\vec{k}_i \neq 0$ are involved; the approach

of BZ is thus invalidated in the case of normal liquids. It is generally accepted, however, that superfluids have a condensate¹⁷ and that the condensate density shows only small fluctuations about its equilibrium value¹⁸; in this case we have $\vec{k}_i = 0$ in a macroscopic fraction of the rows of the permanent in Eq. (1) and $\vec{k_i} \neq 0$ for only a few extremely improbable intermediate states. Thus, in a system with a condensate, the assumption that the $\rho_{\mathbf{i}}$ are independent is justifiable.

Since the excitation spectrum (12) contains V_k , it cannot be appropriate for a strongly interacting system. The interparticle potential for helium is strongly repulsive at short distances; this repulsion gives a large contribution to V_k at small k. The helium atoms never enter the core region, however, so that the wave function and energy levels should not be sensitive to the details or the magnitude of the core repulsion. This point is well understood in other systems; it necessitates a consideration of the higher-order dependences of the wave function on the potential and in some circumstances results simply in the replacement of the interparticle potential by an effective interaction.¹⁹ Such an analysis will not be attempted here; in what follows we shall assume a weak potential having a Fourier transform.

III. THREE-PHONON PROCESSES

The transformation which produced the BZ Hamiltonian (8) was exact, and the derivation of the excitation spectrum did not involve any linearization of an equation of motion. If the corrections to the excitation spectrum coming from the three-phonon terms H_1 are small, then the BZ Hamiltonian is a viable starting point for a microscopic calculation of the sound speed of a Bose-condensed liquid. We will now consider how important these terms will be.

It is not *a priori* obvious that the three-phonon processes are negligible for any finite density, even though they vanish (so far as the ground state and single-phonon states are concerned) in the lowdensity limit. The limit is not uniform: For any density there is a region of k space for which $\lambda_{k} \neq 1$ and thus for which the perturbation must be considered. It will be shown below that for a reasonable example the lowest-order correction to the excitation spectrum is only a small shift of that spectrum which vanishes uniformly in the low-density limit. This suggests that the BZ Hamiltonian provides a reasonable description of the weakly interacting boson gas.

The construction of approximation schemes to take H_1 into account is complicated by the following consideration: It is generally true that a Hamiltonian with only a cubic term does not have a ground state.²⁰ The expectation value of such a Hamiltonian in trial states of the form

$$|\alpha\rangle = \exp[\alpha(b_{\mathbf{k}}^{\dagger} + b_{\mathbf{p}}^{\dagger} + b_{\mathbf{k}+\mathbf{p}}^{\dagger}) - \frac{3}{2}\alpha^{2}] |\operatorname{vac}\rangle \qquad (17)$$

is not bounded below, since the expectation of the cubic term is proportional to $\alpha^3 N^{-1/2}$, which can be made arbitrarily large and negative by suitable choice of α . The magnitude of α required, how-ever, is of order $N^{1/2}$; in this case the expectation of $b_k^{\dagger} b_k$ in the state $|\alpha\rangle$ is of order N. In view of the discussion of Sec. II, it is clear that these states (17) are nonphysical and the argument does not apply.

The BZ Hamiltonian does not conserve phonon number; consequently a matrix Green's-function formalism must be employed.²¹ Let us define

$$b_{q}^{\alpha} = \begin{cases} b_{q}^{\alpha}, & \alpha = -1 \\ b_{q}^{\dagger}, & \alpha = +1 \end{cases}$$
(18)
and
$$D^{\alpha\beta}(q, \omega) = i^{-1} \int e^{i\omega t} dt \langle \Phi_{0} | T b_{q}^{\alpha}(t) b_{q}^{\beta}(0) | \Phi_{0} \rangle ,$$
(19)

where $|\Phi_0\rangle$ is the ground-state wave function for the BZ Hamiltonian. The Green's function for the "unperturbed" system (for which the Hamiltonian is just H_0) is

$$D_0^{\alpha\beta}(q,\omega) = \delta_\beta^{-\alpha} \left[\beta \hbar \omega - E_q + i\delta\right]^{-1}, \qquad (20)$$

where E_q is the excitation spectrum [Eq. (12)]. The equation of motion for D can be written

$$D^{\alpha\beta}(q, \omega) = D_0^{\alpha\beta}(q, \omega) + D_0^{\alpha\gamma}(q, \omega) \Sigma^{\gamma\nu}(q, \omega) D^{\nu\beta}(q, \omega) .$$
(21)

The self-energy matrix Σ can be given a linkedcluster diagrammatic expansion similar to that which has been proposed for the "hydrodynamic" Hamiltonian.²¹ The diagrams are composed of lines, representing the "bare" Green's function D_0 , which are directed from the vertex at which the virtual phonon is created to that at which it is destroyed; the vertices are the matrix elements of H_1 , and always connect exactly three lines. Some care must be exercised in this perturbation scheme: The non-Hermitian nature of H_1 implies that the usual "time reversal" and "crossing" symmetries fail to hold. In particular, it is not true that $\Sigma^{++}(q, \omega)$ equals $\Sigma^{--}(q, \omega)$: Diagrams contributing to Σ^{**} will have at least one vertex at which three phonons are annihilated (three ingoing lines, as occurs at the tops of the appropriate diagrams in Fig. 1), whereas Σ^{--} will have at least one vertex at which three phonons are created: These processes have different amplitudes in H_1 . The symmetry $\Sigma^{+}(q, \omega) = \Sigma^{-+}(q, -\omega)$ does hold, however.

The excitation spectrum is given by the poles of

where

$$A_{q}^{p} = \langle 0 | b_{p} b_{-p-q} H_{1} b_{q}^{\dagger} | 0 \rangle = \Gamma(p, -p-q) g_{p} g_{p+q} + \Gamma(p, q) f_{q} g_{p} + \Gamma(q, -p-q) f_{q} g_{p+q} , \qquad (27)$$



FIG. 1. Lowest-order contributions to $\Sigma^{\alpha\beta}$.

D, which will occur for ω such that

$$\det \left| D_0^{-1\,\alpha\beta}(q,\,\omega) - \Sigma^{\,\alpha\beta}(q,\,\omega) \right| = 0 , \qquad (22)$$

that is,

$$-\left[\hbar\omega + \frac{1}{2}(\Sigma^{*-}(q,\omega) - \Sigma^{-*}(q,\omega))\right]^2 + \left[E_q + \frac{1}{2}(\Sigma^{*-}(q,\omega))\right]^2$$

$$+ \Sigma^{-+}(q, \omega)]^2 - \Sigma^{++}(q, \omega) \Sigma^{--}(q, \omega) = 0.$$
 (23)

Every vertex of every graph in $\sum^{\alpha\beta}$ contains a factor which is small of order $q^{1/2}$ if any one of the momenta q entering the vertex is small. Since every self-energy diagram has two vertices with the external lines, $\sum^{\alpha\beta}(q, \omega) \sim q$ in the long-wavelength limit. Therefore the solution of Eq. (23) will not display a gap, in contrast to some other approaches to the Bose-gap excitation spectrum.²²

The simplest approximation for Σ is the bubble graphs (Fig. 1). They yield the expressions

$$\Sigma^{+-}(q, \omega) = \frac{1}{2n} \int \frac{d^3p}{(2\pi)^3} \left(\frac{A_q^b B_q^b}{\omega - E_p - E_{\vec{q}-\vec{p}} + i\delta} + \frac{C^{b,q} D_{b,q}}{-\omega - E_p - E_{\vec{p}+\vec{q}} + i\delta} \right) , \quad (24)$$

$$\Sigma^{**}(q, \omega) = \frac{1}{2n} \int \frac{d^{3}p}{(2\pi)^{3}} \left(\frac{A_{q}^{b} D_{p, -q}}{\omega - E_{p} - E_{q-p} + i\delta} + \frac{D_{p, q} A_{-q}^{b}}{-\omega - E_{p} - E_{p+q} + i\delta} \right) , \quad (25)$$

$$\Sigma^{--}(q, \omega) = \frac{1}{2n} \int \frac{d^3p}{(2\pi)^3} \left(\frac{B^a_p C^{p,-q}}{\omega - E_p - E_{q-p} + i\delta} + \frac{C^{p,q} B^{-q}_p}{-\omega - E_p - E_{p+q} + i\delta} \right) , \quad (26)$$

$$B_{p}^{q} = \langle 0 | b_{q} H_{1} b_{p}^{\dagger} b_{-p-q}^{\dagger} | 0 \rangle = \Gamma(p, -p-q) f_{q} f_{p+q} + \Gamma(p, q) g_{q} f_{p} + \Gamma(q, -p-q) g_{q} f_{p+q} , \qquad (28)$$

$$C^{p,q} = \langle 0 | b_{p} b_{q} b_{-p-q} H_{1} | 0 \rangle = \Gamma(p,q) g_{p} g_{q} + \Gamma(p,-p-q) g_{p} g_{p+q} + \Gamma(q,-p-q) g_{q} g_{p+q} , \qquad (29)$$

$$D_{p,q} = \langle 0 | H_1 b_p^{\dagger} b_q^{\dagger} b_{-p-q}^{\dagger} | 0 \rangle = \Gamma(p,q) f_p f_q + \Gamma(p,-p-q) f_p f_{p+q} + \Gamma(q,-p-q) f_q f_{p+q} .$$
(30)

Perturbation theory on three-phonon terms has been proposed in the Bose-gas context before²³; the present method has the advantage that it is not necessary to cut off the integrals in (24)-(26) in the large-momentum region: The factor g_p becomes small where V_p/ϵ_p does; if the potential becomes small for large p then so will $C^{p,q}$ and A_p^p .

The integrals in (24)-(26) were evaluated numerically for a gas of bosons having the mass of helium atoms and interparticle potential

$$V_{b} = V_{0} e^{-k^{2} \sigma^{2}/4}$$
(31)

for $\sigma = 2.5$ Å and various choices of V_0 ; the number density *n* was chosen to be 2.1×10²² particles/cm³, a value typical of liquid helium.

The spectrum E_a for this model, for all but unreasonably large V_0 , has the property that the decay of one phonon into two with conservation of energy and momentum is possible; consequently, if Eqs. (24)-(26) are evaluated for $\omega = E_a$ the denominators of some of the integrals may have zeroes and the self-energies may have imaginary parts. Numerical evaluation of the implied principle-value integrals for the real parts of the self-energies is a difficult problem; it was evaded here by evaluating $\Sigma^{\alpha\beta}(q, \omega)$ only for ω such that the integrals are nonsingular. In practice this requires that ω be only slightly less than E_q . The results may be regarded as good approximations to the real parts of the self-energies, since the integrals are quite insensitive to ω near E_q : The integrands are affected only in the singular region, which has very small volume (|p| must be less than |q|, and \overline{p} nearly collinear with \vec{q}), whereas the principle contribution to the integrals comes from p near the cutoff of V_p (for density-of-states reasons). This contention was also verified numerically in the course of the calculation.

Figure 2 shows $\Sigma^{+-}(q, E_q - \Delta)$ for the various choices of V_0 considered. The other energies are of comparable size and therefore unimportant to the solution of (23). For comparison Fig. 3 shows the corresponding spectra E_q . We observe that in the limit that V_0 is small the shift of the spectrum is small, and that the shift becomes appreciable when $nV_0 \sim 8 \ K \sim 4\pi\sigma\hbar n/m = nV_{ps}$, where V_{ps} is the Fermi pseudopotential.²⁴ For potentials stronger than this, multiple scattering (core nonpenetration) becomes important and theories depending on the unrenormalized V_b become automatically suspect.

These simple numerical studies support the con-

tentions that the representation of the low-lying states of the interacting system in terms of the eigenstates of H_0 becomes asymptotically exact in the limit of weak potential and low density, and that no new phenomena arise from the three-phonon perturbation.

IV. CONNECTION TO OTHER APPROACHES

A. Collective-Variable Formulations

There have been other attempts to formulate the interacting-Bose-gas problem in terms of the natural $\rho_{\vec{k}}$ variables: (a) Several workers²⁵ have attempted to use the linearized equations of motion for $\rho_{\vec{k}}$; (b) model "hydrodynamic" Hamiltonians have been formulated in these variables²⁶; and (c) Bohm and Salt²⁷ applied the Bohm-Pines method²⁸ to divide the representation into "particle" and "collective" variables.

These formulations have provided some useful insights into the nature of the excitation spectrum. They are, however, inferior to the BZ approach in two respects:

(i) They have not taken clear account of the nonorthogonality of the $\rho_{\vec{k}}$ variables: The transformations used are unitary, and the resultant Hamilto-



FIG. 2. Self-energy function $\Sigma^{**}(q, \omega)$ evaluated in lowest-order perturbation theory for ω slightly less than E_q . Three choices have been made for the strength of the potential: $nV_0=0.5$, 2, and 8°K.



FIG. 3. Excitation spectrum E_q for $V_k = V_0 e^{-\sigma^2 k^2/4}$, with three values for nV_0 .

nians Hermitian. The discussion above makes it clear that a non-Hermitian representation is necessary even for the noninteracting gas; furthermore, the asymmetry of the Hamiltonian is essential to the convergence of the self-energy-function integrals.²⁹

(ii) The various linearizations and expansions introduced are of uncertain nature. It is not clear that it is possible to do perturbation theory with the terms that are claimed small.

B. Correlated Basis Functions

Let $\Phi(r_1, \ldots, r_N)$ be the exact ground-state wave function, or some good approximation to it. According to Feynman,¹⁰ the function $\rho_k \Phi$ is a good approximation to the one-phonon wave function; this suggests that the nonorthogonal set

$$|\vec{\mathbf{k}}\rangle = \rho_{\vec{\mathbf{k}}} \Phi , \quad |\vec{\mathbf{h}}, \vec{\mathbf{k}}\rangle = \rho_{\vec{\mathbf{h}}} \rho_{\vec{\mathbf{k}}} \Phi , \dots$$
(32)

might be a useful basis in which to formulate the interacting-boson problem. The BZ description is itself a theory of this type, in which the correlating function Φ is given by Eq. (16), and the nonorthogonality has been handled by a certain prescription.

Other ways to use this basis have been proposed. If Φ is chosen to be the exact ground-state wave function, then all matrix elements of the Hamiltonian and the unit operator can be expressed in terms of the radial distribution function and higherorder distribution functions. In this way Jackson and Feenberg,³⁰ Lee,³¹ and Lai, Sim, and Woo³² have performed perturbation expansions in the basis (32), which they use in a Schmidt orthogonalized form. Upon the introduction of approximations for the higher-order distribution functions, their results come to have the form of expansions in the liquid structure factor S(k). This elimination of the interparticle potential in favor of S(k) is an advantage for the extension of the theory to the case of liquid helium, for which S(k)is better known than the potential itself.

For the case of the weakly interacting system, Lee and Feenberg³³ have shown how S(k) is related to the potential; in our notation,

$$S(k) = \lambda_k^2 , \qquad (33)$$

which is essentially the expansion parameter of the BZ theory.

C. Particle-Coordinate Representations

A commonly used approach to the description of the Bose gas is the Green's-function formalism. The method encounters several difficulties.

(a) The perturbation theory is a double expansion in the interparticle potential and the condensate density; the latter must be determined self-consistently. Beliaev³⁴ and Hugenholtz and Pines¹ have described the formalism necessary to handle this problem.

(b) No nontrivial approximation for the selfenergy has been found which yields both a gapless spectrum and self-consistent thermodynamics.³⁵ It has been shown, however, that the spectrum of the exact Green's function will be gapless.¹

(c) In normal systems the spectra of the singleparticle Green's function and the two-particle correlation function are distinct; however, the extremely successful Landau³⁶ description of superfluidity postulates the existence of just one excitation spectrum. This problem has been resolved by Gavoret and Nozières,² Huang and Klein,³⁷ and Hohenberg and Martin,³⁸ who showed how the presence of the condensate couples the Green's functions, resulting in a single spectrum.

The BZ approach leads to a difficulty comparable to point (a) in that it requires the use of perturbation theory for a non-Hermitian three-phonon Hamiltonian. The formalism has not been studied, and so it is not known how serious a difficulty it presents. I have shown above that in this formalism every approximation leads to a gapless spectrum, so difficulty (b) is not encountered.

The Hamiltonian H_0 has only a single spectrum; for the Green's function D no additional structure appears in lowest-order perturbation theory, nor is there reason to believe that other branches should arise. Thus we begin closer to the Landau point of view; that this single spectrum will appear as the principal structure of the spectral weight function of the usual single-particle Green's function and the dynamic-structure factor is readily established since the matrix elements $\langle k(N) | \rho_k |$

<u>6</u>

 $\times 0(N)$ and $\langle k(N+1) | a_{k}^{\dagger} | 0(N) \rangle$ are nonvanishing in the thermodynamic limit (where $|k(N)\rangle$ and $|0(N)\rangle$ are, respectively, the exact single-phonon state and the exact ground state of an N-particle system). The various correlation functions couple to the same dynamical processes with different matrix elements and hence have the same poles with differing residues. Thus difficulty (c) does not arise, and the Gavoret-Nozières theorem arises in a simple way.

V. SUMMARY

An outline of the BZ approach to the interacting Bose gas has been presented, showing that this method is unusually free of formal difficulties. The Hamiltonian is cast into a form which can be interpreted as describing phonons interacting through a non-Hermitian three-phonon process, and which allows a systematic expansion which is asymptotically exact in the limit of weak interactions and low densities. The presence of a condensate was shown to be necessary for the validity of the theory, although it does not play an obtrusive role otherwise. It was also shown that in every ap-

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¹N. M. Hugenholtz and D. Pines, Phys. Rev. <u>116</u>, 489 (1959).

²J.Gavoret and P. Nozières, Ann. Phys. (N.Y.) <u>28</u>, 349 (1964).

³D. Pines, in Proceedings of the 9th International Conference on Low Temperature Physics, edited by Gaunt et al. (Plenum, New York, 1965), p. 61.

⁴W. Gotze and H. W. Wagner, Physica 31, 475 (1965).

⁵K. Kehr, Z. Physik <u>221</u>, 291 (1969).

⁶K. Kehr, Physica <u>33</u>, 620 (1967).

⁷This is implied by Feynman's discussion of the excitation spectrum (Ref. 10).

⁸J. P. Straley, Phys. Rev. A 5, 338 (1972).

⁹N. N. Bogoliubov and D. N. Zubarev, Zh. Eksperim. i Teor. Fiz. 28, 129 (1955) [Sov. Phys. JETP 1, 83 (1955)].

¹⁰R. P. Feynman, Phys. Rev. <u>91</u>, 1301 (1953); <u>94</u>, 262 (1954); R. P. Feynman and M. Cohen, Phys. Rev. 102, 1189 (1956).

¹¹The permanent of an array a_{ij} is the sum $\sum a_{1j_1}a_{2j_2}\dots$ $\times a_{nj_n}$, where (j_1, j_2, \ldots, j_n) ranges over all permutations of $(1, 2, \ldots, n)$. Regarded as a function of its rows or columns, it is the unique totally symmetric multilinear form which assigns unity to the unit matrix.

¹²F. J. Dyson, Phys. Rev. <u>102</u>, 1216 (1955). See pp. 1221-1222.

¹³A. Bijl, Physica <u>7</u>, 869 (1940).

¹⁴R. Jastrow, Phys. Rev. <u>98</u>, 1479 (1955).

¹⁵L. Reatto and G. V. Chester, Phys. Rev. 155, 88 (1967); G.V. Chester, W. P. Francis, and L. Reatto,

Phys. Rev. A 1, 86 (1970).

¹⁶N. N. Bogoliubov, J. Phys. USSR 11, 7 (1942).

proximation one obtains a single gapless phononlike excitation spectrum. The origins of the non-Hermiticity of the BZ Hamiltonian were explored; it proves to be a necessary feature of a representation which treats phonon states as being independent. The lowest-order corrections to the Bogoliubov excitation spectrum were evaluated and shown to be small. Finally, the BZ method was compared with some other approaches that have been suggested.

The principal difficulties with the BZ approach are the need for a Fourier-transformable potential and the non-Hermiticity of the Hamiltonian. The former problem limits the approach to the case of weak potentials until the appropriate analogs of the *t*-matrix method are developed.

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¹⁷L. Onsager and O. Penrose, Phys. Rev. 104, 576 (1956). Onsager and Penrose give $n_0/\rho = 0.08$; model calculations [W. L. McMillan, Phys. Rev. 138, A442 (1965), and Ref. 7] suggest $n_0/\rho = 0.11$.

- ¹⁸A. E. Glassgold and H. Sauermann, Phys. Rev. <u>182</u>, 262 (1969).
- ¹⁹D. Pines, The Many-Body Problem (Benjamin, New York, 1961), p. 16.

²⁰G. Baym, Phys. Rev. 117, 886 (1960).

²¹C. J. Pethick and D. ter Haar, Physica <u>32</u>, 1905 (1966).

²²M.Girardeau and R. Arnowitt, Phys. Rev. 113, 755 (1959); M. Luban, ibid. 128, 965 (1962).

²³S. Eckstein and B. B. Varga, Phys. Rev. Letters

21, 1311 (1968). ²⁴K. Huang and C. N. Yang, Phys. Rev. <u>105</u>, 767 (1957).

²⁵R. P. Etters, Phys. Rev. Letters 16, 119 (1966); S. Sunakawa, S. Yamasaki, and T. Kebukawa, Progr. Theoret. Phys. (Kyoto) 41, 919 (1969); W. Bierter and H. L. Morrison, Nuovo Cimento Letters 1, 701 (1969).

²⁶I. M. Khalatnikov, Introduction to the Theory of

Superfluidity (Benjamin, New York, 1965), Chap. 7. ²⁷D. Bohm and B. Salt, Rev. Mod. Phys. 39, 894

(1967). For further discussion of this approach, see G. Sposito, Phys. Rev. A 2, 948 (1970); and J. P. Straley, Ph.D. thesis (Cornell University, 1970) (unpublished),

pp. 52-69. ²⁸D. Bohm and D. Pines, Phys. Rev. <u>92</u>, 609 (1953). ²⁹Convergence requires that the amplitude for a phonon

of wave vector k splitting into phonons of wave vector $\vec{k} - \vec{p}$ and \vec{p} vanish for p large. Hermiticity would then require that the interaction between phonons of wave vector $\vec{k} - \vec{p}$ and \vec{p} vanish (in the same limit) which is not very reasonable.

³⁰H. W. Jackson and E. Feenberg, Rev. Mod. Phys.

- <u>34, 686 (1962).</u> ³¹D. K. Lee, Phys. Rev. <u>162</u>, 134 (1967).
- ³²H.-W. Lai, H.-K. Sim, and C.-W. Woo, Phys. Rev. A <u>1</u>, 1536 (1970). ³³D. K. Lee and E. Feenberg, Phys. Rev. <u>137</u>, A731
- (1963).
- ³⁴S. T. Beliaev, Zh. Eksperim. i Teor. Fiz. <u>34</u>, 443 (1959) [Sov. Phys. JETP 7, 299 (1958)].

³⁵V. K. Wong, Ph.D. thesis (Berkeley, 1966) (unpublished), p. 44.

³⁶I. M. Khalatnikov, Introduction to the Theory of Superfluidity (Benjamin, New York, 1965), p. 185.

³⁷K. Huang and A. Klein, Ann. Phys. (N.Y.) <u>30</u>, 203 (1964).

³⁸P. Hohenberg and P. C. Martin, Ann. Phys. (N.Y.) 34, 346 (1965).