⁶B. J. Alder and T. E. Wainwright, Phys. Rev. A <u>1</u>, 18 (1970).

⁷T. E. Wainwright and J. A. Viecelli, UCRL Technical Report No. UCRL-72726 (unpublished).

⁸R. Mountain and R. Zwanzig, J. Chem. Phys. <u>44</u>, 2777 (1966).

PHYSICAL REVIEW A

VOLUME 4, NUMBER 1

Phys. 45, 1086 (1966).

Chem. Phys. 53, 3813 (1970).

JULY 1971

Density Fluctuations in an Interacting Bose Gas*

T. H. Cheung and Allan Griffin

Department of Physics, University of Toronto, Toronto 5, Canada (Received 23 December 1970)

The density fluctuation in a Bose gas interacting via a strong short-range repulsive potential and a weak long-range attractive potential is studied by the methods of quantum-field theory. The density-density correlation function is generated by taking the functional derivative of the single-particle matrix Green's function $G_1(1, 2)$ with respect to an auxiliary scalar field. For $G_1(1, 2)$, we use the Hartree approximation for the attractive potential and the Hartree-Fock approximation for the short-range repulsive potential. We show that the density fluctuation spectrum is identical to the Beliaev approximation for the single-particle excitation spectrum.

I. INTRODUCTION

Beginning with Bogoliubov's classic work in 1947, there have been many studies of an interacting Bose gas using field-theoretic techniques. We mention specifically the important work of Beliaev, 1,2 Hugenholtz and Pines, 3 and Hohenberg and Martin.⁴ With few exceptions, these calculations are mainly concerned with the spectrum of the single-particle Green's function $\tilde{G}_1(k,\omega)$. In the present paper, we compute the density-density fluctuation spectrum at finite temperature using the Green's-function method. To be more specific, we study $S(k, \omega)$ for a system of bosons interacting via a strong short-ranged repulsive potential and a weak long-ranged attractive potential in the Hartree-Fock approximation. This model of an interacting Bose gas has been studied by Huang⁵ and more recently by Singh and Kumar.⁶ However, these authors only considered the single-particle spectrum.

We believe our results give further insight into the general question of the equivalence between elementary excitations and density fluctuations in a condensed Bose system. As is well known, it is this equivalence which is at the center of the phenomenological theories of Landau and Feynman. Moreover, it is this equivalence which makes it possible to study the single-particle excitations (which determine the thermodynamics) by neutron scattering. At the present time, the only rigorous nonperturbative results are those of Gavoret and Nozières.⁷ Summing up self-energy contributions to all orders in perturbation theory, they obtained

$$(\omega > 0)$$

$$S(k, \omega) = 2\pi n k^2 \delta(\omega^2 - c_1^2 k^2) ,$$

$$Im \tilde{G}_{1,1}(k, \omega) = (\pi n_0 / n) m c_1^2 \delta(\omega^2 - c_1^2 k^2)$$
(1)

⁹B. J. Berne, J. P. Boon, and S. A. Rice, J. Chem.

¹⁰ P. C. Martin and S. Yip, Phys. Rev. <u>170</u>, 151 (1968).

¹¹B. J. Alder, D. M. Gass, and T. E. Wainwright, J.

in the limit $k \rightarrow 0$ and 0 °K. The phonon velocity c_1 is given by the usual thermodynamic expression. In their derivation, it was assumed that the Dyson-Beliaev self-energies could be expanded in powers of k and ω .

In Sec. II, we use the *Hartree-Fock* (Girardeau-Arnowitt⁸ or GA) approximation to generate the two-particle Green's functions by functional differentiation with respect to an external field. This is an example of a conserving approximation in the sense of Baym and Kadanoff.⁹ The twoparticle potential is assumed to have a Fourier transform V(k) and is split into a short-range repulsive part $V_R(k) \equiv V_R$ and a long-range attractive part $V_A(k)$. The Hartree self-energy involves $V_R(k) + V_A(k)$ but in the exchange term we only consider $V_R(k)$. The neglect of $V_A(k)$ in the exchange term is justified in one limit discussed in Sec. III.

In Sec. III, we solve the equations of motion obtained in Sec. II using perturbation theory and show that the spectrum of the density-density correlation function is phononlike at very low momentum. This is obtained for zero temperature and is identical to the single-particle spectrum in the Singh-Kumar approximation. 6,2

In Sec. IV, the equation determining the density fluctuation spectrum for a purely repulsive shortrange interaction is shown to be identical to the Beliaev expression for the single-particle spectrum. This equivalence is not limited to 0 $^\circ K$ and long wavelengths.

Partly for pedagogic reasons, in the Appendix we compute $S(k, \omega)$ using functional differentiation of the self-consistent *Hartree* approximation for the single-particle Green's function. This gives the so-called random-phase-approximation (RPA) result for $S(k, \omega)$ and corresponds to a special case of the more general results of Sec. II.

II. DENSITY-DENSITY CORRELATION FUNCTION IN HARTREE-FOCK APPROXIMATION

In the following discussion, we assume that the reader is familiar with Sec. VI of Hohenberg and Martin, ⁴ whose notation we follow quite closely. The full 2×2 -matrix Green's function is given by

$$G_{1}(1, 1') = G_{1}(1, 1') + G_{1/2}(1) G_{1/2}^{*}(1'), \qquad (2.1)$$

where

$$G_{1}(1, 1') \equiv -i \langle \{ \Psi(1) \Psi^{\dagger}(1') \}_{*} \rangle,$$

$$G_{1/2}(1) \equiv (-i)^{1/2} \langle \Psi(1) \rangle = \begin{bmatrix} g_{1}(1) \\ g_{2}(1) \end{bmatrix},$$
(2.2)

and

$$\Psi(1) = \begin{bmatrix} \psi(1) \\ \psi^{\dagger}(1) \end{bmatrix}, \quad \Psi^{*}(1) = \begin{bmatrix} \psi^{\dagger}(1), \ \psi(1) \end{bmatrix}. \quad (2.3)$$

In addition to the system's effective Hamiltonian $\hat{\mathcal{K}} = \hat{H} - \mu \hat{N}$, we assume the existence of external fields given by

$$\hat{V}_{\text{ext}}(t_1) = \frac{1}{2} \sum_{\alpha\beta} \int d\vec{\mathbf{r}}_1 \Psi_{\alpha}^{\dagger}(1) U_{\alpha\beta}(1, \overline{2}) \Psi_{\beta}(\overline{2}) + \sum_{\alpha} \int d\vec{\mathbf{r}}_1 \Psi_{\alpha}^{\dagger}(1) \eta_{\alpha}^{\text{ext}}(1), \quad (2.4)$$

where barred coordinates imply a space and (imaginary) time integration and

$$U_{\alpha\beta}(1,2) \equiv \delta_{\alpha\beta} U(1,2) = \delta_{\alpha\beta} \delta(t_1 - t_2) U(\vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2) ,$$

$$\eta^{\text{ext}}(1) \equiv \begin{bmatrix} \eta_1^{\text{ext}}(1) \\ \eta_2^{\text{ext}}(1) \end{bmatrix} .$$
(2.5)

The equations of motion can be written in the form

$$G_{0}^{-1}(1, \overline{2}) \tilde{G}_{1}(\overline{2}, 1') = \delta(1, 1') + \Sigma(1, \overline{2}) \tilde{G}_{1}(\overline{2}, 1') + U(1, \overline{2}) \tilde{G}_{1}(\overline{2}, 1')$$
(2.6)

and

with

$$G_0^{-1}(1, \overline{2}) G_{1/2}(\overline{2}) = (-i)^{1/2} \eta(1) + (-i)^{1/2} \eta^{\text{ext}}(1) + U(1, \overline{2}) G_{1/2}(\overline{2}), \quad (2.7)$$

$$G_0^{-1}(1, 1') \equiv \left(i\tau^{(3)}\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2} + \overline{\mu}\right) \delta(1, 1') . \quad (2.8)$$

We choose units such that $\hbar = m = 1$. Equations (2.6) and (2.7) determine \tilde{G}_1 and $G_{1/2}$ in terms of the self-energy $\Sigma(1, 2)$ and the condensate source function $\eta(1)$.

In the limit $\hat{V}_{ext} \rightarrow 0$, Eqs. (2.6) and (2.7) describe a homogeneous condensed Bose system. In this case we may take

$$G_{1/2}(1) = (-in_0)^{1/2} \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

where n_0 is the number of atoms in the condensate. In this limit, (2.7) reduces to an equation determining the chemical potential $\overline{\mu}$.

We may use functional differentiation with respect to the auxiliary scalar field U(1, 2) to generate the two-particle correlation function

$$L(1, 2; 1', 2') \equiv \frac{\delta G_{11}(1, 1'; U)}{\delta U(2', 2)} \bigg|_{U=0}.$$
 (2.9)

One may easily verify that the equilibrium timeordered density-density correlation function is given by

$$L_{11}(1,2) \equiv -i \left\lfloor \left\langle \left\{ n(1)n(2) \right\}_{+} \right\rangle - \left\langle n(1) \right\rangle \left\langle n(2) \right\rangle \right\rfloor$$

$$=iL(1, 2; 1, 2)$$
 (2.10)

In terms of the Fourier transform of this correlation function, Van Hove's dynamical structure factor is simply

$$S(k, \omega) = -2 [N^{0}(\omega) + 1] \operatorname{Im} L_{11}(k, \omega) , \qquad (2.11)$$

where $N^{0}(\omega) = [e^{\beta \omega} - 1]^{-1}$ and $\beta = (k_{B}T)^{-1}$. Inelastic thermal neutron scattering enables one to directly measure $S(k, \omega)$.

It is useful to define the matrix inverse of $ilde{G}_1$ by

$$\tilde{G}_{1}(1, \overline{2})\tilde{G}_{1}^{-1}(\overline{2}, 1') = \tilde{G}_{1}^{-1}(1, \overline{2})\tilde{G}_{1}(\overline{2}, 1') = \delta_{\alpha\beta} \,\,\delta(1, 1') \,\,.$$
(2.12)

Using (2.6), we have

$$\tilde{G}^{-1}(1, 1'; U) = \tilde{G}_0^{-1}(1, 1') - U(1, 1') - \Sigma(1, 1'; U) .$$
(2.13)

A somewhat lengthy but straightforward calculation gives the identity

$$\frac{\delta \tilde{G}_{\alpha\beta}(\mathbf{1},\mathbf{1}')}{\delta U(\mathbf{2}',\mathbf{2})}\Big|_{U=0} = -\sum_{\alpha, \ \gamma=1,2} \tilde{G}_{\alpha\sigma}(\mathbf{1},\overline{\mathbf{3}}) \frac{\delta \tilde{G}_{\sigma\gamma}^{-1}(\overline{\mathbf{3}},\overline{\mathbf{4}})}{\delta U(\mathbf{2}',\mathbf{2})}\Big|_{U=0}$$
$$\times \tilde{G}_{\gamma\beta}(\overline{\mathbf{4}},\mathbf{1}')$$
$$= \sum_{\sigma=1,2} \tilde{G}_{\alpha\sigma}(\mathbf{1},\mathbf{2}')\tilde{G}_{\sigma\beta}(\mathbf{2},\mathbf{1}')$$

238

$$+\sum_{\sigma, \gamma=1,2} \tilde{G}_{\alpha\sigma}(1,\overline{3}) \left. \frac{\delta \Sigma_{\sigma\gamma}(3,4)}{\delta U(2',2)} \right|_{U=0} \times \tilde{G}_{\gamma\beta}(\overline{4},1'), \qquad (2.14)$$

_ _ .

where we have made use of (2.13) in the last step.

Our major aim is to obtain $S(k, \omega)$ using (2.9) in conjunction with the conserving Hartree-Fock (or GA) approximation for G_1 . The results of such a calculation have been reported by Hohenberg (see Ref. 4) for a purely repulsive potential in the long-wavelength low-temperature limit.

The Hartree-Fock approximation for the Dyson-Beliaev self-energies in the presence of a scalar field U(1, 2) is given by

$$\Sigma(1, 1') = \frac{1}{2} i V(1, \overline{2}) [G_{1/2}(\overline{2}) G_{1/2}^{*}(\overline{2}) + \tilde{G}_{1}(\overline{2}, \overline{2})] \delta(1, 1')$$
$$+ i V_{R}(1, 1') [G_{1/2}(1) G_{1/2}^{*}(1') + \tilde{G}_{1}(1, 1')],$$
(2.15)

where

$$V(1, 2) = \left[V_R \delta(\vec{r}_1 - \vec{r}_2) + V_A (\vec{r}_1 - \vec{r}_2) \right] \delta(t_1 - t_2) ,$$

$$V_A(1, 2) = V_A (\vec{r}_1 - \vec{r}_2) \delta(t_1 - t_2).$$
(2.16)

The Green's functions in (2.15) are the true ones, self-consistently determined by (2.6) and (2.7). By $V_A(\vec{\mathbf{r}})$ we denote the weak long-range potential between two He⁴ atoms. For later purposes, we further specify the form of $V_A(k)$, the Fourier transform of $V_A(\vec{\mathbf{r}})$:

$$V_{A}(k) = -4\pi(a+b), \quad |\vec{k}| < k_{0}$$

= 0,
$$|\vec{k}| > k_{0}$$
 (2.17)

where *a* is the zero-momentum scattering amplitude for the strong repulsive part V_R (= $4\pi a$). This model of an interacting Bose gas was first employed by Huang.⁵ In the self-energy terms due to exchange, we only consider the repulsive potential. Under certain conditions, it can be shown that the exchange term for the long-range attractive potential is of higher order.

Substituting (2.15) into (2.14), we obtain

$$\frac{\delta \sum_{\alpha\beta} (\mathbf{1}, \mathbf{1'})}{\delta U(\mathbf{2', 2)}} \bigg|_{U=0} = i\delta(\mathbf{1}, \mathbf{1'}) V(\mathbf{1}, \overline{\mathbf{3}}) \frac{\delta G_{11}(\overline{\mathbf{3}}, \overline{\mathbf{3}})}{\delta U(\mathbf{2', 2})} \bigg|_{U=0} \delta_{\alpha\beta}$$
$$+ i\delta(\mathbf{1}, \mathbf{1'}) V_R \frac{\delta G_{\alpha\beta} (\mathbf{1}, \mathbf{1'})}{\delta U(\mathbf{2', 2})} \bigg|_{U=0}. \quad (2.18)$$

Inserting this approximate result into (2.14) and setting 1'=1, 2'=2, we find a set of coupled equations for

$$\begin{split} L_{\alpha\beta}(1,2) &\equiv \left. \frac{i \,\delta G_{\alpha\beta}(1,1)}{\delta U(2)} \right|_{U=0} ,\\ \tilde{L}_{\alpha\beta}(1,2) &\equiv \left. \frac{i \,\delta \tilde{G}_{\alpha\beta}(1,1)}{\delta U(2)} \right|_{U=0} . \end{split}$$

$$(2.19)$$

Fourier-transforming this set of equations, we obtain finally

$$\tilde{L}_{11}(k, \omega_{\nu}) = \left[\tilde{\chi}_{1}^{0}(k, \omega_{\nu}) + \tilde{\chi}_{2}^{0}(k, \omega_{\nu})\right] + \left[2V_{R} + V_{A}(k)\right] \left[\tilde{\chi}_{1}^{0}(k, \omega_{\nu}) + \tilde{\chi}_{2}^{0}(k, \omega_{\nu})\right] L_{11}(k, \omega_{\nu}) + V_{R}\tilde{\chi}_{3}^{0}(k, -\omega_{\nu}) L_{12}(k, \omega_{\nu}), \qquad (2.20)$$

$$L_{12}(k, \omega_{\nu}) = 2\tilde{\chi}_{3}^{0}(k, -\omega_{\nu}) + \left[2V_{R} + V_{A}(k)\right] 2\tilde{\chi}_{3}^{0}(k, -\omega_{\nu}) L_{11}(k, \omega_{\nu})$$

$$- V_R \tilde{\chi}_2^0(k,\,\omega_\nu) L_{21}(k,\,\omega_\nu) + V_R \tilde{\chi}_4^0(k,\,\omega_\nu) L_{12}(k,\,\omega_\nu), \qquad (2.21)$$

$$\tilde{L}_{21}(k,\,\omega_{\nu}) = 2\tilde{\chi}_{3}^{0}(k,\,\omega_{\nu}) + \left[2V_{R} + V_{A}(k)\right] 2\tilde{\chi}_{3}^{0}(k,\,\omega_{\nu}) L_{11}(k,\,\omega_{\nu})$$

+
$$V_R \tilde{\chi}_4^0(k, -\omega_\nu) L_{21}(k, \omega_\nu) + V_R \tilde{\chi}_2^0(k, \omega_\nu) L_{12}(k, \omega_\nu),$$
 (2.22)

where we have used the identities

$$G_{12}(1, 2) = G_{21}(1, 2), \quad G_{11}(1, 2) = G_{22}(2, 1)$$
 (2.23)
and introduced the following abbreviations:

$$\begin{split} \tilde{\chi}_{1}^{0}(1, 2) &= i\tilde{G}_{11}(1, 2) \tilde{G}_{11}(2, 1) = \tilde{\chi}_{1}^{0}(2, 1), \\ \tilde{\chi}_{2}^{0}(1, 2) &= i\tilde{G}_{12}(1, 2) \tilde{G}_{12}(2, 1) = \tilde{\chi}_{2}^{0}(2, 1), \\ \tilde{\chi}_{3}^{0}(1, 2) &= i\tilde{G}_{12}(1, 2) \tilde{G}_{11}(2, 1), \\ \tilde{\chi}_{4}^{0}(1, 2) &= i\tilde{G}_{11}(1, 2) \tilde{G}_{11}(1, 2). \end{split}$$

$$(2.24)$$

$$L_{11} = \tilde{L}_{11} + (-in_0)^{1/2} i \left[L_{1/2} + L_{1/2}^* \right], \qquad (2.25a)$$

$$L_{12} = \tilde{L}_{12} + (-in_0)^{1/2} 2iL_{1/2}, \qquad (2.25b)$$

$$L_{21} = \tilde{L}_{21} + (-in_0)^{1/2} 2iL_{1/2}^*, \qquad (2.25c)$$

where the three-point function is defined by

$$L_{1/2}(1, 2) \equiv \frac{\delta g_1(1)}{\delta U(2)} \bigg|_{U=0}$$
, etc. (2.26)

Now in the Hartree-Fock approximation, the source function is given by

 $+iV_{R}[g_{1}(1)\tilde{G}_{11}(1,1)+g_{2}(1)\tilde{G}_{12}(1,1)],$ (2.27a)

 $(-i)^{1/2}\eta_1(1) = iV(1, \overline{2})g_1(1)G_{11}(\overline{2}, \overline{2})$

$$(-i)^{1/2}\eta_2(1) = iV(1, \overline{2})g_2(1)G_{11}(2, \overline{2})$$

+ $iV_R[g_1(1)\tilde{G}_{21}(1,1)+g_2(1)\tilde{G}_{11}(1,1)]$. (2.27b)

Taking the functional derivative of Eqs. (2.7) in conjunction with (2.27) and then Fourier transforming, we obtain

$$\begin{aligned} (\omega_{\nu} - \frac{1}{2} k^{2} + \overline{\mu}) L_{1/2}(k, \omega_{\nu}) &= i V_{R} [G_{11}(1, 1) + \tilde{G}_{11}(1, 1)] L_{1/2}(k, \omega_{\nu}) + i V_{R} \tilde{G}_{12}(1, 1) L_{1/2}^{*}(k, \omega_{\nu}) \\ &+ (-in_{0})^{1/2} \{ V_{R} [L_{11}(k, \omega_{\nu}) + \tilde{L}_{11}(k, \omega_{\nu}) + \tilde{L}_{12}(k, \omega_{\nu})] + 1 \} \\ &+ i V_{A} G_{11}(1, 1) L_{1/2}(k, \omega_{\nu}) + (-in_{0})^{1/2} V_{A}(k) L_{11}(k, \omega_{\nu}), \quad (2.28) \\ (-\omega_{\nu} - \frac{1}{2} k^{2} + \overline{\mu}) L_{1/2}^{*}(k, \omega_{\nu}) &= i V_{R} [G_{11}(1, 1) + \tilde{G}_{11}(1, 1)] L_{1/2}^{*}(k, \omega_{\nu}) + i V_{R} \tilde{G}_{12}(1, 1) L_{1/2}(k, \omega_{\nu}) \\ &+ (-in_{0})^{1/2} \{ V_{R} [L_{11}(k, \omega_{\nu}) + \tilde{L}_{11}(k, \omega_{\nu}) + \tilde{L}_{21}(k, \omega_{\nu})] + 1 \} \\ &+ i V_{A} G_{11}(1, 1) L_{1/2}(k, \omega_{\nu}) + (-in_{0})^{1/2} V_{A}(k) L_{11}(k, \omega_{\nu}). \quad (2.29) \end{aligned}$$

We have made use of $g_1(1) = g_2(1) = (-in_0)^{1/2}$ for a homogeneous system and $V_A \equiv V_A(k=0)$.

Equations (2. 20)-(2. 22), (2. 28), and (2. 29) form a closed set of linear algebraic equations which can be solved for L_{11} , L_{12} , L_{21} , $L_{1/2}$, and $L_{1/2}^*$. The density-density correlation function in (2.11) is directly related to $L_{11}(k, \omega_{\nu})$. The polarization functions $\tilde{\chi}_{i}^{0}(k, \omega_{\nu})$ (*i*=1, 2, 3, 4) are determined by the Hartree-Fock single-particle Green's functions $\tilde{G}_{\alpha\beta}$:

$$\begin{split} \tilde{\chi}_{1}^{0}(k,\,\omega_{\nu}) &= -\frac{1}{\beta} \sum_{\nu'} \int \frac{d\,\vec{k}\,'}{(2\pi)^{3}} \,\tilde{G}_{11}(\vec{k}\,',\,\omega_{\nu'}) \,\tilde{G}_{11}(\vec{k}\,'-\vec{k},\,\omega_{\nu'}-\omega_{\nu}) \\ &= \tilde{\chi}_{1}^{0}(k,\,-\omega_{\nu}), \\ \tilde{\chi}_{2}^{0}(k,\,\omega_{\nu}) &= -\frac{1}{\beta} \sum_{\nu'} \int \frac{d\,\vec{k}\,'}{(2\pi)^{3}} \,\tilde{G}_{12}(\vec{k}\,',\,\omega_{\nu'}) \,\tilde{G}_{12}(\vec{k}\,'-\vec{k},\,\omega_{\nu'}-\omega_{\nu}) \\ &= \tilde{\chi}_{2}^{0}(k,\,-\omega_{\nu}), \end{split}$$
(2.30)
$$\tilde{\chi}_{3}^{0}(k,\,\omega_{\nu}) &= -\frac{1}{\beta} \sum_{\nu'} \int \frac{d\,\vec{k}\,'}{(2\pi)^{3}} \,\tilde{G}_{12}(\vec{k}\,',\,\omega_{\nu'}) \,\tilde{G}_{11}(\vec{k}\,'-\vec{k},\,\omega_{\nu'}-\omega_{\nu}), \\ \tilde{\chi}_{4}^{0}(k,\,\omega_{\nu}) &= -\frac{1}{\beta} \sum_{\nu'} \int \frac{d\,\vec{k}\,'}{(2\pi)^{3}} \,\tilde{G}_{11}(\vec{k}\,,\omega_{\nu'}) \,\tilde{G}_{11}(\vec{k}\,-\vec{k}\,',\,\omega_{\nu}-\omega_{\nu'}). \end{split}$$

In terms of spectral densities, we have (for example)

$$\begin{split} \tilde{\chi}_{1}^{0}(k,\,\omega_{\nu}) &= \int \frac{d\,\vec{\mathbf{k}}\,'}{(2\pi)^{3}} \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \frac{N^{0}(\omega) - N^{0}(\omega')}{\omega - \omega' - \omega_{\nu}} \\ &\times \tilde{A}_{11}(\vec{\mathbf{k}},\,\omega) \tilde{A}_{11}(\vec{\mathbf{k}}\,' - \vec{\mathbf{k}},\,\omega'), \quad (2.31a) \\ \tilde{\chi}_{4}^{0}(k,\,\omega_{\nu}) &= -\int \frac{d\,\vec{\mathbf{k}}\,'}{(2\pi)^{3}} \int \frac{d\omega}{2\pi} \int \frac{d\omega'}{2\pi} \frac{N^{0}(\omega) + N^{0}(\omega') + 1}{\omega + \omega' - \omega_{\nu}} \\ &\times \tilde{A}_{11}(\vec{\mathbf{k}}\,',\,\omega) \tilde{A}_{11}(\vec{\mathbf{k}}\,' - \vec{\mathbf{k}},\,\omega'). \quad (2.31b) \end{split}$$

Finally, the chemical potential $\overline{\mu}$ is determined by inserting (2. 27) into (2. 7). We thus obtain

$$\vec{\mu} = i V_R [G_{11}(1, 1) + \tilde{G}_{11}(1, 1) + \tilde{G}_{12}(1, 1)]$$

 $+iV_A \tilde{G}_{11}(1,1)$ (2.32)

in the Hartree-Fock approximation.

The Hartree-Fock approximation summarized by (2.15) and (2.27) is a so-called "conserving approximation" in the sense that both the self-energy and source function can be generated from the same

240

4

functional $\Phi{\{\vec{G}_1, G_{1/2}\}}$ by differentiation.^{4,9} We are thus ensured that the spectrum exhibited by $L_{\alpha\beta}$ $\times(\vec{k}, \omega)$ will be gapless in the limit of long wavelength. However, the chemical potential $\overline{\mu}$ in (2.32) does not obey the Hugenholtz-Pines equality $\bar{\mu} = \Sigma_{11}(0, 0) - \Sigma_{12}(0, 0)$ (2.33) and hence the spectrum exhibited by $\tilde{G}_{\alpha\beta}$ in the longwavelength limit will have a gap.

Making use of (2.25) and (2.32), we may rewrite Eqs. (2.20)-(2.22), (2.28), and (2.29) as follows:

$$\left[1 - 2\overline{V}\tilde{\chi}_{1}^{0} - 2\overline{V}\tilde{\chi}_{2}^{0}\right]L_{11} - V_{R}\tilde{\chi}_{3}^{0}L_{12} - V_{R}\tilde{\chi}_{3}^{0}L_{21} - i(-in_{0})^{1/2}L_{1/2} - i(-in_{0})^{1/2}L_{1/2}^{*} = \tilde{\chi}_{1}^{0} + \tilde{\chi}_{2}^{0}, \qquad (2.34a)$$

$$-4\overline{V}\tilde{\chi}_{3}^{0*}L_{11} + \left[1 - V_{R}\tilde{\chi}_{4}^{0}\right]L_{12} - V_{R}\tilde{\chi}_{2}^{0}L_{21} - 2i(-in_{0})^{1/2}L_{1/2} = 2\tilde{\chi}_{3}^{0*}, \qquad (2.34b)$$

$$-4\overline{V}\,\tilde{\chi}_{3}^{0}\,L_{11}-V_{R}\,\tilde{\chi}_{2}^{0}\,L_{12}+\left[1-V_{R}\,\tilde{\chi}_{4}^{0*}\right]L_{21}-2i(-in_{0})^{1/2}L_{1/2}^{*}=2\,\tilde{\chi}_{3}^{0}\,,\qquad(2.34c)$$

$$-(-in_0)^{1/2} 2\overline{V}L_{11} - (-in_0)^{1/2} V_R L_{12} + [\omega_\nu - \frac{1}{2}k^2 + iV_R \tilde{G}_{12}(1,1) + 3n_0 V_R]L_{1/2} + [-iV_R \tilde{G}_{12}(1,1) + n_0 V_R]L_{1/2}^* = (-in_0)^{1/2},$$

$$-(-in_0)^{1/2}2\overline{V}L_{11} - (-in_0)^{1/2}V_RL_{21} + [-iV_R\tilde{G}_{12}(1,1) + n_0V_R]L_{1/2} + [-\omega_\nu - \frac{1}{2}k^2 + iV_R\tilde{G}_{12}(1,1) + 3n_0V_R]L_{1/2}^* = (-in_0)^{1/2}, \quad (2.34e)$$

where $2\overline{V} \equiv 2V_R + V_A(k)$ and $\tilde{\chi}_3^{0*} \equiv \tilde{\chi}_3^0(k, -\omega_\nu)$, etc. It is a straightforward but lengthy task to solve this system of five linear algebraic equations and hence determine the density-density correlation function $S(k, \omega)$. Since we are working in a conserving approximation, the resulting expression for $S(k, \omega)$ will satisfy the *f*-sum rule.⁹

In closing this section, we note that the solution of system of equations in (2.34) is very simple for an uncondensed Bose gas $(n_0=0)$, namely,

$$L_{11}(k, \omega_{\nu}) = \frac{\tilde{\chi}_{1}^{0}(k, \omega_{\nu})}{1 - 2\overline{V}(k)\tilde{\chi}_{1}^{0}(k, \omega_{\nu})} \quad .$$
 (2.35)

A more "physical" way of expressing this result is to write it as a sum of polarization bubbles,

$$L_{11}(k, \omega_{\nu}) = \frac{\tilde{\chi}_{E}(k, \omega_{\nu})}{1 - [V_{R} + V_{A}(k)]\tilde{\chi}_{E}(k, \omega_{\nu})} , \qquad (2.36)$$

where each bubble $\tilde{\chi}_{E}(k, \omega_{\nu})$ now contains particlehole multiple scattering arising from the repulsive interaction

$$\tilde{\chi}_E(k,\,\omega_\nu) = \frac{\tilde{\chi}_1^0(k,\,\omega_\nu)}{1 - V_R \tilde{\chi}_1^0(k,\,\omega_\nu)} \quad . \tag{2.37}$$

III. DENSITY FLUCTUATION SPECTRUM INCLUDING ATTRACTIVE INTERACTIONS IN LONG-WAVELENGTH 0°K LIMIT

The spectrum exhibited by $L_{\alpha\beta}(k, \omega)$, $L_{1/2}(k, \omega)$, and $L_{1/2}^*(k, \omega)$ can be obtained from the condition that the determinant $\Delta(k, \omega)$ of the coefficients in (2.34) must vanish. $\Delta(k, \omega)$ is obtained from $\Delta(k, \omega_{\nu})$ by analytic continuation from the discrete set of points ω_{ν} .

A. Lowest-Order Approximation

To begin with, we only keep terms in $\Delta(k, \omega_{\nu})$ which involve explicitly the interaction potentials to first order. We obtain, after a lengthy calculation,

$$\Delta^{(1)}(k, \omega_{\nu}) = \left[-\omega_{\nu}^{2} + (\frac{1}{2}k^{2})^{2}\right]$$

$$\times \left[1 - 2\overline{V}(\tilde{\chi}_{1}^{0} + \tilde{\chi}_{2}^{0}) - V_{R}(\tilde{\chi}_{4}^{0} + \tilde{\chi}_{4}^{0*})\right]$$

$$+ n_{0}[V_{R} + V_{A}(k)]k^{2} - iV_{R}\tilde{G}_{12}(1, 1)k^{2}. \quad (3.1)$$

If we restrict ourselves to a strictly perturbative solution of $\Delta^{(1)}(k, \omega_{\nu}) = 0$, we see immediately that the density fluctuation spectrum is given by

$$-\omega_k^2 + (\frac{1}{2}k^2)^2 + n_0 [V_R + V_A(k)]k^2 = 0.$$
 (3.2)

If we specialize to the use of purely repulsive interactions, this expression reduced to single-particle spectrum derived by Bogoliubov. Equation (3.2) also coincides with the lowest-order results of Singh and Kumar,⁶ who evaluated the singleparticle spectrum in the case of a system of bosons including attractive interactions. However, the total scattering length of the potential (repulsive plus attractive) in the present case is negative, and hence ω_k becomes pure imaginary as k approaches zero. It is therefore necessary to include higher-order terms in $\Delta(k, \omega_{\nu})$. We note in passing that in going from (3.1) to (3.2), we have assumed that the functions $\tilde{\chi}_i^0(k, \omega_{\nu})$ do not exhibit any singular

(2.34d)

structure and hence we can multiply (3.1) through by

$$D(k, \omega_{\nu}) \equiv \left[1 - 2\overline{V}(\tilde{\chi}_{1}^{0} + \tilde{\chi}_{2}^{0}) - V_{R}(\tilde{\chi}_{4}^{0} + \tilde{\chi}_{4}^{0*})\right]^{-1}$$
$$\simeq 1 + 2\overline{V}(\tilde{\chi}_{1}^{0} + \tilde{\chi}_{2}^{0}) + V_{R}(\tilde{\chi}_{4}^{0} + \tilde{\chi}_{4}^{0*}) .$$
(3.3)

B. Higher-Order Approximation

On examining the various high-order terms in $\Delta(k, \omega_{\nu})$, we find that the density fluctuation spectrum is determined by

$$\Delta^{(2)}(k,\omega_{\nu}) = -\omega_{\nu}^{2} + (\frac{1}{2}k^{2})^{2} + 2n_{0}\omega_{\nu} \left[V_{R}^{2}(\tilde{\chi}_{4}^{0} - \tilde{\chi}_{4}^{0*}) + 4\overline{V}V_{R}(\tilde{\chi}_{3}^{0*} - \tilde{\chi}_{3}^{0}) \right] + n_{0}k^{2} \left[V_{R}^{2}(\tilde{\chi}_{4}^{0} + \tilde{\chi}_{4}^{0*}) + 4\overline{V}V_{R}(\tilde{\chi}_{3}^{0*} + \tilde{\chi}_{3}^{0}) + 4\overline{V}^{2}(\tilde{\chi}_{1}^{0} + \tilde{\chi}_{2}^{0}) \right] \\ + k^{2} \left\{ n_{0} \left[V_{R} + V_{A}(k) \right] - i\tilde{G}_{12}(1,1) \right\} - 4n_{0} \left[2V_{R}\overline{V} - V_{R}^{2} \right] i\tilde{G}_{12}(1,1) = 0 .$$

$$(3.4)$$

In the derivation of (3. 4), we have again assumed the functions $\tilde{\chi}_i^0(k, \omega_{\nu})$ are well-behaved functions of k and ω_{ν} and thus $D(k, \omega_{\nu})$ does not introduce any new singularities (see Sec. 5 of Beliaev²).

In the limit $k \rightarrow 0$, the coefficient of ω_{ν} in (3.4) vanishes. Making use of the fact that the last term may be neglected since it is of higher order, we are left with

$$\omega_{k}^{2} = -4\pi b n_{0} k^{2} + A k^{2} - i4\pi a \,\tilde{G}_{12}(1,\,1) k^{2} , \qquad (3.5)$$

where

$$A \equiv n_0 (4\pi a)^2 \left\{ 2\tilde{\chi}_4^0(0, 0) + 4 \left[1 + \frac{V_A(0)}{4\pi a} + \frac{1}{4} \left(\frac{V_A(0)}{4\pi a} \right)^2 \right] \times \left[\tilde{\chi}_1^0(0, 0) + \tilde{\chi}_2^0(0, 0) \right] + 8 \left(1 + \frac{1}{2} \frac{V_A(0)}{4\pi a} \right) \tilde{\chi}_3^0(0, 0) \right\} .$$

$$(3.6)$$

We now assume that $V_A(k)$ is given by (2.17) with $b/a \ll 1$. In this case, we have

$$V_A(0)/4\pi a \approx -1$$
, (3.7)

and (3.6) simplifies to

$$A \approx n_0 (4\pi a)^2 \left[2\tilde{\chi}_4^0(0,0) + \tilde{\chi}_1^0(0,0) + \tilde{\chi}_2^0(0,0) + 4\tilde{\chi}_3^0(0,0) \right] .$$
(3.8)

Proceeding in a perturbative fashion, it is sufficient to use the Bogoliubov propagators in (2.30).

Let us now restrict ourselves to the case of zero temperature, in which case the functions $\bar{\chi}_i^0(k=0, \omega_{\nu}=0)$ can be computed directly from (2.30) using

$$-\frac{1}{\beta}\sum_{\nu'}+i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}$$

It turns out that these integrals have already been evaluated by Singh and Kumar,⁶ to whom we refer the reader for a detailed discussion. One obtains

$$A = \kappa \left[(1 + \nu^2)^{-1/2} + 2(1 + \nu^2)^{1/2} - 2\nu \right],$$

$$i V_R \tilde{G}_{12}(1, 1) = \kappa \left[(1 + \nu^2)^{1/2} - \nu \right],$$

(3.9)

where

$$\kappa = 32n_0 a (\pi n_0 a^3)^{1/2} \tag{3.10}$$

and

$$\frac{1}{\nu = k_0 a / (16\pi n_0 a^3)^{1/2}}.$$
(3.11)

The density fluctuation spectrum at very small momentum is then

$$\omega_k^2 = 4\pi n_0 a [-b/a + 16(n_0 a^3/\pi)^{1/2} G(\nu)]k^2 , \qquad (3.12)$$

where

$$G(\nu) \equiv \frac{1}{2} \left[(1+\nu^2)^{1/2} + (1+\nu^2)^{-1/2} - \nu \right] .$$
 (3.13)

It is phononlike provided

$$b/a < 16(n_0 a^3/\pi)^{1/2} G(\nu)$$
 (3.14)

A plot of $G(\nu)$ can be found in Ref. 6.

In evaluating the integrals involved in $\tilde{\chi}_i^0(0, 0)$, the momentum integrations are restricted to $|\vec{k}'| > k_0$. It can be shown that the contributions from the interval $(0, k_0)$ are of a higher order in b/a than those given in (3.12). It is easily seen that this justifies our neglect of exchange terms for the weak long-range attractive potential in the Dyson-Beliaev self-energies.

This completes our proof that in the long-wavelength 0 $^{\circ}$ K limit, the density fluctuation spectrum in the Hartree-Fock approximation is identical to that of the single-particle spectrum in the Singh-Kumar approximation. While Singh and Kumar did not discuss the density fluctuation spectrum directly, they did show that the thermodynamically defined sound velocity was equal to the velocity of the phononlike single-particle excitations.

While the above discussion was limited to 0 $^{\circ}$ K, we recall that (3.8) is valid at finite temperatures as well. In this connection, we note that Singh and Kumar¹⁰ have recently extended their work on the single-particle excitations to include the lowest-order temperature corrections.

IV. EQUIVALENCE OF DENSITY FLUCTUATIONS AND SINGLE-PARTICLE EXCITATIONS FOR REPULSIVE INTERACTIONS

In this section, we wish to show explicitly that the density fluctuation spectrum predicted by $\Delta(k, \omega)$ = 0 is formally identical to the single-particle excitation spectrum based on the Beliaev approximation,² for arbitrary values of the temperature and

wavelength. We shall set the attractive potential $V_A(k)$ to zero for simplicity.

We recall that the poles of $\tilde{G}_1(k,\,\omega)$ are determined by

$$\left[\omega - \frac{1}{2}(\Sigma_{11}^{*} - \Sigma_{11}^{*})\right]^{2} - \left[\frac{1}{2}k^{2} - \overline{\mu} + \frac{1}{2}(\Sigma_{11}^{*} + \Sigma_{11}^{*})\right]^{2} + \Sigma_{12}^{2} = 0,$$
(4.1)

where $\Sigma_{11}^{\pm} \equiv \Sigma_{11} (k, \pm \omega)$. To second order in the explicit dependence on V_R , the Dyson-Beliaev selfenergies are given by Eq. (6.48) of Ref. 4. This neglects terms of the kind $V_R^2 \tilde{G}_1 \cdot \tilde{G}_1 \cdot \tilde{G}_1$, which turn out to be of higher order in a dilute weakly interacting Bose gas. One may verify after some calculation that

and

$$\Sigma_{12}(k, \omega) = [n_0 + i\tilde{G}_{12}(1, 1)]V_R$$
$$+ n_0 V_R^2 [4\tilde{\chi}_1^0 + 6\tilde{\chi}_2^0 + 4(\tilde{\chi}_3^0 + \tilde{\chi}_3^{0*})] . \quad (4.3)$$

Inserting (4.2) and (4.3) into (4.1) and using

$$\overline{\mu} = V_R[iG_{11}(1,1) + i\tilde{G}_{11}(1,1) + i\tilde{G}_{12}(1,1)]$$
$$= V_R[2n - n_0 + i\tilde{G}_{12}(1,1)], \qquad (4.4)$$

we find that (4.1) can be written as

$$-\omega^{2} + (\frac{1}{2}k^{2})^{2} + \omega(\Sigma_{11}^{+} - \Sigma_{11}^{-}) + \frac{1}{2}k^{2}(\Sigma_{11}^{+} + \Sigma_{11}^{-} - 2\overline{\mu})$$
$$+ n_{0}V_{R}(\Sigma_{11}^{+} + \Sigma_{11}^{-} - 2\overline{\mu} - 2\Sigma_{12}) = 0 \qquad (4.5)$$

or, more explicitly,

$$-\omega^{2} + (\frac{1}{2}k^{2})^{2} + 2n_{0}\omega V_{R}^{2}[(\tilde{\chi}_{4}^{0} - \tilde{\chi}_{4}^{0*}) + 4(\tilde{\chi}_{3}^{0*} - \tilde{\chi}_{3}^{0})] + k^{2}V_{R}[n_{0} - i\tilde{G}_{12}(1, 1)] + n_{0}k^{2}V_{R}^{2}[4(\tilde{\chi}_{3}^{0} + \tilde{\chi}_{3}^{0*}) + 4(\tilde{\chi}_{1}^{0} + \tilde{\chi}_{2}^{0}) + (\tilde{\chi}_{4}^{0} + \tilde{\chi}_{4}^{0*})] - 4n_{0}i\tilde{G}_{12}(1, 1)V_{R}^{2} + 2n_{0}^{2}V_{R}^{3}[(\tilde{\chi}_{4}^{0} + \tilde{\chi}_{4}^{0*}) - 2\tilde{\chi}_{2}^{0}] = 0.$$

$$(4.6)$$

Here we have kept certain terms which are of third order in their explicit dependence on V_R , although we omit terms of the kind $n_0 i \tilde{G}_{12} V_R^3 \tilde{\chi}_i^0$ as giving rise to higher-order corrections. Now, if we work out the determinant $\Delta(k, \omega)$ using (2.34) to third order in V_R , neglecting all terms involving products of two or more $\tilde{\chi}_i^0(k, \omega)$ functions, we find that $\Delta^{(3)}(k, \omega)$ = 0 is *identical* to (4.6). As in Sec. III, this determination of the density fluctuation spectrum is based on the assumption that

$$1 - 2V_R(\tilde{\chi}_1^0 + \tilde{\chi}_2^0) - V_R(\tilde{\chi}_4^0 + \tilde{\chi}_4^{0*}) = 0$$
(4.7)

has no solutions. To the extent that this is true, the *density* fluctuation spectrum using the Hartree-Fock conserving approximation is given by either (4.5) or (4.6).

The reason that we must include terms of order V_R^3 in (4.6) is only clear after we have evaluated the coefficients involving $\tilde{\chi}_i^0(k, \omega)$. We are not dealing with a simple perturbative expansion in powers of the interaction. If we limit ourselves to 0 °K for simplicity, we find that the expansion parameter is $(n_0 V_R^3)^{1/2}$, the condensate gas parameter. Explicit calculation using (4.2) and (4.3) in the long-wavelength limit gives

$$\Sigma_{11}(k, \pm \omega_{k}) = 2n_{0}V_{R} + \frac{14}{3\pi^{2}}n_{0}V_{R}(n_{0}V_{R}^{3})^{1/2} \mp \frac{n_{0}V_{R}^{2}k}{2\pi^{2}} + \frac{79}{720\pi^{2}}(n_{0}V_{R}^{3})^{1/2}k^{2} + \cdots ,$$

$$\Sigma_{12}(k, \omega_{k}) = n_{0}V_{R} + \frac{3}{\pi^{2}}n_{0}V_{R}(n_{0}V_{R}^{3})^{1/2}$$
(4.8)

and

$$\overline{\mu} = n_0 V_R [1 + (5/3\pi^2) (n_0 V_R^3)^{1/2}], \qquad (4.9)$$

 $-\frac{41}{720\pi^2} (n_0 V_R^3)^{1/2} k^{2_+} \cdots ,$

where $\omega_k^2 = (\frac{1}{2}k^2)^2 + (n_0 V_R)k^2$ is the Bogoliubov approximation for the excitations. It is easy to verify that (4.8) and (4.9) satisfy the Hugenholtz-Pines relation (2.33) and hence there is no gap in the single-particle excitation spectrum. This is not surprising since (4.6) also determines the density fluctuation spectrum and the latter was obtained using a conserving approximation. It is interesting to note explicitly that in the long-wavelength limit, the last two terms in (4.6), each of order $n_0^2 V_R^2 (n_0 V_R^3)^{1/2}$, exactly cancel each other.

Making use of (4.8) and (4.9) in (4.5), one may show that in the long-wavelength 0 °K limit, the dispersion relation describes a phononlike excitation with a sound velocity given by

$$c = (n_0 V_R)^{1/2} \left[1 + (7/6\pi^2) (n_0 V_R^3)^{1/2} + \cdots \right], \qquad (4.10)$$

as first obtained by Beliaev.² If we simply used $\Sigma_{11}^{*}(0, 0)$ and $\Sigma_{12}(0, 0)$ in (4.5), we would have found the slightly different expression

$$c = (n_0 V_R)^{1/2} \left[1 + (3/2\pi^2)(n_0 V_R^3)^{1/2} \right].$$
(4.11)

This shows that the last term in (4.6) must be included if we are to obtain the complete lowest-order correction to the Bogoliubov velocity $(n_0 V_R)^{1/2}$. Moreover, it suggests that it may not be adequate to use $\tilde{\chi}_i^0$ ($k = 0, \omega = 0$) in evaluating the phonon velocity in the presence of attractive interactions, such

243

as we used (following Singh and Kumar) in obtaining (3.12). This question requires further investigation.

APPENDIX: DENSITY FLUCTUATIONS IN RPA

In Sec. II, we used functional differentiation of the self-consistent Hartree-Fock single-particle Green's functions to obtain the density-density correlation function. We arrived at a closed set of algebraic equations (2, 34) from which we could obtain $S(k, \omega)$. Since the functions $\tilde{\chi}_i^0(k, \omega_{\nu})$ involve the true Hartree-Fock propagators, the set of equations (2, 34) are really nonperturbative in nature. In Secs. III and IV, we examined the density fluctuation sepctrum using these equations in conjunction with a perturbative approach appropriate to a dilute weakly interacting Bose gas.

If we use the Hartree single-particle Green's functions (neglecting the exchange self-energies completely), the structure of the equations of motion in (2.34) is much simpler, although they still describe a conserving approximation. We find

$$L_{11}(k, \omega_{\nu}) = \frac{\left[-\omega_{\nu}^{2} + (\frac{1}{2}k^{2})^{2}\right]\tilde{\chi}_{1}^{0}(k, \omega_{\nu}) - n_{0}k^{2}}{\left[-\omega_{\nu}^{2} + (\frac{1}{2}k^{2})^{2}\right]\left[1 - V(k)\,\tilde{\chi}_{1}^{0}(k, \omega_{\nu})\right] + n_{0}k^{2}V(k)}$$
(A1)

It is of interest to compare the denominator with the Hartree-Fock expression to lowest order given by (3.1). It is convenient to rewrite (A1) in the form

$$L_{11}(k, \omega_{\nu}) = \frac{\chi_{1}^{0}(k, \omega_{\nu})}{1 - V(k)\chi_{1}^{0}(k, \omega_{\nu})} ,$$

where

$$\chi_1^0(k,\,\omega_\nu) \equiv \tilde{\chi}_1^0(k,\,\omega_\nu) + n_0 k^2 \frac{1}{\omega_\nu^2 - (\frac{1}{2}k^2)^2} \quad . \tag{A2}$$

Since the single-particle propagators are given by the Hartree approximation, we have simply

$$\tilde{\chi}_{1}^{0}(k,\,\omega_{\nu}) = \int \frac{d\tilde{\mathbf{p}}}{(2\pi)^{3}} \, \frac{N_{0}(\epsilon_{\mathfrak{F}}) - N^{0}(\epsilon_{\mathfrak{F}+\vec{k}})}{\omega_{\nu} - [\epsilon_{\mathfrak{F}+\vec{k}} - \epsilon_{\mathfrak{F}}]} \quad . \tag{A3}$$

Finally, we obtain the RPA expression for the density-density correlation function

*Work supported by an operating grant from the National Research Council of Canada.

- ¹S. T. Beliaev, Zh. Eksperim. i Teor. Fiz. <u>34</u>, 417 (1958) [Sov. Phys. JETP <u>7</u>, 289 (1958)].
- ²S. T. Beliaev, Zh. Eksperim. i Teor. Fiz. <u>34</u>, 433 (1958) [Sov. Phys. JETP 7, 299 (1958)].
- ³N. M. Hugenholtz and D. Pines, Phys. Rev. <u>116</u>, 489 (1959).
- ⁴P. C. Hohenberg and P. C. Martin, Ann. Phys. (N. Y.) <u>34</u>, 291 (1965).
- ⁵K. Huang, *Studies in Statistical Mechanics* (North-Holland, Amsterdam, 1964), Vol. II.

$$S_{\text{RPA}}(k,\,\omega) = \frac{-2[N^{0}(\omega)+1]\,\text{Im}\,\chi_{1}^{0}(k,\,\omega)}{[1-V(k)\,\text{Re}\,\chi_{1}^{0}(k,\,\omega)]^{2} + [V(k)\,\text{Im}\,\chi_{1}^{0}(k,\,\omega)]^{2}}$$
(A4)

This result has been derived by many authors using different techniques (see, for example, Etters¹¹).

One sees that the structure in $S_{RPA}(k, \omega)$ comes mainly from structure in $Im\chi_1^0(k, \omega)$ for $V(k) \leq 0$ and from the zeros of the denominator

$$1 - V(k) \operatorname{Re}\chi_1^0(k, \,\omega) = 0 \tag{A5}$$

if V(k) > 0. We note that the single-particle spectrum exhibited by $\tilde{G}_{\alpha\beta}(k, \omega)$ in the shielded potential approximation also has a resonance given by (A5). The reader is referred to Ref. 12 for a detailed discussion of the solutions of Eq. (A5) in connection with the single-particle excitation spectrum.

The complete neglect of the effect of the excited atoms $(\vec{k} \neq 0)$ corresponds to setting $\tilde{\chi}_1^0(k, \omega_{\nu})$ in (A2) to zero. In this case, the RPA result (A4) reduces to

$$S(k, \omega) = 2\pi n_0 k^2 [N^0(\omega) + 1] \delta(\omega^2 - \omega_k^2) \operatorname{sgn}\omega , \quad (A6)$$

where $\omega_k^2 = \epsilon_k^2 + n_0 V(k)k^2$. It is easy to see that this expression is equivalent to using

$$L_{11}(k,\,\omega_{\nu}) = n_0 \sum_{\alpha,\beta} \tilde{G}^B_{\alpha\beta}(k,\,\omega_{\nu}) \,, \tag{A7}$$

where $\tilde{G}^{B}_{\alpha\beta}(k,\omega)$ are the single-particle propagators given by the Bogoliubov approximation.

In concluding this appendix, it might be appropriate to mention the recent work of Kerr, Pathak, and Singwi¹³ on the density fluctuation spectrum for large values of $k (\geq 2.5 \text{ Å}^{-1})$. In analyzing neutron scattering data, ¹⁴ they used what might be called a generalized version of the RPA result in (A4). This involved (a) replacing V(k) by an effective potential $\psi(k)$, (b) using the true momentum distribution n_p in (A3), and (c) replacing the sharp δ functions in $\text{Im}\chi_1^0(k, \omega)$ by Gaussians in order to include the damping. Frequency moments or sum rules were then used to determine the effective potential $\psi(k)$ and the width of the Gaussians.

- ⁶K. K. Singh and S. Kumar, Phys. Rev. <u>162</u>, 173 (1967). ⁷J. Gavoret and P. Nozières, Ann. Phys. (N. Y.) <u>28</u>, 349 (1964).
- ⁸M. Girardeau and R. Arnowitt, Phys. Rev. <u>113</u>, 755 (1959).
- ⁹G. Baym and L. P. Kadanoff, Phys. Rev. <u>124</u>, 287 (1961); G. Baym, *ibid*. <u>127</u>, 1391 (1962).
- ¹⁰K. K. Singh and S. Kumar, Phys. Rev. A <u>1</u>, 497 (1970).
- ¹¹R. D. Etters, Phys. Rev. Letters <u>16</u>, 119 (1966).

¹²T. H. Cheung and A. Griffin, Can. J. Phys. <u>48</u>, 2135 (1970).

4

¹³W. C. Kerr, K. N. Pathak, and K. S. Singwi, Phys. Rev. A (to be published).

¹⁴R. A. Cowley and A. D. B. Woods, Phys. Rev. Letters <u>21</u>, 787 (1968).

PHYSICAL REVIEW A

VOLUME 4, NUMBER 1

JULY 1971

Measurement of Transition Probabilities for O1 in the Vacuum Ultraviolet

W. R. Ott*

National Bureau of Standards, Washington, D. C. 20234 (Received 13 November 1970)

Transition probabilities for OI lines emitted in the vacuum ultraviolet were measured using a wall-stabilized arc discharge operating in a mixture of argon and oxygen. The lines were emitted from a column of plasma which was observed end-on and which was characterized by a nearly uniform temperature. Optically thin conditions were achieved by reducing the relative concentration of oyxgen atoms in the discharge to levels of less than one part per million. Absolute values for the O_I transition probabilities were obtained by determining the oxygen-atom density and plasma length through a measurement of the absolute intensity of the O I λ =7773.4 Å line, whose transition probability is known. The following values were measured for lines in the resonance transition array: $A({}^{1}D_{2}-{}^{1}D_{2}^{2}, \lambda = 1152 \text{ \AA}) = 5.5 \times 10^{8} \text{ sec}^{-1}$; $A({}^{1}S_{0}-{}^{1}P_{1}^{2}, \lambda = 1218 \text{ \AA})$ $=1.8\times10^8 \sec^{-1}; \ A({}^3P_0 - {}^3S_1^\circ, \ \lambda = 1306 \text{ \AA}) = 0.66\times10^8 \sec^{-1}; \ A({}^3P_{2,1,0} - {}^3S_1^\circ, \ \lambda = 1303.5 \text{ \AA}) = 5.9\times10^8 \sec^{-1}.$ These values are in excellent agreement with recent lifetime measurements. Existing discrepancies in the literature concerning a previous arc determination of the OI vacuum ultraviolet oscillator strengths by Boldt and Labuhn are discussed. The present method is considered to be an improvement over the method used by Boldt and Labuhn which relied, first of all, upon extrapolation techniques to reach the linear part of the curve of growth and, secondly, upon a complex calculation of the oxygen-atom number density using basic conservation equations.

I. INTRODUCTION

Transition probabilities for O_I lines emitted in the vacuum ultraviolet have been measured using a wall-stabilized arc discharge. In particular, the following wavelengths associated with the resonance transition array were studied: 1152, 1218, 1302, 1305, and 1306 Å. These lines have previously been investigated using electron excitation phaseshift techniques, absorption spectroscopy, beamfoil lifetime determinations, and arc emission methods. Nevertheless, there exists in the literature a rather wide range of f values for these transitions.

Several measurements of the ${}^{1}D_{2} - {}^{1}D_{2}^{\circ}$ transition at $\lambda = 1152$ Å have been reported. The lifetime measurements¹⁻³ agree almost exactly with one another and correspond to a transition probability value of 5.3×10^{8} sec⁻¹. Boldt and Labuhn, ⁴ using a dc wallstabilized arc discharge, obtained a value of 16.5 $\times 10^{8}$ sec⁻¹, a very puzzling discrepancy since several N r⁵ and C r⁶ transition probabilities obtained using the identical method are in much better agreement with the various lifetime measurements.

There has been only one reported direct measurement of the ${}^{1}S_{0}{}^{-1}P_{1}^{\circ}$ transition at $\lambda = 1218$ Å: Boldt and Labuhn⁴ obtained a transition probability of 4.3×10^{8} sec⁻¹. However, Lawrence² has measured the lifetime of the ${}^{1}P_{1}^{\circ}$ level and, having assumed a branching ratio of 0.34 for ${}^{1}S_{0}{}^{-1}P_{1}^{\circ}$ decay out of the ${}^{1}P_{1}^{\circ}$ level, he has found it to be inconsistent with the arc measurement. If in addition autoionization processes are significant as Lawrence has suggested, the discrepancy between the two experiments is even greater.

The resonance triplet ${}^{3}P-{}^{3}S^{\circ}$ has been the object of much attention mainly because of its aeronomical significance. An accurate determination of its transition probability is useful also for plasma diagnostic purposes, since the resonance triplet is readily observed in laboratory plasmas in which trace amounts of oxygen are present. There exists in the literature an order-of-magnitude spread between the oscillator strength of 0.021 reported by Parkes et al.⁷ using absorption techniques and the oscillator strength of 0.18 reported by Boldt and Labuhn.⁴ Lin *et al*.⁸ have recently repeated the absorption measurement and obtained an oscillator strength of about 0.045 in apparent agreement with the current lifetime measurements of Lawrence.² There still remains, therefore, a discrepancy of about a factor of 4 between these values and the arc measurement. Since the wall-stabilized arc discharge is generally a rather reliable source for determining transition probabilities, it was decided to reexamine the oxygen vacuum ultraviolet (vuv) lines emitted in an arc discharge in order to resolve the existing discrepancies. At the same time it was decided to replace the complex plasma diagnostic method of Boldt and Labuhn with a simpler more