

## Structure of the static pair-correlation function in superfluid $^4\text{He}$

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In 1970, Hyland, Rowlands, and Cummings suggested that one could obtain the condensate fraction  $n_0(T)$  from careful measurements of the static pair-correlation function  $g(r, T)$  in the superfluid and normal phases of  $^4\text{He}$ . Their arguments are critically analyzed by going back to the general structure of  $S(Q)$  and  $S(Q, \omega)$  predicted by the field-theoretic analysis of a Bose-condensed liquid. It is shown that at low temperatures, the single-particle correlation functions, which Hyland *et al.* argue are negligible, in fact make a major contribution to  $g(r, T)$  in the region  $r \geq 4 \text{ \AA}$ .

### I. INTRODUCTION

Ten years ago, Hyland, Rowlands, and Cummings<sup>1,2</sup> discussed how the static density correlation function in superfluid  $^4\text{He}$  depends on the condensate fraction  $n_0(T)$ . Using some assumptions on how certain static two-point correlation functions would decay spatially, they arrived at the following formula for  $4 \leq r \leq 12 \text{ \AA}$ :

$$n^2[g(\bar{r}, T) - 1] = [n - n_0(T)]^2[g(\bar{r}, T^*) - 1], \quad (1)$$

where  $g(\bar{r}, T)$  is the static pair-correlation function for liquid  $^4\text{He}$  and the temperature  $T^*$  is just above the lambda transition temperature  $T_\lambda = 2.17 \text{ K}$ . If this formula is correct, it would mean that careful measurement of the temperature dependence of the static pair-correlation function would enable one to find  $n_0$  as a function of the temperature. Some years ago, Raveché and Mountain<sup>3</sup> summarized the arguments leading to Eq. (1) and attempted to use it to find  $n_0(T)$ . However the available experimental data for  $g(\bar{r}, T)$  were not very accurate and the results for  $n_0(T)$  had a lot of scatter.

Very recently, Svensson, Sears, Woods, and Martel<sup>4</sup> have completed very accurate neutron scattering measurements of the static structure factor  $S(\bar{Q}, T)$  as a function of the temperature. Sears and Svensson<sup>5</sup> have used these results in formula (1) and claim to have thus obtained accurate values for the temperature dependence of the condensate fraction  $n_0(T)$ . The value of  $n_0(T)$  so obtained was about (10–15)% of  $n$  at low temperatures ( $T \sim 1 \text{ K}$ ); which is similar to the value obtained by several direct theoretical calculations<sup>6,7</sup> as well as from an analysis of high momentum inelastic neutron scattering studies (see, for example, Ref. 8). As the temperature increased,  $n_0(T)$  decreased and vanished at  $T_\lambda$ .

The question remains, however, as to the correctness of formula (1) and in this paper, we critically re-

view the arguments which lead Hyland, Rowlands, and Cummings (HRC) to Eq. (1). The original work<sup>1,2</sup> of HRC was based on a theoretical study of a condensed Bose system by Fröhlich.<sup>9</sup> Fröhlich's analysis involved an attempt to understand how the presence of a Bose condensate would modify the structure of static correlation functions. Curiously, neither Fröhlich nor HRC made any contact with the well-developed field-theoretic description of superfluid  $^4\text{He}$  initiated by Beliaev<sup>10</sup> and developed by many workers since then (see, in particular, Refs. 11 and 12).

In this paper, we review what the field-theoretic predictions are for the general structure of the static  $[S(\bar{Q})]$  and dynamic  $[S(\bar{Q}, \omega)]$  structure factors of a Bose-condensed liquid. This approach gives a rigorous basis for the type of decomposition of static correlation functions which Fröhlich tried to obtain. However the effects of the anomalous correlation functions characteristic of a Bose-condensed system are now properly included.

The field-theoretic analysis shows that  $S(\bar{Q}, T)$  and hence  $g(\bar{r}, T)$  can be separated into singular and regular parts.<sup>11,13</sup> The singular part  $S_C(\bar{Q}, T)$  is associated with the contribution arising from single quasiparticles and recent work has shown that<sup>13,14</sup>

$$S_C(\bar{Q}, T) = \frac{\rho_s(T)}{\rho} Z(\bar{Q}), \quad (2)$$

where  $\rho_s(T)$  is the superfluid density [ $\rho_s = \rho$  at  $T = 0 \text{ K}$ ] and  $Z(\bar{Q})$  is the weight of the quasiparticle resonance in  $S(\bar{Q}, \omega)$  at  $T = 0 \text{ K}$ . A crucial argument of HRC in deriving Eq. (1) was that, effectively, the single-particle part of  $g(\bar{r}, T)$  could be neglected in the range  $r \geq 4 \text{ \AA}$ . However, we show that at low temperatures [where  $\rho_s(T)$  is appreciable], a significant contribution in fact is associated with the single-particle part given by Eq. (2). This effectively invalidates the derivation of Eq. (1) given by HRC. This does not preclude the possibility that Eq. (1) is still

essentially correct. As discussed by Sears and Svenson,<sup>5,15</sup> Eq. (1) appears to describe the experimental data quite well and gives values of  $n_0(T)$  which are in good agreement with independent determinations.

In Sec. II, we briefly review the results and implications of the field-theoretic analysis of the structure of  $S(\vec{Q}, T)$ . In Sec. III, we discuss some simple models for a condensed-Bose system (free particle and the Bogoliubov model for a dilute interacting Bose gas) and make contact with the work of Fröhlich<sup>9</sup> as well as Hyland, Rowlands, and Cummings.<sup>1,2</sup>

## II. STRUCTURE OF STATIC CORRELATION FUNCTIONS IN A BOSE-CONDENSED SYSTEM

The static pair-correlation function is defined by

$$\langle \hat{n}(\vec{r}) \hat{n}(\vec{r}') \rangle = n^2 g(\vec{r} - \vec{r}') + n \delta(\vec{r} - \vec{r}') \quad (3)$$

where  $\langle \hat{n}(\vec{r}) \rangle \equiv n$  and the density operator is given in terms of quantum field operators

$$\hat{n}(\vec{r}) \equiv \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \quad (4)$$

The static structure factor  $S(\vec{Q})$ , as measured by neutron scattering, is the Fourier transform of

$$nS(\vec{r} - \vec{r}') \equiv \langle \hat{n}(\vec{r}) \hat{n}(\vec{r}') \rangle - n^2 \quad (5)$$

We have defined  $S(\vec{r} - \vec{r}')$  so that  $S(\vec{Q}) = 1$  for large  $Q$ .

In a Bose-condensed system, it is useful<sup>10</sup> to separate out the condensate part of the field operators

$$\begin{aligned} \hat{\psi}(\vec{r}) &= \langle \hat{\psi}(\vec{r}) \rangle + \tilde{\psi}(\vec{r}) \quad , \\ \hat{\psi}^\dagger(\vec{r}) &= \langle \hat{\psi}^\dagger(\vec{r}) \rangle + \tilde{\psi}^\dagger(\vec{r}) \quad , \end{aligned} \quad (6)$$

where the Bose field expectation values are  $\langle \hat{\psi}(\vec{r}) \rangle = \langle \hat{\psi}^\dagger(\vec{r}) \rangle = \sqrt{n_0}$ . Making use of Eq. (6), we see that

$$\hat{n}(\vec{r}) = n_0 + \sqrt{n_0} \Psi(\vec{r}) + \tilde{n}(\vec{r}) \quad , \quad (7)$$

where we have defined the operators

$$\begin{aligned} \Psi(\vec{r}) &\equiv \tilde{\psi}^\dagger(\vec{r}) + \tilde{\psi}(\vec{r}) \quad , \\ \tilde{n}(\vec{r}) &\equiv \tilde{\psi}^\dagger(\vec{r}) \tilde{\psi}(\vec{r}) \quad . \end{aligned} \quad (8)$$

We note that  $\tilde{n}(\vec{r})$  is the density operator for the noncondensed atoms. This is most clearly seen by taking the Fourier transform of Eq. (9)

$$\tilde{n}(\vec{Q}) = \frac{1}{V} \sum_{p \neq 0, -Q} a_p^\dagger a_{p+Q} \quad (10)$$

and contrasting it with the transform of  $\hat{n}(\vec{r})$ ,

$$\hat{n}(\vec{Q}) = \frac{1}{V} \sum_p a_p^\dagger a_{p+Q} \quad (11)$$

Separating out the condensate part using Eq. (7), one finds Eq. (5) decomposes as follows:

$$\begin{aligned} nS(\vec{r} - \vec{r}') &= n_0^2 + 2n_0 \langle \tilde{n}(\vec{r}) \rangle + n_0 \langle \Psi(\vec{r}) \Psi(\vec{r}') \rangle \\ &\quad + \sqrt{n_0} [ \langle \Psi(\vec{r}) \tilde{n}(\vec{r}') \rangle + \langle \tilde{n}(\vec{r}) \Psi(\vec{r}') \rangle ] \\ &\quad + \langle \tilde{n}(\vec{r}) \tilde{n}(\vec{r}') \rangle - n^2 \quad . \end{aligned} \quad (12)$$

Using the fact that the depletion  $\tilde{n} \equiv \langle \tilde{n}(\vec{r}) \rangle = n - n_0$ , we can write Eq. (12) in the form

$$S(\vec{r} - \vec{r}') = S_C(\vec{r} - \vec{r}') + S_R(\vec{r} - \vec{r}') \quad , \quad (13)$$

where we have defined

$$\begin{aligned} nS_C(\vec{r} - \vec{r}') &\equiv n_0 \langle \Psi(\vec{r}) \Psi(\vec{r}') \rangle \\ &\quad + \sqrt{n_0} [ \langle \Psi(\vec{r}) \tilde{n}(\vec{r}') \rangle \\ &\quad + \langle \tilde{n}(\vec{r}) \Psi(\vec{r}') \rangle ] \quad , \end{aligned} \quad (14)$$

$$nS_R(\vec{r} - \vec{r}') \equiv \langle \tilde{n}(\vec{r}) \tilde{n}(\vec{r}') \rangle - \tilde{n}^2 \quad . \quad (15)$$

Clearly  $S_C$  vanishes if  $n_0 = 0$  and we are left with  $S_R$ . The reason we have grouped the terms in Eq. (12) in this particular way is clear from the discussion given in an earlier paper.<sup>13</sup>  $S(\vec{r} - \vec{r}')$  in Eq. (5) is related to the static limit of the density-density correlation function  $\chi_{nn}$ . A field-theoretic diagrammatic analysis shows that all contributions can be divided into two categories. The contributions of one category are always proportional to the single-particle Dyson-Beliaev Green function  $\tilde{G}_{\alpha\beta}$  and form what is called the condensate (or singular) part of  $\chi_{nn}$ .<sup>11, 12, 16-18</sup> One finds that it is precisely the terms included in Eq. (14) which form this condensate part of  $S(\vec{r} - \vec{r}')$ . Physically,  $S_C(\vec{r} - \vec{r}')$  in Eq. (14) is the part of the static structure factor which is related to density fluctuations in which atoms are put into or taken out of the condensate reservoir. More precisely, the first term in Eq. (14) describes density fluctuations in which *two* atoms with zero momentum are involved, while the second term in Eq. (14) describes density fluctuations in which only *one* condensate atom is involved. It is perhaps surprising but still true that this second term (proportional to  $\sqrt{n_0}$ ) can be proven<sup>11, 17, 18</sup> to be proper in the sense that it is directly proportional to the Dyson-Beliaev single-particle Green's function and hence part of  $S_C$ .

The second category of contributions to the density-density correlation function constitutes the so-called regular part. This regular part of  $S(\vec{r} - \vec{r}')$  is given by Eq. (15), and has a direct physical interpretation.  $S_R(\vec{r} - \vec{r}')$  is the part of the static structure factor which arises from density fluctuations which involve excited atoms (i.e., with nonzero momentum).

The dynamic structure factor  $S(\vec{Q}, \omega)$  can also be decomposed into singular and regular parts. The singular part  $S_C(\vec{Q}, \omega)$  has been shown<sup>13</sup> to have a sharp quasiparticle resonance at  $\omega(Q)$ , with a

temperature-dependent weight which is proportional to the superfluid density  $\rho_s(T)$ , in agreement with the experimental results of Woods and Svensson.<sup>14</sup> The regular part  $S_R(\vec{Q}, \omega)$  is composed of two kinds of terms<sup>19</sup>: (A) exciting *two* quasiparticles out of the ground state [ $\omega = \omega(k) + \omega(k+Q)$ ] and (B) scattering from thermally excited quasiparticles [ $\omega = \omega(k) - \omega(k+Q)$ ]. Contribution B is a broad continuum, vanishes at  $T=0$  K and is proportional to the normal fluid density  $\rho_n(T) = \rho - \rho_s(T)$  in the temperature region  $1 \leq T \leq T_\lambda$  where rotons are the dominant excitations. The fact that contribution B is proportional to  $\rho_n$  is easily seen in a calculation based on the Bogoliubov model<sup>19</sup> but these features have been suggested more generally by Pines and Nozieres<sup>20</sup> some years ago. We identify the B part of  $S_R(\vec{Q}, \omega)$  with what Woods and Svensson<sup>14</sup> call the "normal-fluid" part. In contrast, the A part of  $S_R(\vec{Q}, \omega)$  corresponds to the so-called "multiphonon" part<sup>21</sup> of  $S(\vec{Q}, \omega)$ . It can be shown to vanish if  $n_0=0$  and combines with the condensate part  $S_C(\vec{Q}, \omega)$  to form what is called<sup>14</sup> the "superfluid" part of  $S(\vec{Q}, \omega)$ .

The static structure factor is given by

$$S(\vec{Q}, T) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(\vec{Q}, \omega, T) \quad (16)$$

and moreover, we recall that

$$n^2 g(\vec{r}, T) = n^2 + n \int \frac{d\vec{Q}}{(2\pi)^3} e^{i\vec{Q}\cdot\vec{r}} S(\vec{Q}, T) - n \delta(\vec{r}) \quad (17)$$

It is clear that the results of the last paragraph enable us to decompose  $g(\vec{r}, T)$  into contributions from: (a) excitation of single quasiparticles (one-phonon term); (b) excitation of two quasiparticles (multiphonon term); and (c) scattering of thermally excited quasiparticles. At low temperatures ( $\leq 1$  K), there is a negligible number of quasiparticles present and (c) may be ignored. The contribution of (a) to  $S(\vec{Q})$  has been obtained<sup>21</sup> some years ago at  $T=1.1$  K. This "one-phonon" contribution  $Z(\vec{Q})$  is shown in Fig. 1, in addition to the full  $S(\vec{Q})$  at  $T=1$  K which includes the "multiphonon" contribution  $S_{II}(\vec{Q})$ . In Fig. 2, we have plotted what we call the "one-phonon" contribution to  $g(\vec{r})$ , as defined by

$$n^2 g_Z(\vec{r}) \equiv n^2 + n \int \frac{d\vec{Q}}{(2\pi)^3} e^{i\vec{Q}\cdot\vec{r}} Z(\vec{Q}) \quad (18)$$

The multiphonon contribution to  $g(\vec{r})$  is defined by

$$n^2 g_{II}(\vec{r}) \equiv n \int \frac{d\vec{Q}}{(2\pi)^3} e^{i\vec{Q}\cdot\vec{r}} [S_{II}(\vec{Q}) - 1] \quad (19)$$

with  $g(\vec{r}) = g_Z(\vec{r}) + g_{II}(\vec{r})$ . We know that  $g(\vec{r}) \approx 0$  for  $r \leq 2$  Å due to hard-core effects. The multiphonon contribution  $g_{II}(\vec{r})$  in this region is large and negative, effectively canceling the one-phonon contribution shown in Fig. 2. What is of real interest is the

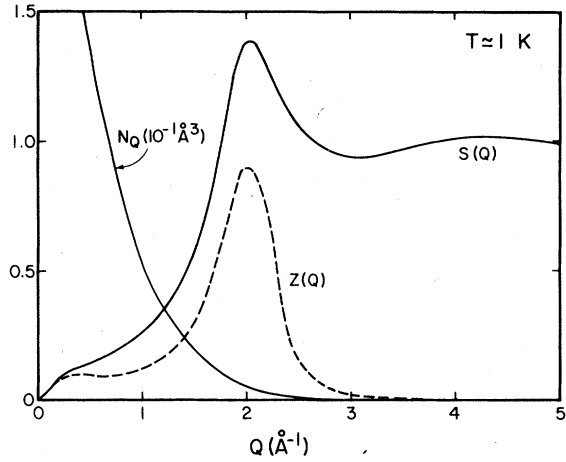


FIG. 1. Comparison between the full static structure factor  $S(\vec{Q})$  (based on Ref. 4) and the one-phonon contribution  $Z(\vec{Q})$  (based on Ref. 21). In addition, the momentum distribution  $N_Q$  of atoms is shown (based on Ref. 8). Some of the results are for  $T=1.1$  K.

region  $r \geq 3$  Å. Figure 2 shows dramatically that a significant part of the oscillations in  $g(\vec{r})$  in this asymptotic region are associated with the one-phonon term. As we shall explain in more detail in Sec. III, one can phrase one key step in the argument of Ref. 1 as being equivalent to the assumption that  $g_Z(\vec{r}) \approx 1$  in the region  $r \geq 4$  Å. Figure 2 shows that this is simply not correct in superfluid  $^4\text{He}$ .

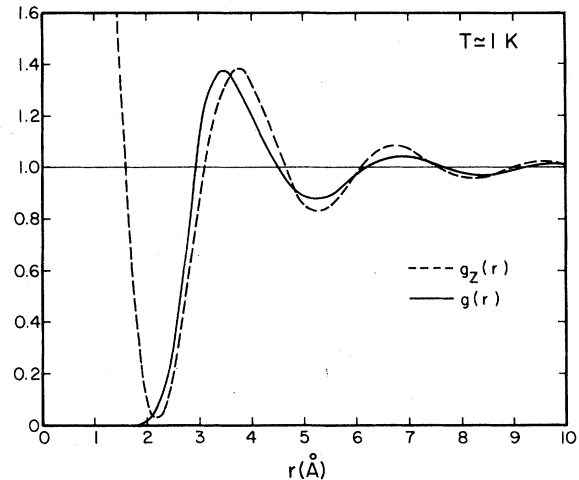


FIG. 2. Comparison between the full pair-correlation function (Ref. 4)  $g(\vec{r})$  and the one-phonon contribution  $g_Z(\vec{r})$  defined in Eq. (18). The difference is due to the multiphonon contribution defined in Eq. (19). Strictly speaking, the curves are  $g(\vec{r}, T=1$  K) and  $g_Z(\vec{r}, T=1.1$  K) but negligible difference is expected to arise from this temperature difference.

The preceding analysis for  $T \leq 1$  K can be generalized to higher temperatures. Using the Woods-Svensson<sup>14</sup> two-component decomposition of  $S(\bar{Q}, \omega)$ , it immediately follows from Eq. (16) that<sup>22</sup>

$$S(\bar{Q}, T) = \frac{\rho_s(T)}{\rho} S(\bar{Q}, 1 \text{ K}) + \frac{\rho_n(T)}{\rho} S(\bar{Q}, T^*) \quad (20)$$

Using Eq. (20) in Eq. (17) gives an analogous Woods-Svensson formula for the static pair-correlation function

$$g(\bar{r}, T) = \frac{\rho_s(T)}{\rho} g(\bar{r}, 1 \text{ K}) + \frac{\rho_n(T)}{\rho} g(\bar{r}, T^*) \quad (21)$$

where we have made use of the identity  $\rho_s + \rho_n = \rho$ . Both Eqs. (20) and (21) have been found to be in good agreement with experimental data.<sup>22</sup> We also note that there is a fairly convincing microscopic basis<sup>13,19</sup> to the Woods-Svensson decomposition for  $S(\bar{Q}, \omega)$  and hence for Eqs. (20) and (21). The expression in Eq. (2) gives the following formula for the temperature dependence of  $g_Z(\bar{r}, T)$ :

$$[g_Z(\bar{r}, T) - 1] = \frac{\rho_s(T)}{\rho} [g_Z(\bar{r}, 1 \text{ K}) - 1] \quad (22)$$

or, equivalently,

$$g_Z(\bar{r}, T) = \frac{\rho_n(T)}{\rho} + \frac{\rho_s(T)}{\rho} g_Z(\bar{r}, 1 \text{ K}) \quad (23)$$

### III. SOME MODEL CALCULATIONS AND THE ANSATZ OF HYLAND, ROWLANDS, AND CUMMINGS

In this section, we want to show how Fröhlich's analysis<sup>2,9</sup> of static correlation functions can be viewed in terms of simple approximations for the singular and regular parts, defined in Eqs. (14) and (15). We first discuss the simple case of a free Bose gas, where  $S_C$  and  $S_R$  can be calculated exactly.<sup>23</sup> This example not only gives a concrete illustration of the difference between  $S_C$  and  $S_R$  but will allow us to see the crucial changes introduced by the effect of interactions. These were not adequately included in Fröhlich's analysis or in the subsequent work of HRC.<sup>1,2</sup>

$$\begin{aligned} \Omega_2(\bar{r}, \bar{r}'; \bar{r}, \bar{r}') &\equiv \langle \psi^\dagger(\bar{r}) \psi^\dagger(\bar{r}') \psi(\bar{r}') \psi(\bar{r}) \rangle \equiv n^2 g(\bar{r} - \bar{r}') \\ &= R(\bar{r} - \bar{r}') [n^2 + 2n_0 \Lambda_1(\bar{r} - \bar{r}') + \Lambda_1(\bar{r} - \bar{r}') \Lambda_1(\bar{r}' - \bar{r})] + \Lambda_2^f(\bar{r} - \bar{r}') \end{aligned} \quad (32)$$

where  $\Lambda_1(\bar{r} - \bar{r}') \equiv \langle \tilde{\psi}^\dagger(\bar{r}) \tilde{\psi}(\bar{r}') \rangle$ . The terms in the square brackets form the "asymptotic part" which was discussed by Fröhlich.<sup>9</sup> It is to be noted that these are identical in structure to that for a free Bose gas discussed above; i.e.,

$$\begin{aligned} n^2 g_0(\bar{r} - \bar{r}') &= n^2 + 2n_0 \Lambda_1^0(\bar{r} - \bar{r}') \\ &+ \Lambda_1^0(\bar{r} - \bar{r}') \Lambda_1^0(\bar{r}' - \bar{r}) \end{aligned} \quad (33)$$

Combining Eqs. (3) and (5), we have

$$n^2 g(\bar{r} - \bar{r}') = n^2 + n S(\bar{r} - \bar{r}') - n \delta(\bar{r} - \bar{r}') \quad (24)$$

where the condensate and regular parts are defined in Eqs. (14) and (15). In a noninteracting Bose gas, all anomalous correlation functions [such as  $\langle \tilde{\psi}(\bar{r}) \tilde{\psi}(\bar{r}') \rangle$  and  $\langle \tilde{\psi}^\dagger(\bar{r}) \tilde{n}(\bar{r}') \rangle$ ] vanish. Calculation of the remaining terms gives

$$n S_C(\bar{r} - \bar{r}') = 2n_0 \Lambda_1^0(\bar{r} - \bar{r}') + n_0 \delta(\bar{r} - \bar{r}') \quad (25)$$

$$n S_R(\bar{r} - \bar{r}') = \Lambda_1^0(\bar{r} - \bar{r}') \Lambda_1^0(\bar{r}' - \bar{r}) + \tilde{n} \delta(\bar{r} - \bar{r}') \quad (26)$$

where the single-particle density matrix is

$$\begin{aligned} \Lambda_1^0(r - r') &\equiv \langle \tilde{\psi}^\dagger(\bar{r}) \tilde{\psi}(\bar{r}') \rangle_0 \\ &= \frac{1}{V} \sum_{p \neq 0} N_p^0 e^{-i\bar{p} \cdot (\bar{r} - \bar{r}')} \end{aligned} \quad (27)$$

and  $N_p^0 \equiv \langle a_p^\dagger a_p \rangle_0$  is the usual Bose factor. Using these results, one finds<sup>23</sup> that  $g(\bar{r}, T)$  starts off from a maximum at  $r = 0$ ,

$$n^2 g(r = 0, T) = n^2 + n^2 - n_0^2(T) \quad (28)$$

and decreases towards unity as  $r$  increases. We also note that the equivalent results in momentum space are

$$n S_C^0(\bar{Q}) = 2n_0 N_Q^0 + n_0 \quad (29)$$

$$n S_R^0(\bar{Q}) = \frac{1}{V} \sum_{(p \neq 0, -Q)} N_p^0 N_{p+Q}^0 + \tilde{n} \quad (30)$$

These combine to give

$$n S^0(\bar{Q}) = \frac{1}{V} \sum_p N_p^0 (N_{p+Q}^0 + 1) \quad (31)$$

where the sum is now unrestricted and  $N_{p=0}^0 \equiv V n_0$ .

We next turn to a general discussion of the second order reduced density matrix  $\Omega_2$  for a Bose-condensed system due to Fröhlich and developed by others.<sup>2,3,9</sup> Fröhlich attempted to find the form of  $\Omega_2$  by requiring that it satisfy various exact symmetry and asymptotic conditions. The form used as the basis of Ref. 1 is

except that the first-order reduced density matrix  $\Lambda_1(\bar{r} - \bar{r}')$  is now for an interacting Bose system.

The factor  $R(\bar{r} - \bar{r}')$  in Eq. (32) was introduced in an *ad hoc* way to make sure that the short-range behavior due to hard-core effects was properly included. The term  $\Lambda_2^f(\bar{r} - \bar{r}')$  was added to describe all the remaining contributions which could not be written in terms of  $\Lambda_1(\bar{r} - \bar{r}')$ . Very little is known

about either  $R(\vec{r})$  or  $\Lambda_2^f(\vec{r})$ . On the other hand, as emphasized by HRC,  $\Lambda_1(\vec{r})$  is the Fourier transform of the momentum distribution [see Eq. (27)]. This can be found by numerical calculations<sup>6,7</sup> as well as from inelastic neutron scattering<sup>8</sup> and one finds  $\Lambda_1$  decays rapidly from the value  $\bar{n}$  at  $r=0$ , with

$$\Lambda_1(\vec{r}) \approx 0 \text{ for } r \geq 4 \text{ \AA} . \quad (34)$$

It is argued also that for  $r \geq 4 \text{ \AA}$ ,  $R(\vec{r})$  is effectively unity. Finally, since it is found that  $g(\vec{r}) = 1$  for  $r \geq 12 \text{ \AA}$ , Eq. (33) implies that

$$\Lambda_2^f(\vec{r}) \approx 0 \text{ for } r \geq 12 \text{ \AA} . \quad (35)$$

To summarize, HRC conclude that Eq. (32) can be approximated by

$$n^2 g(\vec{r}, T) = n^2 + \Lambda_2^f(\vec{r}, T) \quad (36)$$

in the region  $4 \leq r \leq 12 \text{ \AA}$ . We shall call this HRC ansatz I. Effectively it is based on the idea that contributions to  $g(\vec{r}, T)$  arising from the single-particle contributions (unique to a Bose-condensed system) are negligible in the region  $r \geq 4 \text{ \AA}$ .

We note that Eq. (36) is exact if there is no condensate. HRC make the further argument that  $\Lambda_2^f(\vec{r}, T)$  should be similar to that for  $^4\text{He}$  just above  $T_\lambda$ , except that only  $\bar{n}$  atoms are involved. They thus assume

$$\Lambda_2^f(\vec{r} - \vec{r}') \approx \frac{\bar{n}^2}{n^2} \langle n(\vec{r}) n(\vec{r}') \rangle_{T^*} \quad (37a)$$

or, equivalently

$$\Lambda_2^f(\vec{r}, T) \approx \bar{n}^2 [g(\vec{r}, T^*) - 1] , \quad (37b)$$

where  $T^*$  is some temperature just above  $T_\lambda$ . We shall call Eq. (37) the HRC ansatz II. Combining Eq. (36) with Eq. (37b) gives the HRC formula in Eq. (1).

On comparing Eq. (32) with the rigorous field-theoretic decomposition given in Sec. II, it is clear that Eq. (32) corresponds to the following approximations:

$$n S_C(\vec{r}) = 2n_0 \Lambda_1(\vec{r}) , \quad (38)$$

$$n S_R(\vec{r}) = [\Lambda_1(\vec{r})]^2 + \Lambda_2^f(\vec{r}) , \quad (39)$$

where we assume that we are in the asymptotic region with  $R(\vec{r}) \approx 1$ . Unfortunately, when interactions are included, the structure of  $g(\vec{r})$  is quite different from that of a free Bose gas as given by Eq. (33). A key difference, according to the microscopic theory of a Bose-condensed system, is that one must work with a  $2 \times 2$  single-particle density matrix, i.e.,  $\langle \tilde{\psi}(\vec{r}) \tilde{\psi}(\vec{r}') \rangle$  and  $\langle \tilde{\psi}^\dagger(\vec{r}) \tilde{\psi}^\dagger(\vec{r}') \rangle$  are just as important as  $\langle \tilde{\psi}^\dagger(\vec{r}) \tilde{\psi}(\vec{r}') \rangle$  and  $\langle \tilde{\psi}(\vec{r}) \tilde{\psi}^\dagger(\vec{r}') \rangle$ . This crucial feature is *already* present in the Bogoliubov theory of a dilute interacting Bose gas,<sup>24</sup> which we now turn to.

For our purposes, it is sufficient to limit ourselves to the Bogoliubov approximation results at  $T=0 \text{ K}$ .

The momentum distribution in this case is

$$N_Q^{\text{Bog}} = \frac{\epsilon(Q) + n_0 V(Q) - \omega(Q)}{2\omega(Q)} , \quad (40)$$

while the condensate part of  $S(\vec{Q})$  is

$$S_C^{\text{Bog}}(\vec{Q}) = \frac{n_0}{n} \frac{\epsilon(Q)}{\omega(Q)} . \quad (41)$$

Here the quasiparticle energy is given by

$$\omega(Q) = [\epsilon^2(Q) + 2n_0 V(Q)\epsilon(Q)]^{1/2} , \quad (42)$$

where  $\epsilon(Q) = Q^2/2m$  and  $V(Q)$  is the Fourier transform of the interatomic potential. It is easy to see that these model results are quite incompatible with the momentum-space equivalent of the HRC approximation (38), namely,

$$\begin{aligned} S_C(Q) &= \frac{n_0}{n} (2N_Q + 1) \quad (\text{HRC}) \\ &= \frac{n_0}{n} \frac{\epsilon(Q) + n_0 V(Q)}{\omega(Q)} . \end{aligned} \quad (43)$$

Due to the presence of off-diagonal single-particle correlation functions, the small- $Q$  behavior of  $S_C(Q)$  in Eq. (41) is completely different than predicted by Eq. (43).

The completely different long wavelength behavior of  $S_C(Q)$  and  $N_Q$  exhibited by the Bogoliubov model also shows up in exact results of Gavoret and Nozieres<sup>11</sup> as well as in superfluid  $^4\text{He}$ . We recall from Sec. II that at  $T \approx 1 \text{ K}$ ,  $S_C(Q)$  is given by  $Z(Q)$ . In Fig. 1, we compare the results for  $Z(Q)$  and  $N_Q$  as obtained from inelastic neutron scattering data (this momentum distribution<sup>8</sup> is in good agreement with results of direct numerical calculations<sup>6,7</sup>). The Fourier transform of  $N_Q$  gives  $\Lambda_1(\vec{r})$  and this is found to be negligible for  $r \geq 4 \text{ \AA}$ , in marked contrast to the result for  $[g_Z(\vec{r}) - 1]$  shown in Fig. 2.

The preceding results show how the anomalous correlation functions *completely* alter the behavior of  $S_C(\vec{r})$  for large  $r$ . We might note here that while they are neglected in the Bogoliubov approximation, the correlation functions involving *three* field operators in Eq. (14) are also very important in superfluid  $^4\text{He}$ . It is their presence which renormalizes the weight of the single quasiparticle excitations from  $n_0/n$  as in the dilute interacting Bose gas result [Eq. (41)] to  $\rho_s/\rho$  in Eq. (2). This is discussed in more detail in Ref. 13.

We next consider the HRC discussion for the regular part  $S_R$ , as given in Eq. (39). When anomalous correlation functions are properly included, the generalized version of Eq. (39) is<sup>25</sup>

$$\begin{aligned} n S_R(\vec{r} - \vec{r}') &= \langle \tilde{\psi}^\dagger(\vec{r}) \tilde{\psi}(\vec{r}') \rangle^2 \\ &+ \langle \tilde{\psi}^\dagger(\vec{r}) \tilde{\psi}^\dagger(\vec{r}') \rangle \langle \tilde{\psi}(\vec{r}') \tilde{\psi}(\vec{r}) \rangle \\ &+ \Lambda_2^f(\vec{r} - \vec{r}') . \end{aligned} \quad (44)$$

The first term on the right-hand side of Eq. (44) is  $\Lambda_1^2(\vec{r} - \vec{r}')$ , and as HRC have noted,  $\Lambda_1(\vec{r})$  is known to be negligible for  $r \geq 4 \text{ \AA}$  in superfluid  $^4\text{He}$ . The second term involves the square of the "off-diagonal" single-particle density matrix  $\Lambda_{\text{od}}(\vec{r} - \vec{r}') \equiv \langle \tilde{\psi}(\vec{r}) \tilde{\psi}(\vec{r}') \rangle$ . Unfortunately, we do not have a direct way<sup>26</sup> of measuring  $\Lambda_{\text{od}}(\vec{r})$  or its Fourier transform and therefore one cannot say whether it is negligible in the region  $r \geq 4 \text{ \AA}$ . However, we have already noted that the presence of  $\Lambda_{\text{od}}(\vec{r})$  completely changes the structure of  $S_C(\vec{r})$  in the Bogoliubov approximation. One has no justification at the present time for neglecting the second term on the right-hand-side of Eq. (44). This may be just as important as the contributions lumped into  $\Lambda_2^2(\vec{r})$ .

To summarize the preceding analysis, once one generalizes the analysis of Fröhlich to include both diagonal and off-diagonal single-particle density matrices, one is no longer justified in using the approximation (36) in the region  $r \geq 4 \text{ \AA}$ . Thus the HRC

ansatz I is not valid. We have not addressed ourselves to HRC ansatz II, namely, the validity of Eq. (37b). Needless to say, this seems to be also very doubtful. Indeed the importance of the contribution from the single-particle correlation functions means that if Eq. (37b) was valid, we would *not* obtain the HRC formula in Eq. (1). If this formula is correct, we can only conclude that it is for reasons quite different from those originally advanced by Hyland, Rowlands, and Cummings.

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