Exchange effects on the excitation spectrum of liquid helium*

A. Isihara and T. Samulski
Statistical Physics Laboratory, Department of Physics, State University of New York at Buffalo, Buffalo, New York 14214
(Received 24 March 1976)

The contribution to the pair-distribution function from two types of quantum graph is investigated. These graphs have the exchange and collective characters, and are important in the elimination of a divergence and also in the evaluation of the effective mass. A microscopic justification of Landau-type approach with elementary excitations is given. The excitation spectrum and the structure factor are evaluated for a soft potential with a Lennard-Jones–type tail. With the potential parameters chosen so as to have the right sound velocity, and with the effective mass $m^* = 1.71m$, a good agreement with experiments is achieved. The momentum dependence of m^* and the appearance of a particlelike mode in addition to a phononlike mode in the excitation spectrum are discussed.

I. INTRODUCTION

Since Landau's famous phenomenological theory of liquid helium was published, several important microscopic theories have been developed. Bogoliubov[1] proved in early 1947 the existence of a phonon spectrum in an imperfect Bose gas. Feynman and Cohen[2] introduced a variational method, Lee and Yang[3] developed the pseudopotential and binary-kernel methods, and Bogoliubov and Zubarev[1], Pines and others have given collective coordinate methods.[4] More recently, Nishiyama, Kebukawa *et al.*, Iwamoto, Grest, and Rajagopal and others[5] have considered interactions between the quasiparticles.

In treating many-body systems, the evaluation of the pair-distribution function is worthwhile because it yields not only the results which can be derived from the partition function but also information concerning the spatial correlations and the structure factor.[6] The pair-distribution function can be evaluated in several different ways including the diagram method[7] which we are going to adopt in the present paper.

The pair-distribution function in the chain-diagram approximation has been very useful.[7] The formula is

$$\rho_2(r)=n^2+I_2(r)-\frac{1}{(2\pi)^3\beta}\sum_i\int\frac{u(q)\lambda_i^2e^{i\vec{q}\cdot\vec{r}}}{1+u(q)\lambda_i}d\vec{q}\,, \qquad (1.1)$$

where n is the number density, $\beta=1/kT$, $I_2(r)$ represents the ideal quantum-gas contribution, $u(q)$ is the interaction, and λ_i is the ith eigenvalue of the effective propagator representing the unit of a chain. In this equation and in what follows, we shall use the units such that $\hbar=1$ and $2m=1$, where m is the particle mass.

By applying the chain-diagram formula, the screening constants in the classical and quantum-electron gases, the ground-state energy of hard-sphere systems, the phonon spectrum for a hard-sphere Bose gas, and many other interesting results have been obtained.[7] It has been found, however, that there are other equally important graphs of the same order.[7] The present paper discusses the contributions of these graphs.

For convenience, let us classify these graphs into two categories. The first class, to be called chain-exchange graphs, are those graphs in which the two representative particles entering the pair-distribution function have an exchange (Fig. 1). Hence, in this type of graph, an interaction line crosses the exchange. That is, the interaction line ends at both sides of the exchange. On the other hand, in the second class of diagrams, to be called ring-exchange graphs, an interaction line starts and ends at one side of the exchange (Fig. 2).

With respect to interaction, these two types of graph are of the same order as the simple-chain diagrams. They originate from quantum statistics and can be considered important for low temperatures.

In what follows in this paper, we shall give a general description of the contributions of these graphs. We shall remark that our previous treatment requires a modification.[7] We shall then make a specific application of our new results and show that they are indeed important.

The motivation for this particular application comes from our recent trial to apply the chain-diagram formula to liquid helium. Although the chain-diagram formula has reproduced the general form of the elementary-excitation spectrum of liquid helium II, we have found that the structure factor did not fit with experiment as well. Within our trial interaction functions, we have noted that the simple-chain diagram approximation based on Eq. (1.1) is not adequate. Therefore, in the present paper, we shall try to improve the

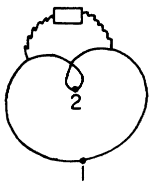

FIG. 1. Chain-exchange graph.

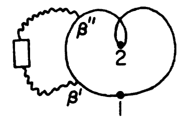

FIG. 2. Ring-exchange graph.

chain-diagram result by considering some other types of graph.

In Sec. II, we shall deal with the chain exchange graphs, i.e., those graphs with exchange between the two representative particles which characterize the pair-distribution function. Section III will give their contribution to the energy. In Sec. IV, we shall treat another type of quantum graphs called ring-exchange graphs. Section IV gives also their contribution to the energy. In Sec. V, we shall combine all these contributions and give a justification of a Landau-type description. The basic rules to treat these graphs have been given before.[7] Therefore, we shall avoid a detailed explanation of the derivation of the pair-distribution function. However, its application to the evaluation of energy will be discussed in detail. Finally, in Sec. VI, we report results of numerical calculations and comment on the momentum dependence of the effective mass of the quasiparticles.

II. CHAIN-EXCHANGE DIAGRAMS

Let us examine the contribution of the chain-exchange diagrams. The closed-form result after summing over chains of all lengths is

$$I_{\mathrm{cx}}(r) \equiv -\frac{1}{\beta}\sum_j \int \frac{d\vec{q}}{(2\pi)^3}\,\frac{u(q)\lambda_j^2(q,r)e^{i\vec{q}\cdot\vec{r}}}{1+u(q)\lambda_j(q)}\,, \tag{2.1}$$

where with $f(p)$ for the Bose distribution function we used

$$\lambda_j(q,r) = \int \frac{d\vec{p}}{(2\pi)^3}\,\frac{f(p)[1+f(\vec{p}+\vec{q})](e^{\beta[\vec{p}^2-(\vec{p}+\vec{q})^2]}-1)e^{i\vec{p}\cdot\vec{r}}}{p^2-(\vec{p}+\vec{q})^2+2\pi ij/\beta}\,. \tag{2.2}$$

Note that $\lambda_j(q, r=0)=\lambda_j(q)$ which is the eigenvalue for simple chains [see Eq. (2.5) below].

We evaluate $\lambda_j(q,r)$, the exchange eigenvalue, as follows: Separation of Eq. (2.2) into two integrals yields

$$\lambda_j(q,r) = \int \frac{d\vec{p}}{(2\pi)^3}\,\frac{f(\vec{p}+\vec{q})e^{i\vec{p}\cdot\vec{r}}}{p^2-(\vec{p}+\vec{q})^2+2\pi ij/\beta} - \int \frac{d\vec{p}}{(2\pi)^3}\,\frac{f(p)e^{i\vec{p}\cdot\vec{r}}}{p^2-(\vec{p}+\vec{q})^2+2\pi ij/\beta}\,. \tag{2.3}$$

Changing variable $\vec{p}\to-(\vec{p}+\vec{q})$ in the first integral and recombining we get

$$\lambda_j(q,r) = \int \frac{d\vec{p}}{(2\pi)^3}\,\frac{2f(p)e^{-i\vec{q}\cdot\vec{r}/2}\{[(\vec{p}+\vec{q})^2-p^2]\cos[(\vec{p}+\vec{q}/2)\cdot\vec{r}]-(2\pi j/\beta)\sin[(\vec{p}+\vec{q}/2)\cdot\vec{r}]\}}{[(\vec{p}+\vec{q})^2-p^2]^2+(2\pi j/\beta)^2}\,. \tag{2.4}$$

For low temperatures, we can expand about $p=0$ to obtain a first-order approximation. This approximation assumes effectively that the excitation spectrum associated with the exchange mode is characterized by momentum transfer q.

The cosine term in Eq. (2.4) has a factor which resembles the eigenvalue expression for the usual chain diagram

$$\lambda_j(q) = \frac{2nq^2}{q^4+(2\pi j/\beta)^2}\,, \tag{2.5}$$

except for the phase factor. [Note that in Eq. (2.3), $r=0$ gives rise to the above form.] The sine term is due to exchange. It behaves well for $j=0$ and $q=0$. In fact, $q=0$ makes the integral vanish due to the asymmetric integrand.

So far, we have not introduced any approximation and Eq. (2.4) is exact. We now introduce a small-momentum approximation and expand the integrand about $p=0$. In the first approximation, we obtain

$$\lambda_j(q,r) = \frac{q^2(1+e^{-i\vec{q}\cdot\vec{r}})+(2\pi ij/\beta)(1-e^{-i\vec{q}\cdot\vec{r}})}{q^4+(2\pi j/\beta)^2}\,G_{3/2}(r)\,, \tag{2.6}$$

where

$$G_{3/2}(r) = \int \frac{d\vec{p}}{(2\pi)^3} f(p)e^{i\vec{p}\cdot\vec{r}}\,. \tag{2.7}$$

This integral can be evaluated approximately as follows[6]:

$$G_{3/2}(r) \approx n_0 + \frac{e^{-2(\pi\alpha)^{1/2}r/\lambda}}{\lambda^2 r}\,, \tag{2.8}$$

where

$$n_0 = (1/V)[z/(1-z)]\,,\qquad \alpha = -\ln z\,,\quad \lambda^2 = 4\pi\beta\,. \tag{2.9}$$

Introducing Eqs. (2.5) and (2.6) into Eq. (2.1) and multiplying through $\exp(i\vec{q}\cdot\vec{r})$, we obtain

$$I_{cx}(r) = -\frac{1}{\beta}\sum_j \int \frac{d\vec{q}}{(2\pi)^3}\left(\frac{G_{3/2}^2(r)u(q)2[q^4-(2\pi j/\beta)^2]\cos\vec{q}\cdot\vec{r}}{[q^4+2nu(q)q^2+(2\pi j/\beta)^2][q^4+(2\pi j/\beta)^2]} + \frac{2G_{3/2}^2(r)u(q)}{q^4+2nu(q)q^2+(2\pi j/\beta)^2} + \frac{G_{3/2}^2(r)u(q)(2\pi q^2 j/\beta)\sin\vec{q}\cdot\vec{r}}{[q^4+2nu(q)q^2+(2\pi j/\beta)^2][q^4+(2\pi j/\beta)^2]}\right). \quad (2.10)$$

Due to asymmetry the last term vanishes. The summation over j is straightforward. We arrive at

$$I_{cx}(r) = \int \frac{d\vec{q}}{(2\pi)^3}\,\frac{G_{3/2}^2(r)}{n}\left(\frac{q\coth\{\beta q/2[q^2+2nu(q)]^{1/2}\}\cos\vec{q}\cdot\vec{r}}{[q^2+2nu(q)]^{1/2}} - \coth(\beta q^2/2)\cos\vec{q}\cdot\vec{r} + \frac{nu(q)\coth\{(\beta q/2)[q^2+2nu(q)]^{1/2}\}(\cos\vec{q}\cdot\vec{r}-1)}{q[q^2+2nu(q)]^{1/2}}\right). \quad (2.11)$$

When the first approximation in Eq. (2.8) is used, we shall have

$$\frac{n_0^2}{n}\left(\frac{q\coth[(\beta q/2)(q^2+2nu)^{1/2}]}{(q^2+2nu)^{1/2}} - \coth\left(\frac{\beta q^2}{2}\right)\right)e^{i\vec{q}\cdot\vec{r}}$$

in the integrand. However, this is exactly the contribution which has already been included in the regular chain diagrams. [Note that in Eq. (2.5) a term which is proportional to n_0 appears. We can easily find that this term contributes the above.] Hence, subtracting the above terms, we find

$$I_{cx}(r) = \int \frac{d\vec{q}}{(2\pi)^3}\left(\frac{g_{3/2}^2(r)q\coth\{(\beta q/2)[q^2+2nu(q)]^{1/2}\}\cos\vec{q}\cdot\vec{r}}{n[q^2+2nu(q)]^{1/2}} - \frac{g_{3/2}^2(r)}{n}\coth\left(\frac{\beta q^2}{2}\right) + \frac{G_{3/2}^2(r)u(q)\coth\{\frac{1}{2}\beta q[q^2+2nu(q)]^{1/2}\}}{q[q^2+2nu(q)]^{1/2}}(\cos\vec{q}\cdot\vec{r}-1)\right), \quad (2.12)$$

where

$$g_{3/2}^2(r) = \frac{2n_0}{\lambda^2 r}e^{-2(\pi\alpha)^{1/2}r/\lambda} + \frac{e^{-4(\pi\alpha)^{1/2}r/\lambda}}{\lambda^4 r^2}.$$

In Eq. (2.8) we have approximated the function $G_{3/2}$ by the two terms on the right side. Of these, we consider that the first term n_0 is dominant. The second term is due to the particles in excited states. Because of these two terms, the chain-exchange contribution can be interpreted graphically as in Fig. 3. Here, dotted curves represent the fictitious propagation of the particles in the condensed state and solid curves the ususal propagation characterized by finite momentum. A simplified version of formula (2.12) is derived in Appendix A.

III. EXCITATION ENERGY DUE TO CHAIN EXCHANGES

From the pair-distribution function, the internal energy can be obtained in accordance with the grand-ensemble formula

$$U = U_0 + \frac{V}{2}\int_0^1 d\xi\, d\vec{r}\phi(r)\,\frac{\partial}{\partial\beta}\,\beta\rho_2(r,\xi)\Big|_z, \quad (3.1)$$

where ξ is a coupling parameter and U_0 is the kinetic energy. The pair-distribution function ρ_2 here is what we obtain by replacing the interaction $u(q)$ by $\xi u(q)$.

The above formula is general and exact. The particular contribution from the chain-exchange graphs to the energy can be obtained by using Eq. (2.12). We then find many terms, but of these we select the important contribution which is proportional to $G_{3/2}^2$. The other terms which are associated with $g_{3/2}^2$ may be neglected because it does not include the major term n_0. We shall also neglect the temperature variation of $G_{3/2}$. Then, the essential part of the integrand for the q integration becomes

$$\frac{G_{3/2}^2(r)}{nq^2}\left[\epsilon\coth(\beta\epsilon/2) - \frac{2}{\beta q^2}\int_a^b dx\left(\frac{2x}{\beta q}\right)^2\coth x\right],$$

where

$$x = \tfrac{1}{2}\beta q[q^2+2n\xi u(q)]^{1/2},$$
$$a = \tfrac{1}{2}\beta q^2,$$
$$b = \beta q[q^2+2nu(q)]^{1/2}/2, \quad (3.2)$$
$$\epsilon = q[q^2+2nu(q)]^{1/2}.$$

Note that ϵ is the Bogoliubov spectrum if the total density n is replaced by n_0, the number density of condensed molecules.

The integral in the domain (a,b) can be partially

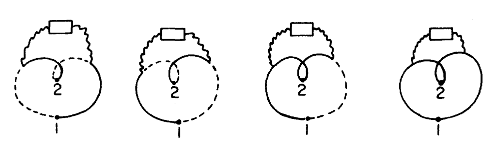

FIG. 3. Four types of chain-exchange graphs. Dotted lines represent a $p=0$ particle.

integrated

$$\int_a^b x^2 \coth x\, dx = \frac{x^3}{3} \coth x \Big|_a^b + \frac{1}{3}\int_a^b x^3(\coth^2 x - 1)\, dx\,.$$

For small q, both a and b are small. Hence, we can have the approximation

$$\coth^2 x/x \simeq \coth x/x\,.$$

Also, in this region the contribution from the x^3 term can be neglected. Thus,

$$\int_a^b x^2 \coth x dx \simeq \frac{x^3}{2} \coth x \Big|_a^b\,.$$

On the other hand, for large q or x, $\coth^2 x - 1$ is close to 0 so that

$$\int_a^b x^2 \coth x\, dx \simeq \tfrac{1}{3} x^3 \coth x \Big|_a^b\,. \tag{3.3}$$

Interpolating these two regions in terms of a parameter $P(q)$, we approximate the integral as follows:

$$\int_a^b dx\, x^2 \coth x = P(q) x^3 \coth x \Big|_a^b\,, \tag{3.4}$$

where

$$P(q) \simeq \begin{cases} \frac{1}{2}, & q<1\,, \\ \frac{1}{3}, & q>1\,, \end{cases} \tag{3.5}$$

$$U_{ex} = \frac{V}{2}\int \frac{d\vec{q}}{2\pi}\left(\frac{n_0^2 u'}{n^2 u}\right) \times\left[\epsilon\left(\frac{nu}{q^2}[1-2P(q)] - P(q)\right)\coth\left(\frac{\beta\epsilon}{2}\right) + P(q) q^2 \coth\left(\beta\,\frac{q^2}{2}\right)\right]\,, \tag{3.6}$$

where

$$u = \int \phi(r) e^{i\vec{q}\cdot\vec{r}} d\vec{r}\,,$$
$$u' = \int \phi(r)(\cos\vec{q}\cdot\vec{r} - 1)\, d\vec{r}\,, \tag{3.7}$$
$$\epsilon = q(q^2 + 2nu)^{1/2}\,.$$

IV. RING-EXCHANGE DIAGRAMS

First, consider a particle propagation clockwise in the graph of Fig. 2. This gives the contribution

$$\sum_j \int \frac{d\vec{p}_1 d\vec{p}_2 d\vec{q}}{(2\pi)^9}\int_0^\beta d\beta''\int_0^{\beta''} d\beta'\left(\frac{u^2(q)\lambda_j(q)}{1+u(q)\lambda_j(q)}\right) e^{i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}} \times\left\{f(p_1) f(\vec{p}_1+\vec{q})[1+f(\vec{p}_1)] f(\vec{p}_2)\exp\left[(\beta''-\beta')\left(p_1^2 - (\vec{p}_1+\vec{q})^2 - \frac{2\pi i j}{\beta}\right)\right]\right\}\,. \tag{4.1}$$

The above result is true only when β' and β'' do not occur during a single propagation interval $(0,\beta)$. For future simplification, we rewrite this contribution for a particle propagating counterclockwise.

$$\sum_j \int \frac{d\vec{p}_1 d\vec{p}_2 d\vec{q}}{(2\pi)^9}\int_0^\beta d\beta''\int_0^{\beta''} d\beta'\left(\frac{u^2(q)\lambda_j(q)}{1+u(q)\lambda_j(q)}\right) e^{i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}} \times\left\{f(\vec{p}_1)[1+f(\vec{p}_1+\vec{q})] f(\vec{p}_1+\vec{q}) f(\vec{p}_2+\vec{q})\exp\left[(\beta''-\beta')\left(p_1^2 - (\vec{p}_1+\vec{q})^2 + \frac{2\pi i j}{\beta}\right)\right]\right\}. \tag{4.2}$$

Next, we consider the special case where β' and β'' do occur in the same propagation interval. For this case we have

$$\sum_j \int \frac{d\vec{p}_1 d\vec{p}_2 d\vec{q}}{(2\pi)^9}\int_0^\beta d\beta''\int_0^{\beta''} d\beta'\left(\frac{u^2(q)\lambda_j(q)}{1+u(q)\lambda_j(q)}\right) e^{i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}} \times\left\{f(p_1)[1+f(p_1)] f(p_2)\exp\left[(\beta''-\beta')\left(p^2 - (\vec{p}_1+\vec{q})^2 + \frac{2\pi i j}{\beta}\right)\right]\right\}\,. \tag{4.3}$$

Here, the unrestricted integration over β' and β'' includes both a clockwise and counterclockwise propagation. The total contribution is then

$$\sum_j \int \frac{d\vec{p}_1 d\vec{p}_2 d\vec{q}}{(2\pi)^9}\int_0^\beta d\beta''\int_0^{\beta'} d\beta'\,\frac{u^2(q)\lambda_j(q)}{1+u(q)\lambda_j(q)}\, e^{i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}}$$
$$\times\{(f(p_1) f(\vec{p}_1+\vec{q})[1+f(p_1)] f(p_2) + f(p_1+q) f(\vec{p}_1)[1+f(\vec{p}_1+\vec{q})] f(\vec{p}_2+\vec{q}) + f(p_1)[1+f(p_1)] f(p_2)\}$$
$$\times\exp\left\{(\beta''-\beta')\left[p_1^2 - (\vec{p}_1+\vec{q})^2 + \frac{2\pi i j}{\beta}\right]\right\}\,. \tag{4.4}$$

(The factor $\frac{1}{2}$ which results from adding the counterclockwise propagation is canceled by a factor of 2 due to the fact that either particle may contain the interaction ring.) Because the factor

$$\{f(p_1)f(\vec{p}_1+\vec{q})[1+f(p_1)]f(p_2)+f(\vec{p}_1+\vec{q})[1+f(\vec{p}_1+\vec{q})]f(\vec{p}_2+\vec{q})+f(p_1)[1+f(p_1)]f(p_2)\}$$
$$\times\exp\left\{\alpha\left[p_1^2-(\vec{p}_1+\vec{q})^2+\frac{2\pi ij}{\beta}\right]\right\}e^{i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}}, \quad (4.5)$$

where $\alpha=|\beta''-\beta'|$, is not symmetric under the transformation, $\alpha\to\beta-\alpha$ the double integration over β'' and β' cannot be reduced to a single interaction over α. This is the point which corrects the previous result.[7] Part of the above factor is symmetric and can be reduced. After doing so we obtain

$$\sum_j\int\frac{d\vec{p}_1d\vec{p}_2d\vec{q}}{(2\pi)^9}\int_0^\beta d\alpha U_{\text{eff}}\exp\left[\alpha\left(\vec{p}_1^2-(\vec{p}_1+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]$$
$$\times\{f(\vec{p}_2+\vec{q})f(p_1)f(\vec{p}_1+\vec{q})[1+f(\vec{p}_1+\vec{q})]+f(p_2)f^2(p_1)[1+f(\vec{p}_1+\vec{q})]\}e^{i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}}$$
$$+\frac{1}{\beta}\sum_j\int\frac{d\vec{p}_1d\vec{p}_2d\vec{q}}{(2\pi)^9}\int_0^\beta d\beta''\int_0^{\beta''}d\alpha U_{\text{eff}}\exp\left[\alpha\left(p_1^2-(\vec{p}_1+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]f(p_2)f(p_1)[1+f(\vec{p}_1+\vec{q})]e^{i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}}$$
$$+\frac{1}{\beta}\sum_j\int\frac{d\vec{p}_1d\vec{p}_2d\vec{q}}{(2\pi)^9}\int_0^\beta d\beta''\int_0^\beta d\alpha U_{\text{eff}}\exp\left[\alpha\left(p_1^2-(\vec{p}_1+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]$$
$$\times\{f(\vec{p}_2+\vec{q})f(p_1)[1+f(\vec{p}_1+\vec{q})]e^{i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}}\}, \quad (4.6)$$

where

$$U_{\text{eff}}\equiv u^2(q)\lambda_j(q)/[1+u(q)\lambda_j(q)].$$

We note that when $\vec{r}=0$, the phase factor $\exp[i(\vec{p}_1-\vec{p}_2)\cdot\vec{r}]$ will vanish and the last two terms in Eq. (4.6) can be combined to give

$$\sum_j\int\frac{d\vec{p}_1d\vec{p}_2d\vec{q}}{(2\pi)^9}\int_0^\beta d\alpha U_{\text{eff}}\{f(p_2)f(p_1)[1+f(\vec{p}_1+\vec{q})]\}\exp\left[\alpha\left(p_1^2-(\vec{p}_1+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]. \quad (4.7)$$

Adding this to the first term gives

$$\sum_j\int\frac{d\vec{p}_1d\vec{p}_2d\vec{q}}{(2\pi)^9}\int_0^\beta d\alpha U_{\text{eff}}\frac{\partial}{\partial\ln z}\{f(p_1)[1+f(\vec{p}_1+\vec{q})]\}f(p_2)\exp\left[\alpha\left(p_1^2-(\vec{p}_1+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]. \quad (4.8)$$

This is the necessary and correct result needed to ensure that the pair-distribution function is correctly normalized and compatible with the Pauli-exclusion principle (for fermions). Finally, for convenience, let us define the following terms:

$$\chi_j(q,r)\equiv\int\frac{d\vec{p}}{(2\pi)^3}\int_0^\beta d\alpha f^2(p)[1+f(\vec{p}+\vec{q})]\exp\left[\alpha\left(p^2-(\vec{p}+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]e^{i\vec{p}\cdot\vec{r}},$$

$$\lambda_j(q,r,\beta'',0)\equiv\int\frac{d\vec{p}}{(2\pi)^3}\int_0^{\beta''}d\alpha f(p)[1+f(\vec{p}+\vec{q})]\exp\left[\alpha\left(p^2-(\vec{p}+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]e^{i\vec{p}\cdot\vec{r}},$$

$$\lambda_j(q,r,\beta'',\beta)\equiv\int\frac{d\vec{p}}{(2\pi)^3}\int_{\beta''}^\beta d\alpha f(p)[1+f(\vec{p}+\vec{q})]\exp\left[\alpha\left(p^2-(\vec{p}+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]e^{i\vec{p}\cdot\vec{r}},$$

$$\rho_1^0(r)\equiv\int\frac{d\vec{p}}{(2\pi)^3}f(p)e^{i\vec{p}\cdot\vec{r}}, \quad (4.9)$$

$$\rho_1^1\equiv-\beta\int\frac{d\vec{p}d\vec{q}}{(2\pi)^6}f(p)f(\vec{p}+\vec{q})[1+f(\vec{p})]u(q)e^{i\vec{q}\cdot\vec{r}},$$

$$\Lambda_j(q,r)\equiv\int\frac{d\vec{p}}{(2\pi)^3}\int_0^\beta d\alpha f(p)f(\vec{p}+\vec{q})[1+f(\vec{p}+\vec{q})]\exp\left[\alpha\left(p^2-(\vec{p}+\vec{q})^2+\frac{2\pi ij}{\beta}\right)\right]e^{i\vec{p}\cdot\vec{r}}.$$

With these definitions, the general contribution or the ring-exchange diagrams to the pair distribution is

$$I_{rx}(r) = -2\rho_1^0(r)\rho_1^1(r) + \rho_1^0(r)\sum_j \int \frac{d\vec{q}}{(2\pi)^3} U_{\rm eff}[\Lambda_j(q,r)e^{i\vec{q}\cdot\vec{r}} + \chi_j(q,r)] + \rho_1^0(r)\sum_j \int \frac{d\vec{q}}{(2\pi)^3}\int_0^\beta d\beta'' U_{\rm eff}[\lambda_j(q,r,\beta'',0) + \lambda_j(q,r,\beta'',\beta)e^{i\vec{q}\cdot\vec{r}}]. \quad (4.10)$$

On the right-hand side of Eq. (4.10), the first term is due to the first-order self-energy-type graphs. It cancels the first term in the expansion of the square of the number density, i.e., the singlet-distribution function, in powers of interaction. The square appears in the cluster expansion of the pair-distribution function as the limiting value for infinite distance. The first term has the form

$$2\rho_1^0(r)\rho_1^1(r) = 2\beta G_{3/2}(r)\frac{1}{(2\pi^3)^2} \times \int f(p)f(\vec{p}+\vec{q})[1+f(p)]u(q)\,e^{i\vec{p}\cdot\vec{r}}d\vec{p}d\vec{q}.$$

A further simplification of the expression may be made by changing the momentum variables. However, since we have been taking only the nonfluctuating, that is, the temperature-independent part of the number density, it is appropriate to neglect the term with $\rho_1^1(r)$.

The real parts of the second and third terms vanish at $r=0$ as can be seen by changing momentum variables in the eigenvalue expressions in Eqs. (4.9) which appear in these terms. The j sums in these expressions shall be performed by expanding the integrand about $p=0$, as we have done in Sec. II. We shall then see that the last term is contributing. The relevance of this term in relation to the chain graphs can be seen if we rewrite the j sum as follows:

$$\sum_j \frac{u^2\lambda_j\psi_j}{1+u\lambda_j} = \sum_j \frac{u\lambda_j}{1+u\lambda_j} - \sum_j u\lambda_j\,, \quad (4.11)$$

where ψ_j is a certain function of j. In the j sum we may use a formula

$$\sum_j \frac{1}{(j+x)^2+y^2} = \left(\frac{\pi}{y}\right)\frac{\sinh 2\pi y}{\cosh 2\pi y - \cos 2\pi x}. \quad (4.12)$$

In momentum space, we then find [apart from the first factor $\rho_1^0(r)$]

$$\frac{1}{(2\pi^3)^2}\int\left[\frac{q\coth[\beta q(q^2+2nu)^{1/2}/2]}{n(q^2+2nu)^{1/2}} + \frac{u\coth[\beta q(q^2+2nu)^{1/2}/2]}{q(q^2+2nu)^{1/2}} - \frac{\coth(\beta q^2/2)}{n}\right] \times f(\vec{p}+\vec{q})[f(\vec{p}+\vec{q}) - f(p)]d\vec{p}d\vec{q} \quad (4.13)$$

as the important contribution. As we might expect, there is a similarity between the chain and ring-exchange contributions. Again, keeping those terms which are proportional to n_0^2 we have

$$I_{rx}(r) = \frac{n_0^2}{n}\int\frac{d\vec{q}}{(2\pi)^3}\left[\frac{q\coth\{\beta q/2[q^2+2nu(q)]^{1/2}\}}{[q^2+2nu(q)]^{1/2}} - \coth\left(\frac{\beta q^2}{2}\right) + \frac{nu(q)\coth\{\beta q/2[q^2+2nu(q)]^{1/2}\}}{q[q^2+2nu(q)]^{1/2}}\right][\cos(\vec{q}\cdot\vec{r}) - 1]. \quad (4.14)$$

The energy can be obtained as before by introducing Eq. (4.14) into Eq. (3.1). We then find

$$U_{rx} = \frac{n_0^2 V}{n}\int\frac{d\vec{q}}{(2\pi)^3}\int_0^1 d\xi\, u'(q^2+n\xi u)\frac{\coth[(\beta/2)\epsilon(\xi)] - [(\beta/2)\epsilon(\xi)]\operatorname{csch}^2[(\beta/2)\epsilon(\xi)]}{\epsilon(\xi)}, \quad (4.15)$$

where $\epsilon(\xi)$ is obtained from ϵ by replacing u by ξu. The ξ integral on the right-hand side consists of

$$I_1 = u'q^2\int_0^1 d\xi\left(\frac{\coth[(\beta/2)\epsilon(\xi)]}{\epsilon(\xi)} - \frac{\beta}{2}\operatorname{csch}^2\frac{\beta}{2}\epsilon(\xi)\right) = \frac{2u'}{\beta nu}x\coth x\Big|_a^b,$$

$$I_2 = nuu'\int_0^1 \xi d\xi\left(\frac{\coth[(\beta/2)\epsilon(\xi)]}{\epsilon(\xi)} - \frac{\beta}{2}\operatorname{csch}^2\left[\frac{\beta}{2}\epsilon(\xi)\right]\right) = \frac{u'}{\beta q^2 nu}\left(\frac{4}{\beta^2q^2}(1-2P)x^2 - q^2\right)x\coth x\Big|_a^b. \quad (4.16)$$

These integrals have been evaluated approximately as before. The integration variable x and the upper and lower bounds a and b have been defined in Eqs. (3.2).

Using Eqs. (4.16) in Eq. (4.15) we obtain

$$U_{rx} = \frac{V}{2}\int\frac{d\vec{q}}{(2\pi)^3}\left(\frac{n_0^2u'}{n^2u}\right) \times\left\{\epsilon\left[1+(1-2P)\left(1+\frac{2nu}{q^2}\right)\coth\frac{\beta}{2}\epsilon\right] - q^2(1-P)2\coth\left(\frac{\beta}{2}q^2\right)\right\}. \quad (4.17)$$

This is the ring exchange equivalence of Eq. (3.6).

V. EXCHANGE EFFECT ON THE EXCITATION SPECTRUM

The chain and ring-exchange contributions to the energy given by Eqs. (3.6) and (4.17) are characterized by

$$\coth\frac{x}{2}=1+2f(x)\ ,\quad f(x)=\frac{e^{-x}}{1-e^{-x}}\ , \tag{5.1}$$

where $f(x)$ is the Bose-distribution function for quasiparticles of energy x. Therefore, the total energy which is obtained by combining these contributions justifies the Landau-type description in which the energy and the distribution function are assumed. Moreover, we note that the elementary excitations consist of a particlelike mode with energy q^2 and a phononlike mode with energy ϵ. The latter reduces to the Bogoliubov spectrum when n is replaced by n_0. At a point at which $u(q)$ vanishes, a cancellation takes place between the two modes. Hence, around such a point particlelike excitations show up as $u(q)$ deviates from the zero point. This may be considered as the situation in which the roton-type spectrum arises.

Combining Eqs. (3.6) and (4.17) we can define

$$\epsilon_x=\epsilon\frac{n_0^2u'}{n^2u}\left(\frac{2nu}{q^2}+1-S_{T=0}\right)(1-2P) \tag{5.2}$$

as the zero-temperature excitation energy due to exchange. Here

$$S_{T=0}(q)=q/(q^2+2nu)^{1/2} \tag{5.3}$$

is the structure factor corresponding to the chain diagrams. These diagrams give rise to the excitation energy

$$\epsilon_c=\epsilon\ , \tag{5.4}$$

where ϵ is given by Eqs. (3.2). Hence, combining this with Eq. (5.2) we obtain

$$\epsilon_x(q)=\epsilon\left[1+\left(\frac{n_0}{n}\right)^2\frac{u'}{u}\left(1-S_{T=0}(q)+\frac{2nu(q)}{q^2}\right)\times[1-2P(q)]\right]. \tag{5.5}$$

Finally, we write this excitation spectrum in the Feynman form bringing out mass

$$\epsilon_x(q)=q^2/2m^*S(q)\ ,$$

where m^* is the effective mass defined by

$$m^*=m\left[1+\left(\frac{n_0}{n}\right)^2\frac{u'}{u}\left(1-S_{T=0}(q)+\frac{2nu(q)}{q^2}\right)\times[1-2P(q)]\right]^{-1} \tag{5.6}$$

and

$$S(q)=S_{T=0}(q)\ . \tag{5.7}$$

VI. CONCLUDING REMARKS

From the above result in Eq. (5.6) we see that if $P(q)$ approaches $\frac{1}{2}$ for small q faster than q^2, then we obtain the original Feynman spectrum with $m^*=m$. For larger values of q, deviations from this spectrum are expected. In general, since $u(q)$ is expected to decrease from its zero-momentum value $u(0)$ and because $P(q)$ approaches $\frac{1}{3}$, the effective mass may increase. If this is the case, the excitation spectrum will be lowered from the case of Feynman and Cohen.[2]

The contributions of the two types of grantum graph are interesting when they are compared with that of simple chain diagrams. The latter diagrams represent collective couplings which can exist even in classical fluids. In these graphs, the momentum q is transfered from one particle to another in a way similar to the propagation of sound. In the exchange-type diagrams, the interaction momentum returns to the original position from which it started. Hence, these graphs may be considered to represent the back-flow effect proposed by Feynman and Cohen. As we mentioned before, these graphs lower the excitation spectrum effectively especially in the roton region.

Equation (5.6) depends on n_0. It is known that the ideal-gas expression for n_0 is not applicable to liquid helium. Therefore, and because we have used the zero-temperature limit, it is difficult to discuss the temperature variation of the effective mass. The effective-mass expression depends also on the potential parameters directly through $u(q)$ and indirectly through $S(q)$. We have taken the simplest step of estimating m^* from the sound velocity by making use of the small momentum limit. Neglecting the momentum dependence of m^*, we have performed some numerical calculations.

The potential which we have adopted is

$$\phi(r)=\begin{cases}\phi(0)\ , & r<a\ ,\\ \epsilon^*[(a/r)^{12}-(a/r)^6]\ , & r>a\ .\end{cases} \tag{6.1}$$

The Fourier transform of this potential is

$$u(q)=4\pi a^3\epsilon^*\left[\sum_{m=0}^{4}\frac{(-a^2q^2)^m}{10\times 9\times\cdots\times(10-2m)}-\left(\frac{1}{4}-\frac{a^2q^2}{4\times 3\times 2}\right)\frac{\sin qa}{qa}+\sum_{m=0}^{4}\frac{(-a^2q^2)^m}{10\times 7\times\cdots\times[10-(2m+1)]}\right.$$
$$\left.-\left(\frac{1}{4\times 3}-\frac{a^2q^2}{4!}\right)\cos qa-\frac{(qa)^3}{4!}\frac{(aq)^6}{10\times 9\times 8\times 7\times 6\times 5}+1\right]\mathrm{Si}(qa)+\frac{\phi(0)4\pi a^3}{a^3q^3}(\sin qa-aq\cos qa)\,. \quad (6.2)$$

We note that for $q=0$, we obtain a phonon spectrum with sound velocity given by (instead of keeping the same unit we restore mass; $\hbar$ is still 1)

$$c=[nu(0)/m^*]^{1/2}\,, \quad (6.3)$$

where for the above potential

$$u(0)=\tfrac{4}{3}\pi\phi(0)a^3-\tfrac{8}{9}\pi a^3\epsilon^*\,. \quad (6.4)$$

Hence, in terms of $\phi(0)$, ϵ^* is

$$\epsilon^*=\tfrac{3}{2}\phi(0)-9c^2m^*/8\pi a^3n\,. \quad (6.5)$$

The sound velocity is determined mainly by $\phi(0)$ and the effective mass. We have determined these and ϵ^* so as to reproduce a satisfactory excitation spectrum for a given value of $a=2.67$ Å and $n=0.0218$. Within our limited trials we found that the following choices give the best result:

$$\phi(0)=30.7\text{ K},\quad m^*=1.71m,\quad \epsilon^*=1.397\text{ K}$$
$$a=2.67\text{ Å},\quad n=0.0218\text{ Å}^{-3}\,.$$

These parameters are close to what Kebukawa *et al.* adopted,[5] although their potential form is different. In their notation, they used

$$V_a=32.7\text{ K},\quad m^*=(1-\gamma)^{-1}m=2.4\text{ m},$$
$$a=2.8\text{ Å},\quad n=0.0218\text{ Å}^{-3}\,.$$

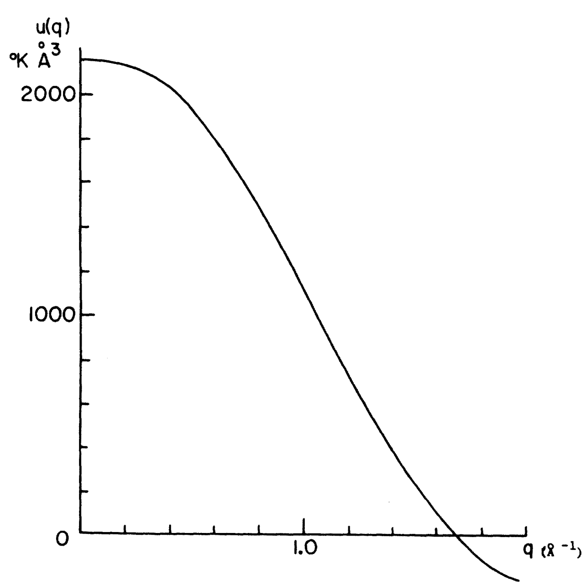

FIG. 4. Fourier transform of the potential, i.e., $u(q)$, as a function of q.

In Fig. 4, we have illustrated $u(q)$. This curve resembles to what Kebukawa *et al.* gave. The feature of these curves are that $u(q)$ is constant for small q and decreases to zero with some wiggles. The potential for $r\gg a$ is not very important in the energy spectrum.

Figure 5 illustrates the excitation spectrum, the solid curve representing our theoretical curve.[8] The agreement with experiment is very good, but since the potential parameters are chosen so as to reproduce the curve we need reservations in accepting the agreement. Nevertheless, without the effective mass and the large initial-potential barrier one cannot reproduce the spectrum.

In Fig. 6 we have given the theoretical structure factor in comparison with experiments. In this figure, the circles correspond to $T=1.94$ and density 0.1628 g/cm³ and the squares to $T=2.02$ and density 0.1528 g/cm³ in the data given by Mozer, De Graaf, and Neindre.[9] The data points are higher than the theoretical curve in the small-momentum region and are lower in the large-momentum region. Earlier, Hallock determined the liquid-structure factor by using x-ray scattering. The triangles in Fig. 6 represent his data. His temperature range was between 0.38 and 4.60 K and the momentum range was from around 0.133 to 1.125 Å^{-1}. He used a weighted least-squares polynomial fit for $S(q)$, and his data agree with our theoretical curve better than the data by Mozer *et al.* in the small momentum region. Around $q=1$, all the data and our theoretical points are close so that we did not plot

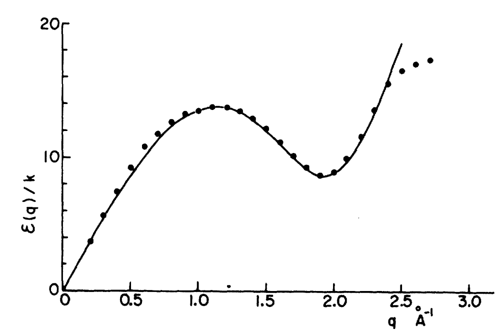

FIG. 5. Excitation spectrum $\epsilon(q)$ divided by the Boltzmann constant k plotted against q in reciprocal angstrom.

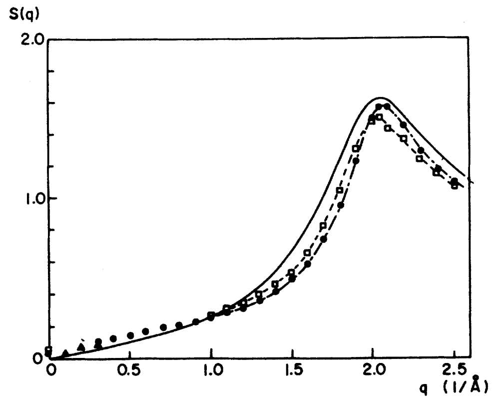

FIG. 6. $S(q)$ as a function of q. The circles and squares represent the data by Mozer, De Graaf, and Le Neindre (Ref. 9) corresponding to 1.94 and 2.02 K, respectively. The triangles represent Hallock's x-ray diffraction data (Ref. 9). For clarity, his data are plotted only in the small-momentum region where differences from the data of Mozer *et al*. are visible.

Hallock's data for clarity. Note that the experiments gave certain values for $S(q)$ at $q=0$. By adopting a slightly different set of potential parameters and trying to make a smooth connection of the two branches of the potential by adding a new term

$$\phi(r)=\epsilon\left[\left(\frac{a}{r}\right)^{12}-\left(\frac{a}{r}\right)^{6}\right]+Ue^{-\alpha(r-a)}\,,\quad r>a\,,$$

$$a=2.75\text{ Å},\quad \epsilon^*=54.20\text{ K},\quad U=\phi(0)=33.12\text{ K},$$

$$a=2.18\text{ Å}\,,\quad \alpha=20\text{ Å}^{-1}\,. \tag{6.6}$$

We have reproduced a somewhat-better structure factor curve. However, this is at the expense of having more adjustable parameters. We are inclined to conclude that a much more extensive numerical calculation with momentum-dependent effective mass would be needed to come to satisfaction.

Concerning the momentum dependence of the effective mass, we remark that if the potential varies in accordance with

$$u(q)=u(0)(1-aq^2)\,, \tag{6.7}$$

and if the sound velocity is c, the effective mass is approximately given by

$$m^*=m[1-(n_0/n)^2c^2a(1-2P)]^{-1}\,. \tag{6.8}$$

Since the parameter P decreases for large q, m^* is expected to increase. If, on the other hand, the potential is more flat around $q=0$ and is given by

$$u(q)=u(0)(1-bq^4)\,, \tag{6.9}$$

the effective mass is approximately given by

$$m^*=m[1-(n_0/n)^2c^2bq^2(1-2P)]^{-1}\,. \tag{6.10}$$

Therefore, we expect a stronger q dependence. It would be very useful if the momentum dependence of the effective mass is determined by experiment. In both Eqs. (6.8) and (6.10), the dependence is dependent also on the sound velocity in the same way.

We have demonstrated that the excitation spectrum in the Bose system consists of particlelike and phononlike modes. We note in Eqs. (3.6) and (4.17) or in the final excitation spectrum of Eq. (5.2) that the energy vanish for $u(q)=0$ and $P(q)=\frac{1}{2}$. That is, the two excitations balance with each other. When the two cancel each other, considerations of the terms which we have neglected become important. We have also retained only the first term in $G_{3/2}(r)$ in order to simplify our result. Improvements on these approximations are possible and should be interesting. We shall aim at these in the near future.

APPENDIX

In this appendix, we derive Eq. (2.11), the chain-exchange contribution, to the pair distibution function by replacing $G_{3/2}(r)$ by n_0.

Using Eq. (2.6) for $\lambda_j(q,r)$, keeping only the part proportional to n_0 from Eq. (2.7) and from Eq. (1.1), we obtain

$$I_{cx}(r)=-\frac{1}{\beta}\sum_j\int\frac{d\vec{q}}{(2\pi)^3}\,\frac{n_0^2u(q)e^{i\vec{q}\cdot\vec{r}}}{1+u(q)\lambda_j(q)}\times\left(q^4(1+2e^{-i\vec{q}\cdot\vec{r}}+e^{-2i\vec{q}\cdot\vec{r}})\left[q^4+\left(\frac{2\pi j}{\beta}\right)^2\right]^{-2}+\frac{4q^2\pi ij(1-e^{-2i\vec{q}\cdot\vec{r}})}{\beta}-\left(\frac{2\pi j}{\beta}\right)^2(1-2e^{-i\vec{q}\cdot\vec{r}}+e^{-2i\vec{q}\cdot\vec{r}})\right)\,. \tag{A1}$$

Using the first-order approximation for $\lambda_j(q)$:

$$\lambda_j(q)=\frac{2(n_0+n_1)q^2}{q^4+(2\pi j/\beta)^2}=\frac{2nq^2}{q^4+(2\pi j/\beta)^2}\,; \tag{A2}$$

we have

$$I_{cx}(r) = -\frac{1}{\beta}\int \frac{d\vec{q}}{(2\pi)^3}\sum_j\left(\frac{u(q)n_0^2}{[q^4+(2\pi j/\beta)^2+2nu(q)q^2]\,[q^4+(2\pi j/\beta)^2]}\right) \times\left\{2\cos(\vec{q}\cdot\vec{r})\left[q^4-\left(\frac{2\pi j}{\beta}\right)^2\right]+2\left[q^4+\left(\frac{2\pi j}{\beta}\right)^2\right]-\frac{8q^2\pi j\,\sin(\vec{q}\cdot\vec{r})}{\beta}\right\}. \quad \text{(A3)}$$

Since $u(q)$ is a function of the magnitude of q only, the integral over $\sin\vec{q}\cdot\vec{r}$ will vanish. Next we can do the summations over j by contour:

$$-\sum_j \frac{u(q)n_0^2[q^4-(2\pi j/\beta)^2]}{[q^4+(2\pi j/\beta)^2+2nu(q)q^2][q^4+(2\pi j/\beta)^2]} = \frac{n_0^2 q\coth\{\beta q/2[q^2+2nu(q)]^{1/2}\}}{2n[q^2+2nu(q)]^{1/2}} + \frac{n_0^2u(q)\coth\{\beta q/2[q^2+2nu(q)]^{1/2}\}}{2q[q^2+2nu(q)]^{1/2}} - \frac{n_0^2}{2n}\coth\left(\frac{\beta q^2}{2}\right) \quad \text{(A4)}$$

and

$$-\frac{1}{\beta}\sum_j \frac{u(q)n_0^2}{q^4+(2\pi j/\beta)^2+2nu(q)q^2} = -\frac{n_0^2u(q)\coth\{\beta q/2[q^2+2nu(q)]^{1/2}\}}{2q[q^2+2nu(q)]^{1/2}}. \quad \text{(A5)}$$

Subtracting out the contribution

$$\sum_j \frac{u\lambda_j^2}{1+u\lambda_j}$$

proportional to n_0^2, which has already been included in the classical chains, removes the term

$$\frac{n_0^2}{n}\left[\frac{q\coth\{(\beta q/2)[q^2+2nu(q)]^{1/2}\}}{[q^2+2nu(q)]^{1/2}} - \coth\left(\frac{\beta q^2}{2}\right)\right], \quad \text{(A6)}$$

and we arrive at

$$I_{cx}(r) = \int\frac{d\vec{q}}{(2\pi)^3}\,\frac{n_0^2u(q)\coth\{(\beta q/2)[q^2+2nu(q)]^{1/2}\}\,[\cos\vec{q}\cdot\vec{r}-1]}{q[q^2+2nu(q)]^{1/2}}. \quad \text{(A7)}$$

---

*Work supported by the NSF under Grant No. DMR 73-02321 A01. Based on the thesis submitted by one of the authors (T.S.) to the SUNY Buffalo for partial fulfillment of the requirements for a Ph.D. degree.

[1]N. N. Bogoliubov, J. Phys. USSR 11, 23 (1947); N. N. Bogoliubov and D. Zubarev, Sov. Phys. 1, 83 (1955).

[2]R. P. Feynman and M. Cohen, Phys. Rev. 102, 1189 (1956).

[3]T. D. Lee and C. N. Yang, Phys. Rev. 112, 1419 (1958).

[4]D. Pines, in *Liquid Helium*, Proceedings of the International School of Physics Course 21 (Academic, New York, 1963), p. 147; D. Pines and P. Nozières, *The Theory of Quantum Fluids* (Benjamin, New York, 1966), Vol. 1; D. Bohm and B. Salt, Rev. Mod. Phys. 39, 894 (1967).

[5]T. Nishiyama, Prog. Theor. Phys. 45, 730 (1971); T. Kebukawa *et al.*, *ibid* 44, 565 (1970); 49, 1802 (1973); G. S. Grest and A. K. Rajagopal, *ibid.* 52, 811 (1974); F. Iwamoto, *ibid.* 44, 1121 (1970).

[6]A. Ishihara, *Statistical Physics* (Academic, New York, 1971), Chap. 11.

[7]A. Ishihara, Prog. Theor. Phys. 44, 1 (1969); Phys. Rev. 172, 166 (1968).

[8]We are grateful to David Y. Kojima for numerical calculations.

[9]B. Mozer, L. A. De Graaf, and B. Le. Neindre, Phys. Rev. A 9, 448 (1974). Earlier neutron diffraction data by Henshaw and others are quoted in this article; Robert B. Hallock, *ibid.* 5, 320 (1972).