

## Liquid Structure Factor of Ground-State He<sup>4</sup>†

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A nonlinear integral equation for the liquid structure factor of ground-state He<sup>4</sup>, constructed from various frequency moments of the density-density correlation function, is proposed. This equation is solved for a particularly simple choice of two-body potential, and the results for the self-consistently-determined particle density are compared with experiment. The energy per particle and the sound velocity are also determined at the calculated density. The density, energy, and sound velocity, as well as the structure-factor curve as a function of  $k$ , all agree quite closely with experimental values. There are no free parameters once the choice of two-body potential has been made.

### I. INTRODUCTION

In this paper we construct a simple theory for the liquid structure factor of He<sup>4</sup> in its ground state. This liquid structure factor  $S(\vec{k})$  and the radial distribution function  $S(\vec{r})$  are in general defined by

$$\begin{aligned} \rho[S(\vec{r}) - 1] &\equiv \rho^{-1} \langle \psi^\dagger(\vec{r}, t) \rho(0, t) \psi(\vec{r}, t) \rangle - \rho^2 \\ &\equiv (2\pi)^{-3} \int d^3k e^{i\vec{k} \cdot \vec{r}} [S(\vec{k}) - 1], \end{aligned} \quad (1.1)$$

where  $\rho(\vec{r}, t) = \psi^\dagger(\vec{r}, t) \psi(\vec{r}, t)$  is the number density operator in the Heisenberg representation and  $\rho = \langle \rho(\vec{r}, t) \rangle$ . The averaging process is taken to be the usual grand canonical one,  $\langle A \rangle \equiv \text{Tr} \exp[-\beta(H - \mu N)] A / \text{Tr} \exp[-\beta(H - \mu N)]$ , and we will be interested ultimately in the zero temperature ( $\beta \rightarrow \infty$ ) or ground-state limit. Since the Hamiltonian  $H$  will have translational and rotational invariance, the functions  $S(\vec{r})$  and  $S(\vec{k})$  will depend only on the magnitudes  $|\vec{r}|$  and  $|\vec{k}|$ , respectively.

We will obtain a nonlinear integral equation for the ground-state structure factor  $S_\rho(k)$  as a function of the number density  $\rho$  and wave number  $k$ . Having obtained a suitable  $S_\rho(k)$ , we may then calculate the energy per particle  $E(\rho)/N$  at a given density and determine the equilibrium density by the condition  $(d/d\rho)E(\rho)/N = 0$ . To do this, we need two familiar expressions. The first relates the total energy to the radial distribution function. We have

$$E/N = \langle KE \rangle / N + \frac{1}{2} \rho \int d^3r V(r) S(r). \quad (1.2)$$

The second familiar result we need is the virial theorem

$$P/\rho = \frac{2}{3} \langle KE \rangle / N - \frac{1}{6} \rho \int d^3r S(r) [\vec{r} \cdot \vec{\nabla} V(r)]. \quad (1.3)$$

In these equations,  $\langle KE \rangle / N$  is the average kinetic energy per particle  $(1/2m\rho) \langle [\vec{\nabla} \psi^\dagger(\vec{r}, t) \cdot [\vec{\nabla} \psi(\vec{r}, t)]] \rangle$ , and  $V(r)$  is the local two-body potential appearing in the Hamiltonian. By eliminating the unknown kinetic energy, we obtain

$$P/\rho = \frac{2}{3} E/N - \frac{1}{3} \rho \int d^3r S(r) \left[ \frac{1}{2} \vec{r} \cdot \vec{\nabla} V(r) + V(r) \right]. \quad (1.4)$$

Equation (1.4) is, of course, a valid relation at any temperature and density. If we restrict our

attention to the zero-temperature limit, we obtain the form necessary for subsequent analysis. Since  $P = \rho^2 (d/d\rho) E(\rho) / N$  at zero temperature, we find

$$\begin{aligned} \rho(d/d\rho)E(\rho)/N &= \frac{2}{3} E(\rho)/N - \frac{1}{3} \rho \int d^3r S_\rho(r) \\ &\times \left[ \frac{1}{2} \vec{r} \cdot \vec{\nabla} V(r) + V(r) \right]. \end{aligned} \quad (1.5)$$

Our aim is then to calculate a suitable  $S_\rho(r)$  [or  $S_\rho(k)$ ], solve the differential equation (1.5) for  $E(\rho)/N$  and  $S_\rho(k)$  for this density, we may then state density at zero pressure by calculating the value of  $\rho$  at the  $E(\rho)/N$  minimum. Having obtained  $E(\rho)/N$  and  $S_\rho(k)$  for this density, we may then find the kinetic energy per particle from Eq. (1.2). Experimental values of  $E/N$ ,  $\rho$ , and the function  $S_\rho(k)$  for low-temperature liquid He<sup>4</sup> can, of course, be compared with the theoretical results.

The integral equation we obtain for  $S_\rho(k)$  in Sec. II, as well as the energy and density to be calculated from Eq. (1.5), will depend on a choice for the two-body potential  $V(r)$ . However, it should be emphasized first that we are not concerned here with the "best" choice of potential. We wish instead to investigate a simple theory which produces familiar results in the weak coupling limit for the boson system, and which is capable of extension to interactions and densities appropriate to the He<sup>4</sup> system. Consequently, for numerical purposes, we will use only a sum of Yukawa potentials for which a reasonable fit to the traditional 12-6 potential can be made and for which the algebraic manipulations are simple. We should also emphasize that our goal is not a variational theory. Having chosen a potential, there will be no free parameters. (It should be noted that some of the most successful calculations for real He<sup>4</sup> parameters have been made with variational theories.<sup>1</sup>)

Because our potential will be simple and will have a Fourier transform, we choose to rewrite Eq. (1.5) in the form

$$\begin{aligned} \rho(d/d\rho)E(\rho)/N &= \frac{2}{3} E(\rho)/N + \frac{1}{6} \rho V(q=0) \\ &+ \frac{1}{3} (2\pi)^{-3} \int d^3q \left[ \frac{1}{2} \vec{q} \cdot \vec{\nabla} q \cdot \{ \vec{q} V(q) \right. \\ &\left. - V(q) \right] [S_\rho(q) - 1], \end{aligned} \quad (1.6)$$

$$\text{where } V(q) = \int d^3r e^{-i\vec{q} \cdot \vec{r}} V(r). \quad (1.7)$$

Equation (1.6) follows from Eq. (1.5) if the Fourier transform  $V(q)$  is finite at  $q=0$ . This condition will be satisfied for the simple potential we use. We might also note that if liquid helium is to be described by a Fourier transformable potential,  $V(q=0)$  must be positive. This fact follows from a simple variational argument, and  $V(q=0) > 0$  obviously does not imply a purely repulsive potential in coordinate space.

The theory for  $S(k)$  discussed in Sec. II can be used for potentials containing a hard core [i. e., the form  $\lambda\theta(a-r) + V(r)$  where  $V(r)$  contains no hard-core part and  $\lambda \rightarrow \infty$  at the end of the calculation]. The self-consistent solution is somewhat more difficult to obtain numerically, of course. Furthermore, the freedom of choice for the core diameter  $a$  is an unnecessary refinement. Even our very rough potential choice gives remarkable agreement with the experimental  $S(k)$  in liquid He<sup>4</sup>. Of course, the fact that the Yukawa form is probably a bit too "soft" at small  $r$  suggests that we should expect our system to bind at slightly higher density and binding energy than the experimental values. This expectation is verified by the calculations in Sec. III. We emphasize again that our choice of potential is dictated by simplicity in both formulation and numerical analysis, and by the obvious connection with the familiar weak coupling theory for the ground-state boson gas.

## II. TIME-DEPENDENT CORRELATIONS AND THE APPROXIMATION SCHEME

The basic correlation function we wish to discuss is the time-dependent density-density commutator and its Fourier transform. This latter spectral function is given by

$$\chi_0(\vec{k}, \omega) = \int d^3r \int_{-\infty}^{\infty} dt e^{-i\vec{k} \cdot \vec{r} + i\omega t} \times \langle [\rho(\vec{r}, t), \rho(0, 0)] \rangle, \quad (2.1)$$

where the average  $\langle \rangle$  is that discussed previously. It is this function which is directly proportional to the differential cross section for inelastic neutron scattering from He<sup>4</sup> with energy and momentum transfer  $(\omega, k)$ . Thus the resonance in this function occurs at the observed excitation energy  $\omega_{\text{ex}}(k)$ . The latter has the familiar Landau-like form.

The quantity  $\chi_0(\vec{k}, \omega)$  satisfies, as a consequence of its definition together with rotational and translational invariance of the Hamiltonian, the following relations:

$$\chi_0(\vec{k}, \omega) = \chi_0^*(\vec{k}, \omega) = \chi_0(|\vec{k}|, \omega) = -\chi_0(k, -\omega),$$

$$\text{with } \omega\chi_0(k, \omega) > 0. \quad (2.2)$$

Furthermore,  $\chi_0$  is related to the structure factor by the familiar equation

$$S(k) = (2\pi\rho)^{-1} \int_0^{\infty} d\omega \chi_0(k, \omega) \coth \frac{1}{2}\beta\omega. \quad (2.3)$$

Two other exact relations satisfied by  $\chi_0$  will

be needed.<sup>2</sup> The first is the well-known  $f$  sum rule

$$(2\pi)^{-1} \int_0^{\infty} d\omega \omega \chi_0(k, \omega) = \rho k^2 / 2m \equiv \rho \omega_0(k), \quad (2.4)$$

and the second is the  $\omega^3$ -moment sum rule

$$(2\pi)^{-1} \int_0^{\infty} d\omega \omega^3 \chi_0(k, \omega) = \rho \omega_0(k) [\omega_I^{\infty}(k)]^2, \quad (2.5)$$

with

$$[\omega_I^{\infty}(k)]^2 = \omega_0^2(k) + 4(\langle KE \rangle / N) \omega_0(k) + 2\rho \omega_0(k) V(k) \\ + (2\pi)^{-3} m^{-1} \int d^3q [V(\vec{k} + \vec{q}) \{\hat{k} \cdot (\vec{k} + \vec{q})\}^2 \\ - V(q) (\hat{k} \cdot \vec{q})^2] [S(q) - 1]. \quad (2.6)$$

The expression (2.6) is valid only for a potential with a Fourier transform such that  $\lim_{q \rightarrow 0} q^2 V(q) = 0$ . In general, the terms on the right-hand side of (2.6) involving the potential should be replaced by  $(\rho/m) \int d^3r S(r) [1 - \cos(\vec{k} \cdot \vec{r})] \{\hat{k} \cdot \vec{\nabla} [(\hat{k} \cdot \vec{\nabla} V(r))]\}$ . In this form, one can include a hard core.

Equations (2.3) and (2.5) together give

$$\left[ [\omega_I^{\infty}(k)]^2 \left( \frac{S(k)}{\omega_0(k)} \right)^2 \right]^{1/3} \\ = \left[ \int_0^{\infty} d\omega \omega^3 f(k, \omega) \right]^{1/3} \\ \times \left[ \int_0^{\infty} d\omega \coth \frac{1}{2}\beta\omega f(k, \omega) \right]^{2/3},$$

where  $f(k, \omega) \equiv \chi_0(k, \omega) / 2\pi\rho\omega_0(k)$ . Since  $f$  is a real positive definite function on the positive  $\omega$  axis, a simple extension<sup>3</sup> of the Schwartz inequality gives

$$\left[ [\omega_I^{\infty}(k)]^2 \left( \frac{S(k)}{\omega_0(k)} \right)^2 \right]^{1/3} \\ \geq \int_0^{\infty} d\omega (\omega^3 f)^{1/3} (f \coth \frac{1}{2}\beta\omega)^{2/3} \\ \geq \int_0^{\infty} d\omega f(k, \omega) \omega = 1, \quad (2.7)$$

where the last equality follows from Eq. (2.4). Thus we have

$$[\omega_I^{\infty}(k)]^2 \geq [\omega_0(k) / S(k)]^2. \quad (2.8)$$

All the relations (2.2)–(2.8) are generally true for any system at any temperature. They depend only on our using a Hamiltonian of the form

$$H = (1/2m) \int [\vec{\nabla}\psi^\dagger(\vec{r})] \cdot [\vec{\nabla}\psi(\vec{r})] d^3r \\ + \frac{1}{2} \int V(|\vec{r}_1 - \vec{r}_2|) \psi^\dagger(\vec{r}_1) \rho(\vec{r}_2) \psi(\vec{r}_1) d^3r_1 d^3r_2. \quad (2.9)$$

In fact, the relations (2.2)–(2.8) are independent of statistics; i. e., the field operators  $\psi$  and  $\psi^\dagger$  may satisfy either commutation or anticommutation relations. In order to make such general relations useful, we need information specific to the condensed Bose system.

The first element of useful information which

should be incorporated in any theory for  $S(k)$  is the result of lowest-order perturbation theory. The unusual features of perturbation theory for the condensed Bose gas arise from the macroscopic occupation of the zero-momentum mode, and the early discussion of these features appears in the work of Bogoliubov.<sup>4</sup> The lowest-order result for  $S(k)$  at  $T=0$ , using the two-body potential  $V(k)$ , is

$$S_{\rho}^{\text{Bog}}(k) = k[k^2 + 4m\rho V(k)]^{-1/2}, \quad (2.10)$$

an expression which can be valid only for low densities and weak potentials. In obtaining the perturbation theory result (2.10), depletion of the zero-momentum mode caused by the interaction is not taken into account.  $\rho_0$ , the number density in the zero-momentum mode, is equal to  $\rho$  to this order. The depletion effect becomes important in higher orders and has been investigated by Belaiev<sup>5</sup> and by Hugenholtz and Pines.<sup>6</sup> In such higher-order calculations,  $\rho_0$  can, in principle, be determined as a function of  $\rho$ , and  $S_{\rho}(k)$  can be expressed as a function of  $\rho$  and  $k$  alone. These calculations are frequently carried out for the hard-core gas, in which case the quantity  $(\rho a^3)$ , where  $a$  is the core diameter, becomes the relevant expansion parameter.

One special feature of Eq. (2.10) should be observed. That is, in the limit of zero interaction,  $S(k)$  goes to the classical free-particle value  $S(k) = 1$  rather than to the zero-temperature limit characteristic of the free Bose gas. This reflects the fact that the limits  $T \rightarrow 0$  and  $\lambda$  (the coupling constant)  $\rightarrow 0$  are not interchangeable. The zero-interaction limit of (2.10) represents the order  $\lim_{\lambda \rightarrow 0} \lim_{T \rightarrow 0}$ , while the free Bose gas result represents the order  $\lim_{T \rightarrow 0} \lim_{\lambda \rightarrow 0}$ . We expect, therefore, that any proposed theory for  $S(k)$  at  $T=0$  should (a) approach the classical free gas limit for zero interaction, and (b) give Eq. (2.10) as a lowest first-order correction for weak potentials. The free classical gas is not entirely irrelevant.

The detailed perturbation-theory calculations mentioned above are all capable of obtaining the excitation spectrum of the weakly coupled Bose system. By this, we mean particularly the spectrum of  $\chi_0$  and not the single-particle spectrum usually emphasized in such theories.<sup>7</sup> The Bogoliubov spectrum

$$\omega_{\text{ex}}^{\text{Bog}}(k) = [\omega_0^2(k) + 2\rho\omega_0(k)V(k)]^{1/2}, \quad (2.11)$$

which in the original work of Bogoliubov referred to the single-particle spectrum, is also the spectrum of  $\chi_0$  in a lowest-order Hartree-like calculation for the condensed Bose gas. The point we wish to emphasize here is that the quantities  $S(k)$  and  $\omega_{\text{ex}}(k)$ , as well as the thermodynamic parameter  $\rho_0$ , are each determined in a complete dynamical theory.

A less complete theory, but one directed more toward the real He<sup>4</sup> problem, was proposed by Feynman.<sup>8</sup> Feynman showed that the variational

trial excited state  $\sum_i f(\vec{r}_i)\Phi_0$ , where  $\Phi_0$  is the ground state, produced the minimum excitation energy  $\omega_{\text{ex}}(k)$  above the ground state if

$$f(\vec{r}_i) = \exp(-i\vec{k} \cdot \vec{r}_i).$$

Thus the trial excited state is the density fluctuation operator  $\rho_k$  (Fourier transform of the density operator) acting on the ground state, and in this case the excitation energy becomes

$$\omega_{\text{ex}}^F(k) = \omega_0(k)/S(k). \quad (2.12)$$

Since this is a variational theory,  $\omega_{\text{ex}}^F(k)$  is known to be greater than or equal to the exact  $\omega_{\text{ex}}(k)$ . The fact that  $S(k)$  is not determined in the variational approach reflects our ignorance of the ground state. In the sense that we obtain neither  $S(k)$  nor  $\rho_0$ , the variational theory is less complete than the dynamical theories referred to above (but it is more relevant to real He<sup>4</sup> since the variational approach is not limited to low densities or weak potentials). As is well known, the use of the experimental  $S(k)$  in Eq. (2.12) produces an excitation energy which agrees with the observed spectrum at low  $k$ , but which is too large by about a factor of 2 in the roton region ( $k \sim 2 \text{ \AA}^{-1}$ ). Considerable improvement in the variational calculation is made possible by a more complicated choice of trial state.<sup>9</sup> In any case, the variational statement of the original Feynman theory allows us to write, with (2.8), the zero-temperature inequality

$$[\omega_{\gamma}^{\infty}(k)]^2 \geq [\omega_0(k)/S(k)]^2 \geq \omega_{\text{ex}}^2(k). \quad (2.13)$$

In spite of the known inadequacies of the original Feynman theory for real He<sup>4</sup>, it is of some interest to ask what the general relations (2.2)–(2.8) for  $\chi_0$  tell us if we assume that the Feynman trial state is an exact excited state. It is clear that if such is the case, the function  $\chi_0$  will have only a single  $\delta$ -function singularity on the positive  $\omega$  axis at the excitation energy  $\omega_{\text{ex}}(k)$ . This follows directly from the definition of  $\chi_0$ . Taking the form

$$\chi_0(k, \omega) = F(k) \{ \delta[\omega - \omega_{\text{ex}}(k)] - \delta[\omega + \omega_{\text{ex}}(k)] \},$$

together with the general relations (2.4) and (2.3) at  $T=0$ , one finds immediately that

$$F(k) = 2\pi\rho\omega_0(k)/\omega_{\text{ex}}(k) \quad \text{and} \quad \omega_{\text{ex}}(k) = \omega_0(k)/S(k).$$

The fact that a single-resonance ansatz produces the Feynman theory has been discussed by Pines.<sup>10</sup> The fact that such an ansatz also uniquely determines  $S(k)$  was observed by one of the authors.<sup>11</sup> That is, the additional sum rule (2.5), together with the single-resonance form associated with the Feynman theory, gives the result  $[\omega_{\gamma}^{\infty}(k)]^2 = [\omega_0(k)/S(k)]^2$ . The inequalities in (2.13) become equalities. Since  $\omega_{\gamma}^{\infty}(k)$  is known as a function of  $S(k)$  [see Eq. (2.6)], it is clear that  $S(k)$  is determined as a function of  $\langle KE \rangle / N$  and  $\rho$  if the potential  $V(k)$  is given. The integral equation  $[\omega_{\gamma}^{\infty}(k)]^2 = [\omega_0(k)/S(k)]^2$  carries the Feynman theory to a more complete stage, in that  $S(k)$  is predicted.

However, even without the experimental evidence which contradicts the Feynman relation between the excitation energy and  $S(k)$ , we know that this integral equation is incorrect. First of all, there are the early observations of Feynman and Cohen<sup>9</sup> concerning the nature of the state  $\rho_k \Phi_0$ . (Such observations led to more suitable variational choices.) Also, even without these observations, we may look at the integral equation  $[\omega_l^\infty(k)]^2 = [\omega_0(k)/S(k)]^2$  itself to see that there can be no system for which it is strictly valid. At high  $k$ , this equation produces an  $|S(k) - 1|$  which falls off as  $1/k^2$ . The resultant  $S(r)$  then is negatively divergent as  $r \rightarrow 0$ . Such difficulties at small  $r$  are not uncommon in calculations for  $S(r)$ . (For example, the pseudopotential results of Lee, Huang, and Yang<sup>12</sup> for the hard-core Bose gas exhibit this small- $r$  divergence.) We can make an *ad hoc* modification by using a cutoff at small  $r$ , but the integral equation is clearly inconsistent without some changes at large  $k$ .

The difficulty has its origin in the term  $4\langle KE \rangle/N \times \omega_0(k)$  in Eq. (2.6). The general inequality (2.8) can be rewritten

$$[\omega_l^\infty(k)]^2 - f(k) = [\omega_0(k)/S(k)]^2$$

where  $f(k) \geq 0$  for all  $k$ . (2.14)

If we seek to use an expression like this as an integral equation for  $S(k)$ , the quantity  $f(k)$  must have, as its leading term at large  $k$ , the value  $4\langle KE \rangle/N \omega_0(k)$ . The kinetic-energy term is then eliminated from the equation at high  $k$ , and a solution for which  $S(r)$  is convergent at the origin is possible. We furthermore see that the choice  $f = 0$  will not give a correct result for the noninteracting case, whereas the choice  $f = 4\langle KE \rangle/N \omega_0(k)$  for all  $k$  gives the correct result  $S(k) = 1$  when the potential is zero.

We have observed that the integral equation

$$[\omega_l^\infty(k)]^2 - 4\langle KE \rangle/N \omega_0(k) = [\omega_0(k)/S(k)]^2$$

gives  $S(k) = 1$  for the zero-potential case. However, if this were *all* we knew about the free gas, we would still not have an excitation energy. Again, just as in the Feynman theory for  $\text{He}^4$ , we need a model form for  $\chi_0$  in order to obtain both the excitation energy and the quantity  $S(k)$ . To illustrate this point, let us use a "model" form for the free-particle classical gas

$$\chi_0^{\text{FP}}(k, \omega) = F(k) \{ \exp\{-[\gamma(k)/4][\omega - \omega_{\text{ex}}(k)]^2\} - \exp\{-[\gamma(k)/4][\omega + \omega_{\text{ex}}(k)]^2\} \}. \quad (2.15)$$

This is a more complicated model than the  $\delta$  function associated with the Feynman theory, since it contains a width (it also happens to be the exact form for this trivial classical free-particle problem). Having chosen (2.15) as a model, we see that

$$F(k) = \rho [\omega_0(k)/\omega_{\text{ex}}(k)] [\pi \gamma(k)]^{1/2}$$

results from the sum rule (2.4). The sum rule

(2.5) then gives

$$\omega_{\text{ex}}^2(k) - [6/\gamma(k)] = \omega_0^2(k) + 4[\langle KE \rangle/N] \omega_0(k) \\ \{ = [\omega_l^\infty(k)]^2 \text{ for free particles} \}, \quad (2.16)$$

while the relation (2.3) yields

$$S(k) = \frac{\omega_0(k)}{\omega_{\text{ex}}(k)} \left[ 1 + \frac{1}{2} \left( \frac{\gamma(k)}{\pi} \right)^{1/2} \right. \\ \times \int_{-\infty}^{\infty} d\omega \frac{\exp\{-[\gamma(k)/4][\omega - \omega_{\text{ex}}(k)]^2\}}{e^{\beta\omega} - 1} \\ \left. \times [1 - \exp\{\beta - \gamma(k)\omega_{\text{ex}}(k)\}] \right]. \quad (2.17)$$

Because of the additional freedom in the "model" (2.15), we now need the *independent* equation

$$[\omega_l^\infty(k)]^2 - 4\langle KE \rangle/N \omega_0(k) = [\omega_0(k)/S(k)]^2$$

or  $\omega_0^2(k) = [\omega_0(k)/S(k)]^2$  to tell us that  $S(k) = 1$ . Knowing that  $S(k) = 1$ , we see that (2.16) and (2.17) yield

$$\omega_{\text{ex}}(k) = \omega_0(k), \quad \gamma(k) = \beta/\omega_0(k) \quad \text{with } \frac{2}{3} \langle KE \rangle/N = 1/\beta.$$

Although this approach may seem like an unnecessarily complicated one for the classical free gas, it is the calculation most analogous to the sum-rule manipulations used to generate the Feynman theory.

We may now conclude that (2.15) is a possible model for some system (i. e., the free gas), whereas the  $\delta$ -function or sharp-resonance model cannot be a consistent possibility for any system. This follows from the fact that the sharp-resonance model forces the  $f(k)$  in Eq. (2.14) to be zero for all  $k$ , whereas  $f(k)$  must behave like  $4\langle KE \rangle/N \omega_0(k)$  at high  $k$ .

We can try to improve the model  $\chi_0$  so as to achieve consistency with (2.14) and a proper  $f$  at high  $k$ . However, it is evident from our discussion of the free-particle gas that we must specify  $f(k)$  *independently* in order to obtain a complete theory for both  $S(k)$  and  $\omega_{\text{ex}}(k)$  whenever the model contains more than two parameters. A specification of  $f(k)$  alone will give  $S(k)$ , but a model for  $\chi_0$  will give a unique  $\omega_{\text{ex}}(k)$  only if that model contains few enough parameters. Instead of attempting to generate a theory complete enough to include a model form for  $\chi_0$ , we may first ask how the independent choice of  $f$  should be made.

Observe that if we take  $f(k) = 4\langle KE \rangle/N \omega_0(k)$  for all  $k$  in the interacting case, the first-order expansion in the potential  $V(k)$  gives

$$\omega_0^2(k) + 2\rho \omega_0(k) V(k) = [\omega_0(k)/S(k)]^2 \\ [\text{lowest order in } V(k)]. \quad (2.18)$$

This result follows from the fact that  $S(q) = 1$  to zeroth order in the last term of (2.6). The solution of (2.18) is  $S(k) = S^{\text{Bog}}(k)$ . Since the Bogoliubov result is known to be correct to first order, we may write

$$[\omega_l^\infty(k)]^2 - 4\frac{\langle KE \rangle}{N} \omega_0(k) + g_2(k) = \left( \frac{\omega_0(k)}{S(k)} \right)^2, \quad (2.19)$$

where  $g_2(k)$  must be higher than first order in the potential and less than order  $k^2$  for large  $k$ . Furthermore, in order to obtain the zero-temperature sound velocity  $c$  from the limit  $S(k) \rightarrow k/2mc$  as  $k \rightarrow 0$  from Eq. (2.19), we must have

$$\lim_{k \rightarrow 0} g_2(k)/k^2 = c^2 - [c_l^\infty]^2 + 2\langle KE \rangle/mN,$$

where  $[c_l^\infty]^2 \equiv \lim_{k \rightarrow 0} [\omega_l^\infty(k)]^2/k^2$ .

Therefore  $g_2(k) \leq O(k^2)$  as  $k \rightarrow 0$ .

On the grounds that the choice  $g_2(k) = 0$  for all  $k$  is the simplest possible modification, consistent with the weak-coupling limit, of the results implicit in the Feynman theory, we will investigate the implications of this choice for real He<sup>4</sup>. We note at the outset that our choice is severely tested by the calculation. For example, even the sound velocity  $c^2 = [c_l^\infty]^2 - 2\langle KE \rangle/mN$  is sensitively dependent on our predicting the high-momentum components of  $S(k)$  correctly, since  $[c_l^\infty]^2$  is given by an integral over the full self-consistent solution to  $S$ .

### III. RESULTS FOR GROUND-STATE He<sup>4</sup>

Our proposed equation for  $S(k)$  [(2.19) with  $g_2 = 0$ ] may now be written, using Eq. (2.6), in the form

$$\begin{aligned} \left( \frac{\omega_0(k)}{S(k)} \right)^2 &= \omega_0^2(k) + 2\rho\omega_0(k)V(k) \\ &+ \frac{1}{m} \int \frac{d^3q}{(2\pi)^3} [V(\vec{k}+\vec{q})[\vec{k} \cdot (\vec{k}+\vec{q})]^2 \\ &- V(q)(\vec{k} \cdot \vec{q})^2][S(q) - 1]. \end{aligned} \quad (3.1)$$

For a solution, we use the simple potential

$$V(r) = E_0(a/r)[e^{-r/a} - \gamma e^{-\beta r/a}], \quad (3.2)$$

with  $E_0 = 8.940 \times 10^5$  K<sup>o</sup>,  $\gamma = 0.2560$ ,  $a = 0.3760$  Å, and  $\beta = 0.8000$ . The constants are chosen to correspond roughly to the traditional Lennard-Jones (12-6) potential<sup>13</sup> by fitting the position and slope at the minimum, the position of the zero on the  $r$  axis, and the value at a point ( $r = 3.60$  Å) corresponding to the interparticle spacing in He<sup>4</sup>. This potential is shown in Fig. 1, together with the 12-6 potential for comparison.

Having made a choice of potential, the only parameter remaining in Eq. (3.1) is the particle density. Furthermore, for our choice of potential, the angular integrals can be done explicitly. The result is a one-dimensional nonlinear integral equation for  $S(k)$ . We have solved this equation with the aid of an IBM 7094 computer, and find the following features of the solution. At sufficiently low density, the solution is indistinguishable from the Bogoliubov result. At "intermediate" densities (still well below those appropriate to He<sup>4</sup>), the quantity  $S_\rho(k)$  continues to remain less than unity for all  $k$ . At densities in the neighborhood of the He<sup>4</sup> density, however, the solution exhibits the oscillatory behavior (with maximum greater than unity) characteristic of the experimentally observed structure. We have calculated  $S_\rho(k)$  for

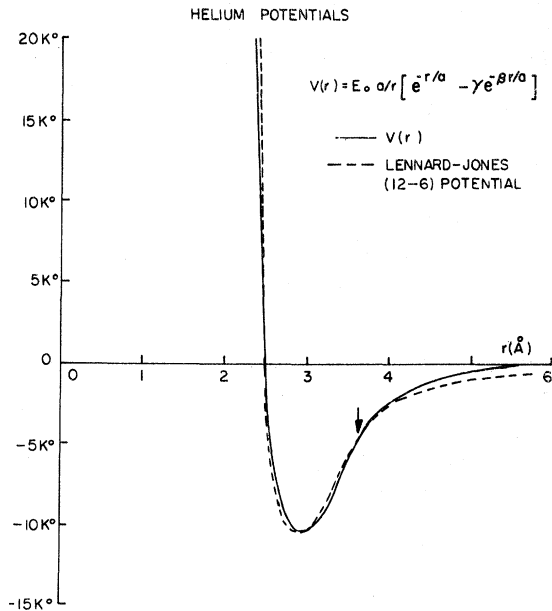


FIG. 1. Comparison between the 12-6 potential and  $V(r)$ .

density values in the appropriate range, and have used these functions to obtain values of  $E(\rho)/N$  by finding a numerical solution of the differential equation (1.6) for densities in this range. Obviously, if our calculated  $E(\rho)/N$  curve did not exhibit a minimum in the chosen density range, we would face an impasse. Fortunately, we find that  $E(\rho)/N$  calculated in this manner does have a minimum at a particular value of  $\rho$  close to the observed helium density. The calculated curve for  $S_\rho(k)$  at this self-consistent-density value is shown in Fig. 2, together with experimental points

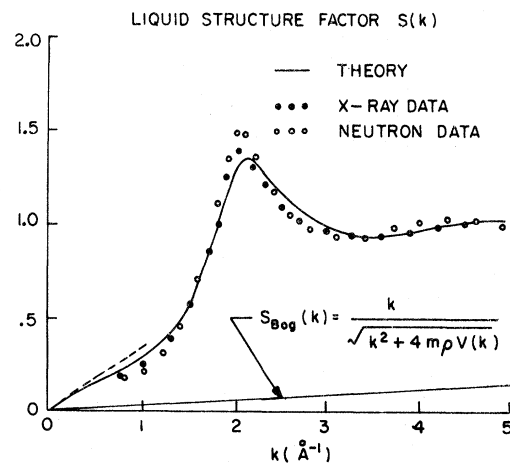


FIG. 2. Comparison of the theoretical ground state  $S_\rho(k)$  at the calculated density with experimental data. The x-ray points are taken from Ref. 14 ( $T = 1.4^\circ$  K) and the neutron points are taken from Ref. 15 ( $T = 1.06^\circ$  K). The dashed line represents a slope taken from the experimental sound velocity. Precise comparison of the calculated slope with the experimental value appears in Table I.

for He<sup>4</sup> taken from the x-ray data of Gordon, Shaw, and Daunt,<sup>14</sup> and from the neutron data of Henshaw.<sup>15</sup> The Bogoliubov solution at the same density for the same potential is also shown in order to emphasize how small the perturbation theory result is for higher densities. The calculated density, energy per particle and sound velocity [taken from the slope of the  $S(k)$  curve] are shown in Table I. The experimental values for these quantities, taken from Atkins' s<sup>16</sup> book, are also shown. We have, in addition, listed the value of the kinetic energy per particle calculated from Eq. (1.2).

One interesting question concerns the behavior of  $S(k)$  at higher densities. The calculation described above requires a knowledge of  $S_\rho(k)$  only very close to the  $E(\rho)/N$  minimum. We could, of course, solve the differential equation for  $E(\rho)/N$  by using the known value at  $\rho=0$  and by computing density integrals of  $S_\rho(k)$  over all densities up to the neighborhood of the  $E(\rho)/N$  minimum. However, we adopted a simpler procedure, involving only the region close to the  $E(\rho)/N$  minimum, in which the boundary condition on the differential equation was supplied by demanding that the sound velocity calculated from the second derivative of the energy be equal to the sound velocity given by the slope of  $S_\rho(k)$  at small  $k$ . [Table I gives the value of this sound velocity, at the  $E(\rho)/N$  minimum, produced by either expression]. However, some calculations of  $S_\rho(k)$  were made at higher densities. As  $\rho$  was increased, the first peak in  $S(k)$  became higher and shifted slightly to smaller  $k$ . The amplitude of the oscillations was also increased. This sort of behavior is to be expected;  $S(k)$  should begin to look more "solid-like" at higher densities. However, the changes do not appear to be pronounced enough to imply that Eq. (3.1) is adequate for the solid. This question remains to be investigated further, but the fact that Fig. 2 shows the first peak in the theoretical  $S(k)$  to be slightly too small at the liquid density might suggest that the approximation (3.1) is not sufficiently "solid-like" and that an increase in  $\rho$  will further emphasize the discrepancy. Although we suspect that our approximation becomes less reliable for higher densities, differences between experimental and theoretical

TABLE I. Comparison between calculated macroscopic parameters and experimental values. The experimental numbers are taken from Ref. 16.

	Theory	Experiment	Unit
$\frac{\langle E \rangle}{N}$	-8.11	-7.20	K°
$m\rho$	0.152	0.145	gms/cm <sup>3</sup>
$C$	248	237	m/sec.
$\frac{\langle KE \rangle}{N}$	10.2		K°

values at liquid densities are too small to supply any obvious clues concerning the errors involved in Eq. (3.1). Indeed, since we have made no attempt at a "best" potential choice, the agreement with experimental values seems extremely good, both for the  $S(k)$  curve itself and for the macroscopic parameters  $E/N$ ,  $\rho$ , and  $c$ . We expect a somewhat large binding energy, density, and sound velocity for this "soft" potential, and this expectation is confirmed by the results in Table I.

To summarize, we note the following: Our proposed equation for  $S_\rho(k)$  [Eq. (3.1)] gives familiar perturbation theory results in the weak-coupling low-density limit, and is capable of extension to interactions and densities appropriate to liquid He<sup>4</sup>. In obtaining this equation, we have lost any knowledge of the density fluctuation spectrum. By this we mean simply that there are many parametrizations of  $\chi_0$  consistent with (2.3)–(2.5). A knowledge of approximate equalities connecting various moments of  $\chi_0$  gives us little information about the shape or resonant position of  $\chi_0$  itself without further drastic assumptions. Therefore we have stressed the calculation of  $S_\rho(k)$  and the macroscopic thermodynamic quantities, and have not attempted to introduce additional assumptions needed for a complete discussion of  $\chi_0$ . In Eq. (3.1) for  $S(k)$ , the density appears as a parameter. The self-consistent density is obtained for He<sup>4</sup> by finding the minimum of  $E(\rho)/N$  as calculated from  $S_\rho(k)$ . Results for He<sup>4</sup> are shown in Fig. 2 and Table I.

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<sup>1</sup> Among the early variational calculations were those of Feynman (Ref. 8) and Feynman and Cohen (Ref. 9). Later calculations by W. L. McMillan [Phys. Rev. 138, A442 (1965)] used a trial state  $\prod_{i < j} f(\mathbf{r}_i - \mathbf{r}_j)$  and determined the relevant integrals numerically by a Monte Carlo technique for 32 and 108 particles. This gave a somewhat low binding energy, with reasonably good results for the structure factor. Another variational approach, for the infinite system, has been discussed by Feenberg, Woo, Wu, and Massey in a series of papers. Results for He<sup>4</sup> using this method are described by

W. E. Massey, Phys. Rev. 151, 153 (1966). In this approach, a seven-constant parametrization of  $S(\mathbf{r})$  was used to calculate and minimize the energy for a trial state whose form is related to  $S(\mathbf{r})$  through the Kirkwood superposition approximation. The 12-6 potential is adjusted slightly to give the correct ground-state energy and density, and the density variation of pressure, energy, and sound velocity are determined. Results compare favorably with experimental values.

<sup>2</sup> We will use units  $\hbar=1$ . The relations given in (2.2)–(2.6) have all been discussed in the literature. A compilation of such relations, for the complete list of ten independent spectral functions formed from the five densities and currents appearing in the microscopic

conservation laws, can be found in a paper by R. D. Puff and N. S. Gillis, *Ann. Phys. (N. Y.)* **46**, 1 (1968).

<sup>3</sup>This extension is called Hölder's inequality. See H. L. Royden, *Real Analysis* (The MacMillan Co., New York, 1963).

<sup>4</sup>N. N. Bogoliubov, *J. Phys. USSR* **11**, 23 (1947).

<sup>5</sup>S. T. Beliaev, *Zh. Eksperim. i Teor. Fiz.* **34**, 417 (1958) [English transl.: *Soviet Phys. JETP* **7**, 289 (1968)].

<sup>6</sup>N. M. Hugenholtz and D. Pines, *Phys. Rev.* **116**, 489 (1959).

<sup>7</sup>For a comparison of the various perturbative calculations, together with a discussion of the distinction between the spectrum of  $\chi_0$  and the single-particle spectrum in these calculations, see P. C. Hohenberg and P. C. Martin, *Ann. Phys. (N. Y.)* **34**, 291 (1965).

<sup>8</sup>R. P. Feynman, *Phys. Rev.* **94**, 262 (1954).

<sup>9</sup>R. P. Feynman and Michael Cohen, *Phys. Rev.* **102**, 1189 (1956).

<sup>10</sup>See, for example, the discussion in D. Pines, *The Many-Body Problem* (W. A. Benjamin, Inc., New York, 1961).

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<sup>12</sup>T. D. Lee, Kerson Huang, and C. N. Yang, *Phys. Rev.* **106**, 1135 (1957).

<sup>13</sup>J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory Of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954), Appendix I.

<sup>14</sup>W. Gordon, C. Shaw, and J. Daunt, *J. Phys. Chem. Solids* **5**, 117 (1958).

<sup>15</sup>D. G. Henshaw, *Phys. Rev.* **119**, 9 (1960).

<sup>16</sup>K. R. Atkins, *Liquid Helium* (Cambridge University Press, Cambridge, 1959).

## Spin Waves in He<sup>3</sup> in the Paramagnon Model\*

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We have estimated the effect on the long-wavelength spin-wave spectrum of the large spin fluctuations in a nearly ferromagnetic Fermi liquid, in order to investigate the possibility of observing spin waves in liquid He<sup>3</sup>. The study is based on a general formula, which we derive from the spin conservation law, for the long-wavelength spin-wave dispersion curve and the paramagnon model. With the parameters of the model fixed by the He<sup>3</sup> susceptibility and the spin-diffusion coefficient data, the width of the spin-wave line and its shift from the Larmor frequency are estimated as functions of the temperature, the pressure, and the wavelength of the spin wave. The spin diffusion coefficient is obtained from the large damping limit of the dispersion formula.

### I. INTRODUCTION

The rapid advances of experimental low-temperature physics leads us to expect that the spin wave, as well as many other phenomena, in liquid He<sup>3</sup> will be observable in the not too distant future. Some theoretical estimate on the spin-wave spectrum of liquid He<sup>3</sup> would therefore be of interest, and it is the purpose of this paper to make such an estimate.

Theoretical investigations of the spin waves in liquid He<sup>3</sup> and in some paramagnetic metals have been largely based on the kinetic equations in the Landau theory.<sup>1</sup> Recently it has been shown that, for He<sup>3</sup>, some of the features of which the Landau theory does not easily give an adequate description can be qualitatively understood, in terms of the paramagnon model,<sup>2</sup> as the consequences of the large spin fluctuations implied by the fact that the He<sup>3</sup> is nearly ferromagnetic. One thus expects that the large spin fluctuations would have important effects on the spin-wave spectrum, and the paramagnon model should provide a reasonable qualitative description. We are aware of the fact

that, unlike the Landau theory, which is a self-consistent phenomenological theory within its domain of application, the paramagnon model is very crude and almost certainly not rigorously self-consistent in its present form.<sup>3</sup> However, because of its simplicity and qualitative success so far, we shall base our investigation on the paramagnon model in spite of its crudeness and ambiguities, which will be discussed in some detail.

Much of our discussion will center around the width of the spin-wave line, to which the previous investigations<sup>1</sup> paid little attention. The physical picture is clarified and the mathematical complication reduced considerably by exploiting the fact that the interaction in the model conserves the total spin and is of very short range. A qualitative discussion of the physical processes involved will precede the analysis of diagrams leading to our results.

An important feature of the spin-wave spectrum is that it must be an infinitely sharp line at the Larmor frequency, i. e., the precessing frequency of a free spin, for  $k \rightarrow 0$ , where  $k$  is the wave number of the spin wave, if the interaction conserves