Results on the quasiparticle model for liquid ^{4}He at finite temperatures*

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Within the interacting-quasiparticle model, we find several identities expressing the thermal energy $\langle \mathcal{H} \rangle$ in terms of parameters entering the thermal-neutron scattering function $S(q,\omega)$ and an unknown interaction term. A new form for $S(q,\omega)$ at finite T is found which should be useful in analyzing neutron experiments. The only approximations are that the self-energies $\Sigma_{ij}(q,\omega)$ are independent of ω, and that the density $\rho_{\vec{q}}$ is linear in the boson operators $\alpha_{\vec{q}}^{\dagger}$ and $\alpha_{\vec{q}}$ of the model.

I. INTRODUCTION

Recently, Donnelly and Roberts[1] (DR) have shown that a surprisingly good fit to thermodynamic data in liquid helium can be obtained by assuming that the energies $\mathcal{E}_q$ which appear in the entropy expression

$$\bar{S} = V \sum_{\vec{q}} \left(k_B \ln(1 + \langle n_{\vec{q}} \rangle) + \frac{\mathcal{E}_{\vec{q}} \langle n_{\vec{q}} \rangle}{T} \right)$$

are temperature dependent. Here, $\langle n_{\vec{q}} \rangle = (e^{\mathcal{E}_{\vec{q}}\beta} - 1)^{-1}$ and $\mathcal{E}_{\vec{q}}$ is assumed to vary with temperature in a manner given by the temperature variation of the single quasiparticle peaks in the neutron-scattering function $S(\vec{q},\omega)$. DR have pointed out that their results bear a resemblance to Fermi-liquid theory and follow from simple assumptions concerning the form of the energy and entropy, but a microscopic justification of their procedure is lacking. Here we explore whether the quasiparticle Hamiltonian

$$\mathcal{H} = E_0 + \sum_{\vec{q}} E(\vec{q})\, \alpha_{\vec{q}}^{\dagger} \alpha_{\vec{q}} + \frac{1}{2} \sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3} [g_3(\vec{k}_1,\vec{k}_2,\vec{k}_3) \alpha_{\vec{k}_1}^{\dagger} \alpha_{\vec{k}_2}^{\dagger} \alpha_{\vec{k}_3} + \text{H.c.}]$$
$$+ \sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} \{ g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4) \alpha_{\vec{k}_1}^{\dagger} \alpha_{\vec{k}_2}^{\dagger} \alpha_{\vec{k}_3} \alpha_{\vec{k}_4} + [g_4'(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4) \alpha_{\vec{k}_1}^{\dagger} \alpha_{\vec{k}_2}^{\dagger} \alpha_{\vec{k}_3}^{\dagger} \alpha_{\vec{k}_4} + \text{H.c.}] \} \quad (1)$$

can account for these results. We have discussed this Hamiltonian[2] critically in a previous publication and have emphasized the difficulties associated with using it to account for neutron and light scattering results. Nevertheless, in view of its wide application to problems in liquid helium[3] and the open nature of the problem of accounting for the DR result, we explore the consequences of Eq. (1) for thermodynamics here.

The theoretical determination, starting with the microscopic Hamiltonian, of the coefficients g_3, g_4, and g_4' [Eq. (1)] can be carried out in principle using the procedure described in Ref. 4 by Jackson. Jackson has evaluated g_3 by this means. In the present paper, we are concerned not with evaluating the coefficients, but rather with determining the phenomenological consequences of Eqs. (1) and (4a) below on the algebraic form of $S(\vec{q},\omega)$ and on the connection between $S(\vec{q},\omega)$ and the thermodynamics. We will find in particular that, at finite T, Eqs. (1) and (4a) imply that one cannot simply use the peak energies in $S(\vec{q},\omega)$ in the noninteracting entropy $\bar{S}$ in order to make this connection. Several workers[1] have essentially done this (though with approaches differing in some details).

We note that, if one derives Eq. (1) by use of the procedures described by Jackson[4] or by Bogoliubov and Zubarev (references in Ref. 7) then a perturbation theory in the resulting interaction terms in Eq. (1) should converge much more rapidly than a perturbation theory in the potential in the microscopic Hamiltonian [Eq. (3) below]. This is because the hard core in the He-He potential causes very serious divergence difficulties in the latter approach. For this reason, we believe that exact conclusions based on Eqs. (1) and (4a) (as drawn here) are more reliable [despite possible problems with Eq. (4a)] than approximate conclusions based on approximate treatment of perturbation theory in the He-He potential.

Cohen[5] has taken this same approach in exploring the same questions considered here. The differences between his work and the present study are as follows: (i) terms involving g_3 and g_4' in Eq. (1) are omitted from Cohen's Hamiltonian. There is no reason to expect that the effects of g_3 and g_4' are small compared to the effects of g_4. Jackson[4] has shown that g_3 does have an important qualitative effect on $S(\vec{q}, \omega)$. (ii) In Ref. 5, only the first terms in a series in $e^{-\Delta\beta}$ are studied (Δ is the roton energy). Here we confine our attention to exact results. If we set $g_4'=g_3=0$ and confine attention to the case of weak interactions, then our results agree with those of Ref. 5. Further discussion of the relationship of this work to Ref. 5 appears in the last section.

Though we have not succeeded in accounting for the Donnelly-Roberts results, we have obtained a number of new results following from the Hamiltonian [Eq. (1)] at finite temperature. These results include a new form for $S(\vec{q}, \omega)$ at finite temperature which should be useful to experimentalists analyzing neutron data and several forms of a well-known theorem[6] relating the thermodynamic internal energy $\langle \mathcal{H} \rangle$ to the same response functions which are involved in $S(\vec{q}, \omega)$. Unfortunately, in contrast to the microscopic case, the energy $\langle \mathcal{H} \rangle$ also involves terms which cannot be determined from $S(\vec{q}, \omega)$.

Our preliminary objective is to establish an analog to the formula

$$\langle \mathcal{H}_m \rangle = \sum_{\vec{q}} \int \frac{d\omega}{2\pi} \frac{\omega + q^2/2m}{2} f(\omega) A_m(\vec{q}, \omega) \tag{2}$$

established by many authors[6] for a system with the Hamiltonian

$$\mathcal{H}_m = \int d\vec{r}\, \frac{\nabla\psi^\dagger(\vec{r})\, \nabla\psi(\vec{r})}{2m} + \frac{1}{2}\int d\vec{r} \int d\vec{r}'\, \psi^\dagger(\vec{r})\, \psi^\dagger(\vec{r}')\, V(\vec{r}-\vec{r}')\, \psi(\vec{r}')\, \psi(\vec{r}) \; . \tag{3}$$

In Eq. (2), $f(\omega) = (e^{\beta\omega} - 1)^{-1}$ and $A_m(\vec{q}, \omega)$ is a spectral weight function given by

$$A_m(\vec{q}, \omega) = i[\, G_m(\omega + i\epsilon, \vec{q}) - G_m(\omega - i\epsilon, \vec{q})] \; , \tag{4}$$

in which $G_m(\omega + i\epsilon, \vec{q})$ is the Fourier transform of the retarded single-particle Green's function, and $G_m(\omega - i\epsilon, \vec{q})$ is similarly the Fourier transform of the advanced Green's function:

$$G_m(\omega + i\epsilon, \vec{q}) = \int d\vec{r} \int dt\, e^{i(\omega t - \vec{q}\cdot\vec{r})} G_R^m(t, \vec{r}) \; ,$$

$$G_m(\omega - i\epsilon, \vec{q}) = \int d\vec{r} \int dt\, e^{i(\omega t - \vec{q}\cdot\vec{r})} G_A^m(t, \vec{r})$$

and

$$G_R^m(t, \vec{r}) = -i\Theta(t) \langle [\, \psi(\vec{r}, t), \psi^\dagger(0,0)] \rangle \; ,$$

$$G_A^m(t, \vec{r}) = i\Theta(-t) \langle [\, \psi(\vec{r}, t), \psi^\dagger(0,0)] \rangle \; .$$

$A_m(\vec{q}, \omega)$ is to be thought of as the density of single-particle states with momentum $\vec{q}$.

In principle, the Hamiltonian [Eq. (3)] is valid for liquid helium and the identity [Eq. (2)] applies directly in the absence of Bose condensation. Further, $A_m(\vec{q}, \omega)$ would be expected to have peaks at the same places where the neutron-scattering function has peaks. In liquid helium, however, one does have a Bose condensation. Nevertheless, one can show that the form of the identity [Eq. (2)] will not be changed essentially.[6] On the other hand, when working with the microscopic system, the residues of the poles in the single-particle Green's function are different from the residues of the poles in the density-density response function as discussed, for example, by Woods and Cowley.[7] These residues, or the term involving the chemical potential which must be added[6] to Eq. (2) in the case of a condensed Bose gas, must play a very important role in changing the basic form of $\langle \mathcal{H}_m \rangle$ at low temperatures. One can see this by inserting an appropriate form [e.g., Eq. (31) of this paper] for $A_m(\vec{q}, \omega)$ into Eq. (2) for $\langle \mathcal{H}_m \rangle$. The poles of $A_m(\vec{q}, \omega)$ will necessarily be near those of the neutron-scattering cross section, so that if the residues or chemical-potential term mentioned above did not play a major role in determining $\langle \mathcal{H}_m \rangle$, then $\langle \mathcal{H}_m \rangle$ would be in error by about a factor of 2 at low temperatures. As a consequence of these difficulties, we proceed from the more phenomenological Hamiltonian (1) together with the relation

$$\rho_{\vec{q}} = [\, \xi(\vec{q})]^{1/2} (\alpha_{\vec{q}} + \alpha^\dagger_{-\vec{q}}) \; , \tag{4a}$$

where $\rho_{\vec{q}}$ is the density operator

$$\rho_{\vec{q}} = \sum_{i=1}^{N} e^{-i\vec{q}\cdot\vec{r}_i(t)} \; .$$

In this framework, $S(\vec{q}, \omega)$, the neutron-scattering function, is directly related to the single-particle Green's functions and the problems of unknown residues do not arise. On the other hand, the terms of order g_3 and g_4' mean that the identity [Eq. (2)] will take a different form for the Hamiltonian (1). In the following, we first find two different expressions analogous to Eq. (2) but following from the Hamiltonian (1). Secondly, we investigate the relationship of the result to the neutron data and to the thermodynamics.

II. QUASIPARTICLE FORMS OF THE IDENTITY DETERMINING $\langle\mathcal{H}\rangle$

We follow the derivation[6] of Kadanoff and Baym, forming the equations of motion of $\alpha_{\vec{q}}$ and $\alpha_{\vec{q}}^\dagger$ in order to relate $\langle\mathcal{H}\rangle$ to the spectral weight associated with a Green's function involving $\alpha_{\vec{q}}$ and $\alpha_{\vec{q}}^\dagger$. We have, using

$$i\frac{\partial X}{\partial t}=[X,\mathcal{H}]$$

that

$$i\frac{\partial\alpha_{\vec{q}}}{\partial t}=E(\vec{q})\alpha_{\vec{q}}+\sum_{\vec{k}_1,\vec{k}_2}\{\tfrac{1}{2}[g_3(\vec{q},\vec{k}_1,\vec{k}_2)+g_3(\vec{k}_1,\vec{q},\vec{k}_2)]\alpha_{\vec{k}_1}^\dagger\alpha_{\vec{k}_2}+g_3^*(\vec{k}_1,\vec{k}_2,\vec{q})\alpha_{\vec{k}_2}\alpha_{\vec{k}_1}\}$$
$$+\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3}[g_4(\vec{q},\vec{k}_1,\vec{k}_2,\vec{k}_3)+g_4(\vec{k}_1,\vec{q},\vec{k}_2,\vec{k}_3)]\alpha_{\vec{k}_1}^\dagger\alpha_{\vec{k}_2}\alpha_{\vec{k}_3}$$
$$+\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3}[3g_4'(\vec{q},\vec{k}_1,\vec{k}_2,\vec{k}_3)\alpha_{\vec{k}_1}^\dagger\alpha_{\vec{k}_2}^\dagger\alpha_{\vec{k}_3}+g_4'(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{q})\alpha_{\vec{k}_1}\alpha_{\vec{k}_2}\alpha_{\vec{k}_3}]\;; \tag{5}$$

together with the Hermitian conjugate of this equation. We use these two equations to form an equation for the quantity

$$\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}\right)\sum_{\vec{q}}{}'\,\alpha_{\vec{q}}^\dagger(t')\,\alpha_{\vec{q}}(t)\;.$$

We use the facts, following from Eq. (1), that

$$g_3(\vec{k}_1,\vec{k}_2,\vec{k}_3)=g_3(\vec{k}_2,\vec{k}_1,\vec{k}_3),\quad g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)=g_4(\vec{k}_2,\vec{k}_1,\vec{k}_3,\vec{k}_4)\;.$$

The resultant equation is

$$\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}\right)\sum_{\vec{q}}{}'\,\alpha_{\vec{q}}^\dagger(t')\,\alpha_{\vec{q}}(t)$$
$$=2\sum_{\vec{q}}{}'E(\vec{q})\,\alpha_{\vec{q}}^\dagger(t')\,\alpha_{\vec{q}}(t)+\frac{3}{2}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3}\{g_3(\vec{k}_1,\vec{k}_2,\vec{k}_3)[\tfrac{2}{3}\alpha_{\vec{k}_1}^\dagger(t')\,\alpha_{\vec{k}_2}^\dagger(t)\,\alpha_{\vec{k}_3}(t)+\tfrac{1}{3}\alpha_{\vec{k}_1}^\dagger(t')\,\alpha_{\vec{k}_2}^\dagger(t')\,\alpha_{\vec{k}_3}(t)]$$
$$+g_3^*(\vec{k}_1,\vec{k}_2,\vec{k}_3)[\tfrac{2}{3}\alpha_{\vec{k}_3}^\dagger(t')\,\alpha_{\vec{k}_2}(t')\,\alpha_{\vec{k}_1}(t)+\tfrac{1}{3}\alpha_{\vec{k}_3}^\dagger(t')\,\alpha_{\vec{k}_2}(t)\,\alpha_{\vec{k}_1}(t)]\}$$
$$+4\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)[\tfrac{1}{2}\alpha_{\vec{k}_1}^\dagger(t')\,\alpha_{\vec{k}_2}^\dagger(t')\,\alpha_{\vec{k}_3}(t')\,\alpha_{\vec{k}_4}(t)+\tfrac{1}{2}\alpha_{\vec{k}_1}^\dagger(t')\,\alpha_{\vec{k}_2}^\dagger(t)\,\alpha_{\vec{k}_3}(t)\,\alpha_{\vec{k}_4}(t)]$$
$$+\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}[3g_4'(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\alpha_{\vec{k}_1}^\dagger(t')\,\alpha_{\vec{k}_2}^\dagger(t)\,\alpha_{\vec{k}_3}^\dagger(t)\,\alpha_{\vec{k}_4}(t)+g_4'^*(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\,\alpha_{\vec{k}_4}^\dagger(t')\,\alpha_{\vec{k}_1}(t)\,\alpha_{\vec{k}_2}(t)\,\alpha_{\vec{k}_3}(t)$$
$$+3g_4'^*(\vec{k}_4,\vec{k}_1,\vec{k}_2,\vec{k}_3)\,\alpha_{\vec{k}_3}^\dagger(t')\,\alpha_{\vec{k}_2}(t')\,\alpha_{\vec{k}_1}(t')\,\alpha_{\vec{k}_4}(t)+g_4'(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\,\alpha_{\vec{k}_3}^\dagger(t')\,\alpha_{\vec{k}_2}^\dagger(t')\,\alpha_{\vec{k}_1}^\dagger(t')\,\alpha_{\vec{k}_4}(t)]\;.$$

Taking a thermal average of this and setting $t=t'$, we have

$$\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}\right)\sum_{\vec{q}}\langle\alpha_{\vec{q}}^\dagger(t')\,\alpha_{\vec{q}}(t)\rangle\Big|_{t=t'}$$
$$=3\langle\mathcal{H}\rangle-\sum_{\vec{q}}E(\vec{q})\langle\alpha_{\vec{q}}^\dagger(t')\,\alpha_{\vec{q}}(t)\rangle|_{t=t'}$$
$$+\sum_{\vec{k}_1\vec{k}_2\vec{k}_3\vec{k}_4}\{g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha_{\vec{k}_1}^\dagger(t')\,\alpha_{\vec{k}_2}^\dagger(t')\,\alpha_{\vec{k}_3}(t')\,\alpha_{\vec{k}_4}(t)\rangle|_{t=t'}+[g_4'^*(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha_{\vec{k}_4}^\dagger\alpha_{\vec{k}_1}\alpha_{\vec{k}_2}\alpha_{\vec{k}_3}\rangle+\text{H.c.}]\}\;. \tag{6}$$

Alternatively, this can be written

$$\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}\right)\sum_{\vec{q}}\langle \alpha_{\vec{q}}^{\dagger}(t')\,\alpha_{\vec{q}}(t)\rangle\Big|_{t=t'}$$

$$=4\langle\mathcal{H}\rangle-2\sum_{\vec{q}}E(\vec{q})\langle\alpha_{\vec{q}}^{\dagger}\alpha_{\vec{q}}\rangle-\frac{1}{2}\sum_{\vec{k}_1\vec{k}_2\vec{k}_3}{}^{\prime}\,[g_3(\vec{k}_1,\vec{k}_2,\vec{k}_3)\langle\alpha_{\vec{k}_1}^{\dagger}\,\alpha_{\vec{k}_2}^{\dagger}\,\alpha_{\vec{k}_3}\rangle+g_3^{*}(\vec{k}_1,\vec{k}_2,\vec{k}_3)\langle\alpha_{\vec{k}_3}^{\dagger}\,\alpha_{\vec{k}_2}\,\alpha_{\vec{k}_1}\rangle]\ . \tag{7}$$

The two expressions [Eqs. (6) and (7)] give different (though equivalent) formal results for the thermal energy $\langle\mathcal{H}\rangle$. From Eq. (6)

$$\langle\mathcal{H}\rangle=\sum_{\vec{q}}\int\frac{2\omega+E(\vec{q})}{3}f(\omega)\,A(\vec{q},\omega)\,\frac{d\omega}{2\pi}-\frac{1}{3}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}\{g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha_{\vec{k}_1}^{\dagger}\,\alpha_{\vec{k}_2}^{\dagger}\,\alpha_{\vec{k}_3}\,\alpha_{\vec{k}_4}\rangle$$
$$+[g_4^{\prime *}(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\,\langle\alpha_{\vec{k}_4}^{\dagger}\,\alpha_{\vec{k}_1}\,\alpha_{\vec{k}_2}\,\alpha_{\vec{k}_3}\rangle+\text{H.c.}]\}\ , \tag{8}$$

while from Eq. (7)

$$\langle\mathcal{H}\rangle=\sum_{\vec{q}}\int\frac{\omega+E(\vec{q})}{2}f(\omega)A(\vec{q},\omega)\,\frac{d\omega}{2\pi}+\frac{1}{8}\sum_{k_1k_2k_3}[g_3(\vec{k}_1,\vec{k}_2,\vec{k}_3)\langle\alpha_{\vec{k}_1}^{\dagger}\,\alpha_{\vec{k}_2}^{\dagger}\,\alpha_{\vec{k}_3}\rangle+\text{H.c.}]\ . \tag{9}$$

Here $A(\vec{q},\omega)$ is defined in a manner analogous to Eq. (4):

$$A(\vec{q},\omega)=i[G_{11}(\omega+i\epsilon,\vec{q})-G_{11}(\omega-i\epsilon,\vec{q})]\ , \tag{10}$$

where

$$\lim_{\epsilon\to 0}G_{11}(\omega+i\epsilon,\vec{q})=\int_{-\infty}^{\infty}dt\,e^{i\omega t}G_r(t,\vec{q})\ ,$$
$$\lim_{\epsilon\to 0}G_{11}(\omega-i\epsilon,\vec{q})=\int_{-\infty}^{+\infty}dt\,e^{i\omega t}G_a(t,\vec{q})\ , \tag{11}$$

$$G_{r,a}(t,\vec{q})=\mp i\Theta(\pm t)\langle[\alpha_{\vec{q}}(t),\alpha_{\vec{q}}^{\dagger}(0)]\rangle=\langle\langle\alpha_{\vec{q}}(t);\alpha_{\vec{q}}^{\dagger}(0)\rangle\rangle_{r,a}\ , \tag{12}$$

where the last expression in Eq. (12) uses the notation of Zubarev.[8] In order to apply Eqs. (8) and (9) to thermodynamics, we need to establish restrictions on $E(\vec{q})$. We get these, together with some other constraints, by requiring that this model satisfy sum rules on $S(\vec{q},\omega)$.

Another form of Eq. (8) can be derived by using the equation for

$$\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}\right)\sum_{\vec{q}}\alpha_{\vec{q}}(t)\,\alpha_{\vec{q}}^{\dagger}(t')$$

formed from Eq. (5) and its Hermitian conjugate. Adding this to the equation for $(i\partial/\partial t-i\partial/\partial t')\sum_{\vec{q}}\alpha_{\vec{q}}^{\dagger}(t')\alpha_{\vec{q}}(t)$ and making manipulations similar to the ones just described, we find

$$\langle\mathcal{H}\rangle=\sum_{\vec{q}}\int\frac{2\omega}{3}f(\omega)\frac{A(\vec{q},\omega)-A'(\vec{q},\omega)}{2}\,\frac{d\omega}{2\pi}+\sum_{\vec{q}}\frac{E(\vec{q})}{3}f(\omega)\frac{A(\vec{q},\omega)+A'(\vec{q},\omega)}{2}\,\frac{d\omega}{2\pi}$$
$$-\frac{1}{3}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}\{g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha_{\vec{k}_1}^{\dagger}\,\alpha_{\vec{k}_2}^{\dagger}\,\alpha_{\vec{k}_3}\,\alpha_{\vec{k}_4}\rangle+[g_4^{\prime *}(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha_{\vec{k}_4}^{\dagger}\,\alpha_{\vec{k}_1}\,\alpha_{\vec{k}_2}\,\alpha_{\vec{k}_3}\rangle+\text{H.c.}]\}$$
$$-\frac{2}{3}\sum_{\vec{k}_1,\vec{k}_2}g_4(\vec{k}_1,\vec{k}_2,\vec{k}_1,\vec{k}_2)\langle\alpha_{\vec{k}_2}^{\dagger}\,\alpha_{\vec{k}_2}\rangle-\sum_{\vec{k}_1,\vec{k}_2}[g_4^{\prime}(\vec{k}_1,\vec{k}_2,-\vec{k}_2,\vec{k}_1)\langle\alpha_{\vec{k}_2}^{\dagger}\,\alpha_{-\vec{k}_2}^{\dagger}\rangle+\text{H.c.}]\ . \tag{12a}$$

Here an infinite, temperature-independent part of the form $\frac{1}{2}\sum_{\vec{q}}E(\vec{q})$ has been dropped. $A'(\vec{q},\omega)$ in Eq. (12a) is defined by

$$A'(\vec{q},\omega)=i[G_{22}(\omega+i\epsilon,\vec{q})-G_{22}(\omega-i\epsilon,\vec{q})]\ , \tag{12b}$$

where

$$G_{22}(z,\vec{q})=\langle\langle\alpha_{\vec{q}}^{\dagger};\alpha_{\vec{q}}\rangle\rangle(z)\ .$$

Although Eq. (12a) looks more complicated than Eq. (8), it might be somewhat easier to use in some cases because the sums and differences in the first two lines of Eq. (12a) have a somewhat simpler form than the individual terms $A(\vec{q},\omega)$ and $A'(\vec{q},\omega)$. $\langle \alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_2}\rangle$ in Eq. (12a) is easily related to $A(\vec{k}_2,\omega)$:

$$\langle \alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_2}\rangle = \int \frac{d\omega}{2\pi} f(\omega) A(\vec{k}_2,\omega) ,$$

while $\langle \alpha_{\vec{k}_1}\alpha_{-\vec{k}_1}\rangle$ is related to the quantity $S(\vec{q},\omega)$ which is measured in neutron scattering. This relation is established in Secs. III and V.

The identity [Eq. (21)] derived in Sec. III can be used to write other forms of the unknown g_4 and g_4' terms in Eqs. (8) and (12a). One such form is presented in the Appendix for the case $g_4'=0$.

III. SUM-RULE RESTRICTIONS ON THE QUASIPARTICLE THEORY AT FINITE T

We get an expression for $E(\vec{q})$ by requiring that

$$\int_{-\infty}^{+\infty} \omega S(\vec{q},\omega)\, d\omega = \frac{q^2}{2m} . \tag{13}$$

Using the definition

$$S(\vec{q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\omega t}\langle \rho_{-\vec{q}}(t)\rho_{\vec{q}}\rangle\, dt . \tag{14}$$

The analysis commonly used to prove Eq. (13) shows that

$$\int_{-\infty}^{+\infty} \omega S(\vec{q},\omega)\, d\omega = \frac{\langle [\rho_{-\vec{q}},[\rho_{\vec{q}},\mathcal{H}]]\rangle}{2} . \tag{15}$$

We require, combining Eqs. (13), (15), and

$$\rho_{\vec{q}} = [\xi(\vec{q})]^{1/2}(\alpha_{\vec{q}} + \alpha^\dagger_{-\vec{q}}) \tag{16}$$

that

$$\frac{q^2}{2m} = \frac{\xi(\vec{q})\langle [(\alpha_{\vec{q}}+\alpha^\dagger_{-\vec{q}}),[(\alpha_{\vec{q}}+\alpha^\dagger_{-\vec{q}}),\mathcal{H}]]\rangle}{2} , \tag{17}$$

in which $\mathcal{H}$ is given by Eq. (1). We require, in addition, that $E(\vec{q})$ and $\xi(\vec{q})$ be temperature independent. (Otherwise, $\mathcal{H}$ is not a meaningful Hamiltonian and $\rho_{\vec{q}}$ is not a microscopic operator.) Working out the commutators in Eq. (17)

$$\frac{q^2}{2m} = \xi(\vec{q})\Big(E(\vec{q}) + \sum_{\vec{k}} \{\{-2[g_4(-\vec{q},\vec{k},-\vec{q},\vec{k}) + g_4(\vec{q},\vec{k},\vec{q},\vec{k})] + 3[g_4'(-\vec{q},\vec{q},\vec{k},\vec{k}) + g_4'^*(\vec{q},-\vec{q},\vec{k},\vec{k})]\}\langle n_{\vec{k}}\rangle$$
$$+\{[g_4(\vec{q},-\vec{q},\vec{k},-\vec{k}) - 3g_4'(-\vec{q},\vec{k},-\vec{k},-\vec{q})]\langle \alpha^\dagger_{\vec{k}}\alpha^\dagger_{-\vec{k}}\rangle + \text{H.c.}\}\}\Big) , \tag{18}$$

where $\langle n_{\vec{k}}\rangle = \langle \alpha^\dagger_{\vec{k}}\alpha_{\vec{k}}\rangle$. Equivalently,

$$E(\vec{q}) = \frac{q^2}{2m\xi(\vec{q})} + \sum_{\vec{k}} (\{2[g_4(-\vec{q},\vec{k},-\vec{q},\vec{k}) + g_4(\vec{q},\vec{k},\vec{q},\vec{k})] - 3[g_4'(-\vec{q},\vec{q},\vec{k},\vec{k}) + g_4'^*(\vec{q},-\vec{q},\vec{k},\vec{k})]\}\langle n_{\vec{k}}\rangle$$
$$-\{[g_4(\vec{q},-\vec{q},\vec{k},-\vec{k}) - 3g_4'(-\vec{q},\vec{k},-\vec{k},-\vec{q})]\langle \alpha^\dagger_{\vec{k}}\alpha^\dagger_{-\vec{k}}\rangle + \text{H.c.}\}) . \tag{19}$$

In deriving Eq. (18), we have used the fact that $\langle n|\alpha_{\vec{k}}|n\rangle = \langle n|\alpha^\dagger_{\vec{k}}|n\rangle = 0$ for any eigenstate $|n\rangle$ of the quasiparticle Hamiltonian if $k\neq 0$ (as a consequence of momentum conservation) in order to eliminate terms depending on g_3. At $T=0$, the relation $\alpha_{\vec{k}}|g\rangle = 0$ for the ground state means that

$$E(\vec{q}) = q^2/2m\xi(\vec{q}) .$$

But $E(\vec{q})$ must be independent of T and $\xi(\vec{q})$ is independent of T. Therefore, the last term in Eq. (19) must be zero for all temperatures. Furthermore, we have previously shown, using $\alpha_{\vec{q}}|g\rangle = 0$ for the ground state $|g\rangle$, that $\xi(\vec{q}) = S(\vec{q},T=0)$. Therefore, we have in summary that

$$E(\vec{q}) = q^2/2mS(\vec{q},T=0) \equiv \omega_F(\vec{q}) \tag{20}$$

and

$$\sum_{\vec{k}} \{2[g_4(-\vec{q},\vec{k},-\vec{q},\vec{k}) + g_4(\vec{q},\vec{k},\vec{q},\vec{k})]$$
$$- 3[g_4'(-\vec{q},\vec{q},\vec{k},\vec{k}) + g_4'^*(\vec{q},-\vec{q},\vec{k},\vec{k})]\}\langle n_{\vec{k}}\rangle$$
$$= \sum_{\vec{k}} \{[g_4(\vec{q},-\vec{q},\vec{k},-\vec{k})$$
$$- 3g_4'(-\vec{q},\vec{k},-\vec{k},-\vec{q})]\langle \alpha^\dagger_{\vec{k}}\alpha_{-\vec{k}}\rangle + \text{H.c.}\} , \tag{21}$$

$\omega_F(\vec{q})$ is the (zero-temperature) Feynman spectrum.

To further establish the meaning of Eqs. (8) and (9), we next consider the relationship of the neutron-scattering function $S(\vec{q},\omega)$ to the function $A(\vec{q},\omega)$ appearing in Eqs. (8) and (9).

IV. DYNAMICAL STRUCTURE FACTOR $S(\vec{q},\omega)$ IN THE QUASIPARTICLE MODEL AT FINITE T

Using the fundamental assumption

$$\rho_{\vec{q}}=[\xi(\vec{q})]^{1/2}(\alpha_{\vec{q}}+\alpha^{\dagger}_{-\vec{q}}) ,$$

we have

$$S(\vec{q},\omega)=\frac{1}{2\pi}\int e^{i\omega t}\langle\rho_{\vec{q}}(t)\rho_{-\vec{q}}(0)\rangle dt$$
$$=\frac{\xi(\vec{q})}{2\pi}\int e^{i\omega t}[\langle\alpha_{\vec{q}}(t)\alpha^{\dagger}_{\vec{q}}(0)\rangle+\langle\alpha^{\dagger}_{-\vec{q}}(t)\alpha_{-\vec{q}}(0)\rangle+\langle\alpha_{\vec{q}}(t)\alpha_{-\vec{q}}(0)\rangle+\langle\alpha^{\dagger}_{-\vec{q}}(t)\alpha^{\dagger}_{\vec{q}}(0)\rangle] . \quad (22)$$

At zero temperature, the first term of this is the only one which contributes by virtue of the assumption that $\alpha_{\vec{q}}|g\rangle=0$. On the other hand, at finite temperature the second pair of terms will contribute in a quasiparticle model. We proceed by expressing the correlation functions in Eq. (22) in terms of Green's functions of the quasiparticle operators $\alpha_{\vec{q}}$, $\alpha^{\dagger}_{\vec{q}}$. This is useful in two ways: First, it permits a connection to be made with the thermodynamic expression for $\langle\mathcal{H}\rangle$ derived in Sec. II. Secondly, it permits us to make a connection with the *formalism* of the Dyson-Beliaev perturbation theory developed for use with the microscopic Hamiltonian $\mathcal{H}_m$ of Eq. (3) in the case that a condensate is present.

This formal connection permits some statements to be made about the form of the Green's function. We will use the new form to propose an alternative form for analysis of the neutron data. We use the following identity, proved, for example, by Zubarev[8]

$$\langle B(0)A(t)\rangle=\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{[\langle\langle A;B\rangle\rangle(\omega'+i\epsilon)-\langle\langle A;B\rangle\rangle(\omega'-i\epsilon)]e^{-i\omega' t}}{e^{\omega'\beta}-1}d\omega' , \quad (23)$$

where A and B are operators in the Heisenberg representation and the definition of the Zubarev notation $\langle\langle\ldots;\ldots\rangle\rangle$ has already been given in Eqs. (11) and (12). Applying Eq. (23) to Eq. (22), we have

$$S(\vec{q},\omega)=-[\xi(q)/\pi(e^{-\omega\beta}-1)]\times[\mathrm{Im}G_{11}(-\omega+i\epsilon)+\mathrm{Im}G_{22}(-\omega+i\epsilon)+\mathrm{Im}G_{12}(-\omega+i\epsilon)+\mathrm{Im}G_{21}(-\omega+i\epsilon)] . \quad (24)$$

Here

$$G_{11}(z)=\langle\langle\alpha_{\vec{q}};\alpha^{\dagger}_{\vec{q}}\rangle\rangle(z) ,$$
$$G_{22}(z)=\langle\langle\alpha^{\dagger}_{\vec{q}};\alpha_{\vec{q}}\rangle\rangle(z) ,$$
$$G_{12}(z)=\langle\langle\alpha_{\vec{q}};\alpha_{-\vec{q}}\rangle\rangle(z) ,$$
$$G_{21}(z)=\langle\langle\alpha^{\dagger}_{-\vec{q}};\alpha^{\dagger}_{\vec{q}}\rangle\rangle(z) ,$$

are the analytic continuations of the Fourier transforms of the retarded and advanced Green's functions as discussed by Zubarev.[8]

We now note that the Hamiltonian Eq. (1) is formally identical to the one studied by Hugenholtz and Pines[10] and others[11] as long as one bears in mind the following features.

First, there are no terms in $\mathcal{H}$ of the form $\alpha_{\vec{q}}\alpha_{-\vec{q}}$ or $\alpha^{\dagger}_{\vec{q}}\alpha^{\dagger}_{-\vec{q}}$. Some terms involving products of three and four α's and $\alpha^{\dagger}$'s in the microscopic $\mathcal{H}$ will also not have analogs in the quasiparticle $\mathcal{H}$. This has consequences in that certain terms of the perturbation theory will not appear, but it does not affect the general form of the Dyson equations.

For example, referring to Figure 69 of the book[11] by Abrikosov, Gorkov, and Dzyaloshinski, the first two terms for Σ_{20} in that figure will be zero in this system, but the third term for Σ_{20} as shown in the same figure of Ref. 11 will not be zero in a perturbation theory for the quasiparticle Hamiltonian. The important point is that anomalous contributions to the Green's functions and self-energies will appear in just the same way that they do in the microscopic theory and the *forms* of the Dyson equations will be the same, even though not all the perturbation theory terms contributing in the microscopic case will contribute in the quasiparticle case.

Secondly, we note that as a consequence of the assumption that $\alpha_{\vec{q}}|g\rangle=0$, the anomalous terms in the Dyson equations will vanish at $T=0$ (as they do not in the microscopic theory). This is why a consideration of these terms was not essential in previous explorations of the quasiparticle model, which focused on $T=0$.

Thirdly, the number of quasiparticles is not conserved, so we cannot meaningfully introduce a chemical potential, and μ should be taken equal to zero in applying expressions valid for the microscopic theory to this case. The arguments leading to the Hugenholtz-Pines theorem (as described, for example, in Sec. 25.2 of Ref. 11) fail. On the other hand, we do have the conclusion (p. 221 of Ref. 11) that, as $q\to 0$, and setting $\mu=0$:

$$[\Sigma_{11}(q=0,\ T)]^2=[\Sigma_{02}(q=0,T)]^2 .$$

We have argued that for the quasiparticle case, $\Sigma_{02}(\vec{q}, T=0)=0$, so that $\Sigma_{11}(q=0, T=0)=0$. Here, we cannot choose the sign in the relation $\Sigma_{11}(q=0, T)=\pm\Sigma_{02}(q=0, T)$ on the basis of the arguments used in the microscopic case.

Fourth, one obviously replaces $\hbar^2 q^2/2m$ by $E(\vec{q})$ in this system. It is very easy to write down replacements for the vertices but we will not need them here.

With these remarks, we can write down the following expressions for the Green's functions appearing in Eq. (24):

$$G_{11}(\omega,\vec{q})=\omega_+/[\omega_+\omega_-+(\Sigma_{20})^2], \tag{25a}$$

$$G_{12}(\omega,\vec{q})=-\Sigma_{20}/[\omega_+\omega_-+(\Sigma_{20})^2], \tag{25b}$$

$$G_{22}(\omega,\vec{q})=G_{11}(-\omega,-\vec{q}), \tag{25c}$$

$$G_{21}(\omega,\vec{q})=G_{12}(\omega,\vec{q}), \tag{25d}$$

where

$$\omega_+=\omega+E(\vec{q})+\Sigma_{11}(-\omega,-\vec{q}), \tag{26a}$$

$$\omega_-=\omega-E(\vec{q})-\Sigma_{11}(\omega,\vec{q}). \tag{26b}$$

Here $\Sigma_{20}(\omega,\vec{q})$, $\Sigma_{11}(\omega,\vec{q})$ are the self-energies defined in Ref. 11. We have assumed, following that reference, that

$$\Sigma_{20}(\omega,\vec{q})=\Sigma_{02}(\omega,\vec{q}). \tag{27}$$

We now make use of the restrictions on the self-energies found to follow from time-reversal invariance by Iachello and Rasetti and others[12]:

$$\Sigma_{11}^*(\vec{q},\omega)=\Sigma_{11}(\vec{q},-\omega), \tag{28a}$$

$$\Sigma_{02}^*(\vec{q},\omega)=\Sigma_{20}(\vec{q},-\omega). \tag{28b}$$

We note that Eqs. (27) and (28b) together imply that Σ_{20} is real, a conclusion not drawn by Iachello and Rasetti, but which we will assume. We are then led to the following forms for the self-energies, following Iachello and Rosetti except for the assumption that Σ_{20} is real:

$$\begin{aligned}\Sigma_{11}(\vec{q},\omega)&=\sigma(\vec{q})+i\tau(\vec{q}),\\ \Sigma_{11}(\vec{q},-\omega)&=\sigma(\vec{q})-i\tau(\vec{q}),\\ \Sigma_{02}(\vec{q},\omega)&=\lambda(\vec{q}),\end{aligned} \tag{29}$$

where the functions σ, τ, and λ are real functions of the three vector $\vec{q}$. These equations contain the consequences of the general results [Eqs. (27) and (28)] and also the important assumption that the self-energies can be regarded as functions of $\vec{q}$ only. This assumption is also made in the analysis of the microscopic case by Iachello and Rasetti.[12] One might hope that this would be a more-reasonable assumption in this quasiparticle case where the perturbing part of the Hamiltonian is expected to be smaller relative to the zero-order part than it is in the microscopic case. On the other hand, calculations of the self-energy using the Hamiltonian[2,3] [Eq. (1)] at $T=0$ have shown that the self-energy Σ_{11} does, in fact, have a very important frequency dependence leading to a qualitative explanation of the multiphonon peak in $S(\vec{q},\omega)$. If, however, we confine attention to frequencies well below the frequency at which this multiphonon peak occurs (about $2\Delta\sim 16\,^\circ$K at low temperatures), then we can expect, on the basis of the $T=0$ calculations, that the assumptions embedded in Eq. (29) would be reasonable. Inserting Eq. (29) into Eq. (25), doing some algebra, and putting the result in Eq. (24), we find the following form for $S(\vec{q},\omega)$:

$$S(\vec{q},\omega)=-[\xi(\vec{q})/\pi](e^{-\omega\beta}-1)^{-1}\times\frac{4\tau(E+\sigma+\lambda)\omega}{[\omega^2-(E+\sigma)^2+\lambda^2]^2+4\tau^2\omega^2}. \tag{30}$$

It is not hard to show that this gives the result used by Dietrich *et al.*[1] in analyzing their data if one takes $\lambda\to 0$ and assumes τ small. In using Eq. (30) to analyze data, one can make use of the following facts: $\xi(q)$ is $S(\vec{q})$ (the static structure factor) at $T=0$ as proved in Sec. III. σ and λ are even functions of q, and τ is an odd function of q as proved on general grounds by Iachello and Rosetti. λ will be zero at zero temperature. The $q\to 0$ limits are such that $\tau\to 0$, and $\sigma\to\lambda$ as $q\to 0$. $E(q)$ is the $T=0$ Feynman spectrum, but in view of the fact that it enters Eq. (30) only in the combination $E'(q)=E+\sigma$, one can also fit data by fitting to the single unknown function E'. Then one can't assume; however, that only even powers of q enter a series for E'.

V. CONNECTION OF THERMODYNAMICS AND THE STRUCTURE FACTOR

To make the connection of Eq. (30) with the thermodynamics, we write out the expressions for $\mathrm{Im}G_{11}(\omega+i\epsilon)$ and $\mathrm{Im}G_{22}(\omega+i\epsilon)$, which follow from Eqs. (25)–(30):

$$\mathrm{Im}G_{11}(\omega+i\epsilon)=\frac{\tau(-3\omega^2-2\omega E'+E'^2-\lambda^2)}{(\omega^2-E'^2+\lambda^2)^2+4\tau^2\omega^2}, \tag{31}$$

$$\begin{aligned}\mathrm{Im}G_{22}(\omega+i\epsilon)&=\mathrm{Im}G_{11}(-\omega-i\epsilon)\\ &=-\mathrm{Im}G_{11}(-\omega+i\epsilon)\\ &=\frac{-\tau(-3\omega^2+2\omega E'+E'^2-\lambda^2)}{(\omega^2-E'^2+\lambda^2)^2+4\tau^2\omega^2}.\end{aligned} \tag{32}$$

We note that, from Eq. (10)

$$A(\vec{q},\omega)=-2\mathrm{Im}G_{11}(\omega+i\epsilon). \tag{33}$$

Inserting Eqs. (33) and (31) in Eq. (8), we find

$$\langle\mathcal{H}\rangle=\sum_{\vec{q}}\int\frac{2\omega+E(\vec{q})}{3}f(\omega)\frac{\tau(3\omega^2+2\omega E'+E'^2-\lambda^2)d\omega}{[(\omega^2-E'^2+\lambda^2)^2+4\tau^2\omega^2]2\pi}-\frac{1}{3}\sum_{\vec{k}_1\vec{k}_2\vec{k}_3\vec{k}_4}\{g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle+[g_4'^*(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha^\dagger_{\vec{k}_4}\alpha_{\vec{k}_1}\alpha_{\vec{k}_2}\alpha_{\vec{k}_3}\rangle+\text{H.c.}]\}. \quad (34)$$

A possible procedure for relating the neutron scattering to the thermodynamics would be to fit the functions E', λ, and τ to the neutron data using Eq. (30), and then use them to compute the first term in Eq. (34). We discuss some details of the relation of Eq. (34) to thermodynamics below. We note that, although the peaks in the function to the right of $f(\omega)$ in the first line of Eq. (34) and those in Eq. (30) will be approximately the same frequencies (because the denominators are the same), the numerators in the two expressions are different. We discuss below (but do not resolve) the problem of what to do about the last term in Eq. (34).

We also write the form of the identity [Eq. (12a)] which follows from Eqs. (31)–(33) together with

$$A'(\vec{q},\omega)=-2\text{Im}G_{22}(\omega+i\epsilon,\vec{q})$$

[from Eq. (12b)]. One finds

$$\langle\mathcal{H}\rangle=\frac{2}{3}\sum_{\vec{q}}\int\omega f(\omega)\frac{(6\omega^2-2E'+2\lambda^2)\tau}{(\omega^2-E'^2+\lambda^2)^2+4\tau^2\omega^2}\frac{d\omega}{2\pi}+\frac{1}{3}\sum_{\vec{q}}E(\vec{q})\int f(\omega)\frac{4\omega E'\tau}{(\omega^2-E'^2+\lambda^2)^2+4\tau^2\omega^2}\frac{d\omega}{2\pi}-\frac{2}{3}\sum_{\vec{k}_1,\vec{k}_2}g_4(\vec{k}_1,\vec{k}_2,\vec{k}_1,\vec{k}_2)\int f(\omega)\frac{3\omega^2+2\omega E'-E'^2+\lambda^2)\tau}{(\omega^2-E'^2+\lambda^2)^2+4\tau^2\omega^2}\frac{d\omega}{2\pi}-\frac{1}{3}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle-(g_4'\text{ terms}). \quad (35)$$

The second term of this equation now contains a term which is quite closely related to $S(\vec{q},\omega)$ [compare with Eq. (30)]. The frequency factor in the first term, however, remains quite different.

We next make some remarks on the detailed connection between thermodynamics and the expression we have found for $\langle\mathcal{H}\rangle$. It is of particular interest to discover the form of the entropy implied by the first term in expressions like Eq. (8), because the theory of Donnelly and Roberts is based on the expression for the entropy appropriate to noninteracting bosons:

$$S_{\text{NI}}=\sum_{\vec{q}}\left(\frac{\mathcal{E}_{\vec{q}}\langle n_{\vec{q}}\rangle}{T}+k_B\ln(1+\langle n_{\vec{q}}\rangle)\right). \quad (36)$$

To find the entropy in terms of $\langle\mathcal{H}\rangle$ given by Eqs. (8) and (12a), we start with the thermodynamic expression

$$\left(\frac{\partial E}{\partial T}\right)_V=T\left(\frac{\partial S}{\partial T}\right)_V$$

and integrate giving

$$S=\int_0^T\frac{1}{T}\left(\frac{\partial\langle\mathcal{H}\rangle}{\partial T}\right)_V dT. \quad (37)$$

To clarify the following remarks, we will first derive Eq. (36) from this, using

$$\mathcal{H}_{\text{NI}}=\sum_{\vec{q}}\mathcal{E}_{\vec{q}}n_{\vec{q}},$$

where $\mathcal{E}_{\vec{q}}$ is temperature independent and $n_{\vec{q}}=\alpha^\dagger_{\vec{q}}\alpha_{\vec{q}}$. We have

$$\left(\frac{\partial E_{\text{NI}}}{\partial T}\right)_v=\sum_{\vec{q}}\frac{\mathcal{E}_{\vec{q}}}{k_BT^2}\frac{e^{\mathcal{E}_{\vec{q}}\beta}}{(e^{\mathcal{E}_{\vec{q}}\beta}-1)^2},$$

so that

$$S_{\text{NI}}=\sum_{\vec{q}}\int_0^T\frac{\mathcal{E}^2_{\vec{q}}}{k_BT^3}\frac{e^{\mathcal{E}_{\vec{q}}\beta}}{(e^{\mathcal{E}_{\vec{q}}\beta}-1)^2}dT. \quad (38)$$

Changing the variable to

$$x=\mathcal{E}/k_BT \quad (39)$$

we have, *because* $\mathcal{E}_{\vec{q}}$ *is T independent*:

$$dx=-\mathcal{E}_{\vec{q}}dT/k_BT^2, \quad (40)$$

so that

$$S_{\text{NI}}=\sum_{\vec{q}}k_B\int_{\mathcal{E}_{\vec{q}}\beta}^\infty\frac{xe^x}{(e^x-1)^2}dx=\sum_{\vec{q}}\left(\frac{\mathcal{E}_{\vec{q}}\langle n_{\vec{q}}\rangle}{T}+k_B\ln(1+\langle n_{\vec{q}}\rangle)\right), \quad (41)$$

where the last line is obtained by an integration by parts.

Now we turn to Eq. (8) [similar remarks could be made for Eq. (12a)]. Using Eq. (37), one has

$$S=\int_0^T\sum_{\vec{q}}\int_{-\infty}^{+\infty}\frac{2\omega+E(\vec{q})}{3}\left[\frac{1}{T}\left(\frac{\partial f}{\partial T}\right)_V A+f\frac{1}{T}\left(\frac{\partial A}{\partial T}\right)_V\right]\times\frac{d\omega}{2\pi}dT+(g_4\text{ term}). \quad (42)$$

To simplify the discussion, we suppose that A can be adequately represented by the form

$$A = 2\tau / [(\omega - \mathcal{E})^2 + \tau^2]$$

which is true if $\lambda \to 0$, τ is small compared to $\mathcal{E}$ in our previous expressions, and the temperature T is much less than $\mathcal{E}$ $(\tau \ll T \ll \mathcal{E})$. Then, if $\tau \ll k_B T$, one can write the first term of Eq. (42) as

$$\int_0^T \frac{2\mathcal{E}_{\vec{q}} + E(\vec{q})}{3} \frac{1}{T} \frac{\partial \langle n_{\vec{q}} \rangle}{\partial T} dT , \tag{43}$$

where

$$\langle n_{\vec{q}} \rangle = (e^{\mathcal{E}_{\vec{q}}\beta} - 1)^{-1} . \tag{44}$$

This looks very much like the first line of Eq. (38) in the noninteracting case. The differences are: first, that $\frac{1}{3}[2\mathcal{E}_{\vec{q}} + E(\vec{q})]$ appears instead of $\mathcal{E}_{\vec{q}}$ in the linear term *but not in the argument of* $\langle n_{\vec{q}} \rangle$. One might try to use Eq. (43) for the entropy assuming that $\mathcal{E}_{\vec{q}}$ was given by the peaks in the neutron-scattering function. The result would not be as poor as simply substituting $\frac{1}{3}[2\mathcal{E}_{\vec{q}} + E(\vec{q})]$ for $\mathcal{E}_{\vec{q}}$ in the noninteracting formula, because most of the temperature dependence is in $\langle n_{\vec{q}} \rangle$. We note, however, that Eq. (43) *cannot* be integrated following steps [Eqs. (38)–(41)] to give an entropy of the same form as that found for the noninteracting case, but with a temperature dependent $\mathcal{E}_{\vec{q}}$. This is because the step [Eq. (40)] fails: $\mathcal{E}_{\vec{q}}$ is T dependent so the differential dx contains both $d\mathcal{E}_{\vec{q}}$ and dT. The result can be expressed in terms of $d\mathcal{E}_{\vec{q}}/dT$ but the resulting integral will not give a result like that in Eq. (41). Thus we have not succeeded in finding a form for the thermodynamics which is the same as the Donnelly-Roberts result, though our form for $\langle \mathcal{H} \rangle$ is suggestive of the philosophy of that paper, which was to express the thermodynamics in terms of the single-particle peaks in $S(\vec{q}, \omega)$.

VI. CONCLUSIONS AND DISCUSSION

We have pointed out that within the quasiparticle model at $T \neq 0$ a new functional form arises for $S(\vec{q}, \omega)$ which is not used in the existing fit to experimental data [Eq. (30)]. In an attempt to account for the success[1] of the approach of Donnelly and Roberts to the thermodynamics, we derived theorems analogous to a well-known[6] one relating $\langle \mathcal{H} \rangle$ to the single-particle propagator for the microscopic Hamiltonian. We can relate a part of the resulting expression to the results of neutron-scattering experiments [Eq. (34) and the following discussion]. As we discuss at the end of Sec. V, however, the expression cannot be used to fully account for the success of the Donnelly-Roberts approach though with an appropriate choice of g_4, g_4'; our results will certainly be numerically consistent with those of Ref. 1.

Comparing Eq. (24) with Eqs. (8) and (12a), one sees that the anomalous Green's functions G_{12} and G_{21} enter $S(\vec{q}, \omega)$, but not our expressions for the energy. It is tempting to try to find an expression for $\langle \mathcal{H} \rangle$ which involves these anomalous Green's functions but not the unknown part depending on g_4 in Eqs. (8) and (12a). One can make some steps in this direction by using the identity [Eq. (21)]. This has been done for the case in which $g_4' = 0$ in the Appendix.

Unfortunately, the terms involving g_4 and g_4' in Eqs. (8) and (12a) are difficult to estimate. The terms involving g_4' are expected to be small in the temperature range of interest. Light-scattering measurements give only very limited information about the terms involving g_4, both because the light-scattering measurements involve a very limited range of momenta and because there are fundamental difficulties with using this approach to describe the light-scattering data.[9] We have emphasized the use of Eqs. (8) and (12a) instead of Eq. (9) because the spirit of the Hamiltonian [Eq. (1)] is that the terms are successively smaller, so that an expression for $\langle \mathcal{H} \rangle$ involving an unknown part depending on g_4 and g_4' is preferable to an expression involving an unknown part depending on g_3. By judicious combined use of Eqs. (8) and (9), it may be possible to learn a substantial amount about the relative importance of three- and four-quasiparticle interactions in the thermodynamics.

We add some further comments on the relationship of this work to that of Cohen[5]: If we accept Cohen's Hamiltonian (equivalent to getting $g_3 = 0$, $g_4' = 0$), then Eqs. (9), (10), (25a), (26a), (26b), (29), (30), and (37) do establish a direct relationship between the thermodynamics and $S(\vec{q}, \omega)$. This represents an advance on Cohen's work, which only established this relationship to leading order in the interactions. On the other hand, this result is not very useful because g_3 cannot be neglected, as shown by Jackson.[4] Secondly, we note that in Cohen's model ($g_3 = 0$, $g_4' = 0$) we would get $\lambda = 0$ in Eq. (30) so that Eq. (30) reduces to a sum of two Lorentzians, which is Cohen's result for $S(\vec{q}, \omega)$. Next we note that both this work and Ref. 5 make the assumption of Eq. (4a). [This is the equation preceding Eq. (20) of Ref. 5 or equivalently the retention of only the first term in Eq. (20).] The assumption in Eq. (4a) is the weakest point in the quasiparticle model used in this paper, as is further discussed below. Finally, our results are consistent with the Cohen result that, at low temperatures when the quasiparticle interactions are weak, the noninteracting entropy $\bar{S}$ can be used with the quasiparticle energies $\mathcal{E}_q$ taken as the positions of the frequency peaks in $S(\vec{q}, \omega)$. At higher temperatures, we agree with Cohen that "there appears to be no simple connection," but in the equations cited at the beginning of this paragraph we have established a connection in closed form within Cohen's model ($g_3 = 0, g_4' = 0$). When $g_3 \neq 0$, and $g_4' \neq 0$, we find no direct connection at elevated temperatures; but we have established that part of the entropy can be related to parameters characterizing $S(\vec{q}, \omega)$ [Eq. (42)].

The calculation of g_4 and g_4' by Jackson's method will eventually make an exact evaluation of all the expressions in this paper possible. Some static correlation functions of the type involved have recently been evaluated from first principles using Monte Carlo techniques.[13] It should be emphasized, however, that the expressions presented here should be useful in analyzing data to yield information about the quasiparticle model, even without knowledge of g_4 and g_4'. Furthermore, Eq. (9) could presently be evaluated using Jackson's result for g_3. We leave this calculation to the future.

In further work, it will be necessary to modify the quasiparticle model in order to take account of excluded volume effects.[9] It is likely that such a modification will result in a change in the assumption [Eq. (4a)] along the lines implicit in Jackson's approach[4] to microscopic justification of the quasiparticle model. We anticipate, however, that at least at low temperatures these modifications may not affect the predictions of the quasiparticle model for frequencies in the neighborhood of the roton energy. Thus Eq. (30) may remain valid. The identities [Eqs. (8) and (12a)] do not depend on Eq. (4a) and we can anticipate that they will remain unchanged.

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APPENDIX: REDUCTION OF g_4 TERM IN EQ. (8) TO SINGLE-PARTICLE TERMS AND A FLUCTUATION TERM

The correlation function in the g_4 term is written

$$\langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle = \langle\alpha^\dagger_{\vec{k}_1}\alpha_{\vec{k}_3}\rangle\langle\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_4}\rangle + \langle\alpha^\dagger_{\vec{k}_1}\alpha_{\vec{k}_4}\rangle\langle\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\rangle + \langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\rangle\langle\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle + \langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle_c\,, \tag{A1}$$

where this equation defines $\langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle_c$. Using the symmetry properties of $g_4(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4)$, the g_4 term in Eq. (8) becomes

$$-\frac{1}{3}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle = -\frac{1}{3}\Bigg(\sum_{\vec{k}_2}\langle n_{\vec{k}_2}\rangle 2\sum_{\vec{k}_1} g_4(\vec{k}_1,\vec{k}_2,\vec{k}_1,\vec{k}_2)\langle n_{\vec{k}_1}\rangle + \sum_{\vec{k}_2}\langle\tilde{n}_{\vec{k}_2}\rangle^*\sum_{\vec{k}_1} g_4(\vec{k}_1,-\vec{k}_1,\vec{k}_2,-\vec{k}_2)\langle\tilde{n}_{\vec{k}_1}\rangle + \sum_{\substack{\vec{k}_1,\vec{k}_2\\ \vec{k}_3,\vec{k}_4}} g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle_c\Bigg)\,. \tag{A2}$$

The first terms in this equation can be evaluated directly from the Green's functions defined in the text and related therein to the neutron-scattering function. Alternatively, one can rewrite Eq. (A2) using Eq. (21) to give

$$-\frac{1}{6}\sum_{\vec{k}_1,\vec{k}_2} g_4(\vec{k}_1,-\vec{k}_1,\vec{k}_2,-\vec{k}_2)[\langle\tilde{n}_{\vec{k}_1}\rangle(\langle\tilde{n}_{\vec{k}_2}\rangle^* - \langle n_{\vec{k}_2}\rangle) + \langle\tilde{n}_{\vec{k}_1}\rangle^*(\langle\tilde{n}_{\vec{k}_2}\rangle - \langle n_{\vec{k}_2}\rangle)] - \frac{1}{3}\sum_{\substack{\vec{k}_1,\vec{k}_2\\ \vec{k}_3,\vec{k}_4}} g_4(\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4)\langle\alpha^\dagger_{\vec{k}_1}\alpha^\dagger_{\vec{k}_2}\alpha_{\vec{k}_3}\alpha_{\vec{k}_4}\rangle_c\,.$$

In these equations,

$$\langle\tilde{n}_{\vec{k}_1}\rangle = \langle\alpha_{\vec{k}_1}\alpha_{-\vec{k}_1}\rangle, \quad \langle n_{\vec{k}_1}\rangle = \langle\alpha^\dagger_{\vec{k}_1}\alpha_{\vec{k}_1}\rangle\,,$$
$$\langle\tilde{n}_{\vec{k}_1}\rangle^* = \langle\alpha^\dagger_{-\vec{k}_1}\alpha^\dagger_{\vec{k}_1}\rangle\,.$$

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