Relation between Inelastic Neutron Scattering and Thermodynamic Functions of Liquid Helium

MICHAEL COHEN
University of Pennsylvania, Philadelphia, Pennsylvania
(Received October 26, 1959)

A model of liquid helium is analyzed, in which the liquid is regarded as a collection of excitations ("rotons" only with energy $\geqslant\Delta$) with an arbitrary pairwise number-conserving interaction. The entropy and normal fluid density of the liquid, and the energy distribution of scattered neutrons are computed as power series in the density of excitations $\exp(-\Delta/kT)$. The first terms containing effects of the interactions are studied. When the interactions are weak, the entropy [through order $\exp(-2\Delta/kT)$] is simply related to the neutron scattering, the connection being correctly given by the formula of Bendt, Cowan, and Yarnell. For strong interactions there appears to be no simple connection. Even when interactions are weak, the first correction to the normal fluid density involves information which is not contained in the neutron scattering.

A method due to Bloch and de Dominicis is used in the analysis, and leads to a new form for the second virial coefficient. This is closely related to a curious new form for the level shift of a particle in a large spherical box, under the influence of a central potential.

I. INTRODUCTION

EXPERIMENTS[1–3] with cold neutrons have provided striking evidence of the existence of elementary excitations in liquid helium, with an energy versus momentum relation of the type envisioned by Landau.[4] The Los Alamos determination of the function $E(p)$ was sufficiently accurate to permit a serious calculation[5] of the thermodynamic properties of the liquid. In making such a calculation one has to reckon with the fact that the measured $E(p)$ curve varies with the helium temperature. According to Yarnell, Arnold, Bendt, and Kerr, the minimum roton energy Δ (measured in temperature units) decreases from 8.65°K at a helium temperature of 1.1°K to 8.15°K at a helium temperature of 1.8°K. Since thermodynamic functions depend on Δ in the combination $\exp(-\Delta/kT)$, neglect of the variation in Δ could cause errors of 30% or more in the thermodynamic functions.

The temperature dependence of the excitation curve seems to indicate that the excitations interact with each other, with the result that the energy needed to produce one more depends on the number already present. For weak interactions, line shifts are proportional to the interaction, and line widths are proportional to the square of the interaction. Yarnell et al. report line widths (full width at half maximum) of 1°K and 2°K, for production of minimum energy rotons at temperatures of 1.6°K and 1.8°K, respectively. Since these widths are several times as large as the line shifts at the same temperature, it would seem superficially that the interactions are not weak.

Bendt, Cowan, and Yarnell give a formula for the entropy of a "gas" of interacting excitations

$$S=k\sum_j \beta E_j(T)[e^{\beta E_j(T)}-1]^{-1}-\ln[1-e^{-\beta E_j(T)}], \quad (1)$$

where k=Boltzmann's constant, $\beta=1/kT$, and j is an index which runs over allowed momentum values in the container; in a box of volume Ω the sum may be replaced by $\Omega h^{-3}\int d^3\mathbf{p}$. The important question, of course, is the meaning of $E_j(T)$; in the absence of a method for computing or measuring $E_j(T)$, Eq. (1) is so general as to be vacuous. BCY identify $E_j(T)$ with the energy loss of neutrons scattered with momentum transfer j at helium temperature T.

Using Eq. (1), BCY fit the observed entropy within $\pm 3\%$ in the range $0.2°\leq T\leq 1.8°$. Numerical differentiation of the entropy curve yields specific heat values within $\pm 4\%$ of observed data in the range $0.2°\leq T\leq 1.7°$. Despite this nice agreement, we still regard it as worthwhile to inquire into the validity[6] and limitations of Eq. (1). The equation is not really meaningful until one decides exactly what is meant by $E_j(T)$. For a given momentum transfer j there is a distribution of energy losses, and it seems doubtful that all the thermodynamic information in the distribution is summarized by picking out one point (e.g., the maximum). One might conjecture that (1) is correct when the "density of excitations" is low, regardless of the strength of their interactions, with $E_j(T)$ defined as the most probable energy loss for momentum transfer j. This proves not to be the case.

The problem of "temperature-dependent energy levels" arises quite frequently in other contexts, and is still in need of clarification. Accordingly it seems worthwhile to construct a model for which neutron scattering and thermodynamic functions can be computed, and to examine the relation between them. The analysis also relates neutron line shapes to the primitive interactions

[1] H. Palevsky, K. Otnes, and K. E. Larsson, Phys. Rev. **112**, 11 (1958).
[2] J. L. Yarnell, G. P. Arnold, P. J. Bendt, and E. C. Kerr, Phys. Rev. **113**, 1379 (1959).
[3] D. G. Henshaw, Phys. Rev. Letters **1**, 127 (1958).
[4] L. Landau, J. Phys. (U.S.S.R.) **5**, 71 (1941); **11**, 91 (1947).
[5] P. J. Bendt, R. D. Cowan, and J. L. Yarnell, Phys. Rev. **113**, 1386 (1959), occasionally called BCY in this text. We are especially indebted to these authors for a preprint.
[6] When we speak of the "validity of Eq. (1)," we henceforth assume that $E_j(T)$ is defined by neutron scattering.

of the excitations. With little additional labor one can compute the "normal fluid density" for the model. The present paper is concerned with the general method of analysis. Numerical results will be given in a second paper.

II. THE MODEL

The system we shall study is defined by the Hamiltonian

$$H=\sum a_k^* a_k E(k)+\sum\langle kl|v|ij\rangle a_k^* a_l^* a_i a_j$$
$$=H_0+V. \tag{2}$$

The indices i, j, k, l run over the allowed momentum states in the quantization box. Occasionally we represent the momenta explicitly by writing $\mathbf{k}_i$ or $\mathbf{k}_j$. The interaction is assumed to conserve momentum, i.e., $\langle kl|v|ij\rangle=0$ unless $\mathbf{k}_k+\mathbf{k}_l=\mathbf{k}_i+\mathbf{k}_j$. The operators obey the usual Bose commutation relations $[a_i,a_j^*]=\delta_{ij}$ and $[a_i,a_j]=0$. The operators should be visualized as creating excitations (e.g., rotons) rather than particles. Accordingly, $E(k)$ is not necessarily quadratic and $\langle kl|v|ij\rangle$ is not necessarily the Fourier transform of a potential. Nevertheless, the momentum-conserving matrix elements $\langle kl|v|ij\rangle$ will be proportional to Ω^{-1}. In the interaction each distinct transition is included exactly once; $(kl;ij)$ is the same as $(lk;ji)$ but distinct from $(lk;ij)$. Although the Hamiltonian conserves the total number of excitations, we assume that excitations can be created and destroyed at the walls, so that in thermodynamic equilibrium the number of excitations is uncertain.

The form of the interaction term is based on the idea that a single excitation should be an eigenstate of the system. In earlier work by Feynman[7] and Feynman and Cohen,[8] fairly successful computations of the $E(p)$ curve were based on the idea of minimizing the energy for a given momentum. Exact minimization would lead to an eigenstate for each possible momentum, and we believe that the energy versus momentum curve thus obtained would coincide with that measured by neutron scattering at zero temperature. Other possibilities can be visualized. For example, the thermodynamics might be dominated not by any small set of stationary states, but rather by some long-lived "compound" states; such is the case for atoms in weak interaction with the radiation field. It is also conceivable that neutrons couple with finite probability to these compound states, and only with infinitesimal probability (proportional to Ω^{-1}) to the true stationary states. In this case the compound states, rather than any set of stationary states, would play the role of elementary excitations. One test of whether neutrons couple to stationary or compound states is the behavior of line widths at zero temperature, the line width approaching zero in the former case and remaining finite in the latter. Experiments suggest that line widths vanish at zero temperature, though the finite resolution of instruments limits the accuracy of this statement. Finally, it is worth mentioning that neutrons couple with finite probability[9] to the approximate roton wave function of Feynman and Cohen, though it is not obvious that this feature persists when the exact lowest wave function is used. We shall require, then, that a single excitation be an eigenstate of H. If $|0\rangle$ is the vacuum state, the requirement that $a_k^*|0\rangle$ be an eigenstate implies that the interaction term in H must contain at least two annihilation operators, and, for Hermiticity, at least two creation operators. The interaction in (2) is the simplest having these properties.

The function $E(k)$ is not temperature-dependent. The energy loss of neutrons scattered by the system will prove to be temperature-dependent, and at zero temperature directly measures $E(k)$. It is useful to assume $E(k)\geq\Delta$ for all k, i.e., that a minimum energy Δ is needed to produce an excitation. This is known to be true for excitations in the roton region ($k\sim 2A^{-1}$) but is not true for phonons ($k\to 0$). Since rotons dominate the thermodynamics of helium at temperatures greater than 1°K, no conceptual violence is done if we neglect the phonons. Then the quantity $\exp(-\beta\Delta)$, which roughly measures the density of excitations, is a natural expansion parameter even when interactions are not weak. Phonons are easily included in the final formulas, though identification of the expansion parameter becomes more difficult. It is important to remember that the roton dispersion curve, of the form $E(k)=\Delta+\hbar^2(k-k_0)^2/2\mu$, does *not* imply that at sufficiently low temperatures all rotons have small momenta and therefore small relative momenta.

III. THERMODYNAMIC FUNCTIONS

A. Method of Bloch and de Dominicis

The entropy is given by

$$S=k\beta^2\partial F/\partial\beta, \tag{3}$$

where

$$e^{-\beta F}=\mathrm{Tr}\{e^{-\beta H}\}. \tag{4}$$

Bloch and de Dominicis[10] have given a diagrammatic expansion for F which is particularly appropriate to this problem. Since we are also interested in obtaining diagrammatic representations of other functions, we shall briefly review their method. One makes the familiar

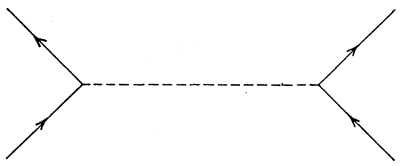

FIG. 1. The fundamental interaction $\langle kl|v|ij\rangle a_k^* a_l^* a_i a_j$.

[7] R. P. Feynman, Phys. Rev. **94**, 262 (1954).
[8] R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).
[9] M. Cohen and R. P. Feynman, Phys. Rev. **107**, 13 (1957).
[10] C. Bloch and C. de Dominicis, Nuclear Phys. **7**, 459 (1958).

expansion

$$e^{-\beta H}=e^{-\beta H_0}\sum_{n=0}^{\infty}(-)^n\int\cdots\int_{\beta>u_n>\cdots>u_1>0}V(u_n)\cdots V(u_1)du_1\cdots du_n, \tag{5}$$

where

$$V(u)=e^{uH_0}Ve^{-uH_0}=\sum\langle kl|v|ij\rangle a_k^*a_l^*a_ia_j\exp[u(E_k+E_l-E_i-E_j)]. \tag{5a}$$

The traces which must be done are of the form $\mathrm{Tr}\{e^{-\beta H_0}A\}$, where A is a product of creation and annihilation operators. If the symbol $\langle\ \rangle$ is defined by

$$\langle A\rangle=\mathrm{Tr}\{e^{-\beta H_0}A\}/\mathrm{Tr}\{e^{-\beta H_0}\}$$

it follows that

$$\langle a_ia_j\rangle=\langle a_i^*a_j^*\rangle=0,$$
$$\langle a_i^*a_j\rangle=\delta_{ij}\exp(-\beta E_i)[1-\exp(-\beta E_i)]^{-1},$$
$$\langle a_ia_j^*\rangle=\delta_{ij}[1-\exp(-\beta E_i)]^{-1}.$$

One readily sees that $\langle A\rangle=0$ unless a_i^* and a_i have the same number of occurrences in A (for every i). Following the method of Wick, Bloch and de Dominicis associate various "factor pairings" with the operator A. A factor pairing is an association of all the operators in A into pairs, each creation operator being associated with an annihilation operator referring to the same state. For each pair of operators one then computes $\langle a_i^*a_i\rangle$ or $\langle a_ia_i^*\rangle$, according as a_i^* stands to the left or right of a_i in A. The product of the numbers thus obtained is the number associated with the factor pairing. The theorem of Bloch and de Dominicis asserts that $\langle A\rangle$ is equal to the sum of the numbers associated with all the distinct factor pairings of A.

Factor pairings can be represented by diagrams; $\langle a_ia_i^*\rangle$ is represented by an arrow (labelled i) directed toward the top of the page, and $\langle a_i^*a_i\rangle$ by an arrow directed toward the bottom of the page. The fundamental interaction $\langle kl|v|ij\rangle a_k^*a_l^*a_ia_j$ is represented by the vertex shown in Fig. 1. Although the arrows have definite directions in the figure, their directions are not really determined until the full factor pairing, of which the vertex is a part, is represented. At this stage we know only that i and j point into the vertex, k and l away from the vertex.

From the definition of $\langle\ \rangle$ we have

$$\mathrm{Tr}\{e^{-\beta H}\}=\mathrm{Tr}\{e^{-\beta H_0}\}\left\langle\sum_{n=0}^{\infty}(-)^n\int\cdots\int_{\beta>u_n>\cdots>u_1>0}V(u_n)\cdots V(u_1)du_1\cdots du_n\right\rangle.$$

The term $n=0$ contributes $\langle 1\rangle=1$. Figure 2(a) and the exchange diagram 2(b) represent the factor pairings arising from the term $n=1$. All arrows in both diagrams point downward, because in V the annihilation operators occur to the right of creation operators. The diagrams shown in Fig. 3 are some of those which come from the term $n=2$. The "time" u increases toward the top of the page. When the unlinked diagram 3(c) is combined with the diagram obtained by exchanging the time ordering of the two vertices, the total time-integrated contribution is just the product of the contributions of the two linked parts separately. One readily sees that the total contribution of all diagrams can be written as the exponential of the contribution of the linked diagrams. It follows that

$$-\beta F=-\beta F_0+\sum A_L, \tag{6}$$

where $e^{-\beta F_0}=\mathrm{Tr}\{e^{-\beta H_0}\}$ and A_L is the contribution of the linked diagram L; explicitly

$$A_L=\prod(\text{matrix elements})\prod_{\uparrow}\frac{1}{1-e^{-\beta E_i}}\prod_{\downarrow}\frac{e^{-\beta E_i}}{1-e^{-\beta E_i}}\times(-)^n\int\cdots\int_{\beta>u_n>\cdots>u_1>0}\exp\sum u_\nu\Delta E_\nu du_1\cdots du_n, \tag{7}$$

where

$\Delta E_\nu=$ (energy of arrows going away from νth vertex) $-$ (energy of arrows going into νth vertex).

A diagram with n vertices has $n-1$ intermediate states I, with which we can associate energies

$E_I=$ (energy of arrows going upward during I) $-$ (energy of arrows going downward during I).

Bloch and de Dominicis show that if all E_I are distinct and not equal to zero, the time integral may be replaced by

$$\beta\prod_I(1/E_I). \tag{8}$$

They do not claim that the time integral for a particular diagram is equal to (8), but they show that when a diagram is considered in conjunction with other diagrams cyclically related to it, the errors due to using (8) exactly cancel out. Equation (8) does not apply to Fig. 3(b), which has an intermediate state with zero energy. The time integral associated with this diagram has the value $\beta^2/2$. Equation (8) is applicable to the diagrams with which we shall be concerned.

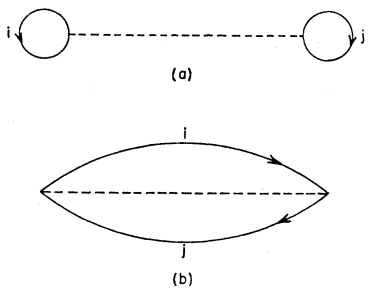

FIG. 2. First order diagrams in thermodynamics.

B. Low-Temperature Expansion

We are interested in expanding F in powers of $\exp(-\beta\Delta)$. Since two rotons are created and two destroyed at each vertex, the time integral in (7) contributes no powers of $\exp(-\beta\Delta)$. Therefore, the dependence on $\exp(-\beta\Delta)$ comes from the statistical factors $[1-\exp(-\beta E_i)]^{-1}$ and $\exp(-\beta E_i)[1-\exp(-\beta E_i)]^{-1}$, and it is evident that a diagram with n downward arrows contributes to the coefficient of $\exp(-\nu\beta\Delta)$ for all $\nu \geq n$. Every diagram involves at least two downward arrows, and the first corrections to F are thus proportional to $\exp(-2\beta\Delta)$. In this order the statistical factors for upward and downward arrows may be taken as 1 and $\exp(-\beta E_i)$, respectively.

Diagrams with two downward lines are all of the "ladder" type shown in Fig. 4, and can be formally summed by an integral equation. It is instructive to exhibit the integral equation in order to compare it with the equation which arises in the line shape calculation. Let us momentarily ignore the fact that (8) fails if any of the E_I are equal or zero, and that denominators can vanish. Then, through order $\exp(-2\beta\Delta)$, the contribution to (6) of the ladder diagrams 4(a) and 4(b) would be given, respectively, by

$$-\tfrac{1}{2}\beta \sum e^{-\beta(E_i+E_j)}\langle ij|T(E_i+E_j)|ij\rangle, \tag{9}$$

and

$$-\tfrac{1}{2}\beta \sum e^{-\beta(E_i+E_j)}\langle ji|T(E_i+E_j)|ij\rangle,$$

where the matrix $T(E)$ is defined by

$$\langle kl|T(E)|ij\rangle=\langle kl|v|ij\rangle+\sum_{i'j'}\langle kl|v|i'j'\rangle \times\frac{1}{E-E_{i'}-E_{j'}}\langle i'j'|T(E)|ij\rangle. \tag{10}$$

In (9) we let both i and j vary over the full range and insert the factor $\frac{1}{2}$ to correct the redundancy.

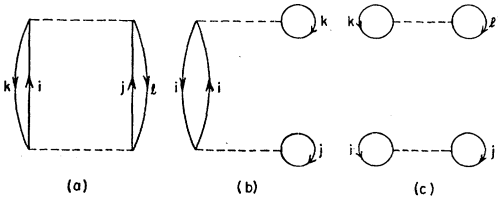

FIG. 3. Some of the second order diagrams in thermodynamics.

If poles are treated by adding a small positive imaginary part $i\epsilon$ to the energy E, then Eq. (10) defines the two-body scattering matrix $T^+(E)$. It is convenient to replace (ij) by a single index a, which lists the two-particle (or two-excitation) eigenstates of H_0. If the objects being scattered had a quadratic energy versus momentum relation[11] $E=\hbar^2k^2/2\mu$, and if v were a central potential, then the states $|a\rangle$ could be taken to have definite total momentum $\mathbf{P}$, relative angular momentum l (with projection m), and relative wave number k. In this case, T^+ would be diagonal in $\mathbf{P}$, l, and m, with diagonal elements related to the scattering phase shifts by

$$\langle a|T^+(E_a)|a\rangle=-(2k\hbar^2/\mu R_0)e^{i\delta_a}\sin\delta_a, \tag{11}$$

where $\delta_a=\delta_l(k)$ and the relative motion is normalized in a sphere of radius R_0. If the poles are treated in the principal value sense, then (10) defines the reaction matrix $G(E)$ with diagonal elements given by

$$\langle a|G(E_a)|a\rangle=-(2k\hbar^2/\mu R_0)\tan\delta_a. \tag{12}$$

Actually, neither (11) nor (12) is the correct recipe for doing thermodynamics. An obvious trouble with (11) is that the diagonal elements of T^+ are complex numbers, and thermodynamic functions are real numbers. We shall shortly see, however, that the temperature-dependent line shifts in neutron scattering are proportional to the real part of the diagonal elements of T^+. Accordingly, one is tempted to try to prove that the real part of T^+ correctly sums the diagrams of Fig. 4, since it would follow that thermodynamics and neutron scattering are simply related. This conjecture is also wrong. The correct recipe (for the case of particles with $E=\hbar^2k^2/2\mu$ interacting through a central potential) is most easily obtained by noting that the diagrams of Fig. 4 are exactly those which must be summed to obtain the second virial coefficient. The Bloch-de Dominicis method can be used to find the grand partition function of a system of Bose particles at fixed density. In the statistical factors $\langle a_i a_i^*\rangle$ and $\langle a_i^* a_i\rangle$, one must replace $\exp(-\beta E_i)$ by $z\exp(-\beta E_i)$, where z is the fugacity. A power series in z is essentially the same as a power series in $\exp(-\beta\Delta)$. If Q is the grand partition

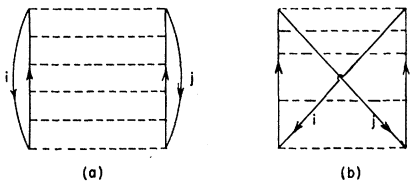

FIG. 4. Ladder diagrams in thermodynamics.

[11] The total momentum $\mathbf{P}$ commutes with our Hamiltonian (2) and can be taken as a constant vector. The resulting one-body Hamiltonian involves the angle between $\mathbf{P}$ and the relative momentum $\mathbf{k}$. Hence a partial-wave analysis of the relative motion is impossible.

function and we write

$$\ln Q=\sum_{l=1}^{\infty} b_l z^l,$$

then b_2 is just the sum of the diagrams in Fig. 4, plus terms arising from F_0. From the equation of state

$$\frac{p}{kT}=\frac{N}{\Omega}-\left(\frac{2\pi\beta\hbar^2}{\mu}\right)^3\frac{b_2}{\Omega}\left(\frac{N}{\Omega}\right)^2+\cdots$$

we obtain the second virial coefficient

$$B=-(2\pi\beta\hbar^2/\mu)^3(b_2/\Omega). \tag{13}$$

The part of the second virial coefficient due to interactions has a well-known[12] representation in terms of scattering phase shifts, namely

$$B_{imp}=-16(\pi)^{\frac{1}{2}}\left(\frac{\beta\hbar^2}{\mu}\right)^{\frac{5}{2}}\sum_{l\ \text{even}}(2l+1)\times\int_0^\infty \exp(-\beta\hbar^2k^2/\mu)\delta_l(k)kdk. \tag{14}$$

Equations (13) and (14) are consistent with (9), provided that T is replaced by a matrix R, the diagonal elements of which are

$$\langle a|R|a\rangle=-(2k\hbar^2/\mu R_0)\delta_a. \tag{15}$$

The Bloch-de Dominicis method does, in fact, imply an unambiguous recipe for treating poles; we shall sketch briefly how this recipe leads to (15), rather than (11) or (12).

For simplicity, let us consider the three cyclically related diagrams of Fig. 5. All involve the same matrix elements, but the time integrals and statistical factors are different for the three diagrams. The contribution of these diagrams is given by (6), (7), and (8) as

$$\frac{e^{-\beta E_c}}{(E_c-E_a)(E_c-E_b)}+\frac{e^{-\beta E_b}}{(E_b-E_c)(E_b-E_a)}+\frac{e^{-\beta E_a}}{(E_a-E_b)(E_a-E_c)}, \tag{16}$$

where $|ij\rangle$, $|kl\rangle$, and $|mn\rangle$ are abbreviated to $|a\rangle$, $|b\rangle$, and $|c\rangle$, respectively, and the uninteresting common factor $-\beta\langle c|v|b\rangle\langle b|v|a\rangle\langle a|v|c\rangle$ is omitted. In Eq. (16) and henceforth, unless otherwise indicated, statistical factors are accurate only through order $\exp(-2\beta\Delta)$. In writing (16), we assumed E_a, E_b, and E_c to be distinct. There are no singularities in (16), however, as any two or all three of the energies approach each other (this follows immediately from the fact that (7) is a well-behaved function of E_ν). Consequently, there is no ambiguity in (16) when the sums over a, b, and c are replaced by integrals, provided that all three terms are kept together. Difficulties arise only when we separate the terms—as we do when we try to sum ladder diagrams by an integral equation.

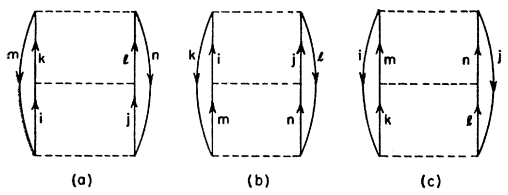

FIG. 5. Cyclically related diagrams.

One way of defining the individual terms of (16) is to add small distinct imaginary parts $i\epsilon_a$, $i\epsilon_b$, and $i\epsilon_c$ to E_a, E_b, and E_c. The value of (16) is unaltered, since (16) is a continuous function of E_a, E_b, and E_c. The same epsilons must be used in all three terms; if we choose $\epsilon_a<\epsilon_b<\epsilon_c$ both denominators in the first term of (16) will have positive imaginary parts, but in the second term one of the denominators will have a negative imaginary part. The expansion of T^+ associates a positive imaginary part with every term in (16) and is therefore not what we want. The reaction matrix G, defined by the principal value recipe in (10), fails for a slightly subtler reason. Since (16) is well-behaved, nothing is changed if we replace the sums over a, b, and c by principal value integrals. But it is important that the integrals be done in the same order in all three terms, since[13]

$$\mathrm{P}\int\frac{dE_c}{E_a-E_c}\mathrm{P}\int\frac{dE_b}{E_b-E_c}\neq\mathrm{P}\int dE_b\mathrm{P}\int\frac{dE_c}{(E_a-E_c)(E_b-E_c)}.$$

Equation (10), with the principal value recipe, implies that in all three diagrams the integral over the state represented by downward lines should be done last; i.e., that in Fig. 5(a) the last integral is over E_c, in 5(b) the last integral is over E_b, and in 5(c) the last integral is over E_a. This is clearly inconsistent with the requirement that the integrals be done in the same order in all three terms.

If the ladder diagrams are to be summed by an integral equation, we need a rule which, upon summation over a, b, and c, associates the same number with all three terms in (16). Then it will be possible to sum diagrams "vertically" rather than "horizontally." A rule which obviously has the required symmetry is simply to omit from the summation any choice of indices for which $E_a=E_b$ or $E_a=E_c$ or $E_b=E_c$. The terms omitted from (16) are all finite and, when the

[12] D. ter Haar, *Elements of Statistical Mechanics* (Rinehart and Company, New York, 1954), p. 196.

[13] N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff, Groningen, 1953), p. 57.

volume Ω is large, form a negligible set. More generally, for a ladder diagram of arbitrary length, we shall omit all choices of indices which give coincidences of energies. The problem is to incorporate this rule, which is essentially non-Markoffian, into an integral equation.

Let us return to the case where an angular momentum decomposition is possible. Riesenfeld and Watson[14] have shown that the phase shift δ_a is given by (15), with the matrix R defined by the nonlinear integral equation

$$R|a\rangle=v|a\rangle+v\frac{1}{E_a-H_0+\langle a|R|a\rangle}(1-\Lambda_a)R|a\rangle, \quad (17)$$

where Λ_a is a projection operator onto $|a\rangle$, and $1-\Lambda_a$ merely eliminates $|a\rangle$ from all intermediate sums.[15] Therefore we are led to conjecture that the diagonal matrix element $\langle a|R|a\rangle$ defined by (17) is the sum of all the terms of the form

$$\left\langle a\left|v\frac{1}{E_a-H_0}v\frac{1}{E_a-H_0}\cdots\frac{1}{E_a-H_0}v\right|a\right\rangle$$

subject to the restriction that $|a\rangle$ does not occur as an intermediate state, and *no intermediate state is repeated.* We have been unable to give a direct proof of this theorem, though the preceding arguments may be regarded as an indirect proof. In Appendix A the theorem is verified in the first five orders of perturbation theory. Verification is not entirely trivial in the fourth and fifth orders. The theorem is useful only in the sense that it relates the present method of computing the second virial coefficient to other "standard" methods.

The angular momentum representation reduces the two-body scattering to a one-dimensional problem, with the immediate consequence that all the information about the scattering can be summarized in a set of phase shifts. In the absence of an angular momentum decomposition, phase shifts can still be defined if the eigenstates $|a\rangle$ of H_0 are properly chosen. For an arbitrary interaction $\langle kl|v|ij\rangle$ one can find the proper eigenstates $|a\rangle$ only after solving the scattering problem. Accordingly, we shall not analyze the scattering in terms of phase shifts, although the phase shift language is useful in distinguishing among the operators T^+, G, and R. If the states are arbitrarily chosen (e.g., as plane wave states), Eq. (17) no longer sums the desired diagrams. For this case, we can still state the low-temperature thermodynamics in the form

$$-\beta F=-\beta F_0-(\beta/2)\sum_a e^{-\beta E_a}\times(\langle a|R|a\rangle+\langle Pa|R|a\rangle), \quad (18)$$

where the states $|a\rangle$ are any complete orthonormal set of two-particle (or two-excitation) eigenstates of H_0, and $P|a\rangle$ is the state obtained from $|a\rangle$ by exchanging the particles (excitations). The matrix $\langle b|R|a\rangle$ is defined to all orders of perturbation theory as the sum of terms of the form

$$\left\langle b\left|v\frac{1}{E_a-H_0}v\cdots v\frac{1}{E_a-H_0}v\right|a\right\rangle, \quad (19)$$

with the restrictions that no intermediate state have the same energy as $|a\rangle$, and no two (or more) intermediate states have the same energy.

IV. LINE SHAPE

A. General Formulation

In order to compute the energy distribution of the scattered neutrons, one needs to know the interaction of a neutron with the liquid. This is just the sum of the short range interactions of the neutron with each of the nuclei in the liquid, and is accurately represented by the pseudopotential[16] $a\sum\delta(\mathbf{r}_j-\mathbf{r})$, where a is a scattering length, $\mathbf{r}$ is the neutron coordinate, and the sum extends over all the atoms in the liquid. Treating the pseudopotential in Born approximation[16] and integrating out the neutron coordinate, one obtains the matrix element for a transition in which the liquid goes from state i to state f, while the neutron gives up momentum $\mathbf{k}$

$$\langle f|M(\mathbf{k})|i\rangle=a\int\psi_f^*(\mathbf{r}_1,\cdots\mathbf{r}_N)\times\sum_{j=1}^{N}e^{i\mathbf{k}\cdot\mathbf{r}_j}\psi_i(\mathbf{r}_1,\cdots,\mathbf{r}_N)d\mathbf{r}_1\cdots d\mathbf{r}_N.$$

We want to write this matrix element in the language of creation and annihilation operators for the excitations. In the limit of small k the system can be treated as a continuous medium; if the potential energy is quadratic in the density one easily finds (omitting trivial factors)

$$\sum e^{i\mathbf{k}\cdot\mathbf{r}_j}=(a_{\mathbf{k}}^*-a_{-\mathbf{k}})/i,$$

where $a_{\mathbf{k}}^*$ creates phonons of momentum $\mathbf{k}$ and $a_{-\mathbf{k}}$ destroys phonons of momentum $-\mathbf{k}$. More generally, for arbitrary $\mathbf{k}$, the operator $M(\mathbf{k})$ can be expanded as a series

$$M(\mathbf{k})=A_{\mathbf{k}}a_{\mathbf{k}}^*+B_{-\mathbf{k}}a_{-\mathbf{k}}+\sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}}C_{\mathbf{k}1\mathbf{k}2}a_{\mathbf{k}1}^*a_{\mathbf{k}2}^*+\sum_{\mathbf{k}_1+\mathbf{k}_2=-\mathbf{k}}D_{\mathbf{k}1\mathbf{k}2}a_{\mathbf{k}1}a_{\mathbf{k}2}+\sum_{\mathbf{k}_1-\mathbf{k}_2=\mathbf{k}}E_{\mathbf{k}1\mathbf{k}2}a_{\mathbf{k}1}^*a_{\mathbf{k}2}+\cdots, \quad (20)$$

[14] W. B. Riesenfeld and K. M. Watson, Phys. Rev. **104**, 492 (1956).

[15] Equation (17) is merely a statement of the Brillouin-Wigner perturbation theory for the energy shift of the state due to the interaction v. To show that this energy shift is equal to $-(2\hbar^2k/\mu R_0)\delta_a$ is nontrivial. Riesenfeld and Watson derived this result by explicitly constructing the solution of (17) from the reaction matrix G.

[16] E. Fermi, Ricerca sci. **7**, 13 (1936); G. Breit, Phys. Rev. **71**, 215 (1947).

where the capital letters are numerical coefficients and the operators a_k^* and a_k are the ones introduced in Eq. (2). We shall retain only the term $A_k a_k^*$, that is, we shall say that a neutron creates a single "bare" excitation. Time-reversal considerations imply that the term $B_{-k}a_{-k}$ also occurs, but this term annihilates an excitation and gives rise to an energy gain in the scattered neutrons. It does not affect the energy distribution of neutrons which have lost energy by creating an excitation, and will therefore be omitted. The next three terms on the right side of (20) also do not contribute to the part of the energy distribution in which we are interested. A term like $a_{k1}^* a_{k2}^* a_{k3}$ (where $\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3=\mathbf{k}$) does contribute to the interesting part of the energy loss curve, but the contribution is down by a factor $\exp(-\beta\Delta)$ relative to the leading term, because the annihilation operator must find something to annihilate. Furthermore, if we study the distribution of energy losses for fixed momentum transfer (or fixed scattering angle) any term involving one or more free momenta contributes to the continuous background; only the leading term contributes a sharp peak which approaches a delta-function at low temperatures. In the present analysis we shall study only the low-temperature behavior (shift and width) of this peak, and therefore shall omit all terms in (20) except a_k^*. The omissions are justified provided we do not try to compute in high orders of $\exp(-\beta\Delta)$, and provided $|A_k|^2$ is not negligible (e.g., of order Ω^{-1}) compared with the sum of the squares of the other coefficients in (20). We remarked earlier that the work of Feynman and Cohen[9] supports the latter assumption. At any rate, it seems possible to conceive of an object whose interaction with the liquid is simply a_k^*, and we shall imagine that $E_j(T)$ in Eq. (1) is measured by scattering these objects.

If the incident neutrons have momentum $\hbar\kappa_0$ and the liquid is initially in state i, then the probability that the liquid is left in one of a group of final states F and the neutron emerges with a momentum in some region G of κ-space is (with trivial factors omitted)

$$\int d\kappa \sum_f |\langle f|M(\kappa_0-\kappa)|i\rangle|^2 \delta\left(\frac{\hbar^2\kappa^2}{2m}-\frac{\hbar^2\kappa_0^2}{2m}+E_f-E_i\right),$$

where the sum and integral extend over the regions F and G, respectively, and m is the neutron mass. The eigenstates of the liquid may be taken to have definite momenta. The matrix element $\langle f|M(\kappa_0-\kappa)|i\rangle$ vanishes unless $\kappa_0+\mathbf{k}_i=\kappa+\mathbf{k}_f$. If the number of neutrons per second emerging in solid angle $d\Omega$ with an energy loss in the range $(E, E+dE)$ is $n(E)dEd\Omega$, the Fourier transform of $n(E)$ is given by

$$f(t)=\int_{-\infty}^{\infty} e^{iEt}n(E)dE$$

$$=(\sum e^{-\beta E_i})^{-1}\int d\kappa\,\kappa^2 \sum_i \sum_f |\langle f|M(\kappa_0-\kappa)|i\rangle|^2$$

$$\times\delta\left(\frac{\hbar^2\kappa^2}{2m}-\frac{\hbar^2\kappa_0^2}{2m}+E_f-E_i\right)e^{-\beta E_i}e^{it(E_f-E_i)}. \quad (21)$$

The statistical factor $e^{-\beta E_i}(\sum e^{-\beta E_i})^{-1}$ is the probability that the liquid was in a particular initial state i. It is also understood that the vector κ in the matrix element has magnitude κ and the direction of the cone $d\Omega$. For fixed i and f, we can perform the κ integration. Since the energy needed to produce a roton is small compared with the energy of the incident neutrons, the term (E_f-E_i) in the argument of the delta function may be ignored with little error, and $\kappa_0-\kappa$ may be replaced by a constant vector $\mathbf{k}$, where $|\mathbf{k}|=2\kappa_0\sin(\theta/2)$. Omitting trivial factors and replacing $M(\mathbf{k})$ by a_k^*, we obtain

$$f(t)=(\sum e^{-\beta E_i})^{-1}\sum_{i,f}|\langle f|a_k^*|i\rangle|^2 e^{itE_f}e^{-(\beta+it)E_i}$$

$$=[\mathrm{Tr}\{e^{-\beta H}\}]^{-1}\,\mathrm{Tr}[e^{-\beta H-itH}a_k e^{itH}a_k^*]. \quad (22)$$

B. Graphical Representation

A diagrammatic representation of $f(t)$ is now possible. Employing the symbol $\langle\ \rangle$ which was introduced earlier, we write

$$f(t)=\langle\exp(\beta H_0)\exp(-\beta H)\rangle^{-1}\langle\exp(\beta H_0)$$
$$\times\exp(-\beta H)\exp(-itH)a_k\exp(itH)a_k^*\rangle. \quad (23)$$

The exponential operators have expansions similar to Eq. (5). Figure 6 represents the type of diagram which occurs in evaluating the second $\langle\ \rangle$ in (23). The lower terminal, from which an arrow issues, represents a_k^*. At the other terminal, representing a_k, the arrow points into the terminal; the horizontal direction of the arrow indicates that it may point up or down, depending on how the diagram is completed. The circles contain the V interactions which occur in the expansion of the indicated exponentials. Each V interaction has two arrows entering and two leaving, the only free ends being those

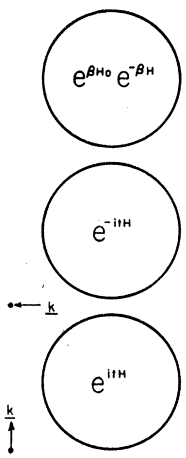

FIG. 6. General structure of diagrams contributing to line shape. The circles contain v interactions.

at the terminals. It follows that the two terminals must be attached to the same linked part of the diagram; a diagram may consist of several disjoint parts not linked to each other, but both terminals must be attached to the same part. This linked part can occur in conjunction with all possible diagrams which can be formed from the contents of the three circles without using the terminals. The contribution of all these diagrams is just the expansion of $\langle\exp(\beta H_0)\exp(-\beta H)\exp(-itH)\exp(itH)\rangle$ and simply cancels the first factor on the right of (23). Introducing the expansions of the exponential operators, we obtain

$$f(t)=\Big\langle\Big[\sum(-)^n\int\cdots\int_{\beta>w_n>\cdots>w_1>0}V(w_n)\cdots V(w_1)dw_1\cdots dw_n\Big]\times e^{-iH_0t}\Big[\sum(-i)^n\int\cdots\int_{t>v_n>\cdots>v_1>0}V'(v_n)\cdots V'(v_1)dv_1\cdots dv_n\Big]\times a_{\mathbf{k}}e^{iH_0t}\Big[\sum(i)^n\int\cdots\int_{t>u_n>\cdots>u_1>0}V''(u_n)\cdots V''(u_1)du_1\cdots du_n\Big]a_{\mathbf{k}}^*\Big\rangle_L, \quad (24)$$

where

$$V'(v)=e^{iH_0v}Ve^{-iH_0v}=\sum\langle kl|v|ij\rangle a_k^*a_l^*a_ia_je^{iv(E_k+E_l-E_i-E_j)},$$
$$V''(u)=e^{-iH_0u}Ve^{iH_0u}=\sum\langle kl|v|ij\rangle a_k^*a_l^*a_ia_je^{iu(E_i+E_j-E_k-E_l)}, \quad (24a)$$

and the subscript L indicates that only linked diagrams attached to the terminals are to be summed.

The simplest diagram (Fig. 7) uses none of the V, V', or V'' interactions, and contributes the term

$$(1-e^{-\beta E_{\mathbf{k}}})^{-1}e^{iE_{\mathbf{k}}t} \quad (25)$$

to $f(t)$. This is just the Fourier transform of a delta function located at $E_{\mathbf{k}}$. At the lowest temperatures $n(E)$ approaches $\delta(E-E_{\mathbf{k}})$, since all other diagrams contain at least one factor of $\exp(-\beta\Delta)$.

Diagrams with a single downward arrow [Fig. 8(a) and the exchange diagram 8(b)] contribute terms to $f(t)$ proportional to $\exp(-\beta\Delta)$. In this order only the V'' interactions (those contained in the lowest circle in Fig. 6) contribute, since any use of the contents of the upper circles would give a diagram with at least two downward arrows. The time integrals associated with Figs. 9(a) and 9(b), which are the simplest cases of 8(a) and 8(b), produce a factor of t. More generally, as will shortly be verified, 8(a) and 8(b) give contributions proportional to t for large t, because the ladder can be attached anywhere along the $\mathbf{k}$ arrow, which runs from $u=0$ to $u=t$. Since the Fourier transform of any reasonable function tends to zero for large t, our expansion seems incorrect. The trouble lies in the neglect of diagrams like Fig. 10(a), which are proportional to $\exp(-2\beta\Delta)$ (for the two downward lines) but also are proportional to $t^2/2$ (because each interaction can occur anywhere along the $\mathbf{k}$ arrow). In order to calculate $n(E)$ correctly, we must calculate $f(t)$ for all t; the neglect of 10(a) is incorrect when t is large.

FIG. 7. Simplest diagram in line shape calculation, contributing a delta function.

To obtain an expansion valid for all t, we expand $\ln f(t)$, rather than $f(t)$, in powers of $\exp(-\beta\Delta)$. If we write

$$f(t)=A_0(t)+A_1(t)e^{-\beta\Delta}+A_2(t)e^{-2\beta\Delta}+\cdots,$$

then we obtain

$$\ln f(t)=\ln A_0+(A_1/A_0)e^{-\beta\Delta}+[(A_2/A_0)-\tfrac{1}{2}(A_1/A_0)^2]e^{-2\beta\Delta}+\cdots. \quad (26)$$

The coefficient of $\exp(-2\beta\Delta)$ in (26) has no term proportional to t^2. For example, the contribution of 10(a) to A_2/A_0 is exactly cancelled by half the square of the contribution of 9(a) to A_1/A_0. More generally, the $t^2/2$ term coming from 10(b) is cancelled by half the square of 8(a). Terms proportional to t still remain, since 10(b) contains terms in t as well as t^2 (the two ladders may overlap and are therefore not completely independent). It is not hard to show that every coefficient in (26) is linear in t for large t; consequently higher terms can be neglected with negligible fractional error. The terms

proportional to t will turn out to have a negative real part, thus assuring that $f(t)$ tends to zero for large t.[17]

C. Calculation at Low Temperatures

To obtain the first deviations of the line shape from a delta-function, we need compute only the first two terms of (26). Only Fig. 7 contributes to A_0, and by (25) we have

$$\ln A_0 = iE(\mathbf{k})t.$$

The contribution of Fig. 7 to A_1/A_0 is independent of t and does not affect the line shape; it merely represents the change in total intensity due to "induced emission" and will be neglected.

None of the V or V' interactions of (24) acts in 8(a) or 8(b). The operator $\exp(-iH_0t)$ acts on the vacuum, producing a factor of unity; the operator $\exp(iH_0t)$ acts just below the upper terminal of 8(a) or 8(b), producing a factor $\exp[iE(\mathbf{k})t]$ which is cancelled in (26) upon division by A_0. To perform the time integrals we use the formula

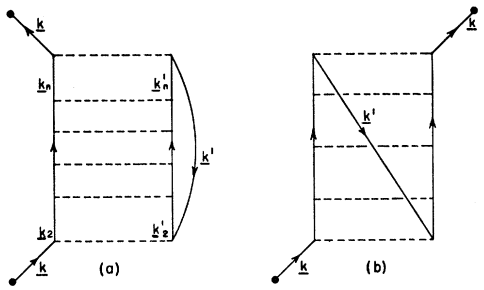

FIG. 8. Ladder diagrams contributing to line shape.

$$\int\cdots\int_{t>t_n>\cdots>t_1>0} dt_1\cdots dt_n \exp i\sum \alpha_i t_i$$

$$= (i)^{n+2}\sum_i \frac{e^{(iA_i-\epsilon_i)t}-1}{A_i+i\epsilon_i}\prod_{j\neq i}\frac{1}{A_j-A_i+i(\epsilon_j-\epsilon_i)} \qquad \left(A_i=\sum_{k=i}^{n}\alpha_k\right), \quad (27)$$

which is easily proved[18] by introducing the Fourier transform of a function which orders the time variables. The ϵ_i are small positive real numbers, all distinct. From (24a) we see that α_i is the sum of the energies of the arrows entering the ith vertex minus the sum of the energies of the arrows leaving. For Figs. 8(a) and 8(b) it follows that

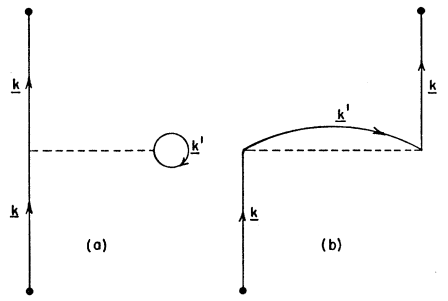

FIG. 9. Simplest versions of Fig. 8.

$$A_i = (\text{energy of arrows entering } i\text{th vertex}) - E(\mathbf{k}) - E(\mathbf{k}'),$$

and, in particular, $A_1=0$. The ϵ_i can be chosen to approach zero in any order, provided we are consistent. We choose $\epsilon_1<\epsilon_2<\cdots<\epsilon_n$.

The term $i=1$ in (27) produces a term proportional to t

$$(i)^{n+3}t\prod_{j=2}^{n}\frac{1}{E(\mathbf{k}_j)+E(\mathbf{k}_j')+i(\epsilon_j-\epsilon_1)-E(\mathbf{k})-E(\mathbf{k}')}, \quad (28)$$

where the intermediate momenta $\mathbf{k}_j$ and $\mathbf{k}_j'$ are defined in Fig. 8(a). Taking note of the factor i^n in (24) and introducing the matrix elements for the interactions, we see that for fixed $\mathbf{k}$ and $\mathbf{k}'$ the terms (28) are summed by $it\langle\mathbf{k}\mathbf{k}'|T^-(E_\mathbf{k}+E_{\mathbf{k}'})|\mathbf{k}\mathbf{k}'\rangle$ for Fig. 8(a), and $it\langle\mathbf{k}'\mathbf{k}|T^-(E_\mathbf{k}+E_{\mathbf{k}'})|\mathbf{k}\mathbf{k}'\rangle$ for Fig. 8(b), where $T^-(E)$ is the scattering matrix defined by (10) with a small negative imaginary part added to E. The contribution of these terms to (26) is

$$it\sum_{\mathbf{k}'} e^{-\beta E_{\mathbf{k}'}}[\langle\mathbf{k}\mathbf{k}'|T^-(E_\mathbf{k}+E_{\mathbf{k}'})|\mathbf{k}\mathbf{k}'\rangle + \langle\mathbf{k}'\mathbf{k}|T^-(E_\mathbf{k}+E_{\mathbf{k}'})|\mathbf{k}\mathbf{k}'\rangle] \equiv iAt-Bt. \quad (29)$$

It is readily shown, using the Hermitian property of H, that B is positive, as was previously stated. The imaginary part of the T^- matrix elements represents the probability of nonforward scattering of roton $\mathbf{k}$ by roton $\mathbf{k}'$, the density of the latter being given by

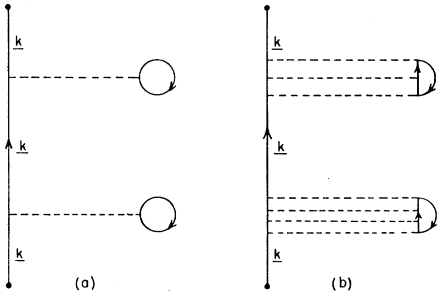

FIG. 10. Diagrams contributing terms proportional to t^2 to Fourier transform of line shape.

[17] Our entire analysis is for positive t. Since $n(E)$ is a real function, we have $f(-t)=\bar{f}(t)$.

[18] The proof in reference 9 contains a sign error, and Eq. (17′) of that paper is wrong by a factor $(-)^r$. Judicious subsequent sign errors lead to the correct Eqs. (19′) and (20′).

$\exp[-\beta E(\mathbf{k}')]$. It follows that $B=\hbar/2t_0$, where t_0 is the lifetime of a roton of momentum $\mathbf{k}$.

The contribution of the remaining terms in (27) is quite complicated, and is evaluated in Appendix B. It is shown there that, within the accuracy of this calculation, these terms do not affect the location or width of the central maximum in $n(E)$. Neglecting these terms and all terms beyond the second in (26), we find (making use of footnote 17)

$$f(t)=\exp[i(E(\mathbf{k})+A)t-B|t|], \tag{30}$$

and

$$n(E)=\frac{1}{\pi}\frac{B}{[E-E(\mathbf{k})-A]^2+B^2}. \tag{31}$$

The line shift A and width B (full width at half maximum$=2B$) are both proportional to $\exp(-\beta\Delta)$.

V. RELATION BETWEEN LINE SHAPE AND THERMODYNAMIC FUNCTIONS

To evaluate the Helmholtz free energy (18), one needs to know the sum of the diagonal matrix elements $\langle a|R|a\rangle$, weighted by the factor $\exp(-\beta E_a)$. Neutron scattering measures the quantity A, which is a weighted average of the real part of $\langle a|T^-|a\rangle$. A simple connection between neutron scattering and thermodynamics exists only when R is almost identical with the real part of T^- (in the language of phase shifts, when $\delta\simeq\sin\delta\cos\delta$). We shall now show this for the case of weak interactions, when both R and T^- may be replaced by v.

Expansion of (18) through terms of order $\exp(-2\beta\Delta)$ yields

$$-\beta F=\sum_{\mathbf{k}}\exp[-\beta E(\mathbf{k})]+\tfrac{1}{2}\sum_{\mathbf{k}}\exp[-2\beta E(\mathbf{k})]-\tfrac{1}{2}\beta\sum_{\mathbf{k}\mathbf{k}'}\exp\{-\beta[E(\mathbf{k})+E(\mathbf{k}')]\}\times[\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}\mathbf{k}'\rangle+\langle\mathbf{k}'\mathbf{k}|v|\mathbf{k}\mathbf{k}'\rangle]+\cdots, \tag{32}$$

where the double sum now extends over all pairs $(\mathbf{k},\mathbf{k}')$ instead of just the distinct pairs. Using (3), we obtain the entropy

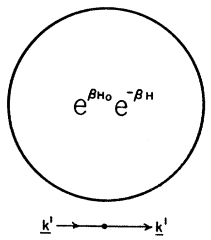

FIG. 11. General structure of diagrams contributing to normal fluid density.

$$S/k=\beta^2\partial F/\partial\beta=\sum\exp[-\beta E(\mathbf{k})]+\beta\sum E(\mathbf{k})\exp[-\beta E(\mathbf{k})]+\tfrac{1}{2}\sum\exp[-2\beta E(\mathbf{k})]+\beta\sum E(\mathbf{k})\exp[-2\beta E(\mathbf{k})]-\beta^2\sum_{\mathbf{k}\mathbf{k}'}E(\mathbf{k})\exp\{-\beta[E(\mathbf{k})+E(\mathbf{k}')]\}\times(\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}\mathbf{k}'\rangle+\langle\mathbf{k}'\mathbf{k}|v|\mathbf{k}\mathbf{k}'\rangle+\cdots). \tag{33}$$

This is to be compared with the expansion of (1) through order $\exp(-2\beta\Delta)$. From (29) we have, for weak interactions

$$E(\mathbf{k},T)=E(\mathbf{k})+A=E(\mathbf{k})+\sum_{\mathbf{k}'}\exp[-\beta E(\mathbf{k}')]\times(\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}\mathbf{k}'\rangle+\langle\mathbf{k}'\mathbf{k}|v|\mathbf{k}\mathbf{k}'\rangle). \tag{34}$$

Substituting (34) into (1), we obtain an expression identical with (33) through order $\exp(-2\beta\Delta)$. We may now state that (1) gives the entropy correctly through order $\exp(-2\beta\Delta)$, provided the interactions are weak. If interactions are not weak, then there is no simple recipe relating the entropy to the neutron scattering.[19] For weak interactions the line width B is proportional to v^2 and (barring cancellations) is small compared to the shift A, which is proportional to v. Since the observed[2] width-to-shift ratio is greater than unity, the use of Eq. (1) seems highly questionable to us. Nevertheless, a good fit of the observed entropy data is obtained by using (1). In a second paper we shall study this situation

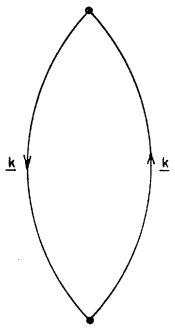

FIG. 12. Simplest version of Fig. 11, giving normal fluid density for noninteracting excitations.

in greater detail and try to learn more about the roton-roton interaction.

VI. NORMAL FLUID DENSITY

The problem of computing the normal fluid density for a system of interacting excitations has not, to our knowledge, been discussed elsewhere. We shall outline a method and study the first corrections due to the interactions.

Following Kramers[20] we imagine a large box of liquid

[19] In an earlier abstract [M. Cohen, Bull Am. Phys. Soc. 4, 245 (1959)] it was erroneously stated that Eq. (1) is correct through order $\exp(-2\beta\Delta)$, regardless of the interaction strength.

[20] H. A. Kramers, Physica **18**, 653 (1952).

at rest, with a small wire cage being dragged through the liquid with velocity $\mathbf{v}$. The cage is such that individual atoms pass through its walls, but excitations are reflected. Kramers shows that the statistical mechanics of the liquid inside the cage is governed by the distribution $\exp[-\beta H+\beta\mathbf{p}\cdot\mathbf{v}]$. The momentum carried by the excitations in the cage is

$$\mathbf{P}=\frac{\mathrm{Tr}\{\mathbf{p}\exp(-\beta H+\beta\mathbf{p}\cdot\mathbf{v})\}}{\mathrm{Tr}\{\exp(-\beta H+\beta\mathbf{p}\cdot\mathbf{v})\}}. \tag{35}$$

For small $\mathbf{v}$ we expand $\exp(\beta\mathbf{p}\cdot\mathbf{v})=1+\beta\mathbf{p}\cdot\mathbf{v}+\cdots$ and obtain $\mathbf{P}=\rho_n\mathbf{v}$ where

$$\rho_n=\tfrac{1}{3}\beta\frac{\mathrm{Tr}\{p^2e^{-\beta H}\}}{\mathrm{Tr}\{e^{-\beta H}\}}. \tag{36}$$

Thus the normal fluid density ρ_n is proportional to the

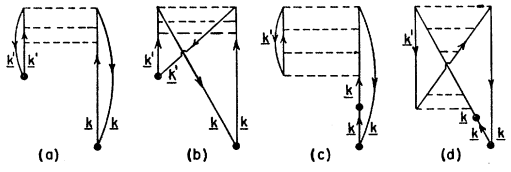

FIG. 13. Diagrams contributing to normal fluid density in order $\exp(-2\beta\Delta)$.

fluctuation of the total momentum in the absence of a moving cage.

The total momentum operator for the liquid is

$$\mathbf{p}=\hbar\sum n(\mathbf{k})\mathbf{k}=\hbar\sum a_{\mathbf{k}}{}^*a_{\mathbf{k}}\mathbf{k}.$$

Returning to the notation of Bloch and de Dominicis, we have

$$\rho_n=\frac{\tfrac{1}{3}\beta\hbar^2\langle e^{\beta H_0}e^{-\beta H}\sum a_{\mathbf{k}'}{}^*a_{\mathbf{k}'}a_{\mathbf{k}}{}^*a_{\mathbf{k}}\mathbf{k}\cdot\mathbf{k}'\rangle}{\langle e^{\beta H_0}e^{-\beta H}\rangle}. \tag{37}$$

Figure 11 shows the structure of the diagrams occurring in the numerator. The horizontal direction of the arrows at the $\mathbf{k}'$ vertex shows that we are uncommitted as to whether they point up or down. No free ends may occur. The circle contains some diagrams which are not attached to either the $\mathbf{k}$ or $\mathbf{k}'$ vertex. These diagrams are exactly cancelled by the denominator. The surviving diagram might still consist of two unlinked parts, one attached to the $\mathbf{k}'$ vertex and one to the $\mathbf{k}$ vertex. Any such diagram gives zero contribution when summed over $\mathbf{k}$ (or $\mathbf{k}'$), because the operator $\mathbf{p}$ is a vector. Accordingly, the only diagrams to be considered are those consisting of a single linked part.

The simplest such diagram is shown in Fig. 12. Inserting the statistical factors for the arrows we obtain the familiar Landau formula for the normal fluid density in a system of noninteracting excitations

$$\rho_n=\tfrac{1}{3}\beta\hbar^2\sum k^2e^{-\beta E(\mathbf{k})}(1-e^{-\beta E(\mathbf{k})})^{-2} \tag{38}$$

$$=\tfrac{1}{3}\beta\hbar^2\sum k^2(e^{-\beta E(\mathbf{k})}+2e^{-2\beta E(\mathbf{k})}+\cdots). \tag{38a}$$

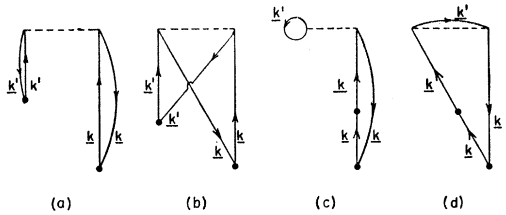

FIG. 14. Simplest versions of Fig. 13.

The only diagrams with two downward arrows, which contribute in order $\exp(-2\beta\Delta)$, are shown in Fig. 13. The associated time integrals are somewhat complicated, and there is no need to exhibit the result here. Equation (8) is no longer useful because the factor $\mathbf{k}\cdot\mathbf{k}'$ destroys the cyclic invariance used in deriving (8). In perturbation theory the lowest order diagrams of type 13(a) and 13(b) are those in Figs. 14(a) and 14(b) which contribute a term

$$-\tfrac{1}{3}\beta\hbar^2\sum_{\mathbf{k}\mathbf{k}'}\mathbf{k}\cdot\mathbf{k}'e^{-\beta E(\mathbf{k})}e^{-\beta E(\mathbf{k}')}\times(\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}\mathbf{k}'\rangle+\langle\mathbf{k}'\mathbf{k}|v|\mathbf{k}\mathbf{k}'\rangle) \tag{39}$$

to the normal fluid density. Similarly, the simplest versions of Figs. 13(c) and 13(d) are Figs. 14(c) and 14(d), which contribute

$$-\tfrac{1}{3}\beta\hbar^2\sum_{\mathbf{k}\mathbf{k}'}k^2e^{-\beta E(\mathbf{k})}e^{-\beta E(\mathbf{k}')}\times(\langle\mathbf{k}\mathbf{k}'|v|\mathbf{k}\mathbf{k}'\rangle+\langle\mathbf{k}'\mathbf{k}|v|\mathbf{k}\mathbf{k}'\rangle). \tag{40}$$

BCY have calculated the normal fluid density by inserting the temperature-dependent $E(\mathbf{k},T)$, measured by neutron scattering, into (38). Inspection of (34), (38), (39), and (40) shows that this recipe does not give the first corrections to ρ_n correctly, even when v is weak. In the special case where v is weak and of such a form as to make (39) vanish, the recipe is correct.

ACKNOWLEDGMENTS

It is a pleasure to thank Professor K. A. Brueckner, Professor J. M. Luttinger, and Dr. R. E. Prange for many valuable discussions.

APPENDIX A. NONREPETITION OF INTERMEDIATE STATES IN PERTURBATION THEORY FOR THE LEVEL SHIFT

We study (17) in the case when v is a spherical potential and the free-particle energy versus momentum relation is $E=\hbar^2k^2/2\mu$. The states $|a\rangle$ are taken to have definite total momentum $\mathbf{P}$, relative angular momentum l (with projection m), and relative wave number k. Since v and R are diagonal in all quantum numbers except k, the problem becomes one-dimensional and states can be labelled by k; explicitly

$$|k\rangle=\frac{\sqrt{2}k}{\sqrt{R_0}}j_l(kr)Y_{lm}(\theta,\varphi). \tag{1'}$$

The normalization in (1′) is asymptotically correct for large values of R_0, the radius of the sphere in which the relative motion is normalized. In order that the wave function vanish on the sphere we need

$$kR_0=n\pi+l\pi/2,$$

which leads to the level density

$$\Delta n/\Delta k=R_0/\pi.$$

Since the mass associated with the relative motion is $\mu/2$, the energy of the state $|k\rangle$ is $\hbar^2k^2/\mu$.

We shall verify a slightly more general theorem than the one stated in Sec. IIIB; namely, that if (17) is written as an explicit power series in v with Schrödinger energy denominators, then $\langle k'|R|k\rangle$ is the sum of all terms of the form

$$\left\langle k'\left|v\frac{1}{E(k)-H_0}v\frac{1}{E(k)-H_0}\cdots\frac{1}{E(k)-H_0}v\right|k\right\rangle \quad (2')$$

subject to the restriction that $|k\rangle$ does not occur as an intermediate state and *no intermediate state is repeated.* When $k=k'$ we have the theorem of Sec. IIIB. Verification will be carried out through the fifth order of v.

By iteration, the solution of (17) can be exhibited as a power series in v, i.e.,

$$R|k\rangle=\rho_1|k\rangle+\rho_2|k\rangle+\rho_3|k\rangle+\cdots,$$

where $\rho_n|k\rangle$ is the part of $R|k\rangle$ involving n matrix elements of v. Iterating (17) we obtain

$$\rho_1|k\rangle=v|k\rangle, \quad (3')$$

$$\rho_2|k\rangle=v\frac{1}{E(k)-H_0}(1-\Lambda_k)\rho_1|k\rangle, \quad (4')$$

$$\rho_3|k\rangle=v\frac{1}{E(k)-H_0}(1-\Lambda_k)\rho_2|k\rangle-v\frac{\langle k|\rho_1|k\rangle}{[E(k)-H_0]^2}(1-\Lambda_k)\rho_1|k\rangle, \quad (5')$$

$$\rho_4|k\rangle=v\frac{1}{E(k)-H_0}(1-\Lambda_k)\rho_3|k\rangle-v\frac{\langle k|\rho_1|k\rangle}{[E(k)-H_0]^2}(1-\Lambda_k)\rho_2|k\rangle$$
$$-v\frac{\langle k|\rho_2|k\rangle}{[E(k)-H_0]^2}(1-\Lambda_k)\rho_1|k\rangle+v\frac{\langle k|\rho_1|k\rangle^2}{[E(k)-H_0]^3}(1-\Lambda_k)\rho_1|k\rangle, \quad (6')$$

$$\rho_5|k\rangle=v\frac{1}{E(k)-H_0}(1-\Lambda_k)\rho_4|k\rangle-v\frac{\langle k|\rho_1|k\rangle}{[E(k)-H_0]^2}(1-\Lambda_k)\rho_3|k\rangle-v\frac{\langle k|\rho_2|k\rangle}{[E(k)-H_0]^2}(1-\Lambda_k)\rho_2|k\rangle$$
$$+v\frac{\langle k|\rho_1|k\rangle^2}{[E(k)-H_0]^3}(1-\Lambda_k)\rho_2|k\rangle-v\frac{\langle k|\rho_1|k\rangle^3}{[E(k)-H_0]^4}(1-\Lambda_k)\rho_1|k\rangle$$
$$+v\frac{\langle k|\rho_1|k\rangle\langle k|\rho_2|k\rangle}{[E(k)-H_0]^3}(1-\Lambda_k)\rho_1|k\rangle-v\frac{\langle k|\rho_3|k\rangle}{[E(k)-H_0]^2}(1-\Lambda_k)\rho_1|k\rangle. \quad (7')$$

We wish to verify that $\langle k'|\rho_n|k\rangle$ is the sum of all nth order terms of the form (2′), subject to the stated restrictions on intermediate states. Verification is immediate for $n=1$ and $n=2$. Rewriting (5′) more explicitly, we have

$$\langle k'|\rho_3|k\rangle=\sum_p{}'\langle k'|v|p\rangle\frac{1}{E(k)-E(p)}\langle p|\rho_2|k\rangle$$
$$-\sum_p{}'\langle k'|v|p\rangle\frac{\langle k|\rho_1|k\rangle}{[E(k)-E(p)]^2}\langle p|\rho_1|k\rangle. \quad (8')$$

The prime on the summation indicates that the term $p=k$ is excluded. The first term in (8′) is almost what we want, except for the unwanted term

$$\sum_p{}'\langle k'|v|p\rangle\frac{1}{E(k)-E(p)}\langle p|v|p\rangle\frac{1}{E(k)-E(p)}\langle p|v|k\rangle, \quad (9')$$

which arises when the intermediate index in $\langle p|\rho_2|k\rangle$ is equal to p. The second term in (8′) would exactly cancel (9′) if $\langle p|v|p\rangle$ could be replaced by $\langle k|v|k\rangle$. At this point we invoke the largeness of R_0. One easily verifies that $\langle k'|\rho_n|k\rangle$ is proportional to R_0^{-1}, with higher order correction terms which we may ignore. The matrix elements v are proportional to R_0^{-1}, but each intermediate summation introduces a compensating factor R_0 arising from the level density. In (9′) however, there are three v matrix elements and only one intermediate summation. One is tempted to throw the term away as being of order R_0^{-2}. This would be wrong, since the energy denominator $E(k)-E(p)$ can become of order R_0^{-1} when p is very close to k. Any such term makes a contribution to (9′) proportional to R_0^{-1}. But in such a term, the index p can be replaced by k in any matrix element (assuming that v is a reasonable function).

Hence, through order R_0^{-1}, the unwanted term (9′) is cancelled by the second term in (8′) and the theorem is also true for $n=3$.

Before going further, it is useful to introduce some shorthand notation. We define

$$(k'rqpk)\equiv\langle k'|v|r\rangle\frac{1}{E(k)-E(r)}\langle r|v|q\rangle\frac{1}{E(k)-E(q)}\times\langle q|v|p\rangle\frac{1}{E(k)-E(p)}\langle p|v|k\rangle, \quad (10')$$

with similar definitions when there are more intermediate indices. For the reasons stated above, any repeated index can be replaced by k in matrix elements. Making use of this result, as well as the results for $n=1, 2, 3$, we rewrite (6′) as

$$\langle k'|\rho_4|k\rangle=\sum_{\substack{pqr\\p\neq q}}{}'(k'rqpk)-\sum_{pq}{}'(k'qqpk)-\sum_{pq}{}'(k'pqpk)+\sum_{p}{}'(k'pppk). \quad (11')$$

The two middle terms are equal. We rewrite (11′) as

$$\langle k'|\rho_4|k\rangle=\sum_{\substack{pqr\\\text{distinct}}}{}'(k'rqpk)+\sum_{\substack{qr\\q\neq r}}{}'(k'rqrk)+\sum_{\substack{pr\\p\neq r}}{}'(k'rrpk)-2\sum_{\substack{pq\\p\neq q}}{}'(k'qqpk)-\sum_{p}{}'(k'pppk). \quad (12')$$

The first term of (12′) is the one we hope will survive. The second and third terms are equal and are cancelled by the fourth. In the last term we need only consider wave numbers p which are very close to k, i.e., $p=k-n\pi/R_0$ and $E(k)-E(p)=(2\pi\hbar^2k/\mu R_0)n$. With trivial factors omitted, the last term in (12′) is

$$\sum_{\substack{n=-\infty\\n\neq 0}}^{\infty}\frac{1}{n^3}=0, \quad (13')$$

and the theorem is true for $n=4$.

The case $n=5$ illustrates the nontrivial nature of the theorem. Using the results for $n=1, 2, 3, 4$ we rewrite (7′)

$$\langle k'|\rho_5|k\rangle=\sum_{\substack{pqrs\\p,\,q,\,r\ \text{distinct}}}{}'(k'srqpk)-\sum_{\substack{pqr\\p\neq q}}{}'(k'rrqpk)-\sum_{pqr}{}'(k'qrqpk)+\sum_{pq}{}'(k'qqqpk)-\sum_{p}{}'(k'ppppk)+\sum_{pq}{}'(k'qpppk)-\sum_{\substack{pqr\\q\neq r}}{}'(k'prqpk). \quad (14')$$

The fourth and sixth terms vanish as a consequence of (13′). The remaining terms can be rewritten

$$\langle k'|\rho_5|k\rangle=\sum_{\substack{pqrs\\\text{distinct}}}{}'(k'srqpk)+2\sum_{\substack{pqr\\\text{distinct}}}{}'(k'prqpk)+\sum_{\substack{pqr\\\text{distinct}}}{}'(k'qrqpk)-\sum_{\substack{pqr\\\text{distinct}}}{}'(k'rrqpk)-2\sum_{\substack{pq\\p\neq q}}{}'(k'qqqpk)-\sum_{\substack{pqr\\\text{distinct}}}{}'(k'qrqpk)-\sum_{pr}{}'(k'prppk)-\sum_{pr}{}'(k'rrrpk)-\sum_{pq}{}'(k'qpqpk)+\sum_{p}{}'(k'ppppk)-\sum_{\substack{pqr\\\text{distinct}}}{}'(k'prqpk)-\sum_{\substack{pr\\p\neq r}}{}'(k'prppk)-\sum_{\substack{pq\\p\neq q}}{}'(k'ppqpk). \quad (15')$$

The third and sixth terms cancel; the seventh and eighth terms vanish by (13′); the second term is cancelled by the fourth and eleventh terms. The fifth, twelfth, and thirteenth terms can be simplified by writing

$$\sum_{\substack{pq\\p\neq q}}{}'(k'qqqpk)=\sum_{pq}{}'(k'qqqpk)-\sum_{p}{}'(k'ppppk), \quad (16')$$

and noting that the first term on the right vanishes as a consequence of (13′). We obtain

$$\langle k'|\rho_5|k\rangle=\sum_{\substack{pqrs\\\text{distinct}}}{}'(k'srqpk)+5\sum_{p}{}'(k'ppppk)-\sum_{pq}{}'(k'qpqpk). \quad (17')$$

The first term in (17′) is the one we hope will survive. The other terms contain the common factor $\langle k'|v|k\rangle\langle k|v|k\rangle^4$. Omitting trivial factors, the sum of these terms is

$$5\sum_{\substack{n=-\infty\\n\neq 0}}^{\infty}\frac{1}{n^4}-\left(\sum_{\substack{n=-\infty\\n\neq 0}}^{\infty}\frac{1}{n^2}\right)^2=5\left(\frac{\pi^4}{45}\right)-\left(\frac{\pi^2}{3}\right)^2=0, \quad (18')$$

and the theorem is verified for $n=5$. We wish to emphasize that the theorem is not intuitively obvious, since its verification depends on the truth of numerical identities like (18′).

We have not been able to produce a general proof of the theorem.

APPENDIX B. TERMS OMITTED IN LINE SHAPE CALCULATION

In evaluating the contribution of Figs. 8(a) and 8(b) to the line shape, all terms in (27) except $i=1$ were neglected. We shall show below that the contribution of

the omitted terms to $\log f(t)$ is of the form $\exp(-\beta\Delta)g(t)$ where the function $g(t)$ is bounded for all t. Anticipating this result, we can then write, through the first order of $\exp(-\beta\Delta)$ and for all t,

$$f(t)=\exp\{i(E(\mathbf{k})+A)t-B|t|\}\times[1+\exp(-\beta\Delta)g(t)]. \quad (19')$$

The Fourier transform of (19′) is the resonance curve (31), plus another term which is smaller by a factor $\exp(-\beta\Delta)$. Elementary geometrical considerations show that the location and width of the resonance are not affected, through order $\exp(-\beta\Delta)$, by the second term. It remains to show that $g(t)$ has the advertised form.

The omitted terms in (27) contribute

$$i^n\sum_{i=2}^{n}\frac{\exp[i(E(\mathbf{k}_i)+E(\mathbf{k}_i')-E(\mathbf{k})-E(\mathbf{k}'))t]-1}{E(\mathbf{k}_i)+E(\mathbf{k}_i')-E(\mathbf{k})-E(\mathbf{k}')}\frac{1}{E(\mathbf{k}_i)+E(\mathbf{k}_i')-E(\mathbf{k})-E(\mathbf{k}')+i(\epsilon_i-\epsilon_1)}$$
$$\times\prod_{j\neq 1,i}\frac{1}{E(\mathbf{k}_j)+E(\mathbf{k}_j')-E(\mathbf{k}_i)-E(\mathbf{k}_i')+i(\epsilon_j-\epsilon_i)}. \quad (20')$$

Introducing matrix elements and the factor i^n, and noting the ordering of the ϵ_i, we can sum the contribution of these terms to (26) in the form

$$\sum_{\mathbf{k}'}e^{-\beta E(\mathbf{k}')}\sum_{\boldsymbol{\kappa},\boldsymbol{\kappa}'}\frac{\exp\{i[E(\boldsymbol{\kappa})+E(\boldsymbol{\kappa}')-E(\mathbf{k})-E(\mathbf{k}')]t\}-1}{E(\boldsymbol{\kappa})+E(\boldsymbol{\kappa}')-E(\mathbf{k})-E(\mathbf{k}')}$$
$$\times\left\{P\frac{1}{E(\boldsymbol{\kappa})+E(\boldsymbol{\kappa}')-E(\mathbf{k})-E(\mathbf{k}')}-i\pi\delta[E(\boldsymbol{\kappa})+E(\boldsymbol{\kappa}')-E(\mathbf{k})-E(\mathbf{k}')]\right\}$$
$$\times\{\langle\mathbf{k}\mathbf{k}'|T^{-}[E(\boldsymbol{\kappa})+E(\boldsymbol{\kappa}')]|\boldsymbol{\kappa}\boldsymbol{\kappa}'\rangle+\langle\mathbf{k}'\mathbf{k}|T^{-}[E(\boldsymbol{\kappa})+E(\boldsymbol{\kappa}')]|\boldsymbol{\kappa}\boldsymbol{\kappa}'\rangle\}\langle\boldsymbol{\kappa}\boldsymbol{\kappa}'|T^{+}[E(\boldsymbol{\kappa})+E(\boldsymbol{\kappa}')]|\mathbf{k}\mathbf{k}'\rangle. \quad (21')$$

The direct and exchange terms come from 8(a) and 8(b), respectively. We have used the identity

$$\frac{1}{x+i\epsilon}=P\left(\frac{1}{x}\right)-i\pi\delta(x).$$

The factor $\exp[-\beta E(\mathbf{k}')]$ makes (21′) proportional to $\exp(-\beta\Delta)$. With an appropriate definition of the function $h(E)$ we can rewrite (21′) in the form

$$\int_{-\infty}^{\infty}\frac{e^{iEt}-1}{E}\left[P\left(\frac{1}{E}\right)-i\pi\delta(E)\right]h(E)dE. \quad (22')$$

If T^{+} and T^{-} are not pathological, $h(E)$ and its derivatives are well-behaved. Writing

$$e^{iEt}-1=-2\sin^2(Et/2)+i\sin(Et)$$

we first examine the term

$$P\int_{-\infty}^{\infty}\frac{\sin(Et)}{E^2}h(E)dE, \quad (23')$$

which can be rewritten as

$$\int_{-\infty}^{-1}+\int_{-1}^{-\epsilon}+\int_{\epsilon}^{1}+\int_{1}^{\infty}. \quad (24')$$

The first and last terms in (24′) tend to zero for large t. In the middle terms we can write

$$h(E)=h(0)+h'(0)E+\tfrac{1}{2}h''(\alpha)E^2, \quad (25')$$

where α is somewhere between 0 and E, and $|h''(\alpha)|$ is bounded by some constant A. We obtain

$$\int_{-1}^{-\epsilon}\frac{\sin(Et)}{E^2}h(0)dE+\int_{\epsilon}^{1}\frac{\sin(Et)}{E^2}h(0)dE=0,$$

$$\int_{-1}^{-\epsilon}\frac{\sin(Et)}{E}h'(0)dE+\int_{\epsilon}^{1}\frac{\sin(Et)}{E}h'(0)dE\underset{\substack{t\to\infty\\ \epsilon t\to 0}}{\longrightarrow}h'(0)\int_{-\infty}^{\infty}\frac{\sin x}{x}dx=\pi h'(0),$$

$$\left|\frac{1}{2}\int_{-1}^{-\epsilon}\sin(Et)h''(\alpha)dE+\frac{1}{2}\int_{\epsilon}^{1}\sin(Et)h''(\alpha)dE\right|<A,$$

and hence (23′) is bounded for all t.

We must now show that the difference between (22′) and (23′)

$$\pi th(0)-2\int_{-\infty}^{\infty}\frac{\sin^2(Et/2)}{E^2}h(E)dE \quad (26')$$

is bounded for all t. Again we break the range of integration

$$\int_{-\infty}^{\infty}=\int_{-\infty}^{-1}+\int_{-1}^{1}+\int_{1}^{\infty}, \quad (27')$$

and use the expansion (25′). The first and third terms in

(27′) are bounded under reasonable assumptions on $h(E)$. To estimate the second term we note

$$h(0)\int_{-1}^{1}\frac{\sin^2(Et/2)}{E^2}dE=h(0)\int_{-\infty}^{\infty}\frac{\sin^2(Et/2)}{E^2}dE+B$$
$$=(\pi t/2)h(0)+B,$$

where B is bounded for all t and, in fact, $|B|<|2h(0)|$. The other terms in (25′) give

$$h'(0)\int_{-1}^{1}\frac{\sin^2(Et/2)}{E}dE=0,$$

and

$$\left|\frac{1}{2}\int_{-1}^{1}\sin^2(Et/2)h''(\alpha)dE\right|<A.$$

This completes the proof that (22′) is bounded for all t.

PHYSICAL REVIEW VOLUME 118, NUMBER 1 APRIL 1, 1960

Ground-State Energy of a Many-Fermion System*

W. KOHN
Carnegie Institute of Technology, Pittsburgh, Pennsylvania

AND

J. M. LUTTINGER
University of Pennsylvania, Philadelphia, Pennsylvania

(Received October 19, 1959)

This paper contains a critique of the Brueckner-Goldstone perturbation series for the ground-state energy of an interacting gas of fermions. We have calculated this energy by first constructing the grand partition function at finite temperature, and then carefully taking the limit as $T\to 0$. In general this leads to a series which differs from that of Brueckner and Goldstone. An exception is the case where both the unperturbed single-particle energy as well as the interaction potential have spherical symmetry. Reasons for the breakdown of the Brueckner-Goldstone formalism are briefly discussed.

I. INTRODUCTION

IN this brief paper we shall consider the problem of calculating the ground-state energy of a collection of many identical, interacting particles obeying Fermi-Dirac statistics. This problem has already been investigated by many authors,[1] and an explicit formula as a power series in the strength of the interaction between the particles has been obtained. The resulting formula—which we shall call the Brueckner-Goldstone (BG) formula—may be obtained by doing ordinary perturbation theory on the ground state of the noninteracting fermions, as if the levels of the system were discrete and well separated. In addition, a rearrangement of the resulting series is made which expresses it very simply in terms of so-called "linked-clusters."

Now we reopen the question for the following reason. In attempting to apply the BG technique to study the effect of interactions on the shape of the Fermi surface in a metal, we became convinced that effects corresponding to a distortion of the Fermi surface are not described by this technique. Of course to discuss this it is necessary to know precisely what one means by the Fermi surface of an interacting system. We do not want to enter into this question here, but hope to return to it in a later publication. The important thing for our present purpose is that one is lead by such considerations to question the validity of the BG formula for those cases where no symmetry exists which would require that the Fermi surface (if it exists) to have the same shape for the unperturbed and perturbed systems. An example of a situation where such symmetry does exist is a gas of free fermions interacting via a potential which is spherically symmetric. In this case both the perturbed and unperturbed Fermi surfaces must be spherical, by symmetry considerations. On the other hand, if, for example, the interaction potential is nonspherical, there is no reason for the perturbed Fermi surface to remain spherical. Another case of the latter type is electrons in metals. Here the interaction is spherically symmetric (Coulomb interaction), but the original unperturbed Fermi surface has only the symmetry of the lattice. Again, we would certainly expect the electron-electron interaction to change the shape of the Fermi surface. As we shall show below, the above conjectures about the limitations of the BG formula have been verified up to the second order in the perturbation by what we consider to be a more correct treatment of the ground-state energy

* This work was supported in part by the Office of Naval Research.

[1] See, for example, K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958); J. Goldstone, Proc. Roy. Soc. (London) **A293**, 267 (1957); N. M. Hugenholtz, Physica **23**, 481 (1957); **23**, 533 (1957); J. Hubbard, Proc. Roy. Soc. (London) **240**, 539 (1957); **243**, 336 (1958).