turbation series. The validity of these approximations has already been mentioned in Sec. III except the following one: In the two particle Green's function (3.8), the two particles are assumed to be excited to the intermediate states from zero-momentum states. This approximation makes the screening factors D_l momentum-independent, and it seems to be a poor approximation especially for large momentum. However, its effect on the excitation spectrum can not be known until a numerical procedure is applied to find out the momentum dependence of D_l. This investigation is presently being carried out and the results will be reported separately.

In summary, we have derived an excitation spectrum in liquid helium in good qualitative agreement with experiments by assuming a hard-sphere-model potential. It is, therefore, hopeful that by taking a more realistic potential for helium including an attractive tail and by improving some of our calculational procedures, mainly the momentum dependence of the screening factors, we may even achieve a quantitative agreement between the spectrum calculated from first principles and that from experiments.

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Finite Superconductors and their Infinite Volume Limit*

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It is demonstrated that the standard applications of the BCS theory to finite systems does not possess the proper asymptotic behavior as the size of the system becomes infinite. In particular, no coupling exists from discrete states to those of positive energy unless the two-body potential is very strong (i.e., stronger than nuclear potentials). Two methods of correcting this deficiency are suggested: (a) a generalization of the BCS variational wave function, and (b) an extension of the Bogoliubov principle of compensating dangerous diagrams.

I. INTRODUCTION

With the introduction of phenomenological pairing interactions, the theory of superconductivity, as adapted to finite systems[1] is successful in explaining the spectra of low-lying states of many nuclei and the thermodynamic properties of finite metallic superconductors. We wish to point out that no coupling exists from discrete to continuum states in this theory, and consequently it does not approach the normal BCS[2] theory as the size of the system becomes infinite. We show, however, that this failure can be rectified to order $(\Delta/E_F)^2$ by either (a) a generalization of the BCS variational-type wave function, or (b) an extension of the Bogoliubov principle of compensating dangerous diagrams.

The BCS "integral" equation for the energy gap of a finite or infinite system is

$$\Delta_\alpha = -\tfrac{1}{2}\sum_{\alpha'} \frac{\langle \alpha - \alpha | V | \alpha' - \alpha' \rangle \Delta_{\alpha'}}{(\Delta_{\alpha'}^2 + \epsilon_{\alpha'}^2)^{1/2}}, \tag{1}$$

where $|-\alpha\rangle$ denotes the single-particle state time reversed with respect to the state $|\alpha\rangle$, and ϵ_α is the single-particle energy measured with respect to the Fermi energy E_F. For a finite system, the eigenstates we consider are those of fermions bound in a self-consistent single-particle potential well of dimension l. The energy spectrum consists of a discrete part, labeled by quantum numbers n, m and a continuum set labeled by indices k, l. Equation (1) can be separated as follows:

$$\Delta_n = -\tfrac{1}{2}\textstyle\sum_{n'} V_{nn'}\Delta_{n'}/E_{n'} - \dfrac{1}{2}\displaystyle\int_{k'} V_{nk'}\Delta_{k'}/E_{k'}, \tag{2a}$$

$$\Delta_k = -\tfrac{1}{2}\textstyle\sum_{n'} V_{kn'}\Delta_{n'}/E_{n'} - \dfrac{1}{2}\displaystyle\int_{k'} V_{kk'}\Delta_{k'}/E_{k'}, \tag{2b}$$

where $V_{\alpha\alpha'} = \langle \alpha - \alpha | V | \alpha' - \alpha' \rangle$ and $E_\alpha = (\Delta_\alpha^2 + \epsilon_\alpha^2)^{1/2}$. Here $\int_k \equiv \sum_k \to (L/2\pi)^3 \int d^3k$, where L is the dimen-

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[1] S. T. Belyaev, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **31**, No. 11 (1959); see also, L. S. Kisslinger and R. A. Sorensen, *ibid.* **32**, No. 9 (1960); J. M. Blatt and C. J. Thompson, Phys. Rev. Letters **10**, 332 (1963); R. C. Kennedy, L. Wilets, and E. M. Henley, *ibid.* **12**, 36 (1964).

[2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

sion of the box used for quantizing the continuum states, and we let $L \rightarrow \infty$. If the range and depth of the two-body potential are a and V_0, then the orders of magnitude of the various matrix elements are

$$V_{nn'} \sim (a/l)^3 V_0, \quad V_{nk} \sim (a/L)^3 V_0, \quad V_{kk'} \sim (a/L)^3 V_0. \quad (3)$$

It is the dependence on L which is of primary interest. In the limit $L \rightarrow \infty$ the discrete sum in Eq. (2b) vanishes as L^{-3}, whereas the integral over the continuum approaches a finite limit. Thus, the continuum decouples from the discrete states, and the resultant integral equation (2b) for Δ_k is formally the same as that which determines the existence of a two-particle bound state with a binding energy greater than E_F. Nuclear forces are not sufficiently strong to satisfy this condition, and we will restrict our general consideration to such forces. Thus, the dependence of Δ_k on the characteristic dimensions is determined by the first (homogeneous) term on the right-hand side of (2b), and we find

$$\Delta_k / \Delta_n = \mathcal{O}(V_0 a^3 / |E_F| L^3). \quad (4)$$

For this reason the integral over k' in Eq. (2a) vanishes as L^{-3} and only matrix elements to discrete states contribute in the evaluation of Δ_n. If we now let the system become infinitely large, $l \rightarrow \infty$ but $l/L = 0$, matrix elements to "continuum" states ($\epsilon > |E_F|$) still fail to contribute. Coupling to "continuum" states does obtain if we let $l \rightarrow \infty$, $L \rightarrow \infty$ with $l/L = 1$; this yields the usual BCS theory. Since any physical system is finite, only the limit with $l/L = 0$ is appropriate.

Before discussing what we believe to be improved formulations for the finite problem, we recast the BCS gap equation by separating the states lying near the Fermi surface (N) from those far away (K). These states could be bound (n) and continuum states (k), respectively, but some of the discrete states could be included in K, for instance. The resulting equations are the same as Eqs. (2a) and (2b) with $n \rightarrow N$, $k \rightarrow K$. We introduce $g_K^{(N)}$, where $\Delta_K = -\frac{1}{2} \sum_N g_K^{(N)} \Delta_N / E_N$, and $g_K^{(N)}$ satisfies

$$g_K^{(N)} = V_{KN} - \frac{1}{2} \sum_{K'} \frac{V_{KK'} g_{K'}^{(N)}}{E_{K'}}. \quad (5a)$$

In terms of $g_K^{(N)}$ the solution of Eq. (2a) for Δ_N becomes

$$\Delta_N = -\frac{1}{2} \sum_{N'} \frac{\Delta_{N'}}{E_{N'}} \left(V_{NN'} - \frac{1}{2} \sum_{K'} \frac{V_{NK'} g_{K'}^{(N')}}{E_{K'}} \right)$$
$$\equiv -\frac{1}{2} \sum_{N'} \frac{\Delta_{N'} G_{NN'}}{E_{N'}}. \quad (5b)$$

It can be verified by iteration of Eq. (5a) that G satisfied

$$G = V_R + V_R (Q/D) G, \quad (6)$$

where Q is a projection operator onto the set (K); the operator V_R (R for reduced) is restricted to allow matrix elements between time-reversed states only, and $D = -2E_K$. Since the states (K) are far removed from the Fermi surface, $E_K \approx |\epsilon_K|$, and G is independent of Δ_K. It follows that the nonlinear Eq. (5b) involves only the energy-gap parameters in the set (N). If the set K is identified as the continuum set k, the iteration of Eq. (6) shows that $G_{NN'} = G_{nn'} = V_{nn'}$, as demonstrated earlier.

II. MODIFIED VARIATIONAL WAVE FUNCTION

In order to include coupling to the continuum states in the BCS gap equation, we have reformulated the pairing problem in two ways which yield similar results. The first is a variational method, based on a generalization of the BCS trial wave function,

$$|\psi\rangle = \prod_{KL} (\bar{u}_{KL} + \bar{v}_{KL} a_K^\dagger a_L^\dagger) \prod_N (u_N + v_N a_N^\dagger a_{-N}^\dagger) |0\rangle, \quad (7)$$

where $|0\rangle$ is the vacuum state, $u_N^2 + v_N^2 = 1$, and we have fixed the normalization of the $\bar{u}_{KL}$ and $\bar{v}_{KL}$ by choosing $\bar{u}_{KL}^2 + \bar{v}_{KL}^2 = 1$. The set KL identifies two fermion states far away from the Fermi surface, and are not necessarily time-reversed; they may, in particular, be thought to belong to the continuum.

The Hamiltonian for the system is

$$H = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{4} \sum_{\alpha,\alpha',\alpha'',\alpha'''} \langle \alpha' \alpha | V | \alpha'' \alpha''' \rangle a_\alpha^\dagger a_{\alpha'}^\dagger a_{\alpha''} a_{\alpha'''}, \quad (8)$$

with ϵ_α measured with respect to the chemical potential (Fermi energy). Variation of the energy $\langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$ with respect to v_N and $\bar{v}_{KL}$ leads to the coupled equations

$$\Delta_N = -\frac{1}{2} \sum_{N'} \langle N - N | V | N' - N' \rangle \Delta_{N'} / E_{N'} - \int_K \int_L \langle N - N | V | KL \rangle \bar{v}_{KL} + \mathcal{O}\left(V_0 \int \int \bar{v}\bar{v}\bar{v} \right), \quad (9a)$$

$$(\epsilon_K + \epsilon_L) \bar{v}_{KL} = -\frac{1}{2} \sum_N \langle N - N | V | KL \rangle \Delta_N / E_N - \int_{K'} \int_{L'} \langle K'L' | V | KL \rangle \bar{v}_{K'L'} + \mathcal{O}\left(V_0 \int \int \bar{v}\bar{v}\bar{v} \right) + \mathcal{O}\left(E_F \int \int (\epsilon / E_F) \bar{v}\bar{v}\bar{v} \right), \quad (9b)$$

where Δ_N is introduced through

$$\begin{pmatrix} u_N^2 \\ v_N^2 \end{pmatrix} = \frac{1}{2} (1 \pm \epsilon_N / E_N),$$

with $E_N = (\epsilon_N^2 + \Delta_N^2)^{1/2}$. To lowest order in $\bar{v}_{KL}$, we find

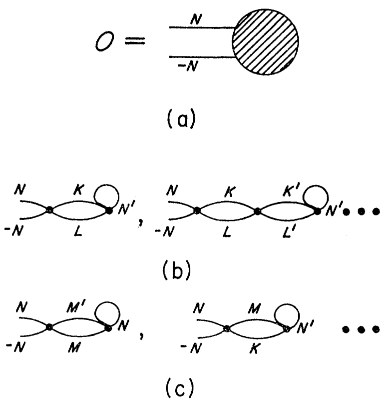

FIG. 1. Diagrammatic representation of the compensation condition. Figure (a) is the general condition; Fig. (b) displays some contributions from two-particle nontime-reversed distant intermediate states, and Fig. (c) some other two-particle intermediate-state contributions. (NM) denote particle states near the Fermi surface and (KL) represent distant states.

an expression identical to Eq. (5b), but with G satisfying

$$G=V+V(Q/D)G. \qquad (10)$$

Here V is the interparticle potential operator connecting to intermediate states which need not be time-reversed pairs (unlike V_R). Only in the limit of an infinite system does momentum conservation restrict V to connect time reversed states. To the same order in $\bar{v}_{KL}$, we see that

$$\bar{v}_{KL}=-\frac{1}{2(\epsilon_K+\epsilon_L)}\sum_N \langle N-N|G|KL\rangle\frac{\Delta_N}{E_N}. \qquad (11)$$

Utilizing Eq. (3) and defining the far states by $|\epsilon_K|>w$, we find that

$$\bar{v}_{KL}\lesssim\frac{\Delta}{2w}\times\begin{cases}(l/L)^3 & \text{for } K,L \text{ continuous,}\\ 1 & \text{for } K,L \text{ discrete,}\end{cases} \qquad (12)$$

where Δ is characteristic of the energy gap near the Fermi surface. Even though $\bar{v}_{KL}$ is of the order $(l/L)^3$ for the continuum, these states do contribute to the energy gap Δ_N because the number of such nonreversed states is greater than the number of reversed states by a factor L^3. Equation (12) allows us to estimate the error made by neglecting terms of higher order in $\bar{v}_{KL}$. We note that the kernels of our integral Eq. (9) are an expansion in $(\Delta/2w)^2$. The neglect of higher order terms is therefore certainly justified in the limit of weak two-particle forces.

III. MODIFIED BOGOLIUBOV PRINCIPLE

The other formulation of the theory invokes the Bogoliubov principle of compensating dangerous diagrams. Following the standard Bogoliubov-Valatin transformation[3] the compensation condition is stated as follows: All ground-state diagrams containing a time-reversed pair [see Fig. 1(a)] sum to zero. For the infinite system, this is equivalent to the statement that all diagrams containing an isolated pair sum to zero.[4] But in the finite system, momentum need not be conserved and we must include diagrams of the kind shown in Figs. 1(b) and 1(c). Note that no isolated time-reversed pairs can appear as intermediate states. Omission of the diagrams corresponding to Fig. 1(c), and others not shown, leads to the variational result, Eqs. (5b) and (10). The omission of diagrams (c) is in the spirit of the ordinary BCS theory. The "consistency" of including nonreversed continuum states but only reversed discrete states is as follows: Discrete time-reversed states have an uncertainty in center-of-mass momentum of the order of h/l, and nontime-reversed discrete pairs have center-of-mass momentum (roughly) greater than h/l. The continuum pairs which couple effectively to the time-reversed discrete pairs will also have center-of-mass momentum of the order or less than h/l.

IV. CONCLUSIONS

A result formally similar to that reported here has been presented by Bando, Murota, and Nagata.[5] Their motivation was not based on the loss of coupling between discrete and continuum states, but rather on the desire to treat hard cores and to include the diagrams of the Bethe-Goldstone[6] perturbation expansion. They obtain an effective pairing interaction based on a Brueckner-type T matrix which can include coupling to the continuum. By contrast, we have shown that we are forced to the present formulation in order to obtain the correct limit for an infinite system.

Applications to finite nuclei are in progress.

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[6] H. A. Bethe and J. Goldstone, Proc. Roy. Soc. (London) **A238**, 551 (1957).