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Treatment of Pairing in Many-Body Systems by an Equation-of-Motion Method*

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A completely unambiguous prescription is presented for extending the equation-of-motion method, including pairing, beyond the random-phase approximation. When combined with the idea of a generalized effective field, this prescription leads to a simple, self-consistent treatment of pairing, lifetime, and renormalization effects in many-body systems.

I. INTRODUCTION

The essence of the equation-of-motion method consists of searching for a quantum-mechanical operator $\mathcal{O}$ such that the commutator of $\mathcal{O}$ with the many-body Hamiltonian is proportional to $\mathcal{O}$. The proportionality constant is necessarily equal to some excitation energy of the system. If $\mathcal{O}$ is approximated by a single-particle creation or destruction operator (in the case of normal systems) or by a linear combination of two such operators (in the case of superfluid systems with pairing), then we have the so-called *random-phase approximation*. If $\mathcal{O}$ is approximated by a linear combination of both single-particle operators and products of single-particle operators, then we have the *extended random-phase approximation* of Suhl and Werthamer.[1] One of the difficulties[2] with this latter approach lies in the ambiguity in choice of *which* products of single-particle operators should be kept in the expansion of $\mathcal{O}$.

In this paper we propose a scheme for the expansion of $\mathcal{O}$ that is (1) completely unambiguous and well defined for any many-body system, (2) reasonably easy to apply, and (3) when combined with Nambu's idea of a generalized effective field,[3] leads to a remarkably simple treatment of pairing, lifetime, and renormalization effects in a self-consistent fashion.

In Sec. II, we set up the scheme for a many-fermion system (electrons). In Sec. III, we show how the scheme can be readily generalized to include many-boson systems, or mixed systems involving both bosons and fermions. In Sec. IV, we consider the example of a superconductor with disorder scattering.

II. THEORY

In general, any quantum-mechanical operator $\mathcal{O}$ has a time dependence given by

$$i\hbar(d\mathcal{O}/dt)=i\hbar(\partial\mathcal{O}/\partial t)+[\mathcal{O},H], \tag{2.1}$$

where $[\mathcal{O},H]$ is the commutator of $\mathcal{O}$ with H, the Hamiltonian of the system. We wish to look for an $\mathcal{O}$ such that

$$i\hbar(d\mathcal{O}/dt)=\hbar\omega\mathcal{O}. \tag{2.2}$$

Of course, a trivial example is $\mathcal{O}=e^{-i\omega t}$. Here, however, we want an operator that contains no explicit time dependence. Therefore, we must have

$$[\mathcal{O},H]=\hbar\omega\mathcal{O}. \tag{2.3}$$

For the time being, we assume $\hbar\omega$ is *real* and *positive*.

Let Ψ_G be the *exact* ground-state wave function associated with H, i.e.,

$$H\Psi_G=E_0\Psi_G, \tag{2.4}$$

E_0 being the ground-state energy. Consider the wave function $\mathcal{O}^\dagger\Psi_G$. We have

$$\begin{aligned} H(\mathcal{O}^\dagger\Psi_G)&=\mathcal{O}^\dagger H\Psi_G+[H,\mathcal{O}^\dagger]\Psi_G\\ &=\mathcal{O}^\dagger H\Psi_G+[\mathcal{O},H]^\dagger\Psi_G\\ &=(E_0+\hbar\omega)\mathcal{O}^\dagger\Psi_G. \end{aligned} \tag{2.5}$$

Thus $\mathcal{O}^\dagger\Psi_G$ is an exact excited-state wave function, with excitation energy $\hbar\omega$. In a similar fashion, we have

$$H(\mathcal{O}\Psi_G)=(E_0-\hbar\omega)\mathcal{O}\Psi_G. \tag{2.6}$$

The only way this can be consistent with Ψ_G being the ground state is by having

$$\mathcal{O}\Psi_G=0. \tag{2.7}$$

As we shall see presently, there may be solutions to Eq. (2.3) where the proportionality constant $\hbar\omega$ is *negative*. If this is the case, the $\mathcal{O}\Psi_G$ is an exact excited-state wave function, with excitation energy $|\hbar\omega|=-\hbar\omega$. Under such conditions, Eq. (2.7) is replaced by

$$\mathcal{O}^\dagger\Psi_G=0. \tag{2.8}$$

An operator which transforms Ψ_G into an excited-state wave function is called a quasiparticle creation operator; the Hermitian conjugate of this operator is the quasiparticle destruction operator. Having found a complete set of quasiparticle operators, in the process having simultaneously determined the corresponding excitation energies, we can determine Ψ_G from the conditions that each of the quasiparticle destruction operators, acting on Ψ_G, gives zero. Once one has determined Ψ_G, one can determine the ground-state energy E_0, and the excited-state wave functions.

Since H is Hermitian, we see that for any $\mathcal{O}$ that *exactly* satisfies Eq. (2.3), the proportionality constant must be *real* (since H has real eigenvalues). In practice, however, we are going only *approximately* to satisfy

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[1] H. Suhl and N. R. Werthamer, Phys. Rev. **122**, 359 (1961).

[2] L. M. Roth, Phys. Rev. Letters **20**, 1431 (1968); R. A. Young, Phys. Rev. **184**, 601 (1969).

[3] Y. Nambu, Phys. Rev. **117**, 648 (1960).

Eq. (2.3), thereby finding an approximate $\mathcal{O}$. In such a case, the corresponding proportionality constant may be *complex*. This indicates a finite *lifetime* to the *approximate* exited-state wave function $\mathcal{O}^\dagger\Psi_G$ (if $\mathrm{Re}\,\omega$ is positive) or $\mathcal{O}\Psi_G$ (if $\mathrm{Re}\,\omega$ is negative). If we write

$$\omega=\omega_1-i\omega_2\,, \tag{2.9}$$

ω_1 and ω_2 being real, then we want ω_1 and ω_2 to have the same signature. Thus, if ω_1 is positive, then the excited-state wave function is $\mathcal{O}^\dagger\Psi_G$ and $|\mathcal{O}^\dagger\Psi_G|^2$ is proportional to $e^{-2\omega_2 t}$, which will damp out with increasing time if ω_2 is positive. Similarly, if ω_1 is negative, then the excited-state wave function is $\mathcal{O}\Psi_G$, and $|\mathcal{O}\Psi_G|^2$ is proportional to $e^{+2\omega_2 t}$, which will damp out with increasing time if ω_2 is negative. In either case,

$$\tau=(2|\omega_2|)^{-1} \tag{2.10}$$

is the *lifetime* of the excited state.

The process of finding an $\mathcal{O}$ which approximately satisfies (2.3) leads to a secular equation for ω. It may be necessary to make the replacement

$$\omega \to \omega+i\eta_\omega\,, \tag{2.11}$$

where

$$\eta_\omega\equiv\eta(\omega_1/|\omega_1|)=\eta\ \mathrm{sgn}\,\omega_1\,, \tag{2.12}$$

η being a positive infinitesimal, in the secular equation. This ensures that any roots lying near the real axis in the complex ω plane will be in either the second or the fourth quadrant, in agreement with the discussion of the previous paragraph. This replacement of ω by $\omega+i\eta_\omega$ will actually need to be done during the process of evaluating certain integrals involving energy denominators containing ω. In evaluating such integrals, it is convenient to use the formal relation

$$\lim_{\eta\to 0^+}(x\pm i\eta)^{-1}=\mathcal{P}(1/x)\mp\pi i\delta(x)\,, \tag{2.13}$$

where $\mathcal{P}$ denotes "principal part of."

In the usual second-quantized notation, the many-electron Hamiltonian H is expressed in terms of the one-electron creation and destruction operators $c_{k,\sigma}{}^\dagger$ and $c_{k,\sigma}$, obeying the anticommutation relations

$$\begin{aligned}[][c_{k,\sigma},c_{k',\sigma'}{}^\dagger]_+&=\delta_{k,k'}\delta_{\sigma,\sigma'}\,,\\ [c_{k,\sigma},c_{k',\sigma'}]_+&=[c_{k,\sigma}{}^\dagger,c_{k',\sigma'}{}^\dagger]_+=0\,.\end{aligned} \tag{2.14}$$

It will be necessary to take thermal averages of various products of the c's, in a manner to be described in detail later. We shall assume that the only nonvanishing thermal averages are

$$n_{k,\sigma}\equiv\langle c_{k\sigma}{}^\dagger c_{k\sigma}\rangle \tag{2.15}$$

and

$$b_k\equiv\langle c_{-k\downarrow}c_{k\uparrow}\rangle\,. \tag{2.16}$$

If H commutes with the time-reversal operator, then we can usually take $n_{k,\sigma}=n_{-k,\sigma}=n_k$ to be independent of the direction of wave vector $\mathbf{k}$ and spin σ. The assumption of finite b_k is, of course, what leads to the possibility of pairing.

It is convenient to associate the one-electron creation and destruction operators in groups or families, such that the $\mathbf{k}$th group consists of the four operators[4]

$$c_{k\uparrow}\,,\ c_{k\uparrow}{}^\dagger\,,\ c_{-k\downarrow}\,,\ c_{-k\downarrow}{}^\dagger\,.$$

Any term of the many-electron Hamiltonian which is proportional to two or more operators from a given group is defined as a *pairing* term. (Note that the proportionality coefficients may also be products of operators.) We thus can break up our Hamiltonian into two parts,

$$H=H_0+H_1\,, \tag{2.17}$$

where H_0 is the *pairing* part of the Hamiltonian (i.e., all pairing terms) and H_1 is the *nonpairing* part. We shall consistently make the approximation of replacing the proportionality coefficients in H_0 by their thermal averages, so that H_0 is bilinear in the operators of each group.

Let

$$H(i)\equiv H\begin{pmatrix} i_1, & i_2, & \ldots, & i_n \\ i_{n+1}, & i_{n+2}, & \ldots, & i_{2n}\end{pmatrix}$$

be that portion of H_1 which is proportional to

$$(c_{-i_1}c_{-i_2}\cdots c_{-i_n})^\dagger(c_{i_{n+1}}c_{i_{n+2}}\cdots c_{i_{2n}})\,.$$

Here we are using the shorthand notation $i=(\mathbf{k},\sigma)$, $-i=(-\mathbf{k},-\sigma)$. In general, $H(i)$ will contain $(n!)^2$ terms of H_1. Since H_1 is nonpairing, no two i's in $H(i)$ can be the same or opposites. In other words, there is one operator from each of $2n$ distinct groups of operators. Now consider *all* the terms of H_1 composed of operators from the *same set* of $2n$ distinct groups. We can write

$$H_1=\sum_l H_{1l}\,, \tag{2.18}$$

where H_{1l} is the terms of H_1 composed of operators from the lth set of distinct groups.

In order to express this idea more formally, we define the permutation operator $P(\mu,\nu)$ which, when acting on $H(i)$, exchanges the μth index of the top row with the νth index of the bottom row, i.e.,

$$\begin{aligned}&P(\mu,\nu)H\begin{pmatrix} i_1, & \ldots, & i_{\mu-1}, & i_\mu, & i_{\mu+1}, & \ldots \\ i_{n+1}, & \ldots, & i_{n+\nu-1}, & i_{n+\nu}, & i_{n+\nu+1}, & \ldots\end{pmatrix}\\ &\qquad\equiv H\begin{pmatrix} i_1, & \ldots, & i_{\mu-1}, & i_{n+\nu}, & i_{\mu+1}, & \ldots \\ i_{n+1}, & \ldots, & i_{n+\nu-1}, & i_\mu, & i_{n+\nu+1}, & \ldots\end{pmatrix}.\end{aligned} \tag{2.19}$$

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[4] We do *not* wish to imply that these four operators form the elements of a *group* in the mathematical sense of the word.

Next we define the operator Q such that

$$Q\equiv 1+\sum_{\mu,\nu} P(\mu,\nu)+\sum_{\mu_i,\nu_i}{}' P(\mu_1,\nu_1)P(\mu_2,\nu_2) +\sum_{\mu_i,\nu_i}{}' P(\mu_1,\nu_1)P(\mu_2,\nu_2)P(\mu_3,\nu_3)+\cdots. \tag{2.20}$$

The prime on the summation indicates that $\mu_i>\mu_{i-1}$, $\nu_i>\nu_{i-1}$. The expression for Q is understood to terminate with a series involving a product of n P's. The total number of terms in Q is

$$\sum_{\nu=0}^{n} [n!/\nu!(n-\nu)!]^2=(2n)!(n!)^{-2}. \tag{2.21}$$

If we assume that H_1 conserves momentum and/or spin, then we have[5]

$$H_{1l}=QH(i)+QH^\dagger(i). \tag{2.22}$$

Returning to Eq. (2.17), let us replace H by

$$H'\equiv H_0'+H_1', \tag{2.23}$$

where

$$H_0'\equiv H_0+H_2,\quad H_1'\equiv\lambda(H_1-H_2). \tag{2.24}$$

Note that H' becomes H when $\lambda=1$. It is convenient to keep λ as a parameter, and set it equal to 1 at the end of the calculation. The additional Hamiltonian H_2, which has been added to H_0 and subtracted from H_1, is assumed to be a *pairing* Hamiltonian. Following Nambu,[3] the basic idea is to find that pairing Hamiltonian H_2 which most nearly cancels the nonpairing Hamiltonian H_1. Having made the optimum choice for H_2, we *assume* that H_1' can be treated as a small perturbation. This is the *key* assumption of this paper. There are certainly situations where it is a poor assumption, but there are many other cases where it appears to be an excellent assumption. It will usually turn out that the optimum choice for H_2 is *non-Hermitian.* This is related to the finite lifetimes of the quasiparticle excitations.

The operator $\mathcal{O}$ is expanded in terms of a set of operators $\psi_{l,\alpha}(\alpha=1,2;\, l=0,1,2,\ldots,N)$,

$$\mathcal{O}=\sum_{l=0}^{N}\sum_{\alpha=1}^{2} a_{l,\alpha}^*\psi_{l,\alpha}, \tag{2.25}$$

where the $a_{l,\alpha}^*$ are arbitrary coefficients. The operators $\psi_{l,\alpha}$, which will be defined presently, are chosen to have the property

$$\begin{gathered}\langle[\psi_{l,\alpha},\psi_{l',\alpha'}^\dagger]_+\rangle=\delta_{l,l'}\delta_{\alpha,\alpha'},\\ \langle[\psi_{l,\alpha},\psi_{l',\alpha'}]_+\rangle=\langle[\psi_{l,\alpha}^\dagger,\psi_{l',\alpha'}^\dagger]_+\rangle=0,\end{gathered} \tag{2.26}$$

so that they are fermionlike operators. As before, $[\ ,\ ]_+$ denotes the anticommutator, and $\langle\ \rangle$ denotes a thermal average. Because of the fact that we are *not* expanding $\mathcal{O}$ in terms of a *complete* set of operators, it follows that we can at best solve Eq. (2.3) approximately.

Again following Nambu,[3] we introduce the matrix notation

$$\begin{gathered}P=\begin{pmatrix}p_1\\p_2\end{pmatrix},\qquad P^\dagger=(p_1^\dagger,p_2^\dagger),\\ M=\begin{pmatrix}m_{11}&m_{12}\\m_{21}&m_{22}\end{pmatrix},\quad M^\dagger=\begin{pmatrix}m_{11}^\dagger&m_{21}^\dagger\\m_{12}^\dagger&m_{22}^\dagger\end{pmatrix}.\end{gathered} \tag{2.27}$$

An arbitrary M can be expanded in terms of the four matrices

$$\begin{gathered}\tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad i\tau_2=\begin{pmatrix}0&1\\-1&0\end{pmatrix},\\ \tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\quad \tau_4=\begin{pmatrix}1&0\\0&1\end{pmatrix}.\end{gathered} \tag{2.28}$$

If P and Q are two column vectors, we define

$$\begin{gathered}[P;Q]_+\equiv\begin{pmatrix}[p_1,q_1]_+&[p_1,q_2]_+\\ [p_2,q_1]_+&[p_2,q_2]_+\end{pmatrix},\\ [P;Q^\dagger]_+\equiv\begin{pmatrix}[p_1,q_1^\dagger]_+&[p_1,q_2^\dagger]_+\\ [p_2,q_1^\dagger]_+&[p_2,q_2^\dagger]_+\end{pmatrix}.\end{gathered} \tag{2.29}$$

If we now define

$$A_l\equiv\begin{pmatrix}a_{l1}\\a_{l2}\end{pmatrix},\quad \Psi_l\equiv\begin{pmatrix}\psi_{l1}\\\psi_{l2}\end{pmatrix}, \tag{2.30}$$

then we can rewrite (2.25) as

$$\mathcal{O}=\sum_{l=0}^{N} A_l^\dagger\Psi_l, \tag{2.31}$$

and (2.26) as

$$\begin{gathered}\langle[\Psi_l;\,\Psi_{l'}^\dagger]_+\rangle=\delta_{l,l'}\tau_4,\\ \langle[\Psi_l;\,\Psi_{l'}]_+\rangle=0.\end{gathered} \tag{2.32}$$

We will also need the notation

$$\langle[[\Psi_l,H];\,\Psi_{l'}^\dagger]_+\rangle\equiv K(l,l';H). \tag{2.33}$$

For given l, l', and H, K is a 2×2 matrix whose matrix elements are various thermal averages. If H is Hermitian, note that [using Eq. (2.35) below]

$$K^\dagger(l,0';H)=K(0',l;H). \tag{2.34}$$

Next we turn to the crucial question of defining the set of operators Ψ_l. We choose

$$\Psi_0=\begin{pmatrix}c_{k,\uparrow}\\c_{-k,\downarrow}^\dagger\end{pmatrix}. \tag{2.35}$$

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[5] In case H_1 conserves neither momentum nor spin, there will be additional terms coming from the possibility of changing the sign of one or both of the i's being interchanged in each permutation. Although it does not appear to occur in practice, in principle there may be additional terms for a sufficiently complicated many-body interaction which does conserve momentum and/or spin. These terms are associated with changing the signs of several of the i's among those involved in a multiple permutation.

This choice means (at least approximately) that $\mathcal{O}$ is either the destruction operator for a quasiparticle of momentum $\hbar\mathbf{k}$ and spin up, or, alternatively, the creation operator for a quasiparticle of momentum $-\hbar\mathbf{k}$ and spin down. We define Ψ_l $(l\neq 0)$ in terms of H_{1l} appearing in Eq. (2.18); namely,

$$[\Psi_0,H_{1l}]=R_l\Psi_l\,,\quad l\neq 0 \tag{2.36}$$

where R_l is a 2×2 matrix. Note that, because of the definition of H_{1l}, it follows that Eqs. (2.32) are satisfied for $l'\neq l$, quite independently of the form of R_l. Also, because of (2.14), Eqs. (2.32) are satisfied for $l=l'=0$. We now choose R_l in order that Eqs. (2.32) be satisfied for $l'=l\neq 0$. Obviously, $R_l=0$ unless the wave vector $\mathbf{k}$ lies in the set $\{l\}$. In the notation of Eq. (2.33), we have

$$R_l=K(0,l;H_{1l})\,. \tag{2.37}$$

Note that this can be rewritten

$$R_l=K(0,l;H_1)\,. \tag{2.38}$$

Let H_P be an arbitrary pairing Hamiltonian, treated in the approximate fashion discussed earlier [immediately after Eq. (2.17)]. It follows that

$$K(l,l';H_P)=0\,,\quad l\neq l'\,. \tag{2.39}$$

Note finally that

$$K(0,0;H_1)=0\,. \tag{2.40}$$

We next replace H by H' [as given by Eq. (2.23)] in our equation of motion, Eq. (2.3), as has already been discussed. Substitute in the expression for $\mathcal{O}$ [Eq. (2.31)]. Take the anticommutator of the equation with $\Psi_{l'}{}^\dagger$, and thermally average. Finally, we make use of Eqs. (2.32) and (2.33) to get

$$\sum_{l=0}^{N} A_l{}^\dagger[K(l,l';H')-\hbar\omega\delta_{l,l'}\tau_4]=0\,. \tag{2.41}$$

The work of Roth,[2] suitably generalized to include pairing, would formally resemble Eq. (2.41). There is the following important difference, however: In addition to the use of a generalized effective field, the present approach goes beyond that of Roth in presenting a prescription [Eq. (2.36)] for choosing an optimum set of operators Ψ_l for expanding $\mathcal{O}$. With the aid of Eqs. (2.23), (2.24), (2.34), (2.38), (2.39), and (2.40), this can be rewritten more explicitly. For $l'=0$, we have

$$A_0{}^\dagger[K(0,0;H_0')-\hbar\omega\tau_4]=\lambda A_0{}^\dagger K(0,0;H_2)-\lambda\sum_{l=1}^{N}A_l{}^\dagger R_l{}^\dagger\,. \tag{2.42}$$

For $l'\neq 0$, we have

$$A_{l'}{}^\dagger[K(l',l';H_0')-\hbar\omega\tau_4]+\lambda A_0{}^\dagger R_l=\lambda A_{l'}{}^\dagger K(l',l';H_2)-\lambda\sum_{l=1}^{N}A_l{}^\dagger K(l,l';H_1)\,. \tag{2.43}$$

Since H_2 will be chosen to make $H_1'=\lambda(H_1-H_2)$ small, we expect $A_l{}^\dagger$ $(l\neq 0)$ to be much smaller than $A_0{}^\dagger$. In particular, we expect $A_l{}^\dagger$ $(l\neq 0)$ to be linear in λ, whereas $A_0{}^\dagger$ is independent of λ. Thus, the left-hand side of Eq. (2.43) is linear in λ; the right-hand side is quadratic in λ. We thus discard the right-hand side and solve for $A_l{}^\dagger$ $(l\neq 0)$ in terms of $A_0{}^\dagger$:

$$A_l{}^\dagger=\lambda A_0{}^\dagger R_l[\hbar\omega\tau_4-K(l,l;H_0')]^{-1}\,. \tag{2.44}$$

We now choose H_2 such that

$$K(0,0;H_2)=\lambda\sum_{l=1}^{N}R_l[\hbar\omega\tau_4-K(l,l;H_0')]^{-1}R_l{}^\dagger\,. \tag{2.45}$$

Equations (2.44) and (2.45) imply that the right-hand side of (2.42) vanishes, or

$$A_0{}^\dagger[K(0,0;H_0')-\hbar\omega\tau_4]=0\,. \tag{2.46}$$

Corresponding to Eq. (2.46), we have the secular equation

$$\det[K(0,0;H_0')-\hbar\omega\tau_4]=0\,. \tag{2.47}$$

This equation has the form

$$\begin{vmatrix} a-\hbar\omega & c \\ d & b-\hbar\omega \end{vmatrix}=0\,, \tag{2.48}$$

the roots of which are

$$\hbar\omega=\tfrac{1}{2}(a+b)\pm[\tfrac{1}{4}(a-b)^2+cd]^{1/2}\,. \tag{2.49}$$

(It should be remembered that a, b, c, d may be complex and may be functions of both $\mathbf{k}$ and ω.) Corresponding to these two roots, there are two possibilities for $\mathcal{O}$, which we designate as $\mathcal{O}(+)$ and $\mathcal{O}(-)$, respectively. In either case, if ω_1 (the real part of ω) is positive, $\mathcal{O}$ is the destruction operator for a quasiparticle of momentum $\hbar\mathbf{k}$ and spin up. If ω_1 is negative, $\mathcal{O}$ is the creation operator for a quasiparticle of momentum $-\hbar\mathbf{k}$ and spin down. If H commutes with the time-reversal operator, it will usually turn out that $\omega(-)=-\omega(+)$. This occurs by virtue of $(a+b)$ being proportional to ω in Eqs. (2.48) and (2.49). In this case, $\mathcal{O}(+)$ is a quasiparticle destruction operator, $\mathcal{O}(-)$ a quasiparticle creation operator.[6]

In general, we want $\mathcal{O}$ normalized such that

$$\langle[\mathcal{O},\mathcal{O}^\dagger]_+\rangle=1\,. \tag{2.50}$$

To the accuracy to terms linear in λ, we can approximate $\mathcal{O}$ in this equation by

$$\mathcal{O}=A_0{}^\dagger\Psi_0\,, \tag{2.51}$$

thereby getting

$$A_0{}^\dagger A_0=1\,. \tag{2.52}$$

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[6] Even with Hamiltonians not invariant to time-reversal, it may happen that $\omega(-)=-\omega(+)$. An example is a superconductor with paramagnetic impurity atoms, *provided the magnetic moments of the impurities are randomly oriented.* This example will be discussed briefly in Sec. IV.

We define the column vector

$$\tilde{O}\equiv\begin{pmatrix}\Theta(+)\\ \Theta(-)\end{pmatrix},\tag{2.53}$$

and the square matrix

$$U^{-1}\equiv\begin{pmatrix}A_0{}^\dagger(+)\\ A_0{}^\dagger(-)\end{pmatrix},\tag{2.54}$$

[$A_0{}^\dagger(+)$ goes with $\Theta(+)$; $A_0{}^\dagger(-)$ goes with $\Theta(-)$.] Equation (2.51) can be rewritten

$$\Psi_0=U\tilde{O}.\tag{2.55}$$

If H_0' were Hermitian, then U would be a unitary matrix, but H_2, and thus H_0', will not be Hermitian when there are lifetime effects. For either $\Theta(+)$ or $\Theta(-)$, we have

$$\langle\Theta^\dagger\Theta\rangle=f(\omega)\equiv\pi^{-1}|\omega_2|\times\int d\omega'[(\omega'-\omega_1)^2+\omega_2{}^2]^{-1}[e^{\beta\hbar\omega'}+1]^{-1},\tag{2.56}$$

while

$$\langle\Theta^\dagger(+)\Theta(-)\rangle=0.\tag{2.57}$$

If $\omega_1>0$, then $f(\omega)$ is the thermodynamic probability of occurrence of the quasiparticle excitation. If $\omega_1<0$, then $1-f(\omega)=f(-\omega)$ is the thermodynamic probability.[7] With the aid of Eqs. (2.55)–(2.57), we can evaluate the thermodynamic averages $n_{k\sigma}$ and b_k, defined in Eqs. (2.15) and (2.16). Writing

$$f_\pm\equiv f[\omega(\pm)],\tag{2.58}$$

we have

$$\begin{aligned}n_{k\uparrow}&=|U_{11}|^2f_++|U_{12}|^2f_-,\\ n_{-k\downarrow}&=|U_{21}|^2(1-f_+)+|U_{22}|^2(1-f_-),\\ b_k&=U_{21}{}^*U_{11}f_++U_{22}{}^*U_{12}f_-.\end{aligned}\tag{2.59}$$

The form of the matrix $K(l,l;H_2)$, and thus that of H_2 itself, is determined implicitly by Eq. (2.45). Let us consider what happens when we make certain assumptions about the form of R_l. First, consider the case where R_l is proportional to a *unitary matrix*, the proportionality constant being a complex number. Equation (2.45) is now consistent with the assumption that $K(l,l;H_0)$ contains no terms proportional to τ_4 and that $K(l,l;H_2)$ has every term which is proportional to τ_4 also proportional to ω. But these are just the assumptions that lead to $n_{k,\sigma}=n_{-k,-\sigma}=n_k$ and $\omega(-)=-\omega(+)$.

Secondly, we consider the case where R_l is proportional to a *real matrix*, the proportionality constant being a complex number. (A real matrix is one with *real* matrix elements.) Equation (2.45) is now consistent with the assumption that neither $K(l,l;H_0)$ nor $K(l,l;H_2)$ contains terms proportional to τ_2. $K(l,l;H_0)$ containing no terms proportional to τ_2 means that b_k is *real*.

III. EXTENSION TO MANY-BOSON AND MIXED SYSTEMS

If we are dealing with a many-boson system rather than a many-fermion system, we still define the groups of operators in the same fashion as before. A group contains the four creation and destruction operators associated with a single-particle state and the corresponding time-reversed single-particle state. Spin indices are suppressed if the bosons have zero spin. In this latter case, the $\mathbf{k}=0$ group has only two operator members, and thus must be treated with special care. (The possibility of a bose condensation is another reason for treating the $\mathbf{k}=0$ group with special care.) Any term of the many-particle Hamiltonian which is proportional to two or more operators from a given group is defined as a pairing term. The nonpairing part of the Hamiltonian is broken up into portions H_{1l}, the latter being the terms of H_1 composed of operators from the lth set of distinct groups. In case particle number is not conserved (e.g., phonons), then Eqs. (2.19)–(2.22) are no longer applicable, since $H(i)$ does not necessarily contain the same number of creation and destruction operators.

Because of the change in statistics, we must replace the *anticommutators* by *commutators* in Eqs. (2.14), (2.26), (2.29), (2.32), (2.33), (2.50). This means that τ_4 should be replaced by τ_3 in Eqs. (2.32) and (2.41)–(2.48) and in the discussion of the next to last paragraph of Sec. II. The factor 1 on the right-hand side of Eqs. (2.50) and (2.52) should be replaced by $\mathrm{sgn}\omega_1$. (This implies that U is not necessarily unitary even in the absence of lifetime effects.) In addition, the thermodynamic factor $f(\omega)$ of Eq. (2.56) must be redefined as

$$f(\omega)\equiv(\mathrm{sgn}\omega_1)\pi^{-1}|\omega_2|\times\int d\omega'[(\omega'-\omega_1)^2+\omega_2{}^2]^{-1}[e^{\beta\hbar\omega'}-1]^{-1}.\tag{3.1}$$

If $\omega_1>0$, then $f(\omega)$ is the thermodynamic probability of occurrence of the quasiparticle excitation. If $\omega_1<0$, then $-1+f(\omega)=f(-\omega)$ is the thermodynamic probability. In the second of Eqs. (2.59), the factors $(1-f_+)$ and $(1-f_-)$ must be replaced by $[\mathrm{sgn}\omega_1(+)+f_+]$ and $[\mathrm{sgn}\omega_1(-)+f_-]$, respectively.

The present approach is well suited to a calculation of the condensate-induced effective attractive interaction between helium atoms in superfluid He^4, first

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[7] The quantity $f(\omega)$ is a weighted average of the Fermi factor $(1+e^{\beta\hbar\omega'})^{-1}$, the weighting factor associated with frequency ω' being the *intensity* of the ω' component in the Fourier decomposition, for $t>0$, of the function $e^{-i\omega t}$. This function contains the time dependence of the quasiparticle-excited-state wave function $\Theta^\dagger\Psi_G$, if $\omega_1>0$, or of the complex conjugate of the excited-state wave function $(\Theta\Psi_G)^*$, if $\omega_1<0$. Such a choice of $f(\omega)$ ensures that detailed balancing will hold in any transfer of electrons between the system and a reservoir of free electrons in thermal equilibrium (a transfer by tunneling, for example). See L. P. Kadanoff, in *Lectures on the Many-Body Problem*, edited by E. R. Caianiello (Academic Press Inc., New York, 1964), Vol. II, p. 77.

calculated by the writer[8] using a canonical-transformation technique. The present scheme is more satisfactory in that it takes into account lifetime and renormalization effects. In treating this problem, it is necessary to replace the two-body interaction matrix elements by an equivalent scattering matrix, in the fashion discussed in Ref. 8.

There are no additional difficulties in principle with treating many-body systems of interacting bosons and fermions. There are now groups composed of fermion operators and groups composed of boson operators. The pairing Hamiltonian H_0 and the nonpairing Hamiltonian H_1 are defined just as before. H_1 is broken up into portions H_{1l} as previously, only now the set $\{l\}$ may contain both boson groups and fermion groups. One looks for a set of bosonlike quasiparticle excitations in the manner described in this section, while simultaneously looking for a set of fermionlike quasiparticle excitations in the manner described in Sec. II. The self-consistency equations for the two classes of excitations will be coupled—this being the difficulty in practice.

Physical examples are the interacting electrons and phonons of a superconducting metal, and the interacting He^3 and He^4 atoms of a superfluid He^3-He^4 solution. It is generally believed that pairing occurs among the electrons of the former example and among the He^4 atoms of the latter example. It would be interesting to investigate the possibility of simultaneous pairing of the phonons of the former example and the He^3 atoms of the latter example. If one ignores the possibility of phonon pairing, it appears that the present scheme gives results for the electron-phonon system equivalent to those obtained from the Green's-function approach.[9]

IV. EXAMPLE: SUPERCONDUCTING ALLOYS

We illustrate the application of the formalism of Sec. II by treating the problem of a dilute superconducting alloy. Initially we consider the case of *nonmagnetic* impurity atoms.[10] The pairing part of the many-electron Hamiltonian is assumed to be the Hamiltonian of the Bardeen-Cooper-Schrieffer (BCS) theory[11]:

$$H_0=\sum_k \epsilon_k(c_{k\uparrow}{}^\dagger c_{k\uparrow}+c_{-k\downarrow}{}^\dagger c_{-k\downarrow}) - V\sum_{k,k'} c_{k'\uparrow}{}^\dagger c_{-k'\downarrow}{}^\dagger c_{-k\downarrow}c_{k\uparrow}\,. \tag{4.1}$$

The nonpairing part of the Hamiltonian is

$$H_1={\sum_{k,k'}}' V_{a,k'-k}(c_{k'\uparrow}{}^\dagger c_{k\uparrow}+c_{-k\downarrow}{}^\dagger c_{-k'\downarrow})\,. \tag{4.2}$$

Since the scattering is nonmagnetic, the terms $c_{k'\uparrow}{}^\dagger c_{k\uparrow}$ and $c_{-k\downarrow}{}^\dagger c_{-k'\downarrow}$ enter with the same sign. The prime over the summation sign indicates $\mathbf{k}'\neq\mathbf{k}$. In other words, any *forward* scattering has been removed from H_1 and incorporated in the one-electron kinetic energy. The matrix element $V_{a,k'-k}$, for $\mathbf{k}'$ and $\mathbf{k}$ lying in the vicinity of the Fermi surface, will be assumed to be a function of the magnitude of momentum transfer $|\mathbf{k}'-\mathbf{k}|$. We have

$$H_{1l}=V_{a,k'-k}(c_{k'\uparrow}{}^\dagger c_{k\uparrow}+c_{-k\downarrow}{}^\dagger c_{-k'\downarrow}) + V_{a,k-k'}(c_{k\uparrow}{}^\dagger c_{k'\uparrow}+c_{-k'\downarrow}{}^\dagger c_{-k\downarrow})\,, \tag{4.3}$$

so that the set $\{l\}=\{\mathbf{k},\mathbf{k}'\}$. Defining the order parameter

$$\Delta=V\sum_k b_k\,, \tag{4.4}$$

we have

$$[\Psi_k,H_0]=[\epsilon_k\tau_3-\tfrac{1}{2}(\Delta+\Delta^*)\tau_1-\tfrac{1}{2}(\Delta-\Delta^*)i\tau_2]\Psi_k\,, \tag{4.5}$$

or

$$K(0,0;H_0)=[\epsilon_k\tau_3-\tfrac{1}{2}(\Delta+\Delta^*)\tau_1-\tfrac{1}{2}(\Delta-\Delta^*)i\tau_2]\,. \tag{4.6}$$

Similarly,

$$[\Psi_k,H_{1l}]=V_{a,k-k'}\tau_3\Psi_{k'}\,. \tag{4.7}$$

It follows that, for $l=0$,

$$\Psi_0=\Psi_k\,, \tag{4.8}$$

and, for $l\neq 0$, $\mathbf{k}'\neq\mathbf{k}$,

$$\Psi_l=\Psi_{k'}\,, \tag{4.9}$$

$$R_l=V_{a,k-k'}\tau_3\,. \tag{4.10}$$

Note that R_l is proportional to a *real*, *unitary* matrix. This means, first of all, that $K(0,0;H_0)$ and $K(l,l;H_0)$ contain nothing proportional to τ_2. In other words, b_k and Δ may be taken *real*. Thus,

$$\begin{aligned} K(0,0;H_0)&=\epsilon_k\tau_3-\Delta\tau_1\,,\\ K(l,l;H_0)&=\epsilon_{k'}\tau_3-\Delta\tau_1\,. \end{aligned} \tag{4.11}$$

Secondly, $K(0,0;H_2)$ and $K(l,l;H_2)$ contain nothing proportional to τ_2, and anything proportional to τ_4 is simultaneously proportional to ω. Let us assume the form (for all l, including $l=0$)

$$K(l,l;H_2)=W'\tau_3+(1-Z)(\Delta\tau_1+\hbar\omega\tau_4)\,. \tag{4.12}$$

The parameter W' is assumed real, but Z is not necessarily so. Defining

$$\alpha=[(\hbar\omega)^2-\Delta^2]^{1/2}\,, \tag{4.13}$$

we have

$$\begin{aligned} R_l[\hbar\omega\tau_4-K(l,l;H_0')]^{-1}R_l{}^\dagger &=|\mathrm{V}_{a,k-k'}|^2\tau_3[Z(\Delta\tau_1+\hbar\omega\tau_4)-(\epsilon_{k'}+W')\tau_3]^{-1}\tau_3\\ &=|V_{a,k-k'}|^2[(Z\alpha)^2-(\epsilon_{k'}+W')^2]^{-1}\\ &\qquad\times[Z(\Delta\tau_1+\hbar\omega\tau_4)+(\epsilon_{k'}+W')\tau_3]\\ &=(2\alpha)^{-1}|V_{a,k-k'}|^2[(\epsilon_{k'}+W'+Z\alpha)^{-1}\\ &\qquad\times(\Delta\tau_1+\hbar\omega\tau_4-\alpha\tau_3)-(\epsilon_{k'}+W'-Z\alpha)^{-1}\\ &\qquad\times(\Delta\tau_1+\hbar\omega\tau_4+\alpha\tau_3)]\,. \end{aligned} \tag{4.14}$$

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[8] R. H. Parmenter, Phys. Rev. **170**, 194 (1968).

[9] J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964), Chap. 7.

[10] D. Markowitz and L. P. Kadanoff, Phys. Rev. **131**, 563 (1963).

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

We assume that α and $Z\alpha$ lie in the same quadrant of the complex plane as does ω. (This will later be checked.) Thus, replacing ω by $\omega+i\eta_\omega$ is equivalent to replacing α by $\alpha+i\eta_\alpha$. Replacing the sum over l, which is the same as a sum over $\mathbf{k}'$, by the equivalent integration, we get

$$\begin{aligned}K(0,0;H_2)&=(2\pi)^{-3}(2\alpha)^{-1}(\Delta\tau_1+\hbar\omega\tau_4-\alpha\tau_3)\\&\quad\times\Big[\mathcal{P}\int d^3k'\,|V_{a,k-k'}|^2(\epsilon_{k'}+W'+(Z\alpha)_1)^{-1}\\&\quad-\pi i\operatorname{sgn}(Z\alpha)_1\int d^3k'\,|V_{a,k-k'}|^2\delta(\epsilon_{k'}+W'+(Z\alpha)_1)\Big]\\&\quad-(2\pi)^{-3}(2\alpha)^{-1}(\Delta\tau_1+\hbar\omega\tau_4+\alpha\tau_3)\\&\quad\times\Big[\mathcal{P}\int d^3k'\,|V_{a,k-k'}|^2(\epsilon_{k'}+W'-(Z\alpha)_1)^{-1}\\&\quad+\pi i\operatorname{sgn}(Z\alpha)_1\int d^3k'\,|V_{a,k-k'}|^2\delta(\epsilon_{k'}+W'-(Z\alpha)_1)\Big].\end{aligned}\tag{4.15}$$

The above integrals are insensitive to $\mathbf{k}$, W', and $(Z\alpha)_1$ as long as $\mathbf{k}$ lies in the vicinity of the Fermi surface, and W' and $(Z\alpha)_1$ are much smaller in magnitude than the Fermi energy. Thus we approximate the above integrals by

$$W\equiv-(2\pi)^{-3}\mathcal{P}\int d^3k\,|V_{a,k}|^2\epsilon_k^{-1},\tag{4.16}$$

$$\begin{aligned}\tau^{-1}&\equiv(2\pi)^{-2}\hbar^{-1}\int d^3k\,|V_{a,k}|^2\delta(\epsilon_k)\\&=N(0)\int_{-1}^{1}|V_a(\mu)|^2d\mu.\end{aligned}\tag{4.17}$$

Here μ (the cosine of the angle between $\mathbf{k}$ and $\mathbf{k}'$) is a measure of the momentum transfer at the Fermi surface. $N(0)$, the density of one-electron states of a given spin per unit energy at the Fermi surface, is the same as in the BCS theory. We get

$$\begin{aligned}&K(0,0;H_2)\\&\quad=-(2\alpha)^{-1}(\Delta\tau_1+\hbar\omega\tau_4-\alpha\tau_3)\\&\qquad\qquad\times[W+i(\hbar/2\tau)\operatorname{sgn}(Z\alpha)_1]\\&\qquad+(2\alpha)^{-1}(\Delta\tau_1+\hbar\omega\tau_4+\alpha\tau_3)\\&\qquad\qquad\times[W-i(\hbar/2\tau)\operatorname{sgn}(Z\alpha)_1]\\&\quad=W\tau_3-i(\hbar/2\tau\alpha)(\Delta\tau_1+\hbar\omega\tau_4)\operatorname{sgn}(Z\alpha)_1.\end{aligned}\tag{4.18}$$

Comparing this with (4.12), we see that self-consistency requires

$$W'=W,\tag{4.19}$$

$$Z=1+i(\hbar/2\tau\alpha)\operatorname{sgn}(Z\alpha)_1.\tag{4.20}$$

This last equation shows that (for τ^{-1} small) αZ lies in the same quadrant of the complex plane as does α and ω. Thus

$$\begin{aligned}Z&=1+i(\hbar/2\tau\alpha)\operatorname{sgn}\alpha_1\\&=1+i(\hbar/2\tau\alpha)\operatorname{sgn}\omega_1.\end{aligned}\tag{4.21}$$

Equation (2.47) now becomes

$$\det[Z\hbar\omega\tau_4+Z\Delta\tau_1-(\epsilon_k+W)\tau_3]=0,\tag{4.22}$$

the roots of which are

$$\pm(\epsilon_k+W)=Z\alpha=\alpha+i(\hbar/2\tau)\operatorname{sgn}\alpha_1.\tag{4.23}$$

This gives immediately

$$\alpha=\pm[|\epsilon_k+W|-i(\hbar/2\tau)],\tag{4.24}$$

$$\hbar\omega=\pm\{[|\epsilon_k+W|-i(\hbar/2\tau)]^2+\Delta^2\}^{1/2}.\tag{4.25}$$

Next we must solve Eq. (2.46) for the row-vector coefficients $A_0^\dagger(+)$ and $A_0^\dagger(-)$. The amplitudes of the coefficients are chosen to satisfy Eq. (2.52). From the $A_0^\dagger$'s, we can determine the matrix U. The phases of the coefficients are chosen such that, when U is substituted into Eqs. (2.59), the resultant b_k is *real*. Finally, this expression for b_k is substituted into Eq. (4.4), resulting in an integral equation for a *self-consistent* value of Δ. In the limit of small τ^{-1}, the integral equation is just the BCS gap equation. These results are consistent with those of Ref. 10.

Finally, let us mention briefly what happens when the impurity atoms are paramagnetic.[12] We assume that the spins of the impurity atoms are *randomly oriented*. The pairing part of the Hamiltonian is still given by (4.1), but the nonpairing part is

$$\begin{aligned}H_1=&\sum_{k,k'}{}'\,V_{a,k'-k}(c_{k'\uparrow}{}^\dagger c_{k\uparrow}+c_{-k\downarrow}{}^\dagger c_{-k'\downarrow})\\&+\sum_{k,k'}{}'\,V_{b,k'-k}(c_{k'\uparrow}{}^\dagger c_{k\uparrow}-c_{-k\downarrow}{}^\dagger c_{-k'\downarrow}).\end{aligned}\tag{4.26}$$

The first line represents the nonmagnetic scattering due to the electrostatic fields of the impurity atoms; the second line represents the magnetic scattering due to the magnetic moments of the impurity atoms. V_a is independent of the orientation of the impurity-atom spins, but V_b is not. Denoting an average over all possible random orientations by $\langle\ \rangle_S$, we have

$$\langle V_a{}^\dagger V_b\rangle_S=0,\tag{4.27}$$

$$\langle V_b{}^\dagger V_b\rangle_S\neq0.\tag{4.28}$$

Equations (4.8) and (4.9) are still true, but Eq. (4.10) is replaced by

$$R_l=V_{a,k-k'}\tau_3+V_{b,k-k'}\tau_4.\tag{4.29}$$

The very different effect on superconductivity of paramagnetic impurities as contrasted with nonmagnetic

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[12] S. Skalski, O. Betbeder-Matibet, and P. R. Weiss, Phys. Rev. **136**, A1500 (1964).

impurities results entirely from the difference between Eqs. (4.10) and (4.29), and in particular from the fact that the second term on the right-hand side of (4.29) is proportional to τ_4 rather than τ_3. Because of (4.27), it is still possible to take b_k and Δ real, and to assume that $K(0,0;H_2)$ and $K(l,l;H_2)$ contain nothing proportional to τ_2 and something proportional to $\omega\tau_4$. However, it is necessary to modify (4.12) by taking *different* coefficients for the two terms $\Delta\tau_1$ and $\hbar\omega\tau_4$. This leads to the results discussed in detail in Ref. 12.

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Destruction of Superconductivity in Disordered Near-Monolayer Films*

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Severe decreases are observed in the superconducting transition temperatures of metallic films as they are made thinner and more disordered. Explanations for these decreases in the transition temperature are discussed. These include changes in the phonon spectrum, the effect of the metal-insulator boundary, size quantization in small particles, the effect of an activated conduction mechanism in the normal state, and, finally, the effect of order-parameter fluctuations.

I. INTRODUCTION

In recent years, there has been much speculation about the properties of ultrathin film superconductors and, especially, the possibility of achieving higher transition temperatures T_c than those presently attained in such systems. Buckel and Hilsch[1] and Zavaritsky[2] initially showed that soft metals deposited at cryogenic temperatures had T_c's significantly above the bulk value in fairly thick films, which electron diffraction work indicated were composed of small metallic grains. With recent work[3–5] on the effects of softening the phonon spectrum, we seem to understand why T_c goes up, and a discussion of this work will not be presented here. Instead, we consider the problem of the decreasing T_c found in the thinnest films. Throughout the literature, there have been various reports that T_c decreases in the very thinnest metallic films.[6,7] In this paper, we present a systematic experimental investigation of this problem along with the effect of dielectric overlayers, and a discussion is given of the physical mechanisms that can affect T_c in this regime.

As mentioned, the general substance of this paper is the severe decrease in the T_c of superconducting films

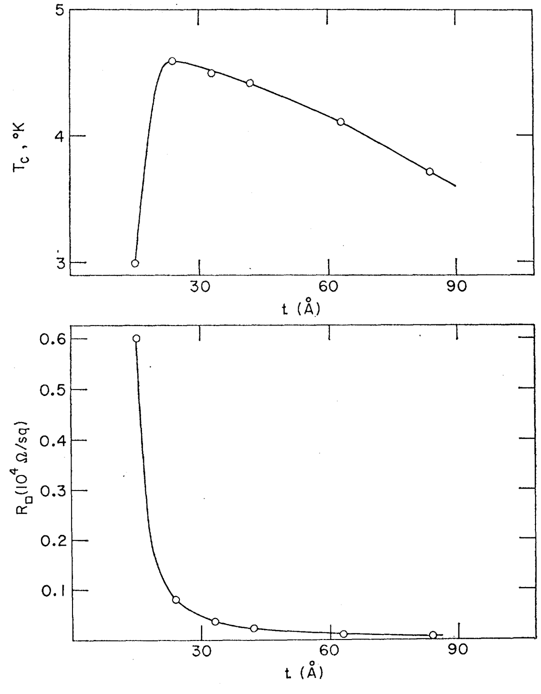

FIG. 1. T_c versus thickness for Al film deposited on previously deposited SiO. Lower graph shows sharply increased resistance at small thicknesses.

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