Ground-State Energy and Green's Function for Reduced Hamiltonian for Superconductivity*

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(Received December 14, 1959)

In their theory of superconductivity, Bardeen, Cooper, and Schrieffer made use of a reduced Hamiltonian which included only scattering of pairs of particles of opposite momentum and spin. It is shown that the solution they obtained by a variational method is correct to $O(1/n)$ for a large system. The single particle Green's function is derived and used to calculate the interaction energy.

IN their theory of superconductivity, Cooper, Schrieffer, and one of the authors[1] made use of a reduced Hamiltonian which included only scattering of pairs of particles of opposite momentum and spin. They suggested that the solution obtained by a variational method might well be correct to $O(1/n)$ in the number of particles, n. They showed in particular that $\langle H_{\rm red}{}^p\rangle$ differs from $\langle H_{\rm red}\rangle^p$ by $O(1/n)$ for $p=2,3$ and very likely for $p\ll n$, where the averages are taken with respect to the variational wave function for the ground state. If this were true for all p, the energy would be exact. Anderson[2] showed that the reduced problem is analogous to one of a system of interacting spins and gave a physical argument, based on the correspondence principle, which also indicated that the solution is correct to $O(1/n)$. Particularly because the validity of the solution has been questioned, we thought it desirable to give a direct proof based on the structure of the wave functions. We also derive the single particle Green's function for the system and use it to calculate the energy of $H_{\rm red}$ from an expression given by Galitskii and Migdal.[3]

The reduced Hamiltonian may be written in the form:

$$H_{\rm red}=\sum_{\mathbf{k},\sigma}(\epsilon_k+\mu)c_{\mathbf{k}\sigma}{}^*c_{\mathbf{k}\sigma}+\sum V_{\mathbf{k}\mathbf{k}'}b_{\mathbf{k}'}{}^*b_{\mathbf{k}}, \quad (1)$$

where $c_{\mathbf{k}\sigma}{}^*$ is a creation operator for a particle in a state of wave vector $\mathbf{k}$ and spin σ, $b_{\mathbf{k}}=c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}$ destroys the pair $\mathbf{k}\equiv(\mathbf{k}\uparrow,-\mathbf{k}\downarrow)$ and $\epsilon_{\mathbf{k}}$ is the Bloch energy measured from the Fermi energy, μ. For simplicity we assume that the interaction $V_{\mathbf{k}\mathbf{k}'}=V_{\mathbf{k}'\mathbf{k}}$ is real. The ground-state wave function Ψ_0 of $H_{\rm red}$ is a linear combination of configurations in which the single particle states are occupied in pairs of opposite momentum and spin.

Following BCS it is convenient to decompose Ψ_0 into parts with definite occupancy of a particular pair, $\mathbf{k}$:

$$\Psi_0=u_{\mathbf{k}}b_{\mathbf{k}}{}^*\varphi_{0\mathbf{k}}(n-2)+v_{\mathbf{k}}\varphi_{0\mathbf{k}}(n), \quad (2)$$

where $u_{\mathbf{k}}{}^2=1-v_{\mathbf{k}}{}^2=h(\mathbf{k})$ is the probability of occupancy of $\mathbf{k}$. Here $\varphi_{0\mathbf{k}}(n)$ is a function of n particles in which the pair $\mathbf{k}$ is not occupied.

The functions $\varphi_{0\mathbf{k}}$ may be further decomposed into parts with definite occupancy of some other pair $\mathbf{k}'$:

$$\varphi_{0\mathbf{k}}(n)=u_{\mathbf{k}\mathbf{k}'}b_{\mathbf{k}}{}^*\varphi_{0\mathbf{k}\mathbf{k}'}(n-2)+v_{\mathbf{k}\mathbf{k}'}\varphi_{0\mathbf{k}\mathbf{k}'}(n). \quad (3)$$

This function is similar to Ψ_0 except that it contains no configurations in which the pair $\mathbf{k}$ is occupied. To terms of $O(1/n)$, the coefficients of this second decomposition must be independent of $\mathbf{k}$ and the same as those in (2), i.e.,

$$u_{\mathbf{k}\mathbf{k}'}=u_{\mathbf{k}'}+O(1/n), \quad (4a)$$

$$v_{\mathbf{k}\mathbf{k}'}=v_{\mathbf{k}'}+O(1/n). \quad (4b)$$

This is true because the occupancy of $\mathbf{k}'$ depends on the interaction of pairs in $\mathbf{k}'$ with all other pairs, and can be changed only to $O(1/n)$ if configurations with one pair state, e.g., $\mathbf{k}$, are omitted. In the BCS solution, there is no correlation between the coefficients of the first and second decomposition, which corresponds to omitting the terms of $O(1/n)$ in (4). The interaction energy to this order is:

$$U=\sum(0|V_{\mathbf{k}\mathbf{k}'}b_{\mathbf{k}'}{}^*b_{\mathbf{k}}|0)=\sum V_{\mathbf{k}\mathbf{k}'}[u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'}+O(1/n)]. \quad (5)$$

As the size of the system is increased, keeping the particle density constant, the matrix element $V_{\mathbf{k}\mathbf{k}'}$ is inversely proportional to volume and thus to n, so that the total interaction energy is proportional to n. The terms of $O(1/n)$ would contribute only a constant energy, independent of volume.[4]

To calculate the Green's function,[5] we need the

* This research was supported in part by the Office of Ordnance Research, U. S. Army.

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[2] P. W. Anderson, Phys. Rev. **110**, 827 (1958).

[3] V. M. Galitskii and A. B. Migdal, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 139 (1958) [translation: Soviet Phys.—JETP **34(7)**, 96 (1958)]. V. M. Galitskii, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 145 (1958) [translation: Soviet Phys.—JETP **7**, 104 (1958)].

[4] It should be noted that a similar argument cannot be applied to the complete Hamiltonian. There are then n^2 interaction terms and errors of $O(1/n)$ can pile up to give a correction proportional to n. In fact, almost the entire normal-superconducting transition energy comes from the interaction terms in $H_{\rm red}$, and these contain only $O(1/n)$ of the total interaction.

[5] The Green's function for $H_{\rm red}$ has been derived by others, e.g., L. P. Gorkov, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 735 (1958) [translation: Soviet Phys.—JETP **34(7)**, 505 (1958)], by use of wave functions with variable numbers of particles. It is believed that the present derivation is new.

matrix elements of $c_{\mathbf{k}\sigma}^*$ and $c_{\mathbf{k}\sigma}$ which connect the ground-state Ψ_0 of n particles with excited states of $n+1$ and $n-1$ particles, respectively. The excited states of interest are what are called single particle excitations in BCS and consist of linear combinations in which one state of a given pair is occupied in all configurations and the other is not. Thus, we shall denote by $\Psi(\mathbf{k}\sigma, n+1)$ an excited state of a system of $n+1$ particles in which $\mathbf{k}\sigma$ is certainly occupied and the remaining particles are in ground pair configurations. It should be noted that there are no terms in H_{red} which scatter an electron in a singly occupied state. It is this fact which makes possible the determination of the excitation energies and matrix elements to $O(1/n)$ from the structure of the wave functions without use of a perturbation or diagram expansion.

We shall use Lehmann's expression for the momentum-energy representation of the single-particle Green's function in a form given by Galitskii[3]:

$$G(k,\epsilon)=\int_0^\infty dE\left(\frac{\rho^+(\mathbf{k},E)}{E-\epsilon-i\delta}-\frac{\rho^-(\mathbf{k},E)}{E+\epsilon-i\delta}\right), \tag{6}$$

where $\rho^+(\mathbf{k},E)$ and $\rho^-(\mathbf{k},E)$ are defined by

$$\rho^+(\mathbf{k},E)dE=\sum_{\mathbf{k}}|(\mathbf{k}, n+1|c_{\mathbf{k}}^*|0)|^2, \quad E<E_{\mathbf{k}}<E+dE; \tag{7a}$$

$$\rho^-(\mathbf{k},E)dE=\sum_{\mathbf{k}}|(\mathbf{k}, n-1|c_{\mathbf{k}}|0)|^2, \quad E<E_{\mathbf{k}}<E+dE. \tag{7b}$$

The single particle energies, $E_{\mathbf{k}}$ are defined by[6]

$$E_{\mathbf{k}}=W(\mathbf{k}, n+1)-W_0(n)-\mu, \tag{8a}$$

$$E_{\mathbf{k}}=W(\mathbf{k}, n-1)-W_0(n)+\mu, \tag{8b}$$

in which $W(\mathbf{k}, n\pm1)$ are energies of $\Psi(\mathbf{k}, n\pm1)$ and W_0 is the ground-state energy of H_{red}.

To terms of $O(1/n)$,

$$\Psi(\mathbf{k}\uparrow, n+1)=c_{\mathbf{k}\uparrow}^*\varphi_{0\mathbf{k}}(n),$$
$$\Psi(\mathbf{k}\uparrow, n-1)=c_{-\mathbf{k}\downarrow}\varphi_{0\mathbf{k}}(n), \tag{9}$$

so that the matrix elements are

$$(\mathbf{k}\uparrow, n+1|c_{\mathbf{k}\uparrow}^*|0)=u_{\mathbf{k}}=[1-h(\mathbf{k})]^{\frac{1}{2}}, \tag{10a}$$

$$(\mathbf{k}\uparrow, n-1|c_{-\mathbf{k}\uparrow}|0)=v_{\mathbf{k}}=h(\mathbf{k})^{\frac{1}{2}}. \tag{10b}$$

Thus

$$G(\mathbf{k},\epsilon)=\frac{1-h(\mathbf{k})}{E_{\mathbf{k}}-\epsilon-i\delta}-\frac{h(\mathbf{k})}{E_{\mathbf{k}}+\epsilon-i\delta}. \tag{11}$$

The energies $W_0(n)$ and $W(\mathbf{k}, n+1)$ may be expressed in the form:

$$W_0(n)=W_{0\mathbf{k}}(n)+2\epsilon_{\mathbf{k}}h(k)+U_{\mathbf{k}}, \tag{12}$$

$$W(\mathbf{k}, n+1)=W_{0\mathbf{k}}(n)+\epsilon_{\mathbf{k}}+\mu. \tag{13}$$

Here $W_{0\mathbf{k}}(n)$ is the energy corresponding to $\varphi_{0\mathbf{k}}(n)$ and is what the ground-state energy of the system would be if the state $\mathbf{k}$ were omitted from the Hamiltonian. The last two terms of (12) represent the contributions of the kinetic energy and of the interaction energy $U_{\mathbf{k}}$ from the pair state $\mathbf{k}$ to W_0. The expression (13) follows because the singly occupied state $\mathbf{k}$ cannot contribute to the pair interaction energy of H_{red} and the Fermi energy μ is unchanged to $O(1/n)$ if one particle or one state is added or subtracted from the system. From (8) we find

$$E_{\mathbf{k}}-\epsilon_{\mathbf{k}}=-2\epsilon_{\mathbf{k}}h(k)-U_{\mathbf{k}}. \tag{14}$$

The explicit expression for $U_{\mathbf{k}}$ is

$$U_{\mathbf{k}}=(0|\Sigma_{\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}b_{\mathbf{k}'}^*b_{\mathbf{k}}+\Sigma_{\mathbf{k}'}V_{\mathbf{k}'\mathbf{k}}b_{\mathbf{k}}^*b_{\mathbf{k}'}|0)$$
$$=2\Sigma_{\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}[h(1-h)h'(1-h')]^{\frac{1}{2}}+O(1/n). \tag{15}$$

Another expression for $U_{\mathbf{k}}$ can be obtained from the equations of motion for G, or, perhaps more directly, for $c_{\mathbf{k}}$. For a pair interaction,

$$U_{\mathbf{k}}=[0|(H,c_{\mathbf{k}}^*)c_{\mathbf{k}}-c_{\mathbf{k}}^*(H,c_{\mathbf{k}})-2(\epsilon_{\mathbf{k}}+\mu)c_{\mathbf{k}}^*c_{\mathbf{k}}|0]$$
$$=[0|Hc_{\mathbf{k}}^*c_{\mathbf{k}}-2c_{\mathbf{k}}^*Hc_{\mathbf{k}}+c_{\mathbf{k}}^*c_{\mathbf{k}}H-2(\epsilon_{\mathbf{k}}+\mu)c_{\mathbf{k}}^*c_{\mathbf{k}}|0]. \tag{16}$$

For our case, this reduces to

$$U_{\mathbf{k}}=h(\mathbf{k})[2W_0-2(E_{\mathbf{k}}-\mu+W_0)-2(\epsilon_{\mathbf{k}}+\mu)]$$
$$=-2(\epsilon_{\mathbf{k}}+E_{\mathbf{k}})h(\mathbf{k}). \tag{17}$$

The same result may be obtained by an expression derived by Galitskii and Migdal[3] for pair interactions in terms of the Green's function:

$$U_{\mathbf{k}}=\frac{i}{2\pi}\int_C(\epsilon-\epsilon_{\mathbf{k}})G(\mathbf{k},\epsilon)d\epsilon. \tag{18}$$

The integral is over a contour C in the complex ϵ plane which consists of the real axis and a semicircle over the upper half-plane.

By combining (14) and (17), we get the same relation between $E_{\mathbf{k}}$ and $h(\mathbf{k})$ that was found by BCS from their variational method:

$$h(\mathbf{k})=\tfrac{1}{2}[1-(\epsilon_{\mathbf{k}}/E_{\mathbf{k}})]. \tag{19}$$

Finally, from (14), (15), and (17), we obtain an integral equation for $h(\mathbf{k})$ which is the same as Eq. (2.33) of BCS.

ACKNOWLEDGMENT

The authors wish to thank Dr. J. R. Schrieffer for helpful discussions.

[6] Our $E_{\mathbf{k}}$ is identical with E_s of Galitskii (reference 3).