Effect of Coulomb interaction on the formation of Cooper pairs in superconducting systems

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A study has been made of coupling of Cooper-pair states of different binding energies by treating the intercarrier Coulomb interaction and the pairing interaction within a mean-field approximation. Illustrative calculations have been made of the Cooper-pair binding energies and their coupling effects. It is found that the Cooper-pair formation is affected in a complicated manner by the Coulomb interaction. General features of the method are discussed.

I. INTRODUCTION

The role of Coulomb interaction in superconducting systems has remained unclear even though more than three decades have passed after the successful microscopic theory of superconductivity formulated by Bardeen, Cooper, and Schrieffer[1] (BCS) in 1957. A few years later Morel and Anderson[2] gave a theory to account for the role of the Coulomb interaction when the attractive interaction, which causes formation of Cooper pairs of electrons, originates from the electron-phonon interaction. During the past decade, a number of superconducting systems—organic superconductors[3] (including the recently discovered K_3C_{60} and Rb_3C_{60} superconductors[4]), heavy-fermion superconductors,[5] and copper oxide superconductors[6]—have been discovered in which the interaction mechanism for superconductivity is believed to be different from the electron-phonon interaction.

In such superconductors,[3-6] where the electron-phonon interaction is not the sole source of the pairing interaction between carrier fermions, the Coulomb interaction has been treated in a number of different ways.[7-11] In most[7-10] of these methods, the role of the Coulomb interaction is not so transparent. Furthermore, except for the approach of Mila and Abraham,[10] and of Lal and Joshi,[11] the Cooper pairs formed because of a suitable attractive interaction correspond to a single binding energy at a given temperature. One consequence of such Cooper pairs of a single binding energy is that the properties of the superconducting systems involving such pairs will be similar to the properties of BCS superconductors. However, in systems such as the cuprate superconductors,[6] the behavior of the superconducting state is quite different[12] from BCS superconductors. In a recent study of superconductivity in cuprate systems, Lal and Joshi[11] treated the Coulomb interaction with use of a scattering theoretic approach and by this method they find Cooper pairs with a finite range of binding energies, ranging from the BCS value to zero value. The calculations made by Lal and Joshi[11] for the specific heat and tunneling spectra of cuprate systems show good agreement with the observed behavior of these properties. However, Lal and Joshi have used a phenomenological approach to obtain the values of the various binding energies of Cooper pairs. As the modified BCS approach of Lal and Joshi is reasonably successful in explaining the behavior of cuprate superconductors, it would be interesting to formulate a microscopic method for the calculation of various binding energies of Cooper pairs. Such an effort has been made in this Brief Report.

We have developed in this Brief Report a mean-field method to incorporate the Coulomb interaction between fermions along with an effective pairing interaction. Details of the formalism are given in Sec. II. In Sec. III we present results of calculation for a one-dimensional system. Conclusions are given in the last section.

II. FORMALISM

In general, a superconductor will be described by a Hamiltonian containing three terms: the kinetic-energy, Coulomb-interaction, and pairing-interaction terms. The kinetic-energy term is given by

$$H_0=\sum_{k,\sigma}\varepsilon_{\mathbf{k}}C^\dagger_{\mathbf{k}\sigma}C_{\mathbf{k}\sigma} . \tag{1}$$

Here $C^\dagger_{\mathbf{k}\sigma}$ and $C_{\mathbf{k}\sigma}$ are creation and annihilation operators of the carrier fermions of energy $\varepsilon_{\mathbf{k}}$, momentum $\mathbf{k}$, and spin σ.

The Coulomb-interaction term is given by

$$H_{\text{Coul}}=U\sum_{\mathbf{k},\mathbf{k}',q}C^\dagger_{\mathbf{k}+\mathbf{q}\uparrow}C^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow}C_{\mathbf{k}'\downarrow}C_{\mathbf{k}\uparrow} . \tag{2}$$

Here U is the on-site Coulomb interaction between fermions. It is independent of momentum, and here it is treated as an instantaneous interaction.

The pairing-interaction term of the Hamiltonian, which will be due to an indirect interaction mediated by those bosons that are relevant to a given superconductors, is given by

$$H_{\text{ind}}=\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}V(\mathbf{q},\omega_{\mathbf{q}})C^\dagger_{\mathbf{k}+\mathbf{q}\uparrow}C^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow}C_{\mathbf{k}'\downarrow}C_{\mathbf{k}\uparrow} . \tag{3}$$

Here $V(\mathbf{q},\omega_{\mathbf{q}})$ is an indirect interaction between fermions. This interaction is mediated by a boson of frequency $\omega_{\mathbf{q}}$. In cuprate and organic superconductors, the exciton is one of the possible excitations[3,13] for mediating the interaction $V(\mathbf{q},\omega_{\mathbf{q}})$ between two fermions.

It is clear from the above description that the origin and nature of the Coulomb interaction U and the indirect interaction $V(\mathbf{q},\omega_{\mathbf{q}})$ are different. A straightforward way to treat these interactions is to combine H_{Coul} and H_{ind} and to work out the effect of this net interaction $U+V(\mathbf{q},\omega_{\mathbf{q}})$. However, it is interesting to use a method in which the effects of U and $\mathbf{V}(\mathbf{q},\omega_{\mathbf{q}})$ are evaluated separately[10] and then combined to see their net effect. Here we adopt this latter approach. In fact, we consider the Coulomb interaction U to scatter an electron between band states $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$ and the indirect interaction $V(\mathbf{q},\omega_{\mathbf{q}})$ to promote pairing between fermions. The scattering caused by U may be conveniently taken through the mean-field parameters

$$n_\sigma(\mathbf{k},\mathbf{q})=\langle C^\dagger_{\mathbf{k}+\mathbf{q}/2,\sigma}C_{\mathbf{k}-\mathbf{q}/2,\sigma}\rangle \ . \tag{4}$$

Here $\langle \cdots \rangle$ denotes an average in terms of the states of H_{eff} (see below). The pairing effect of V may be described through the mean-field parameters

$$\nu^\dagger(\mathbf{k},\mathbf{q})=\langle C^\dagger_{\mathbf{k}+\mathbf{q}/2\uparrow}C^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow}\rangle \tag{5a}$$

and

$$\nu(\mathbf{k},\mathbf{q})=\langle C_{-\mathbf{k}+\mathbf{q}/2\downarrow}C_{\mathbf{k}+\mathbf{q}/2\uparrow}\rangle \ . \tag{5b}$$

The parameters $\nu^\dagger(\mathbf{k},\mathbf{q})$ and $\nu(\mathbf{k},\mathbf{q})$ correspond to Cooper pairs of zero as well as nonzero center-of-mass momenta. The stabilization of Cooper pairs in zero as well as nonzero center-of-mass momenta states will be determined by the Coulomb interaction U through the parameters $n_\sigma(\mathbf{k},\mathbf{q})$. More clearly, the interaction U scatters an electron from the band state $\mathbf{k}-\mathbf{q}/2$ to the band state $\mathbf{k}+\mathbf{q}/2$. The scattering effect is given by the mean-field parameter[14] $n_\sigma(\mathbf{k},\mathbf{q})$. Because of these scattering and pairing processes (caused by the interaction V), a Cooper pair will be scattered from a zero center-of-mass momentum state [characterized by the parameters $\nu^\dagger(\mathbf{k},0)$ and $\nu(\mathbf{k},0)$] to a nonzero center-of-mass momentum state [characterized by $\nu^\dagger(\mathbf{k},\mathbf{q})$ and $\nu(\mathbf{k},\mathbf{q})$]. In this way, while the interaction V leads to the formation of Cooper pairs, the interaction U couples Cooper-pair states of different center-of-mass momenta. This treatment is quite different from that of Morel and Anderson.[2]

It is notable here that when $U=0$, $n_\sigma(\mathbf{k},\mathbf{q})=n_\sigma(\mathbf{k},0)\delta_{\mathbf{q}0}$, so that there will be no coupling of Cooper-pair states of nonzero center-of-mass momenta with a zero center-of-mass momentum state. In fact, in the case of $U=0$ (which is the case of BCS superconductors), Cooper pairs with $q\neq 0$ will also be formed, but since the $q=0$ pairs correspond to minimum energy and since there is nothing to couple Cooper-pair states of various momenta, the ground state of the system will involve $q=0$ pairs only.

With the above plan for the treatment of the Coulomb interaction U and pairing interaction V, we may reduce the Hamiltonian H to the form

$$\begin{aligned}H_{\text{eff}}=&\sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}C^\dagger_{\mathbf{k}\sigma}C_{\mathbf{k}\sigma}+\tfrac{1}{2}U\sum_{\mathbf{k},\mathbf{q},\sigma}[n_{-\sigma}(-\mathbf{q})C^\dagger_{\mathbf{k}+\mathbf{q}/2,\sigma}C_{\mathbf{k}-\mathbf{q}/2,\sigma}+n_\sigma(\mathbf{q})C^\dagger_{\mathbf{k}-\mathbf{q}/2,-\sigma}C_{\mathbf{k}+\mathbf{q}/2,-\sigma}]\\&+V\sum_{\mathbf{k},q}[\nu^\dagger(\mathbf{k},\mathbf{q})C_{-\mathbf{k}+\mathbf{q}/2\downarrow}C_{\mathbf{k}+\mathbf{q}/2\uparrow}+\nu(\mathbf{k},\mathbf{q})C^\dagger_{\mathbf{k}+\mathbf{q}/2\uparrow}C^\dagger_{-\mathbf{k}+\mathbf{q}/2\downarrow}] \ .\end{aligned} \tag{6}$$

In this equation we have assumed, for simplicity, that V is independent of $\mathbf{q}$ and $\omega_{\mathbf{q}}$. For such a V, we shall have s-wave pairing, which is the case, for example, in cuprate superconductors.[15] The mean-field parameters $n_\sigma(\mathbf{q})$ are given by

$$n_\sigma(\mathbf{q})=\sum_{\mathbf{k}}n_\sigma(\mathbf{k},\mathbf{q}) \ . \tag{7}$$

When the mean-field parameters $n_\sigma(\mathbf{q})$, $\nu^\dagger(\mathbf{k},\mathbf{q})$, and $\nu(\mathbf{k},\mathbf{q})$ are determined, the effective Hamiltonian H_{eff} will provide a framework for the calculation of the physical properties of superconducting systems. It may be noted that this type of effective Hamiltonian has not been used earlier in the study of superconducting systems.

A superconductor based on such Cooper-pair states, in which pairs of nonzero center-of-mass momenta are coupled with the pairs of zero center-of-mass momentum states, will show a Andreev reflection spectrum different from that expected from BCS superconductors. Such a deviation from BCS predictions for the Andreev reflection spectrum has indeed been observed[16] in cuprate superconductors. Thus the above idea of mixing nonzero center-of-mass momenta Cooper-pair states with the zero center-of-mass momentum Cooper-pair state is quite reasonable in cuprate superconductors. In fact, the main effect of this kind of mixing will be that a property of the cuprate superconductor will be determined by a range of Cooper-pair binding energies.[11] It may here be noted that the success of Mila and Abrahams[10] in interpreting the tunneling density of this state is also due to the fact that they have worked in terms of a range of Cooper-pair binding energies. However, the validity of the work of Mila and Abrahams with respect to cuprates is questionable because these authors have considered odd pairing, which is not[15] the case in cuprates.

In order to diagonalize the Hamiltonian H_{eff}, we proceed as follows. First of all, we define the correlation functions

$$\mathcal{G}_{\mathbf{p}}(\mathbf{k},\tau-\tau')=-\langle T_\tau C_{\mathbf{k}-\mathbf{p}/2,\sigma}(\tau)C^\dagger_{\mathbf{k}+\mathbf{p}/2,\sigma}(\tau')\rangle \ , \tag{8}$$

$$\mathcal{F}^\dagger_{\mathbf{p}}(\mathbf{k},\tau-\tau')=\langle T_\tau C^\dagger_{\mathbf{k}+\mathbf{p}/2\uparrow}(\tau)C^\dagger_{-\mathbf{k}+\mathbf{p}/2\downarrow}(\tau')\rangle \ . \tag{9}$$

Here T_τ is the time-ordering operator. The Fourier transforms of $\mathcal{G}_{\mathbf{p}}(\mathbf{k},\tau-\tau')$ and $\mathcal{F}^\dagger_{\mathbf{p}}(\mathbf{k},\tau-\tau')$ are given by the usual relations

$$\mathcal{G}_{\mathrm{p}}(\mathbf{k},\tau-\tau')=\frac{1}{\beta}\sum_{\omega_n}\exp(-i\omega_n\tau)\mathcal{G}_{\mathrm{p}}(\mathbf{k},i\omega_n) \tag{10}$$

and

$$\mathcal{F}^{\dagger}_{\mathrm{p}}(\mathbf{k},\tau-\tau')=\frac{1}{\beta}\sum_{\omega_n}\exp(-i\omega_n\tau)\mathcal{F}^{\dagger}_{\mathrm{p}}(\mathbf{k},i\omega_n) . \tag{11}$$

Here $\omega_n=(2n+1)\pi/\beta$ is the Matsubara energy; $\beta=1/k_BT$, with k_B as the Boltzmann constant and T as the temperature.

Using the method of the equation of motion[17] and employing Eqs. (10) and (11), we obtain

$$\begin{aligned}(i\omega_n-\varepsilon_{\mathbf{k}-\mathbf{p}/2})&\mathcal{G}_{\mathrm{p}}(\mathbf{k},i\omega_n)\\ &-U\sum_{\mathbf{q}}n_{-\sigma}(-\mathbf{q})\mathcal{G}_{\mathrm{p}-\mathrm{q}}(\mathbf{k}+\mathbf{q}/2,i\omega_n)\\ &+V\sum_{\mathbf{q},\sigma}\nu\left[\mathbf{k}\sigma-\frac{\mathbf{p}+\mathbf{q}}{2}\sigma,\mathbf{q}\right]\\ &\qquad\times\mathcal{F}^{\dagger}_{\mathrm{p}+\mathrm{q}}(\mathbf{k}\sigma-\mathbf{q}\sigma/2,i\omega_n)=\delta_{\mathrm{p},0}\end{aligned} \tag{12}$$

and

$$\begin{aligned}(i\omega_n+\varepsilon_{\mathbf{k}+\mathbf{p}/2})&\mathcal{F}^{\dagger}_{p}(\mathbf{k},i\omega_n)\\ &+U\sum_{\mathbf{q}}n_{\downarrow}(-\mathbf{q})\mathcal{F}^{\dagger}_{\mathrm{p}+\mathrm{q}}(\mathbf{k}+\mathbf{p}/2,i\omega_n)\\ &+V\sum_{\mathbf{q}}\nu^{\dagger}\left[\mathbf{k}+\frac{\mathbf{p}+\mathbf{q}}{2},\mathbf{q}\right]\mathcal{G}_{-\mathrm{p}+\mathrm{q}}(-\mathbf{k}+\mathbf{q}/2,i\omega_n)=0 .\end{aligned} \tag{13}$$

We may express the parameters $n_{\sigma}(\mathbf{q})$, $\nu^{\dagger}(\mathbf{k},\mathbf{q})$, and $\nu(\mathbf{k},\mathbf{q})$ in terms of $\mathcal{G}_{\mathrm{q}}(\mathbf{k},i\omega_n)$ and $\mathcal{F}^{\dagger}_{\mathrm{q}}(\mathbf{k},i\omega_n)$ by using Eqs. (5) and (7)–(9). We obtain

$$n_{\sigma}(\mathbf{q})=\sum_{\mathbf{k}}\mathcal{G}_{\mathrm{q}}(\mathbf{k},\tau=0)=\frac{1}{\beta}\sum_{\mathbf{k},\omega_n}\mathcal{G}_{\mathrm{q}}(\mathbf{k},i\omega_n) , \tag{14}$$

$$\nu^{\dagger}(\mathbf{k},\mathbf{q})=\mathcal{F}^{\dagger}_{\mathrm{q}}(\mathbf{k},\tau=0)=\frac{1}{\beta}\sum_{\omega_n}\mathcal{F}^{\dagger}_{\mathrm{q}}(\mathbf{k},i\omega_n) , \tag{15}$$

and

$$\nu(\mathbf{k},\mathbf{q})=\mathcal{F}_{\mathrm{q}}(\mathbf{k},\tau=0)=\frac{1}{\beta}\sum_{\omega_n}\mathcal{F}_{\mathrm{q}}(\mathbf{k},i\omega_n) . \tag{16}$$

The binding-energy parameters of Cooper pairs may be written as

$$\Delta^{\dagger}(\mathbf{q})=-V\sum_{\mathbf{k}}\nu^{\dagger}(\mathbf{k},\mathbf{q}) . \tag{17}$$

From Eqs. (12) and (13), it is clear that when there exists a solution of these equations, Cooper pairs will exist with a range of binding energies. A self-consistent solution of Eqs. (12) and (13) may be obtained by using a method similar to the methods used for solving the Fredholm equation.[18]

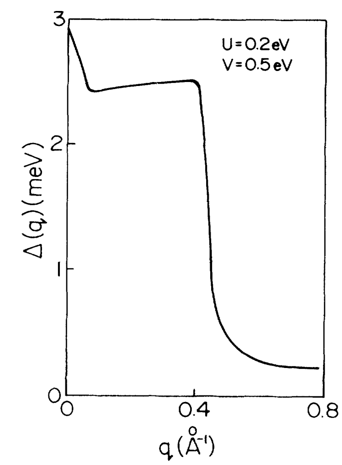

FIG. 1. Cooper-pair binding energy $\Delta(q)$ for $q=0$–0.78 Å^{-1} and for $U=0.2$ eV and $V=0.5$ eV.

III. RESULTS AND DISCUSSION

In order to find out the nature of the variation of pair-binding energies $\Delta(\mathbf{q})$ with different parameters of the model (U and V), we have calculated the values of $\Delta^{\dagger}(\mathbf{q})=\Delta(\mathbf{q})$ at zero temperature for different values of parameters U and V in a one-dimensional case. We deal with a one-dimensional system for the sake of simplicity. The calculation may be extended to a two- and higher-dimensional systems in a straightforward manner.

In the following calculations, the lattice constant is taken to be equal to $a=4$ Å. The band structure is assumed to be given by a parabolic band with the effective band mass of the hole equal to $m^*=10m$, where m is the bare mass of an electron. The Fermi energy is assumed to correspond to the Fermi momentum $k_F=0.75k_{\mathrm{BZ}}$, where k_{BZ} is the momentum at the Brillouin-zone boundary.

The results of our calculations are shown in Figs. 1–3. In Fig. 1 we show values of $\Delta(q)$ for $q=0$ to π/a for $U=0.2$ eV and $V=0.5$ eV. It is clear from this figure

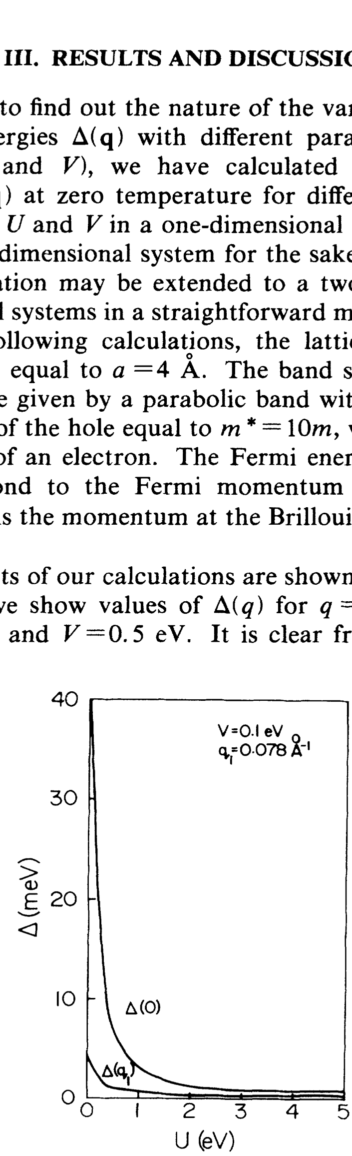

FIG. 2. Cooper-pair binding energies $\Delta(0)$ and $\Delta(q_1)$ for $U=0$–5 eV and $V=0.01$ eV. Here $q_1=0.078$ Å^{-1}.

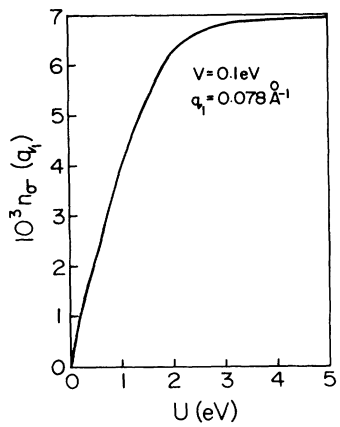

FIG. 3. Coupling parameter $n_\sigma(q_1)$ for coupling of Cooper-pair states of binding energies $\Delta(0)$ and $\Delta(q_1)$ for $U=0$–5 eV and $V=0.1$ eV. Here $q_1=0.078$ Å^{-1}.

that $\Delta(q\neq 0)<\Delta(0)$ for all q and that after a certain q, say, q_0, $\Delta(q)$ drops suddenly to negligibly small values. From Fig. 1 we find that $q_0=0.4$ Å^{-1}. Yet another feature of the $\Delta(q)$ values is that, for $q\neq 0$ and $q<q_0$, $\Delta(q)$ increases with q.

In Fig. 2 we have shown the variation of $\Delta(0)$ and $\Delta(q_1)$ with U for $V=0.1$ eV. Here $q_1=0.078$ Å^{-1}. We see from this figure that both $\Delta(0)$ and $\Delta(q_1)$ decrease monotonically with increasing U for the considered value of V.

In our treatment the role of the Coulomb interaction U is to couple Cooper-pair states of various binding energies $\Delta(q\neq 0)$ with the Cooper-pair state of the binding energy $\Delta(0)$. This coupling is characterized by the parameter $n_\sigma(q)$—the higher the values of $n_\sigma(q)$, the more the coupling of $\Delta(q)$ states with the $\Delta(0)$ state. In Fig. 3 we show the variation of $n_\sigma(q)$ with U. It is clear from this figure that for $U=0$, $n_\sigma(q)=0$, so that the Cooper-pair state of $\Delta(q\neq 0)$ will not be coupled with the Cooper-pair state of $\Delta(0)$. From Fig. 3 we see that $n_\sigma(q)$ increases with increasing U, and so the coupling between $\Delta(q\neq 0)$ Cooper-pair states and the $\Delta(0)$ state will be enhanced with U.

IV. CONCLUSIONS

In the present investigation, we have made a study of the role of the Coulomb interaction on the formation of Cooper pairs in a superconducting system. This study shows that the formation of Cooper pairs in the case where U and V are comparable is quite a complicated process. The present study provides a microscopic method for the calculation of coupling of Cooper pairs of various binding energies. Having calculated the values of the mean-field parameters $n_\sigma(\mathbf{q})$, $\nu^\dagger(\mathbf{k},\mathbf{q})$, and $\nu(\mathbf{k},\mathbf{q})$, we may use the effective Hamiltonian [Eq. (6)] to calculate various properties of superconducting systems in a manner similar to that described by us elsewhere.[11]

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