New type of Cooper pairing in systems with strong electron-phonon interaction

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We have investigated the ground-state properties of a model system with a strong electron-phonon interaction. It is found that as long as the renormalized intersite electron correlation is attractive, a new type of Cooper pairing will occur whether the renormalized on-site electron correlation is repulsive or attractive. Furthermore, we have shown that a new phonon coherent state, named a two-phonon coherent state, must be introduced to serve as the ground state of the phonon subsystem, so that the ground-state energy of the interacting system can be made a stable minimum and an appropriate condensation energy of the superconducting ground state may be obtained. We have performed numerical calculations for the $n=1$ case.

I. INTRODUCTION

As is well known, in the famous BCS theory of superconductivity Cooper pairing forms between the electrons near the Fermi surface.[1] This is a **k**-space pairing but in real space the distance between the electrons in pairing is uncertain. In recent years many authors have dealt with systems of strong electron-phonon interaction.[2-11] They have found that if the interaction is strong enough for the on-site electron-electron correlation to be renormalized attractive the small polarons form spatially overlapping Cooper pairs with superconducting properties similar to ordinary BCS superconductivity except for a few differences in the gap equations as well as in the expressions for the critical temperature T_c.[4-6] Furthermore, if the electron-phonon interaction is strong enough for the on-site or off-site polaron-polaron interaction to be attractive and strong,[2,3,7-11] a new type of superconductivity, so-called bipolaronic superconductivity, will occur; its properties are different from those of BCS superconductivity but are something like those of the superfluidity of ^{3}He.[7-11]

Because the on-site Coulomb replusion between the electrons should be much stronger than the off-site one the phonon-induced attraction between electrons is more likely to be of the off-site type than of the on-site one. Robaszkiewicz *et al.*[5] pointed out that an attractive correlation between intersite electrons would stabilize another type of superconductiving phase. As we know, the possibility and the detail of such a superconducting phase, especially when the renormalized on-site correlation between electrons is still repulsive, have not been investigated by any author(s).

In this paper, starting from a strong electron-phonon interaction, we shall show that so long as there exists a renormalized real-space attraction between intersite electrons a new type of Cooper pairing will occur whether the renormalized on-site correlation between electrons is repulsive or attractive. In order to arrive at our results we shall point out that a new phonon coherent state, named a two-phonon coherent state, must be introduced for the total energy of the interacting system to be a stable minimum and for an appropriate condensation energy of a superconducting state to be obtained.

II. THEORETICAL ANALYSIS

The Hamiltonian of our interacting system is given by

$$H=H_e+H_{\rm ph}+H_{e\text{-ph}}\ , \tag{1}$$

where H_e, $H_{\rm ph}$, and $H_{e\text{-ph}}$ are the electron, phonon, and electron-phonon interacting terms. The electron term is

$$H_e=\sum_{i,\sigma}\varepsilon_0 n_{i\sigma}-\sum_{i,\sigma}\sum_{\delta}T_0 d^{\dagger}_{i\sigma}d_{i+\delta,\sigma}+\sum_i U_0 n_{i\uparrow}n_{i\downarrow}+\frac{1}{2}\sum_i\sum_{\delta}V_0(n_{i\uparrow}+n_{i\downarrow})(n_{i+\delta,\uparrow}+n_{i+\delta,\downarrow})$$
$$-\frac{1}{2}\sum_i\sum_{\delta}\sum_{\sigma,\sigma'}J d^{\dagger}_{i\sigma}d^{\dagger}_{i+\delta,\sigma'}d_{i\sigma'}d_{i+\delta,\sigma}\ , \tag{2}$$

where δ is a nearest-neighboring vector, ε_0 is the unperturbed site level, T_0 is the usual hopping integral, U_0 and V_0 are the on-site and nearest-neighboring intersite Coulomb repulsions, respectively, $d^{\dagger}_{i\sigma}$ and $d_{i\sigma}$ are the usual creation and annihilation operators for electrons on site i, $n_{i\sigma}=d^{\dagger}_{i\sigma}d_{i\sigma}$. The last term in (2) is the exchange interaction between electrons and in this paper only the $J>0$ case will be discussed, which corresponds to an antiferromagnetic coupling between electrons.

The phonon term represents the harmonic energies of the lattice vibrations,

$$H_{\rm ph}=\sum_i \hbar\omega_0 b_i^\dagger b_i \ , \tag{3}$$

where $b_i^\dagger$ and b_i are usual creation and annihilation operators for local phonons and ω_0 is the frequency of phonons, which has been assumed to be dispersionless for simplicity. The electron-phonon interaction term is written as

$$H_{e\text{-ph}}=\sum_{i,\sigma} g_1 n_{i\sigma}(b_i^\dagger+b_i)+\sum_{i,\sigma}\sum_\delta g_2 n_{i\sigma}(b_{i+\delta}^\dagger+b_{i+\delta}) \ , \tag{4}$$

where the first term is the on-site electron-phonon interaction and the second term is the nearest-neighboring intersite one as we consider that the electrons should interact with their nearest-neighboring local phonons.

Applying an unitary transformation of the displaced-operator type to H,[8]

$$\bar{H}=\exp(R)H\exp(-R) \ , \tag{5}$$

$$R=\sum_{i,\sigma}(g_1/\hbar\omega_0)n_{i\sigma}(b_i^\dagger-b_i)+\sum_{i,\sigma}\sum_\delta (g_2/\hbar\omega_0)n_{i\sigma}(b_{i+\delta}^\dagger-b_{i+\delta}) \ , \tag{6}$$

we can obtain

$$\begin{aligned}\bar{H}=&\sum_i \hbar\omega_0 b_i^\dagger b_i+\sum_{i,\sigma}\varepsilon_0 n_{i\sigma}+\sum_i U_0 n_{i\uparrow}n_{i\downarrow}\\
&-\sum_{i,\sigma}\sum_\delta T_0 d_{i\sigma}^\dagger d_{i+\delta,\sigma}\exp\left[(g_1/\hbar\omega_0)[(b_i^\dagger-b_i)-(b_{i+\delta}^\dagger-b_{i+\delta})]+(g_2/\hbar\omega_0)\sum_{q'}[(b_{i+\delta'}^\dagger-b_{i+\delta'})-(b_{i+\delta+\delta'}^\dagger-b_{i+\delta+\delta'})]\right]\\
&+\tfrac{1}{2}\sum_{i,\delta}V_0(n_{i\uparrow}+n_{i\downarrow})(n_{i+\delta,\uparrow}+n_{i+\delta,\downarrow})-\tfrac{1}{2}\sum_{i,\delta}\sum_{\sigma,\sigma'}J d_{i\sigma}^\dagger d_{i+\delta,\sigma'}^\dagger d_{i\sigma'}d_{i+\delta,\sigma}\\
&-\sum_i\left[\sum_\sigma\left[(g_1/\hbar\omega_0)n_{i\sigma}+(g_2/\hbar\omega_0)\sum_\delta n_{i+\delta,\sigma}\right]\right]^2 .\end{aligned} \tag{7}$$

At this point one could suppose that when the temperature is low enough (in this paper only the zero-temperature case will be discussed) the phonon occupation numbers do not change as electrons move, so that the electron and the phonon subsystems can be decoupled by making an average of $\bar{H}$ over the vacuum state of the phonons subsystem and a Holstein reduction factor,[12,2,3,8,10] which is of the form $\exp[-g^2/(\hbar\omega_0)^2]$, may be obtained. However, if the electron-phonon interaction is strong, as we consider in this paper, the ratio $g/\hbar\omega_0$ would be larger than 1 and the reduction effect would be fairly strong. This kind of reduction effect must make the total energy of the interacting system under consideration increase as the mass center of the electronic energy band is not influenced by the electron-phonon interaction (without considering the polaron binding energy of the form $g^2/\hbar\omega_0$). If the average number of the electrons per unit cell, N_e/N, is a negligibly small quantity, the increase of the total energy is also negligible. But it is the completely different case when the ratio N_e/N is a finite quantity. In this paper, via the discussion of a possible solution of the model Hamiltonian we want to develop a variational treatment to make the total energy to be a stable minimum and illustrate that in practice the reduction effect should be much weaker than what the factor $\exp[-g^2/(\hbar\omega_0)^2]$ indicates.

Our variational state vector for the ground state of the phonons subsystem is

$$|\Psi_{\rm ph}\rangle=\exp(-S)|\,{\rm vac}\rangle \ , \tag{8}$$

$$S=\sum_i \alpha(b_i b_i-b_i^\dagger b_i^\dagger) \ , \tag{9}$$

in which α is a variational parameter and, if $\alpha=0$, $|\Psi_{\rm ph}\rangle$ returns to the vacuum state $|\,{\rm vac}\rangle$. As long as $\alpha\neq 0$ $|\Psi_{\rm ph}\rangle$ is a new and special state of the phonons subsystem other than any eigenstates of phonon number operators. Because the unitary operator $\exp(-S)$ is similar to that of the two-photon coherent state in quantum optics proposed firstly by Yuen,[13] we call $|\Psi_{\rm ph}\rangle$ the two-phonon coherent state[14] in which the average values of phonon number operators are nonzero but the average values of phonon creation and annihilation operators are zero. In Sec. III we shall show that a minimum of the total energy of the interacting system could be obtained indeed when the adjustable parameter α is equal to some nonzero value.

Making an average of $\bar{H}$ over the state $|\Psi_{\rm ph}\rangle$ and using the relations

$$\exp(S)(b_i^\dagger\pm b_i)\exp(-S)=(b_i^\dagger\pm b_i)\exp(\pm 2\alpha) \tag{10}$$

and

$$\begin{aligned}\exp(S)b_i^\dagger b_i\exp(-S)&=[b_i^\dagger\cosh(2\alpha)+b_i\sinh(2\alpha)](b_i^\dagger\sinh(2\alpha)\\
&\quad+b_i\cosh(2\alpha)) \ ,\end{aligned} \tag{11}$$

we get an effective Hamiltonian $H_{\rm eff}$ for the electron subsystem,

$$H_{\text{eff}}=\langle \text{vac} \mid \exp(S)H\exp(-S) \mid \text{vac}\rangle = N\hbar\omega_0[\sinh(2\alpha)]^2+\sum_{i,\sigma}\varepsilon_e n_{i\sigma}-\sum_{i,\sigma}\sum_{\delta}T_e d^{\dagger}_{i\sigma}d_{i+\delta,\sigma}+\sum_i U_e n_{i\uparrow}n_{i\downarrow}$$
$$+\tfrac{1}{2}\sum_i\sum_{\delta}V_e(n_{i\uparrow}+n_{i\downarrow})(n_{i+\delta,\uparrow}+n_{i+\delta,\downarrow})-\tfrac{1}{2}\sum_{i,\delta}\sum_{\sigma,\sigma'}Jd^{\dagger}_{i\sigma}d^{\dagger}_{i+\delta,\sigma'}d_{i\sigma'}d_{i+\delta,\sigma}\ , \tag{12}$$

where $\varepsilon_e=\varepsilon_0-g_1^2/(\hbar\omega_0)-zg_2^2/(\hbar\omega_0)$,

$$T_e=T_0\rho=T_0\exp\{-[(g_1-g_2)^2/(\hbar\omega_0)^2+(z-1)g_2^2/(\hbar\omega_0)^2]\exp(-4\alpha)\}\ ,$$
$$U_e=U_0-2g_1^2/\hbar\omega_0-2zg_2^2/\hbar\omega_0,\quad V_e=V_0-4g_1g_2/\hbar\omega_0\ , \tag{13}$$

in which z is the coordination number. We have neglected in H_{eff} the phonon-induced next-nearest and third-nearest neighboring electronic correlations because they are of less importance and do not influence our solution qualitatively. ε_e, T_e, U_e, and V_e are parameters renormalized by the electron-phonon interaction and it is obvious that V_e could be negative whether U_e is positive or negative. In what follows we would consider the case that $V_e<0$ but $U_e>0$. It should be noted that the reduced hopping integral T_e is connected with the adjustable parameter α of the two-phonon coherent state.

Within the generalized Hartree-Fock approximation the effective Hamiltonian H_{eff} can be changed into the following form:

$$H_{\text{eff}}\simeq N\hbar\omega_0[\sinh(2\alpha)]^2-NU_en^2/4+Nzn^2(2\mid V_e\mid +J)/4-\tfrac{1}{4}\sum_{\mathbf{k},\sigma}z(\mid V_e\mid +2J)n_{\mathbf{k}}\langle d^{\dagger}_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}\rangle$$
$$-\tfrac{1}{2}\sum_{\mathbf{k}}\Delta_{\mathbf{k}}\langle d^{\dagger}_{\mathbf{k}\uparrow}d^{\dagger}_{-\mathbf{k}\downarrow}+d_{-\mathbf{k}\downarrow}d_{\mathbf{k}\uparrow}\rangle+\sum_{\mathbf{k},\sigma}E(\mathbf{k})d^{\dagger}_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}+\sum_{\mathbf{k}}\Delta_{\mathbf{k}}(d^{\dagger}_{\mathbf{k}\uparrow}d^{\dagger}_{-\mathbf{k}\downarrow}+d_{-\mathbf{k}\downarrow}d_{\mathbf{k}\uparrow})\ , \tag{14}$$

$$E(\mathbf{k})=E_e-\mu-zT_e\gamma(\mathbf{k})+\tfrac{1}{2}z(\mid V_e\mid +2J)n_{\mathbf{k}}\ , \tag{15}$$

in which the Bloch representation has been introduced and μ is the chemical potential. In (14) and (15) we have used the following definitions:

$$E_e=\varepsilon_e+\tfrac{1}{2}U_en-\tfrac{1}{2}z(2\mid V_e\mid +J)n,\quad \gamma(\mathbf{k})=\frac{1}{z}\sum_{\gamma}\exp(i\mathbf{k}\cdot\boldsymbol{\delta})\ ,$$
$$n=\frac{2}{N}\sum_{\mathbf{k}}\langle d^{\dagger}_{k\sigma}d_{k\sigma}\rangle,\quad n_{\mathbf{k}}=\frac{2}{N}\sum_{\mathbf{k}'}\gamma(\mathbf{k}-\mathbf{k}')\langle d^{\dagger}_{\mathbf{k}'\sigma}d_{\mathbf{k}'\sigma}\rangle\ , \tag{16}$$
$$\Delta_{\mathbf{k}}=\frac{1}{2N}\sum_{\mathbf{k}'}[U_e-z(\mid V_e\mid +J)\gamma(\mathbf{k}-\mathbf{k}')]\langle d^{\dagger}_{\mathbf{k}'\uparrow}d^{\dagger}_{-\mathbf{k}'\downarrow}-d^{\dagger}_{\mathbf{k}'\downarrow}d^{\dagger}_{-\mathbf{k}'\uparrow}\rangle\ ,$$

and assumed that the singlet Cooper pairing is energetically more favorable than the triplet one as the exchange interaction is supposed to be antiferromagnetic. The triplet Cooper pairing will be discussed in a forthcoming paper.

By using the method of the Green's function we have

$$\langle d^{\dagger}_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}\rangle=\tfrac{1}{2}-\tfrac{1}{2}E(\mathbf{k})/\sqrt{E^2(\mathbf{k})+\Delta_{\mathbf{k}}^2},\quad \langle d^{\dagger}_{\mathbf{k}\sigma}d^{\dagger}_{-\mathbf{k}\bar{\sigma}}\rangle=-\tfrac{1}{2}\sigma\Delta_{\mathbf{k}}/\sqrt{E^2(\mathbf{k})+\Delta_{\mathbf{k}}^2}\ . \tag{17}$$

Thus, n, $n_{\mathbf{k}}$, and $\Delta_{\mathbf{k}}$ may be written out as

$$n=\frac{1}{N}\sum_{\mathbf{k}}[1-E(\mathbf{k})/\sqrt{E^2(\mathbf{k})+\Delta_{\mathbf{k}}^2}]\ , \tag{18}$$

$$n_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{k}'}\gamma(\mathbf{k}-\mathbf{k}')[1-E(\mathbf{k}')/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2}]\ , \tag{19}$$

$$\Delta_{\mathbf{k}}=\frac{-1}{2N}\sum_{\mathbf{k}'}[U_e-z(\mid V_e\mid +J)\gamma(\mathbf{k}-\mathbf{k}')]\Delta_{\mathbf{k}'}/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2}\ . \tag{20}$$

In Appendix A we have proved that Eq. (19) can be rewritten as

$$n_{\mathbf{k}}=2\xi\gamma(\mathbf{k})\ ,$$

where

$$\xi=-\frac{1}{2N}\sum_{\mathbf{k}'}\gamma(\mathbf{k}')E(\mathbf{k}')/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2}\ . \tag{21}$$

Hence, from Eq. (15) we have

$$E(\mathbf{k})=E_e-\mu-[zT_e-z(\mid V_e\mid +2J)\xi]\gamma(\mathbf{k}) . \tag{22}$$

We have also obtained in Appendix A the following integral equations for $\Delta_{\mathbf{k}}$:

$$\Delta_{\mathbf{k}}=\Delta_0-\Delta_1\gamma(\mathbf{k}) ,$$
$$\Delta_0=\frac{1}{2N}\sum_{\mathbf{k}'} U_e[\Delta_1\gamma(\mathbf{k}')-\Delta_0]/\sqrt{E^2(\mathbf{k}')+[\Delta_0-\Delta_1\gamma(\mathbf{k}')]^2} , \tag{23}$$
$$\Delta_1=\frac{1}{2N}\sum_{\mathbf{k}'} z(\mid V_e\mid +J)\gamma(\mathbf{k}')[\Delta_1\gamma(k')-\Delta_0]/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2} .$$

Equations (18), (21), and (23) are starting points for calculating the chemical potential μ and parameters ξ, Δ_0, and Δ_1. In general, these equations must be solved by numerical methods.

III. NUMERICAL RESULTS

In what follows only the $n=1$ case will be considered because in this case the above equations could be solved analytically. When $n=1$ it can be easily verified that $\mu=E_e$ and $\Delta_0=0$ but

$$\xi=-\frac{1}{2N}\sum_{\mathbf{k}'}\gamma(\mathbf{k}')E(\mathbf{k}')/\sqrt{E^2(\mathbf{k}')+\Delta_1^2\gamma^2(\mathbf{k}')} \tag{24}$$

and

$$\Delta_1=\frac{1}{2N}\sum_{\mathbf{k}'} z(\mid V_e\mid +J)\gamma^2(\mathbf{k}')\Delta_1/\sqrt{E^2(\mathbf{k}')+\Delta_1^2\gamma^2(\mathbf{k}')} , \tag{25}$$

where

$$E(\mathbf{k})=-z\gamma(\mathbf{k})[T_e-(\mid V_e\mid +2J)\xi] . \tag{26}$$

It is obvious that $\Delta_1=0$ is a trivial solution of Eq. (25).

Introducing a definition that

$$\gamma=\frac{1}{N}\sum_{\mathbf{k}}\mid\gamma(\mathbf{k})\mid , \tag{27}$$

Eqs. (24) and (25) can be changed into the following form

$$\xi=\tfrac{1}{2}\gamma z[T_e-\xi(\mid V_e\mid +2J)]/\sqrt{[zT_e-z\xi(\mid V_e\mid +2J)]^2+\Delta_1^2} , \tag{24'}$$
$$1=\tfrac{1}{2}\gamma z(\mid V_e\mid +J)/\sqrt{[zT_e-z\xi(V_e+2J)]^2+\Delta_1^2} . \tag{25'}$$

The solutions of these two equations are

$$\xi=T_e/(2\mid V_e\mid +3J) \tag{28}$$

and

$$\Delta_1^2=[\tfrac{1}{2}\gamma z(\mid V_e\mid +J)]^2-[(1-\eta)\rho zT_0]^2$$

or

$$\Delta_1=0, \quad \text{if } [\tfrac{1}{2}\gamma z(\mid V_e\mid +J)]^2-[(1-\eta)\rho zT_0]^2<0 , \tag{29}$$

where

$$\eta=(\mid V_e\mid +2J)/(2\mid V_e\mid +3J) . \tag{30}$$

After μ, ξ, Δ_0, and Δ_1 have been obtained the ground-state energy E_g, which is an average of the effective Hamiltonian H_{eff} over the ground state of the electrons subsystem, can be derived from Eqs. (14) and (17). If $\Delta_1>0$,

$$E_g/N=\hbar\omega_0[\sinh(2\alpha)]^2-\tfrac{1}{4}U_e+\tfrac{1}{4}z(2\mid V_e\mid +J)$$
$$-\tfrac{1}{4}\gamma^2 z(\mid V_e\mid +J)$$
$$-(1-\eta)z^2T_e^2/z(\mid V_e\mid +J) ; \tag{31}$$

but if $\Delta_1=0$,

$$E_g/N=\hbar\omega_0[\sinh(2\alpha)]^2-\tfrac{1}{4}U_e+\tfrac{1}{4}z(2\mid V_e\mid +J)$$
$$+\tfrac{1}{4}\gamma^2 z(\mid V_e\mid +2J)-zT_e\gamma . \tag{32}$$

The actual value of γ [Eq. (27)] could be obtained by numerical integration and the result is

$$\gamma=0.258 \quad \text{for body-centered cubic (bcc) lattice}$$

or (33)

$$\gamma=0.331 \quad \text{for simple cubic (sc) lattice} .$$

In numerical calculations all quantities being of the energy dimension are expressed in the unit of half bandwidth zT_0 of bare electrons: $\hbar\bar{\omega}_0=\hbar\omega_0/zT_0$, $\bar{U}_0=U_0/zT_0$, $\bar{V}_0=V_0/zT_0$, $\bar{U}_e=U_e/zT_0$, $\bar{V}_e=V_e/zT_0$, $\bar{J}=J/zT_0$, $\bar{g}_1=g_1/zT_0$, $\bar{g}_2=g_2/zT_0$, $\bar{E}_g=E_g/zT_0$, etc. The employed values of the parameters in the calculations are given in the following figures.

In Fig. 1 the $\bar{E}_g/N$ and $\bar{\Delta}_1$ versus the two-phonon coherent state parameter $\tau=\exp(-2\alpha)$ relations in the bcc lattice are illustrated. In the figure curve (1) corresponds to the $\bar{E}_g/N$ versus τ relation when $\Delta_1>0$ [Eq. (31)], curve (2) that when $\Delta_1=0$ [Eq. (32)] and curve (3) represents $\bar{\Delta}_1$ versus τ relation. We can see from the figure that when $\tau=\tau_0(1)=0.56$ curve (1) passes through its stable minimum $\bar{E}_g/N=\bar{E}_{g0}(1)/N=0.4314$ and so does curve (2) at $\tau=\tau_0(2)=0.52$, at which $\bar{E}_g/N=\bar{E}_{g0}(2)/N=0.4335$.

In Fig. 2, the same relations as in Fig. 1 are illustrated for the sc lattice but the employed parameters are somewhat different from those of Fig. 1. We can see that when $\tau=\tau_0(1)=0.47$ curve (1) ($\Delta_1>0$) passes through its stable minimum $\bar{E}_g/N=\bar{E}_{g0}(1)/N=0.3677$ and so does curve (2) at $\tau=\tau_0(2)=0.435$, at which $\bar{E}_g/N=\bar{E}_{g0}(2)/N=0.3710$.

Because in the ground state the total energy of the interacting system must be as low as possible, we infer that in the cases of Figs. 1 and 2 the ground states of the interacting systems are the superconducting states with $\bar{\Delta}_1=0.158$ (Fig. 1) and $\bar{\Delta}_1=0.183$ (Fig. 2). The condensation energy[1] of the superconducting state, which should be

$$\delta\bar{E}_{g0}/N=\bar{E}_{g0}(1)/N-\bar{E}_{g0}(2)/N\ , \tag{34}$$

is -0.0021 (Fig. 1) or -0.0033 (Fig. 2). However, if $\alpha=0$ and $\tau=1$, that is, if the two-phonon coherent state were not introduced, the condensation energy of the superconducting state would be -0.0558 (Fig. 1) or -0.0942 (Fig. 2). These two values are too large in magnitude. For comparison, in the weak coupling approximation of the BCS theory the condensation energy is of the order of 10^{-8}–10^{-7} eV.[1]

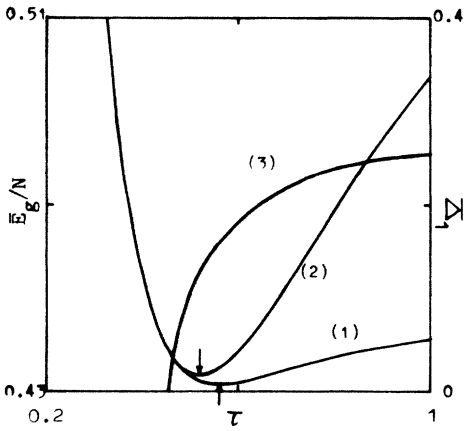

FIG. 1. $\bar{E}_g/N$ and $\bar{\Delta}_1$ vs τ relations in the bcc lattice. The employed values of the parameters are $\hbar\bar{\omega}_0=0.1$, $\bar{U}_0=2$, $\bar{U}_e=1.293$, $\bar{V}_0=0.1$, $\bar{V}_e=-0.15$, $\bar{J}=0.1$, $\bar{g}_1=0.133$, $\bar{g}_2=0.047$. The two arrows indicate the stable minimums of curves (1) and (2), respectively. See the text for details.

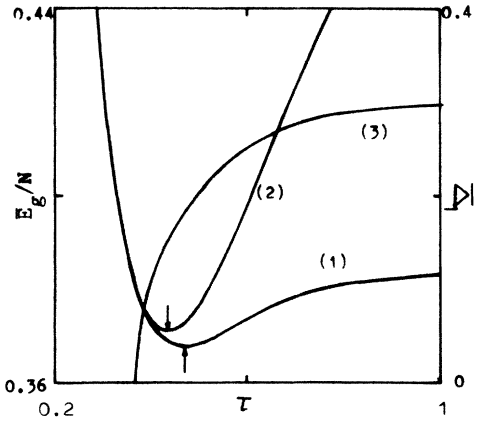

FIG. 2. $\bar{E}_g/N$ and $\bar{\Delta}_1$ vs τ relations in the sc lattice. The employed values of the parameters are $\hbar\bar{\omega}_0=0.08$, $\bar{U}_0=2$, $\bar{U}_e=1.265$, $\bar{V}_0=0.1$, $\bar{V}_e=-0.2$, $\bar{J}=0.1$, $\bar{g}_1=0.121$, $\bar{g}_2=0.050$. The two arrows indicate the stable minimums of curves (1) and (2), respectively. See the text for details.

Furthermore, since in the superconducting ground state the phonons subsystem should be in the two-phonon coherent state with $\alpha\neq 0$, the reduction effect of phonons must be more weaker than the one when the phonons subsystem is in the vacuum state. For the parameters of Fig. 1, the reduction factor ρ, which is given out in Eq. (13), is equal to 0.4883 when $\tau=\tau_0(1)=0.56$ but to 0.1017 when $\tau=1$ ($\alpha=0$). For the parameters of Fig. 2, ρ is equal to 0.5486 when $\tau=\tau_0(1)=0.47$ but to 0.0660 when $\tau=1$ ($\alpha=0$).

At the end of this section we should point out the fact that $\Delta_0=0$ in $n=1$ case indicates that in this case the on-site Cooper pairing does not exist because we can derive the on-site abnormal average value by

$$\langle d_{i\uparrow}^{\dagger}d_{i\downarrow}^{\dagger}-d_{i\downarrow}^{\dagger}d_{i\uparrow}^{\dagger}\rangle=\frac{1}{N}\sum_{\mathbf{k}}\langle d_{\mathbf{k}\uparrow}^{\dagger}d_{-\mathbf{k}\downarrow}^{\dagger}-d_{\mathbf{k}\downarrow}^{\dagger}d_{-\mathbf{k}\uparrow}^{\dagger}\rangle$$
$$=\frac{1}{N}\sum_{\mathbf{k}}\Delta_1\gamma(\mathbf{k})/\sqrt{E^2(\mathbf{k})+\Delta_1^2\gamma^2(\mathbf{k})}=0\ . \tag{35}$$

Hence, in $n=1$ case only the off-site Cooper pairing exists.

We emphasize that the results obtained in this section are not influenced, qualitatively, by the renormalized on-site electron correlation U_e, which may be positive or negative.

IV. DISCUSSIONS

(1.) We have investigated the ground-state properties of a model system with strong electron-phonon interaction. It is found that so long as the renormalized intersite electron correlation is attractive, a new type Cooper pairing would occur, whose occurrence is indicated by the

nonzero function $\Delta_{\mathbf{k}}$ as $\Delta_{\mathbf{k}}$ is connected with the abnormal average values $\langle d^{\dagger}_{\mathbf{k}\uparrow}d^{\dagger}_{-\mathbf{k}\downarrow}-d^{\dagger}_{\mathbf{k}\downarrow}d^{\dagger}_{-\mathbf{k}\uparrow}\rangle$'s, whether the renormalized on-site electron correlation is repulsive or attractive.

(2.) From the method of the Green's function and its result Eq. (17) it can be inferred that the excited energy of the quasiparticle in superconducting ground state is

$$W(\mathbf{k})=\sqrt{E^2(\mathbf{k})+\Delta^2_{\mathbf{k}}}\ . \tag{36}$$

Thus, $\Delta_{\mathbf{k}}$ may be regarded as a gap function.[1] However, as $\Delta_{\mathbf{k}}$ is a function of $\mathbf{k}$, in the Brillouin zone it is not a constant but changing from point to point. For instance, in $n=1$ case $\Delta_{\mathbf{k}}$ can be equal to zero at the point at which $\gamma(\mathbf{k})=0$.

(3.) We have also shown that as a result of the electron-phonon interaction the ground state of the phonons subsystem must be a new phonon coherent state, named as a two-phonon coherent state, for the ground-state energy of the interacting system to be a stable minimum and for an appropriate condensation energy of the superconducting ground state to be obtained. Besides, in such a coherent state the reduction effect of phonons would be more weaker than what the Holstein factor indicates.

(4.) We have made numerical calculations in the $n=1$ case and shown concretely that in this case the ground state of the interacting system may be superconducting with the gap function $\Delta_{\mathbf{k}}=-\Delta_1\gamma(\mathbf{k})$. Moreover we have pointed out that in this case the Cooper pairing would be of an off-site type.

The discussions of the finite temperature case, especially the critical temperature T_c, will be given in a forthcoming paper.

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APPENDIX

It can be easily verified that

$$\frac{1}{N}\sum_{\mathbf{k}'}\gamma(\mathbf{k}-\mathbf{k}')=0\ , \tag{A1}$$

because

$$\gamma(\mathbf{k}-\mathbf{k}')=\frac{1}{z}\sum_{\delta}\exp[i(\mathbf{k}-\mathbf{k}')\cdot\delta]$$

and the $\mathbf{k}'$ summation is over the first Brillouin zone. Thus, from Eq. (19)

$$n_{\mathbf{k}}=-\frac{1}{N}\sum_{\mathbf{k}'}\gamma(\mathbf{k}-\mathbf{k}')E(\mathbf{k}')/\sqrt{E^2(\mathbf{k}')+\Delta^2_{\mathbf{k}'}}\ . \tag{A2}$$

Then, as $E(\mathbf{k}')$ and $\Delta_{\mathbf{k}'}$ must be invariable when symmetry operations of the point group of the crystal are applied to the wave vector $\mathbf{k}'$, we may let the $\mathbf{k}'$ summation in Eq. (A2) be rewritten as

$$\begin{aligned}n_{\mathbf{k}}&=-\frac{1}{Nz}\sum_{l=1}^{z}\sum_{\mathbf{k}'}\gamma(\mathbf{k}-P_l\mathbf{k}')E(P_l\mathbf{k}')/\sqrt{E^2(P_l\mathbf{k}')+\Delta^2_{P_l\mathbf{k}'}}\\&=-\frac{1}{Nz}\sum_{l=1}^{z}\sum_{\mathbf{k}'}\frac{1}{z}\sum_{\delta}\exp[i(\mathbf{k}-P_l\mathbf{k}')\cdot\delta]E(\mathbf{k}')/\sqrt{E^2(\mathbf{k}')+\Delta^2_{\mathbf{k}'}}\ ,\end{aligned} \tag{A3}$$

where P_l's are some symmetry operations of the point group and they satisfy the condition that $P_l\delta$, $P_2\delta,\ldots,P_z\delta$ are all nearest-neighboring vectors, that is,

$$\gamma(\mathbf{k})=\frac{1}{z}\sum_{l=1}^{z}\exp(i\mathbf{k}\cdot P_l\delta)\ . \tag{A4}$$

Because the scalar product of vectors is invariable under the symmetry operations of the point group, from (A3) we can derive

$$n_{\mathbf{k}}=-\frac{1}{N}\gamma(\mathbf{k})\sum_{\mathbf{k}'}\gamma(\mathbf{k}')E(\mathbf{k}')/\sqrt{E^2(\mathbf{k}')+\Delta^2_{\mathbf{k}'}}\ . \tag{A5}$$

If we denote

$$\xi=-\frac{1}{2N}\sum_{\mathbf{k}'}\gamma(\mathbf{k}')E(\mathbf{k}')/\sqrt{E^2(\mathbf{k}')+\Delta^2_{\mathbf{k}'}}\ , \tag{A6}$$

we have

$$n_{\mathbf{k}}=2\xi\gamma(\mathbf{k})\ . \tag{A7}$$

Furthermore, we can verify that

$$\Delta_{\mathbf{k}}=\Delta_0-\Delta_1\gamma(\mathbf{k})\ , \tag{A8}$$

where Δ_0 and Δ_1 are independent of $\mathbf{k}$. Substituting (A8) into Eq. (A20),

$$\Delta_0-\Delta_1\gamma(\mathbf{k})=-\frac{1}{2N}\sum_{\mathbf{k}'}[U_e-z(\mid V_e\mid+J)\gamma(\mathbf{k}-\mathbf{k}')][\Delta_0-\Delta_1\gamma(\mathbf{k}')]/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2}\ .$$

Via the same method as above we can obtain

$$\Delta_0-\Delta_1\gamma(\mathbf{k})=-\frac{1}{2N}\sum_{\mathbf{k}'}U_e[\Delta_0-\Delta_1\gamma(\mathbf{k}')]/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2}$$
$$+\frac{1}{2N}\gamma(\mathbf{k})\sum_{\mathbf{k}'}z(\mid V_e\mid+J)\gamma(\mathbf{k}')[\Delta_0-\Delta_1\gamma(\mathbf{k}')]/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2}\ , \tag{A9}$$

that is

$$\Delta_0=-\frac{1}{2N}\sum_{\mathbf{k}'}U_e[\Delta_0-\Delta_1\gamma(\mathbf{k}')]/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2}\ , \tag{A10}$$

$$\Delta_1=-\frac{1}{2N}\sum_{\mathbf{k}'}z(\mid V_e\mid+J)\gamma(\mathbf{k}')[\Delta_0-\Delta_1\gamma(\mathbf{k}')]/\sqrt{E^2(\mathbf{k}')+\Delta_{\mathbf{k}'}^2}\ . \tag{A11}$$

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