Many-polaron theory for superconductivity and charge-density waves in a strongly coupled electron-phonon system with quasi-two-dimensionality: An interpolation between the adiabatic limit and the inverse-adiabatic limit

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The phase diagram of a two-dimensional N-site N-electron system ($N \gg 1$) with site-diagonal electron-phonon (e-ph) coupling is studied in the context of polaron theory, so as to clarify the competition between the superconducting (SC) state and the charge-density wave (CDW) state. The Fermi surface of noninteracting electrons is assumed to be a complete circle with no nesting-type instability in the case of weak e-ph coupling, so as to focus on such a strong coupling that even the standard "strong-coupling theory" for superconductivity breaks down. Phonon clouds moving with electrons as well as a frozen phonon are taken into account by a variational method, combined with a mean-field theory. It covers the whole region of three basic parameters characterizing the system: the intersite transfer energy of electron T, the e-ph coupling energy S, and the phonon energy ω. The resultant phase diagram is given in a triangular coordinate space spanned by T, S, and ω. In the adiabatic region $\omega \ll (T,S)$ near the T-S line of the triangle, each electron becomes a large polaron with a thin phonon cloud, and the system changes discontinuously from the SC state to the CDW state with a frozen phonon as S/T increases. In the inverse-adiabatic limit $\omega \gg (T,S)$ near the ω vertex of the triangle, on the other hand, each electron becomes a small polaron, and the SC state is always more stable than the CDW state, because the retardation effect is absent. Thus, the polaron radius decreases and the SC region expands in the triangle as T/ω decreases. It is found, for the first time, that the energy gap of the SC state for a given T and S becomes maximum at the intermediate region $\omega \sim T$, indicating the importance of the polaron effect. The collective excitation within the gap of the SC state is also studied by the random-phase approximation, and is found to change its nature continuously from the pair-breaking type to the superfluid type as S/T increases.

I. INTRODUCTION

An electron coupling with phonons in a crystal forms a polaron, composed of the original electron dressed with a phonon cloud that moves along with the electron. This concept was born of experimental and theoretical studies on the electron transport in ionic crystals and semiconductors,[1] and afterwards was extended to molecular crystals.[2,3] At present, we already have a well-established knowledge of its nature. When the electron phonon (e-ph) coupling is of short range, it is determined by three main quantities: the intersite transfer energy of electron T, the e-ph coupling energy S, and the phonon energy ω.

In most inorganic materials the e-ph coupling is nearly adiabatic, in the sense that T and S far exceed ω, and hence quantum effects for the phonons are relatively small. In this case the nature of the polaron is determined through the competition between S and T.[4] When the coupling is weak, $S \ll T$, the electron becomes a large polaron whose phonon cloud is very thin but extends over a wide region. The increase of its mass due to this cloud is also very small. When the coupling is strong, $S \gg T$, on the other hand, the electron becomes a small polaron, whose cloud is very thick and is always in the same site as that of the electron. Its mass enhancement also becomes considerable.

As ω increases, however, the differences between the large and small polaron become obscure, because of the quantum effect of the phonon.[5] Furthermore, when ω far exceeds T and S, the electron always becomes a small polaron with no mass enhancement, because, in this limit, the phonon can follow the motion of the electron without delay. This situation, called the inverse-adiabatic limit hereafter, is expected to be realized in some molecular crystals. In these materials the motion of an electron from one molecule to the other is a kind of tunneling with small T, while the energy of intramolecular vibration associated with a carbon or hydrogen atom is relatively large.[2,3] Moreover, if an electron couples with a quasi-boson such as an exciton[6] or a plasmon[7] through the screened Coulombic interaction, the situation is almost inverse-adiabatic.

As is well known, an attraction acts between two polarons through the overlap of their phonon clouds. The range and the strength of this attraction also change with changes in the cloud. If this attraction exceeds the direct Coulombic repulsion, the two electrons make a bound state, called a singlet bipolaron.[8] This bipolaron, once formed, can give rise to a spinless conductive charge, as is observed in amorphous solids,[9] conducting polymers,[10] Ti_4O_7,[11] and $Na_{0.33}V_2O_5$.[12]

Thus, the one- and two-body natures of polarons have been well clarified, and the purpose of the present paper is to extend these concepts to many-body systems. As is

well known, a metallic state of a many-electron system is always unstable with respect to the e-ph coupling and becomes a superconducting (SC) state. In this state, according to Schrieffer,[13] the electrons only around the Fermi level make singlet bound states, called BCS pairs, through the attraction mediated by phonons. However, most of the theoretical studies for this problem are restricted to a weak-coupling region where perturbation theory works well. Even the so-called strong coupling theory[14] has not included such a strong region that the polaron effect becomes very important.

If we restrict ourselves only to the limit of strong coupling, $S \gg T$, on the other hand, the perturbation theory with respect to T works well, and several theoretical studies have been devoted to this case.[15,16] According to their results, the many-polaron system, in this limit, is in a superfluid-type state rather than the BCS state. However, it is still uncertain how the state changes its nature from the BCS type to the superfluid type. For this reason, we are especially interested in clarifying the interrelation between the two types of states as a function of T, S, and ω.

There is another candidate for the ground state of a many-electron system coupling strongly with phonons. That is, the e-ph coupling can make a certain phonon-mode to be a frozen lattice distortion. It can raise and lower the energy level of electrons at each lattice site periodically. In this state, two electrons with opposite spins tend to occupy lower-energy sites, resulting in a crystalline order of bipolarons. If this order is sufficiently strong, it causes a metal-insulator transition. This is nothing but the charge-density-wave (CDW) state with a structural change of the crystal.

In the SC state, the phonon clouds will move from site to site according to the motion of electrons so as to keep them in a bound state, resulting in no frozen phonons. The crystalline state of bipolarons, on the other hand, has a frozen phonon that is not greatly influenced by instantaneous motions of individual electrons, but is dependent mainly on the average static charge density.

As Chakraverty conjectured,[17] these two states are always competing with each other, and this reflects the competition between the adiabatic nature and the inverse-adiabatic one of the e-ph coupling. In the adiabatic limit, the frozen part of the phonon will be dominant, since the motion of the phonon is too slow to follow the electron, while in the inverse-adiabatic limit, the moving part will be dominant, because the phonon can follow the electron without retardation. One of the main purposes of the present paper is to clarify this competition.

There are several kinds of superconducting materials wherein the e-ph coupling is so strong as to be in the critical region. In $BaPb_{1-x}Bi_xO_3$ ($x=1\sim0$), the breathing motions of oxygen atoms around a bismuth atom are inferred to contribute both to the pairing order and the structural change involving the metal-insulator transition.[18] According to the recent theoretical studies[19] on $A15$-type compounds, it is shown that the e-ph couplings in these materials are too strong to be described even by the standard "strong-coupling theory."[14] Typical examples for the material with the crystalline order of bipolarons are the transition-metal oxides such as Ti_4O_7 (Ref. 11) and $Na_{0.33}V_2O_5$ (Ref. 12), wherein the metal-insulator transition occurs at low temperatures.

In the present paper, we will study the competition between the SC-type pairing order and the CDW-type crystalline order of bipolarons in a two dimensional N-site N-electron system ($N \gg 1$) with a site-diagonal e-ph coupling. We will assume that the Fermi surface of noninteracting electrons is a complete circle with no nesting-type instability in the case of weak e-ph coupling, so as to focus mainly on the strong-coupling region. Phonon clouds moving with the electrons as well as a frozen phonon will be taken into account by a variational method, combined with a mean-field theory. It will cover the whole region of T, S, and ω, and the resultant phase diagram will be shown in a triangular coordinate space spanned by these three quantities. The nature of the collective excitation within the energy gap of the SC state will also be studied by the random-phase approximation, so as to clarify the crossover between the BCS type and the superfluid type.

II. MANY-POLARON SYSTEM

Let us consider a two-dimensional square lattice composed of N sites ($N \gg 1$), and of N electrons interacting with each other and with phonons. Its Hamiltonian ($\equiv H$) is given as ($\hbar=1$),

$$H=-\sum_{l,l',\sigma} T(l-l')\eta_{l\sigma}^{\dagger}\eta_{l'\sigma}+U\sum_{l} n_{l\alpha}n_{l\beta}+(S\omega/2)^{1/2}\sum_{l,\sigma}(\zeta_l^{\dagger}+\zeta_l)n_{l\sigma}+\omega\sum_{l}\zeta_l^{\dagger}\zeta_l \ . \tag{2.1}$$

$T(l-l')$ denotes the transfer energy of an electron between two lattice sites specified by l' and l, where l denotes a two-dimensional position vector, $l\equiv(l_x,l_y)$, $l_x,l_y=1,2,\ldots,N^{1/2}$, represented in a Cartesian coordinate space spanned by two crystal axes of square lattice. The unit of the length is the lattice constant. $\eta_{l\sigma}^{\dagger}$ ($\eta_{l\sigma}$) denotes the creation (annihilation) operator of electron at site l with spin σ ($=\alpha,\beta$), where α and β denote up and down spin, respectively. U is the energy of intrasite Coulombic repulsion, and $n_{l\sigma}\equiv\eta_{l\sigma}^{\dagger}\eta_{l\sigma}$. S is the site-diagonal coupling energy between an electron and a site-localized phonon with an energy ω. $\zeta_l^{\dagger}$ (ζ_l) is its creation (annihilation) operator. This phonon mode corresponds to the intramolecular vibration in the case of molecular crystals, and in the case of inorganic solids it corresponds to a breathing mode of a ligand around a metallic atom with a conducting electron.

To focus our attention mainly on the strong region of

e-ph coupling, we assume that the Fermi surface of noninteracting electrons is a complete circle, with no nesting-type instability in the case of weak e-ph coupling. Hence, we assume that the transfer energy between nearest-neighbor sites is T, that between the next-nearest-neighbor sites is gT ($g=0.35$), and zero otherwise. This provides us with an almost completely round Fermi surface, and its density of states has no singularity around this Fermi level, as shown in Fig. 1. Although we are concerned with only the two-dimensional square lattice throughout this paper, we tacitly assume that there is a small interlayer interaction which makes long-range order stable.

It is expedient to cast all quantities into dimensionless forms: $h \equiv H/\omega$, $t(l-l') \equiv T(l-l')/\omega$, $u \equiv U/\omega$, $s \equiv S/\omega$, where h becomes

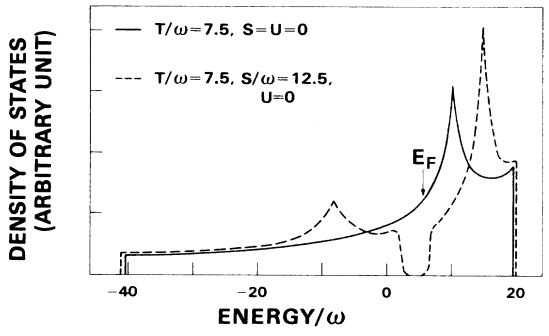

FIG. 1. The density of states of the noninteracting electron (solid line), and of the bipolaronic insulator (dashed line).

$$h = -\sum_{l,l',\sigma} t(l-l')\eta^{\dagger}_{l\sigma}\eta_{l'\sigma} + u\sum_{l} n_{l\alpha}n_{l\beta} + (s/2)^{1/2}\sum_{l,\sigma} n_{l\sigma}(\zeta^{\dagger}_{l}+\zeta_{l}) + \sum_{l}\zeta^{\dagger}_{l}\zeta_{l} \ . \tag{2.2}$$

As mentioned in Sec. I, the state of the phonon can be qualitatively divided into two parts: the frozen part that follows only the static charge density, and the moving part that follows the instantaneous motion of each electron. In the adiabatic limit the frozen part will be dominant, while in the inverse-adiabatic limit, the moving one will be important. Our main idea of describing the intermediate region is an interpolation between these two limits. That is, the two parts are assumed to coexist with a ratio determined by a variational method. For this sake, we introduce a displacement operator ($\equiv M$) for the phonon:

$$M \equiv \exp\left[-is^{1/2}\sum_{l} P_l\left[\bar{q}_l + \sum_{l',\sigma'}\Delta q(l-l')n_{l'\sigma'}\right]\right] ,$$
$$P_l \equiv i(\zeta^{\dagger}_{l}-\zeta_{l})/2^{1/2} , \tag{2.3}$$

which can transform $\eta^{\dagger}_{l\sigma}$ and $\zeta^{\dagger}_{l}$ as

$$a^{\dagger}_{l\sigma} \equiv M^{-1}\eta^{\dagger}_{l\sigma}M = \exp\left[is^{1/2}\sum_{l'}\Delta q(l-l')P_{l'}\right]\eta^{\dagger}_{l\sigma} , \tag{2.4}$$

$$b^{\dagger}_{l} \equiv M^{-1}\zeta^{\dagger}_{l}M = \zeta^{\dagger}_{l} + (s/2)^{1/2}\left[\bar{q}_l + \sum_{l',\sigma'}\Delta q(l-l')n_{l'\sigma'}\right] . \tag{2.5}$$

Here, $\bar{q}_l$ denotes the frozen displacement of phonon at site l, being not directly related to the occupation $n_{l\sigma}$, while $\Delta q(l-l')$, assumed to be an even function of $(l-l')$, denotes the moving displacement of phonons at site l created by electrons at site l'. $\eta^{\dagger}_{l\sigma}$ is now transformed into a creation operator of localized polaron $a^{\dagger}_{l\sigma}$ with a phonon cloud whose spatial extent is given by $\Delta q(l)$. $b^{\dagger}_{l\sigma}$ denotes the creation operator of a new phonon whose equilibrium position is already displayed by aforementioned two parts. Although the original e-ph coupling is of short range, we cannot assume $\Delta q(l)=\delta_{l0}$, because the electron is moving through the effect of $T(l-l')$. Moreover the degree of the spatial extension of $\Delta q(l)$, usually called the polaron radius, plays very important roles as is seen in following sections.

Substituting Eqs. (2.4) and (2.5) into Eq. (2.2), we get

$$\begin{aligned} h = &-\sum_{l,l',\sigma} t(l-l')\exp\left[-is^{1/2}\sum_{l''}[\Delta q(l-l'')-\Delta q(l'-l'')]P_{l''}\right]a^{\dagger}_{l\sigma}a_{l'\sigma} \\ &-s\sum_{l,\sigma}\bar{q}_l n_{l\sigma} + s\sum_{l}(\bar{q}^{\,2}_{l}/2) + u\sum_{l} n_{l\alpha}n_{l\beta} - s\sum_{l,\sigma,l',\sigma}[\Delta q(l-l')-\Delta q_2(l-l')/2]n_{l\sigma}n_{l'\sigma'} \\ &+\sum_{l} b^{\dagger}_{l}b_{l} + (s/2)^{1/2}\sum_{l,l',\sigma}(b^{\dagger}_{l}+b_{l})[\delta_{ll'}-\Delta q(l-l')-\bar{q}_l/N]n_{l'\sigma'} , \end{aligned} \tag{2.6}$$

$$\Delta q_2(l) \equiv \sum_{l'}\Delta q(l-l')\Delta q(l') , \tag{2.7}$$

where we have assumed the orthogonality between two parts of displacements

$$\sum_{l'} \bar{q}_{l'} \Delta q(l'-l)=0 \quad \text{for any } l \ , \tag{2.8}$$

so that their roles do not entangle with each other in the variational method. The first term of Eq. (2.6) denotes the transfer of a polaron, the second one is the potential given by the frozen part, and the third is its elastic energy. The fifth one is the attraction between polarons, subtracted by the increase of elastic energy to create the phonon cloud: $\Delta q_2(l-l')/2$. The sixth one is the Hamiltonian of the new phonon, and the last one denotes the interaction between the polaron and the new phonon. If we assume $\Delta q(l) \equiv \delta_{l0}$ and $\bar{q}_l=0$, this interaction term disappears. However, such a transformation will be useful only in the inverse-adiabatic limit where each electron always becomes a small polaron with no frozen phonon.

Since the displacement of the equilibrium position of the phonon has already been taken into account by Eq. (2.5), the new phonon vacuum [$\equiv |0)$)] becomes our reference state. Using this state, we define an averaged reduction factor ($\equiv X$) of the transfer energy, including the overlap integral between phonon clouds localized at each site [here, $((\cdots)) \equiv ((0|\cdots|0))$],

$$X=\sum_{l,l'} t(l-l') \left\{ \left[\exp\left[-is^{1/2} \sum_{l''} [\Delta q(l-l'')-\Delta q(l'-l'')] P_{l''} \right] \right] \right\} \Big/ \sum_{l,l'} t(l-l') \ . \tag{2.9}$$

It can be easily calculated and we get

$$X=\sum_{l} t(l) \exp\{-s[\Delta q_2(0)-\Delta q_2(l)]/2\} \Big/ \sum_{l} t(l) \ . \tag{2.10}$$

We should note that X^{-1} is nothing but the mass enhancement. In terms of X, thus obtained, we can rewrite h and divide it into four parts as,

$$h=h_0+\sum_{l} b_l^{\dagger} b_l + \Delta h_1 + \Delta h_2 \ . \tag{2.11}$$

h_0 is the Hamiltonian of the many-polaron system whose transfer energy is replaced by its averaged value as

$$\begin{aligned} h_0 \equiv & -X \sum_{l,l',\sigma} t(l-l') a_{l\sigma}^{\dagger} a_{l'\sigma} - s \sum_{l,\sigma} \bar{q}_l n_{l\sigma} + s \sum_{l} (\bar{q}_l^{\,2}/2) - \sum_{l,l'} \{ s[2\Delta q(l-l')-\Delta q_2(l-l')] - u\delta_{ll'} \} n_{l\alpha} n_{l'\beta} \\ & - s \sum_{l,l',\sigma} \{ [2\Delta q(l-l')-\Delta q_2(l-l')] - [2\Delta q(0)-\Delta q_2(0)] \} n_{l\sigma} n_{l'\sigma}/2 - sN[2\Delta q(0)-\Delta q_2(0)]/2 \ , \end{aligned} \tag{2.12}$$

where the last term is the self-energy of the polarons. Δh_1 is the linear interaction term mentioned before,

$$\Delta h_1 \equiv (s/2)^{1/2} \sum_{l,l',\sigma'} (b_l^{\dagger}+b_l)[\delta_{ll'}-\Delta q(l-l')-\bar{q}_l/N] n_{l'\sigma'} \ , \tag{2.13}$$

and Δh_2 is the difference between the true transfer and the averaged one,

$$\Delta h_2 \equiv -\sum_{l,l',\sigma} t(l-l') \left[\exp\left[-is^{1/2} \sum_{l''} [\Delta q(l-l'')-\Delta q(l'-l'')] P_{l''} \right] - X \right] a_{l\sigma}^{\dagger} a_{l'\sigma} \ . \tag{2.14}$$

It is not our purpose to study all possible ground states brought about by the model Hamiltonian h, but rather to clarify the nature of the competition between the SC type pairing order and the crystalline order of bipolarons in the region where the e-ph coupling is strong and the Coulombic repulsion U is weak enough to play only a minor role. Since our system is the square lattice with N sites and N electrons, the crystalline phase of bipolarons in the strong coupling region, $s \gg t$, is inferred to be such that the frozen displacement occurs with twice the period of the original square lattice, both in two directions of the crystal axes,

$$\bar{q}_l = q \cos(Q \cdot l) + 1, \quad Q \equiv (\pi,\pi) \ . \tag{2.15}$$

Here, q (>0) denotes the amplitude of this frozen displacement, Q denotes its wave vector with two dimensions, and the constant term denotes the uniform displacement corresponding to the uniform charge density. $\bar{q}_l$ raises and lowers the site-energy of the electrons alternately along the two axes, and two electrons with opposite spins from each other tend to occupy lower-energy sites. This is the bipolaronic crystal with twice the period schematically shown in Fig. 2. We can also think of other possibilities such as $Q=(\pi,0)$ and $(0,\pi)$, which result in an array of bipolarons with the original period in one direction and with twice the period in the other direction. This state, however, is more unstable than the former one, because Pauli's exclusion principle acts between two bipolarons in neighboring sites, through the second-order perturbation of T.

In the case of weak e-ph coupling, $t \gg s$. On the other

hand, a frozen displacement will occur with such Q that two parts of the Fermi surface can nest, so long as this is possible. As mentioned occasionally, however, the Fermi surface is a circle, any two parts of which cannot nest with each other so efficiently as to make this CDW state more stable than the metallic one. For these reasons, we assume that the frozen displacement only of the type given by Eq. (2.15) can occur, so long as the frozen displacement can occur.

Let us now approximate that the total wave function ($\equiv |\varphi\rangle$) of our system is composed only of the new phonon vacuum as

$$|\varphi\rangle \rightarrow |\varphi_0\rangle\rangle\ |0))\ , \tag{2.16}$$

where $|\varphi_0\rangle\rangle$ is the wave function of the polaron part. We should note $|\varphi_0\rangle\rangle$ or $|0))$ is an operand on which only $a_{l\sigma}^{\dagger}$ ($a_{l\sigma}$) or $b_l^{\dagger}$ (b_l) acts, respectively, and hence this approximation is equal to hold only h_0 in Eq. (2.11), by neglecting Δh_1 and Δh_2. The effects of the neglected parts will be studied in later sections.

The wave-vector representation of h_0 is given by

$$\begin{aligned} h_0 = &-\sum_{k,\sigma} e_k a_{k\sigma}^{\dagger} a_{k\sigma} - sq \sum_{k,\sigma} a_{k+Q,\sigma}^{\dagger} a_{k\sigma} + (sq^2 N/2) - \sum_{k,p} \sum_{k'(\neq k)} N^{-1}[s(2\Delta q_{k-k'} - \Delta q_{k-k'}^2) - u] \\ &\times a_{k+p/2,\alpha}^{\dagger} a_{-k+p/2,\beta}^{\dagger} a_{-k'+p/2,\beta} a_{k'+p/2,\alpha} \\ &+ s \sum_{k,p} \sum_{k'(\neq k)} \sum_{\sigma} N^{-1} \left[(2\Delta q_{k-k'} - \Delta q_{k-k'}^2) - \sum_{p'} N^{-1}(2\Delta q_{p'} - \Delta q_{p'}^2) \right] \Big/ 2 \\ &\times a_{k+p/2,\sigma}^{\dagger} a_{k-p/2,\sigma} a_{k'-p/2,\sigma}^{\dagger} a_{k'+p/2,\sigma} - (sN/2) + (uN/4) - s \sum_{p} (2\Delta q_p - \Delta q_p^2)/4\ , \end{aligned} \tag{2.17}$$

where k, k', and p are two-dimensional wave vectors in the first Brillouin zone shown in Fig. 3, and $a_{k\sigma}$, Δq_p, and e_k are defined as

$$\begin{aligned} &a_{k\sigma} \equiv \sum_l N^{-1/2} e^{-ik\cdot l} a_{l\sigma}, \quad \Delta q_p \equiv \sum_l \Delta q(l) e^{-ip\cdot l}\ , \\ &t_k \equiv \sum_l e^{-ik\cdot l} t(l), \quad e_k \equiv X t_k\ . \end{aligned} \tag{2.18}$$

The quantity t_k, thus defined, is the Fourier component of the transfer energy $t(l)$ which is given as

$$t_k = 2t[\cos(k_x) + \cos(k_y) + 2g\cos(k_x)\cos(k_y)], \quad t \equiv T/\omega\ , \tag{2.19}$$

where k_x and k_y are two components of k; $k = (k_x, k_y)$. We should also note that there is a relation $\sum_k e_k = \sum_k t_k = 0$, since $t(0) = 0$.

In Eq. (2.17), all uniform interactions are eliminated from fourth and fifth terms and are summarized in the last three terms. The attraction between two polarons with a same spin is also rewritten in a form of exchange repulsion in its appearance. We should also note that

$$\Delta q_0 = 0 \ \text{ and } \ \Delta q_Q = 0\ , \tag{2.20}$$

which come from Eq. (2.8). In terms of Δq_p and t_k, X can be rewritten as

$$X = \sum_l t(l) \exp\left[-s \sum_p N^{-1} \Delta q_p^2 [1 - \cos(p\cdot l)]/2 \right] \Big/ t_0\ , \tag{2.21}$$

where we can see that the frozen displacement has no effect on X.

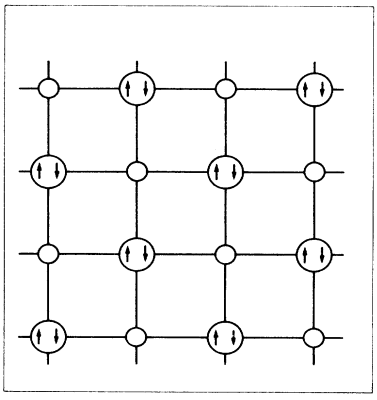

FIG. 2. The schematic nature of the crystalline bipolarons.

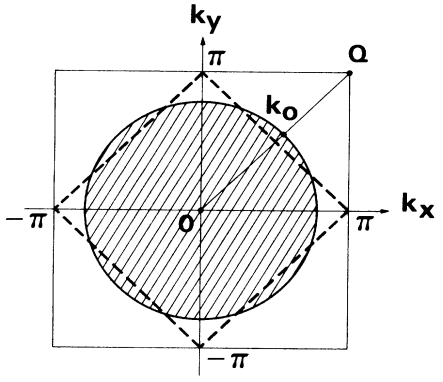

FIG. 3. The first Brillouin zone of the square lattice. The shaded area is occupied in the metallic state. The square surrounded by dashed lines is the half zone (HZ) defined in relation to Eq. (3.13).

III. MEAN-FIELD THEORY

Let us calculate the energy of the ground state of a many-polaron system characterized by h_0, within the mean-field theory for interpolaron interactions and by a variational method for q and Δq_p. So as to reduce the two-body terms of h_0 into one-body terms, we define the partial amplitude of the SC type pairing order ($\equiv f_k$), the crystalline order ($\equiv d_k$), and the average occupation number ($\equiv \Delta n_k$) as

$$f_k = \langle\langle a^\dagger_{k\alpha} a_{-k\beta} \rangle\rangle, \quad d_k = \langle\langle a^\dagger_{k+Q,\sigma} a_{k\sigma} \rangle\rangle ,$$
$$\Delta n_k \equiv \langle\langle a^\dagger_{k\sigma} a_{k\sigma} \rangle\rangle - 1/2 , \tag{3.1}$$

where $\langle\langle \cdots \rangle\rangle \equiv \langle\langle \varphi_0 | \cdots | \varphi_0 \rangle\rangle$ and $\sum_k \Delta n_k = 0$. These quantities are also expected to be even functions of k. In terms of them, h_0 can be reduced as

$$\begin{aligned} h_0 = & -\sum_{k,\sigma} e_k a^\dagger_{k\sigma} a_{k\sigma} - sq \sum_{k,\sigma} a^\dagger_{k+Q,\sigma} a_{k\sigma} + (sq^2 N/2) - \sum_{k,p} N^{-1}[s(2\Delta q_p - \Delta q_p^2) - u] f_{k+p} (a^\dagger_{k\alpha} a^\dagger_{-k,\beta} + a_{-k,\beta} a_{k\alpha} - f_k) \\ & + \sum_{k,p,\sigma} N^{-1}[u + s(2\Delta q_p - \Delta q_p^2)] d_{k+p} (a^\dagger_{k+Q,\sigma} a_{k\sigma} - d_k/2) \\ & + s \sum_{k,p,\sigma} N^{-1}(2\Delta q_p - \Delta q_p^2) \Delta n_{k+p} (a^\dagger_{k\sigma} a_{k\sigma} - \Delta n_k/2) - (sN/2) + (uN/4) - s \sum_p (2\Delta q_p - \Delta q_p^2)/4 , \end{aligned} \tag{3.2}$$

where there is no two-body term. However, f_k, d_k, Δn_k, q, and Δq_p, as well as $|\varphi_0\rangle\rangle$ are unknown at the present stage, and should be determined later self-consistently.

The condition of energy extremum $\partial \langle\langle h_0 \rangle\rangle / \partial q = 0$ combined with the Feynman-Hellman's theorem gives the relation

$$q = 2 \sum_k N^{-1} d_k , \tag{3.3}$$

which is the balance equation between the static charge density and the frozen displacement. Substituting this into Eq. (3.2), we can rewrite h_0 as

$$\begin{aligned} h_0 = & -\sum_{k,\sigma} E_k a^\dagger_{k\sigma} a_{k\sigma} - \sum_k F_k (a^\dagger_{k\alpha} a^\dagger_{-k,\beta} + a_{-k,\beta} a_{k\sigma}) - \sum_{k,\sigma} D_k a^\dagger_{k+Q,\sigma} a_{k\sigma} \\ & + \sum_k [F_k f_k + (E_k - e_k)\Delta n_k + D_k d_k] - (sN/2) + (uN/4) - s \sum_p (2\Delta q_p - \Delta q_p^2)/4 , \end{aligned} \tag{3.4}$$

$$E_k \equiv e_k - s \sum_p N^{-1}(2\Delta q_p - \Delta q_p^2) \Delta n_{k+p} , \tag{3.5}$$

$$F_k \equiv \sum_p N^{-1}[s(2\Delta q_p - \Delta q_p^2) - u] f_{k+p} , \tag{3.6}$$

$$D_k \equiv \sum_p N^{-1}[(2s - u) - s(2\Delta q_p - \Delta q_p^2)] d_{k+p} , \tag{3.7}$$

where E_k is an effective one-polaron energy including the interactions between polarons, F_k is the off-diagonal mixing due to the SC type pairing order, and D_k is the mixing between k and $k+Q$ due to the crystalline order of bipolarons. From Eqs. (3.6) and (3.7), we can see that u contributes to suppress both kinds of orders, while Δq_p contributes positively to F_k, but negatively to D_k. That is, the moving displacement is the origin of the SC type order, while in the crystal phase of bipolarons, it contributes to partially cancel the energy difference between the sites, sq, coming from the frozen displacement. This is a typical aspect of the competition between the adiabatic nature and the inverse-adiabatic one of e-ph coupling.

From Eq. (3.4) we get the total energy as

$$\begin{aligned} \langle\langle h_0 \rangle\rangle = & -\sum_k [F_k f_k + (E_k + e_k)\Delta n_k + D_k d_k] \\ & - (sN/2) + (uN/4) - s \sum_p (2\Delta q_p - \Delta q_p^2)/4 , \end{aligned} \tag{3.8}$$

and the condition of energy extremum $\partial \langle\langle h_0 \rangle\rangle / \partial \Delta q_p = 0$ for fixed Δn_k, d_k, and f_k gives

$$\Delta q_p = \left[1 + 4(t_0 - t_p) t_0^{-1} \sum_k N^{-1} \Delta n_k e_k \Big/ \left[1 + 4 \sum_k N^{-1}(f_{k+p} f_k - \Delta n_{k+p} \Delta n_k - d_{k+p} d_k) \right] \right]^{-1} . \tag{3.9}$$

In this derivation we have used the same approximation as we did in Eq. (2.12). That is, the reduction factor of the transfer energy, which appeared in $\partial X / \partial \Delta q_p$, is replaced by its average as

$$\frac{\partial X}{\partial \Delta q_p} = -2sN^{-1}\Delta q_p \sum_l t(l)\sin^2(p\cdot l/2)\exp\left[-s\sum_{p'} N^{-1}[\Delta q_{p'}\sin(p'\cdot l/2)]^2\right]\Big/ t_0 ,$$

$$\rightarrow -sN^{-1}\Delta q_p X(t_0 - t_p)/t_0 .$$

Thus we have described q and Δq_p in terms of Δn_k, d_k, and f_k, and in the next step, we must derive a self-consistency equation for these three. For this purpose, we first define the Fermi level ($\equiv E_F$) of this many-polaron system by the following equation, assuming E_k is a continuous function of k,

$$\int_{E_F}^{\infty} dE \sum_k N^{-1}\delta(E - E_k) = \tfrac{1}{2} . \tag{3.10}$$

Using E_F, we redefine the one-polaron energy ($\equiv \Delta E_k$) from the Fermi level as

$$\Delta E_k = E_k - E_F ,$$

and transform the present electron picture into an asymmetric electron-hole picture, wherein up-spin electrons are represented by the electron picture, while down-spin electrons are represented by the hole picture as

$$A_k \equiv a_{k\alpha}, \quad B^{\dagger}_{-k} \equiv a_{k\beta} . \tag{3.11}$$

In terms of A_k and B_k, h_0 can be written as

$$\begin{aligned} h_0 = &-\sum_k \Delta E_k (A_k^{\dagger}A_k - B_k^{\dagger}B_k) - \sum_k F_k (A_k^{\dagger}B_k + B_k^{\dagger}A_k) \\ &- \sum_k D_k (A_{k+Q}^{\dagger}A_k - B_k^{\dagger}B_{k+Q}) \\ &+ \sum_k [F_k f_k + (E_k - e_k)\Delta n_k + D_k d_k] \\ &- (sN/2) + (uN/4) - s\sum_p (2\Delta q_p - \Delta q_p^2)/4 , \end{aligned} \tag{3.12}$$

where we have used the relation $\sum_k E_k = 0$ which comes from the formula $\sum_k e_k = \sum_k \Delta n_k = 0$. Restricting the summation over k within the half of the first Brillouin zone (HZ) written by dashed lines in Fig. 3, and denoting such k as $k \in \mathrm{HZ}$, we can rewrite h_0 in a 4×4 matrix form as

$$\begin{aligned} h_0 = &-\sum_{k\in \mathrm{HZ}} \mathbf{A}_k^{\dagger}\underline{M}(k)\mathbf{A}_k \\ &+ \sum_k [F_k f_k + (E_k - e_k)\Delta n_k + D_k d_k] \\ &- (sN/2) + (uN/4) - s\sum_p (2\Delta q_p - \Delta q_p^2)/4 , \end{aligned} \tag{3.13}$$

where $\mathbf{A}_k^{\dagger}$ is the four-dimensional row vector

$$\mathbf{A}_k^{\dagger} \equiv (A_k^{\dagger}, B_k^{\dagger}, A_{k+Q}^{\dagger}, B_{k+Q}^{\dagger}) , \tag{3.14}$$

and $\underline{M}(k)$ is the matrix

$$\underline{M}(k) = \begin{bmatrix} \Delta E_k & F_k & D_k & 0 \\ F_k & -\Delta E_k & 0 & -D_k \\ D_k & 0 & \Delta E_{k+Q} & F_{k+Q} \\ 0 & -D_k & F_{k+Q} & -\Delta E_{k+Q} \end{bmatrix} . \tag{3.15}$$

From the equation

$$\underline{M}(k)\mathbf{V}_i(k) = \xi_i(k)\mathbf{V}_i(k), \quad i = 1, \ldots, 4 \tag{3.16}$$

we get eigenvalue $\xi_i(k)$ and eigenvector $\mathbf{V}_i(k)$ of $\underline{M}(k)$, where $i = 1, \ldots, 4$ is the index of eigenvector, numbered according to its energy,

$$\xi_1(k) \geqq \xi_2(k) \geqq \xi_3(k) \geqq \xi_4(k) . \tag{3.17}$$

However, from the mathematical nature of $\underline{M}(k)$, we can infer that

$$\xi_4(k) \equiv -\xi_1(k), \quad \xi_3(k) = -\xi_2(k) .$$

$V_i^{\dagger}(k)$ in Eq. (3.16) is a four-dimensional row vector

$$\mathbf{V}_i^{\dagger}(k) = (V_{1i}^*(k), V_{2i}^*(k), V_{3i}^*(k), V_{4i}^*(k)) , \tag{3.18}$$

where $V_{mi}^*(k)$ ($m = 1, \ldots, 4$) denotes its component corresponding to the four operators in Eq. (3.14). The unitary transformation $\underline{W}(k)$ that diagonalizes $\underline{M}(k)$ is given by

$$\underline{W}(k) = (\mathbf{V}_1(k), \ldots, \mathbf{V}_4(k)) , \tag{3.19}$$

and a new vector operator $\mathbf{Z}_k^{\dagger}$, defined in terms of $\underline{W}(k)$ as,

$$\mathbf{Z}_k^{\dagger} = \mathbf{A}_k^{\dagger}\underline{W}(k) , \tag{3.20}$$

can diagonalize h_0. Thus we get our final form

$$\begin{aligned} h_0 = &-\sum_{k\in \mathrm{HZ}} [\xi_1(k)(Z_{1k}^{\dagger}Z_{1k} - Z_{4k}^{\dagger}Z_{4k}) \\ &+ \xi_2(k)(Z_{2k}^{\dagger}Z_{2k} - Z_{3k}^{\dagger}Z_{3k})] \\ &+ \sum_k [F_k f_k + (E_k - e_k)\Delta n_k + D_k d_k] \\ &- (sN/2) + (uN/4) - s\sum_p (2\Delta q_p - \Delta q_p^2)/4 , \end{aligned} \tag{3.21}$$

where $Z_{ik}^{\dagger}$ ($i = 1, \ldots, 4$) is the ith component of $\mathbf{Z}_k^{\dagger}$. Since $\xi_1(k)$ and $\xi_2(k)$ are positive, our ground state can now be written as

$$|\varphi_0\rangle\rangle \rightarrow \prod_{k\in \mathrm{HZ}} Z_{1k}^{\dagger}Z_{2k}^{\dagger}\prod_l a_{l\beta}^{\dagger}|0\rangle\rangle ,$$

$$(|0\rangle\rangle \rightarrow \text{true polaron vacuum}) . \tag{3.22}$$

From Eqs. (3.22) and (3.1), we can obtain a set of self-consistency equations as

$$\Delta n_k=\sum_{j=1,2}|V_{1j}(k)|^2-1/2,\quad \Delta n_{k+Q}=\sum_{j=1,2}|V_{3j}(k)|^2-\tfrac{1}{2},(k\in \mathrm{HZ}),$$
$$f_k=\sum_{j=1,2}V_{1j}(k)V_{2j}(k),\quad f_{k+Q}=\sum_{j=1,2}V_{3j}(k)V_{4j}(k),(k\in \mathrm{HZ}), \tag{3.23}$$
$$d_k=\sum_{j=1,2}V_{1j}(k)V_{3j}(k).$$

What we have to do hereafter is to solve a set of equations for X, Δq_p, Δn_k, f_k, and d_k, that is, Eqs. (2.21), (3.5), (3.6), (3.7), (3.9), (3.16), and (3.23). Although it is complicated, we can solve it numerically making use of an iteration procedure, and the total energy can be obtained from Eq. (3.8). We can easily see that F_k at the Fermi level gives a half of the energy gap due to the SC-type order, while D_k gives a half of the energy gap due to the crystalline order of bipolarons if $\Delta E_k=\Delta E_{k+Q}$, and when D_k is large enough to open up the energy gap all over the Fermi surface, we get the bipolaronic insulator.

Generally speaking, the two order parameters D_k and F_k may coexist, however, if one of them is zero, we can simplify Eqs. (3.15), (3.16), and (3.23):

(a) In the case of the SC state; $d_k=0$, $\underline{M}(k)$ is decoupled into two 2×2 matrices, which can be diagonalized by the following unitary transformation,

$$V_{11}(k)=V_{22}(k)=\cos(\phi_k),\quad V_{33}(k)=V_{44}(k)=\cos(\phi_{k+Q}),$$
$$-V_{12}(k)=V_{21}(k)=\sin(\phi_k),\quad -V_{34}(k)=V_{43}(k)=\sin(\phi_{k+Q}), \tag{3.24}$$
$$\phi_k\equiv\arctan[(Y_k-\Delta E_k)/(Y_k+\Delta E_k)]^{1/2},\quad Y_k\equiv(\Delta E_k^2+F_k^2)^{1/2}. \tag{3.25}$$

Other elements in Eq. (3.19) are zero. In this case, Δn_k, f_k, and $\xi_i(k)$ are given by

$$\Delta n_k=\Delta E_k/2Y_k,\quad f_k=F_k/2Y_k,\quad \xi_1(k)=Y_k,\quad \xi_2(k)=Y_{k+Q}. \tag{3.26}$$

(b) In the case of the bipolaronic insulator with $f_k=0$, the unitary transformation is given as

$$V_{11}(k)=V_{22}(k)=V_{33}(k)=V_{44}(k)=\cos(\theta_k),\quad -V_{13}(k)=-V_{24}(k)=V_{31}(k)=V_{42}(k)=\sin(\theta_k),$$
$$\theta_k\equiv\arctan[(\Theta_k-R_{k2})/(\Theta_k+R_{k2})]^{1/2},\quad R_{ki}\equiv(\Delta E_k-(-1)^i\Delta E_{k+Q})/2,(i=1,2)$$
$$\Theta_k\equiv(R_{k2}^2+D_k^2)^{1/2}. \tag{3.27}$$

Other elements in Eq. (3.19) are zero. In this case, Δn_k, d_k, and $\xi_i(k)$ are given as

$$\xi_1(k)=R_{k1}+\Theta_k,\quad \xi_2(k)=-R_{k1}+\Theta_k,$$
$$\Delta n_k=R_{k2}/2\Theta_k,\quad d_k=D_k/2\Theta_k, \tag{3.28}$$

where $\xi_1(k)$ corresponds to the up-spin electron and $\xi_2(k)$ corresponds to the down-spin hole.

IV. EFFECT OF POLARON-PHONON INTERACTION

Let us reinforce the method developed in Sec. III by including effects coming from Δh_1 and Δh_2. At first, we will be concerned with Δh_1, which denotes the interaction between the polaron and the new phonon. In this case, h becomes

$$h\rightarrow h_0+\sum_p b_p^\dagger b_p+\Delta h_1, \tag{4.1}$$

where b_p is the Fourier transform of b_l

$$b_p\equiv\sum_l N^{-1/2}e^{-ip\cdot l}b_l, \tag{4.2}$$

and Δh_1 can be rewritten in terms of b_p as

$$\Delta h_1=(s/2)^{1/2}\sum_{p(\neq 0)}N^{-1/2}(b_p^\dagger+b_{-p})(1-\Delta q_p)\left[\sum_{k,\sigma}a_{k+p/2,\sigma}^\dagger a_{k-p/2,\sigma}-q\delta_{pQ}\right]. \tag{4.3}$$

In the adiabatic limit, it gives a perturbation to the many-polaron system due to the quantum fluctuation of phonons around the frozen displacement, and its effect will be small because of the great difference between the velocity of the electron and that of the phonon. In the inverse-adiabatic limit, on the other hand, the electron becomes a small polaron $\Delta q_p\approx 1$, and Δh_1 denotes a small residual part of e-ph coupling not included in this polaron effect, as seen from the factor $(1-\Delta q_p)$ of Eq. (4.3). For these reasons, we take effects of Δh_1 into account within the second-order perturbation theory. Our theory for describing the intermediate region between these two lim-

its is an interpolation in this sense, too.

Assuming that our ground state is composed not only by the new phonon vacuum but also by a fractional one phonon state, we can write $|\varphi\rangle$ as

$$|\varphi\rangle \rightarrow \left[|\varphi_0\rangle\rangle + \sum_p |\varphi_p\rangle\rangle b_p^\dagger \right] |0\rangle) , \tag{4.4}$$

where $|\varphi_p\rangle\rangle$ is the wave function of the polaron part associated with the one-phonon state. What we must now do is solve the equation $h|\varphi\rangle = E|\varphi\rangle$, where E is the new total energy, and within the second-order perturbation, $|\varphi_p\rangle\rangle$ is given in terms of $|\varphi_0\rangle\rangle$ as

$$|\varphi_p\rangle\rangle = -(h_0 + 1 - \langle\langle h_0 \rangle\rangle)^{-1}((b_p \Delta h_1))|\varphi_0\rangle\rangle . \tag{4.5}$$

From this, we can eliminate $|\varphi_p\rangle\rangle$ and reduce h into an effective Hamiltonian $(h_0 + \Delta h_e)$ which acts only on $|\varphi_0\rangle\rangle$ as,

$$(h_0 + \Delta h_e)|\varphi_0\rangle\rangle = E|\varphi_0\rangle\rangle , \tag{4.6}$$

where Δh_e is defined by

$$\Delta h_e \equiv -\sum_p [(\Delta h_1 b_p^\dagger)](h_0 + 1 - \langle\langle h_0 \rangle\rangle)^{-1}[(b_p \Delta h_1)]$$
$$= -s \sum_{p(\neq 0)} N^{-1}(1-\Delta q_p)^2 \left[\sum_{k',\sigma'} a^\dagger_{k'-p/2,\sigma'} a_{k'+p/2,\sigma'} - q\delta_{pQ} \right] (h_0 + 1 - \langle\langle h_0 \rangle\rangle)^{-1} \left[\sum_{k,\sigma} a^\dagger_{k+p/2,\sigma} a_{k-p/2,\sigma} - q\delta_{pQ} \right] \Big/ 2 . \tag{4.7}$$

This equation gives a solution for $|\varphi_0\rangle\rangle$ which is different from the previous one obtained by Eq. (3.22). However, the effect of Δh_e can be estimated on the basis of the previous solution. For this sake, we introduce a new particle-hole picture taking the ground state given by Eq. (3.22) as our new vacuum. In this picture, h_0 given by Eq. (3.21) is rewritten as

$$h_0 \equiv \sum_k \xi(k)(\tilde{Z}^\dagger_k \tilde{Z}_k + Z^\dagger_k Z_k) + \langle\langle h_0 \rangle\rangle , \tag{4.8}$$

where

$$\xi(k) \equiv \xi_1(k), \quad \tilde{Z}_k \equiv Z^\dagger_{1k} ,$$
$$Z_k \equiv Z_{4k} \quad (k \in \mathrm{HZ}) ,$$
$$\xi(k) \equiv \xi_2(k-Q), \quad \tilde{Z}_k \equiv Z^\dagger_{2,k-Q} ,$$
$$Z_k \equiv Z_{3,k-Q} \quad (k \notin \mathrm{HZ}) ,$$

and $\tilde{Z}^\dagger_k$ ($Z^\dagger_k$) is the creation operator of a hole (particle) above the new vacuum. This new particle-hole picture should not be confused with the old one defined by Eq. (3.11). When the gap due to two kinds of orders is very small: (F_k and D_k) $\ll t$, our system is almost same as the noninteracting metallic system with $\xi(k) \sim |\Delta E_k|$. In this case, $a_{k\alpha}$ is described in terms of $\tilde{Z}^\dagger_k$ and Z_k and $a_{-k\beta}$ is described in terms of $Z^\dagger_k$ and $\tilde{Z}_k$. Hence, $(h_0 + 1 - \langle\langle h_0 \rangle\rangle)^{-1} a^\dagger_{k\sigma} a_{k'\sigma} |\varphi_0\rangle\rangle$ appeared in Eqs. (4.6) and (4.7) can be denoted by a linear combination of following four types of terms

$$\begin{aligned}
&(1+\xi(k)+\xi(k'))^{-1}\tilde{Z}^\dagger_k Z^\dagger_{k'}|\varphi_0\rangle\rangle , \\
&(1-\xi(k)-\xi(k'))^{-1}\tilde{Z}_k Z_{k'}|\varphi_0\rangle\rangle , \\
&(1+\xi(k)-\xi(k'))^{-1}\tilde{Z}^\dagger_k \tilde{Z}_{k'}|\varphi_0\rangle\rangle , \\
&(1+\xi(k)-\xi(k'))^{-1} Z^\dagger_k Z_{k'}|\varphi_0\rangle\rangle .
\end{aligned} \tag{4.9}$$

They correspond to a particle-hole pair creation, a pair annihilation, and scatterings of a hole or a particle. However, all four of these parts are equally important only in a narrow region around the Fermi level; $(\xi(k), \xi(k')) \approx 0$, and hence we can replace all energy denominators by $[1+\xi(k)+\xi(k')]^{-1}$ without serious numerical errors. When the gap is very large, F_k or $D_k \gg t$, on the other hand, we can also rewrite

$$(h_0 + 1 - \langle\langle h_0 \rangle\rangle)^{-1} a^\dagger_{k\sigma} a_{k'\sigma} |\varphi_0\rangle\rangle$$

by using similar terms as shown in Eq. (4.9). In this case, however, only the particle-hole pair creation term is important because of the large gap, and $\xi(k)$ becomes almost independent of k. For these reasons we can replace $(h_0 + 1 - \langle\langle h_0 \rangle\rangle)^{-1}$ in Eq. (4.7) by

$$\{[1+\xi(k'+p/2)+\xi(k'-p/2)]^{-1} + [1+\xi(k+p/2)+\xi(k-p/2)]^{-1}\}/2 .$$

After this replacement, we apply the mean-field approximation to $h_0 + \Delta h_e$ and can get a very similar form to Eq. (3.4) as,

$$h_0 + \Delta h_e = -\sum_{k,\sigma} E'_k a^\dagger_{k\sigma} a_{k\sigma} - \sum_k F'_k (a^\dagger_{k\sigma} a^\dagger_{-k\beta} + a_{-k\beta} a_{k\alpha}) - \sum_{k,\sigma} D'_k a^\dagger_{k+Q,\sigma} a_{k\sigma} + \sum_k [F'_k f_k + (E'_k - e_k)\Delta n_k + D'_k d_k]$$
$$-(sN/2) + (uN/4) - s \sum_p \left[(2\Delta q_p - \Delta q_p^2) + \sum_k N^{-1} G(k,p)(4n_k + 1) \right] \Big/ 4 , \tag{4.10}$$

$$G(k,p) \equiv (1-\Delta q_p)^2 / [1 + \xi(k) + \xi(k+p)] , \tag{4.11}$$

where E'_k, F'_k, and D'_k are defined as

$$E'_k \equiv e_k - s\sum_p N^{-1}[(2\Delta q_p - \Delta q_p^2) + G(k,p)]\Delta n_{k+p} , \tag{4.12}$$

$$F'_k \equiv \sum_p N^{-1}\{s[(2\Delta q_p - \Delta q_p^2) + G(k,p)] - u\} f_{k+p} , \tag{4.13}$$

$$D'_k \equiv \sum_p N^{-1}\{(2s-u) - s[(2\Delta q_p - \Delta p_q^2) + G(k,p)]\} d_{k+p} . \tag{4.14}$$

The total energy of the system also becomes different from Eq. (3.8), and it is given by

$$\langle\langle h_0 + \Delta h_e \rangle\rangle = -\sum_k [F'_k f_k + (E'_k + e_k)\Delta n_k + D'_k d_k] - (sN/2) + (uN/4) - s\sum_p \left[(2\Delta q_p - \Delta q_p^2) + \sum_k N^{-1} G(k,p)\right] \Big/ 4 . \tag{4.15}$$

From Eqs. (4.12), (4.13), (4.14), and (4.15), we can easily see that the effect of Δh_1 is almost same as that of the moving displacement Δq_p, but makes its role more complete, since it contributes positively to F'_k and negatively to D'_k. Using these results, we can determine q, Δq_p, Δn_k, f_k, d_k, E'_k, F'_k, and D'_k, using the almost same procedure as we did in Sec. III. The main difference between the previous case and the present one is that we must prepare $\xi(k)$ in Eq. (4.11) beforehand by solving relevant equations given in Sec. III. However, we omit the detail of this procedure. After numerical calculations according to this theory, we can finally complete our phase diagram. These results will be shown in the following section.

Incidentally, we can also estimate the effects of Δh_2 which comes from the difference between the averaged transfer and the true one. However, its contribution to the total energy is smaller than that of Δh_1.

V. NUMERICAL RESULTS AND EXTREME CASES

In this section, we will be concerned with extreme cases at first, and after that, we will proceed to more general cases.

In the adiabatic limit; $(t,s) \gg 1$, we get $\Delta q_p \ll 1$ and $X = 1$, as seen from Eq. (3.9), since in this equation Δn_k, f_k, and d_k are the quantities of the order of unity, while e_k is proportional to t. Thus, the electron is almost bare with only a thin phonon cloud, and moving in a potential due to the frozen phonon, so long as the frozen part can exist. Since the Fermi surface is a circle with no nesting-type instability, the region with small S/T is the SC state with a very small gap. In this case, our gap equation Eq. (4.13) gives the same result as that of the standard BCS Theory.[13] As S/T increases under the condition $(t,s) \gg 1$, this state changes to the crystalline phase of bipolarons with a frozen phonon, at a certain threshold value of S/T.

In the inverse-adiabatic limit, $(t,s) \ll 1$; on the other hand, we can regard the first three terms of Eq. (2.2) as a perturbation to the eigenstates given by its last term. In this case, the e-ph coupling can be eliminated by the second-order perturbation theory, and it results in an attraction between polarons as

$$h = -\sum_{l,l',\sigma} t(l-l') a^\dagger_{l\sigma} a_{l\sigma} - (s-u)\sum_l n_{l\alpha} n_{l\beta} - sN/2 . \tag{5.1}$$

In other words, we can put $\Delta q_p = 1$ [or $\Delta q(l) = \delta_{l0}$] and $X = 1$ in Eqs. (2.12) and (2.21). That is, the electron is always a small polaron with no mass enhancement. Since the Fermi surface is a complete circle we always have the SC state except the special case with $t = 0$.

For other general cases, we have solved the equations derived in Secs. IV and III numerically, and the resultant phase diagram is shown in Fig. 4. Because of the great mathematical complexities, we have assume that $U = 0$. However, the calculation is performed for all combinations of T, S, and ω. We can see that the phase diagram is separated into the SC state ($d_k = 0$, $f_k \neq 0$) and the bipolaronic insulator ($d_k \neq 0$, $f_k = 0$). Although we have solved the equations for d_k and f_k under the coexistent condition, we could not obtain a new energy gain due to this coexistence. This is mainly because our Fermi surface is perfectly round. We should also note that the SC state, just on the T-S and T-ω lines in the triangle, is the same as the metallic state.

In the adiabatic region, the boundary between the two phases is given by $S/T = 1.47$ (point C), while, as ω increases, the region of the SC phase expands in the phase diagram, and becomes dominant in the region around the ω vertex except on the S-ω line. In Figs. 5–8, we have shown how the state changes according to the change of ω/S (or ω/T) when S/T is fixed at 5/3. As seen in Fig. 5, the bipolaronic insulator becomes more unstable than the SC state at $\omega/S \sim 0.3$. This is mainly because the moving displacement $\Delta q(l)$ increases according to the increase of ω/S (or ω/T) as seen from Fig. 6, and hence the bipolaronic crystal is forced to melt. In fact, q also decreases as ω/T increases. It is also very interesting that the reduction factor X, being unity in both limits, is reduced most distinctly in the intermediate region, where the velocity of the electron is of the same order as that of the phonon. In Fig. 7, we have shown half of the energy gap ($D'_{Q/2})\omega/S$ and ($F'_{k_0})\omega/S$(, k_0 denotes the Fermi level on the $0Q$ line in Fig. 3). In the region of bipolaronic insulator, ($D'_{Q/2})\omega/S$ decreases as ω/S (or ω/T) increases.

Strictly speaking, this energy gap is somewhat larger than the half of the true energy gap written in Fig. 7 by the dashed line, which is obtained after calculating such a density of states as shown in Fig. 1. However $(D'_{Q/2})\omega/S$ and the true energy gap have a same (ω/S) dependence.

As for $(F'_{k_0})\omega/S$, it increases rapidly according to the increase of ω/S (or ω/T). However, it takes its broad maximum in the intermediate region $S\sim\omega$ $(T\sim\omega)$. This maximum, although it depends on S/T, always appears in the intermediate region, as far as the SC state is more stable than the bipolaronic insulator.

In Fig. 8 we have shown the Δq_p as a function p, where we can see that the electron becomes a large polaron in the adiabatic limit, since Δq_p is finite only when $|p| \ll \pi$. As ω/S (or ω/T) increases, however, the components with large $|p|$ increase, and finally they become $\Delta q_p = 1$. That is, the polaron shrinks its radius as ω/T increases.

We have also clarified how the state changes along the line $(S+T)/\omega = 1$. As shown in Fig. 9, the transition occurs at $S/T\sim 2.1$. According to the increase of S/T, F'_{k_0} and $\Delta q(0)$ increase, and X decreases as shown in Figs. 10 and 11. However, it is stopped by the phase transition.

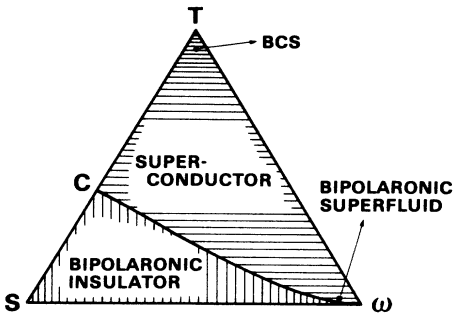

FIG. 4. The phase diagram on the "T-S-ω triangle". The ratios between the three parameters are denoted by the lengths of the perpendiculars from a given point to three vertices.

VI. COLLECTIVE EXCITATION IN THE GAP

In this section we study the nature of the lowest collective excitation in the energy gap of the SC state, by making use of the random-phase approximation (RPA). For simplicity we consider this problem in the region around the ω vertex of the phase diagram, where h can be approximated as given by Eq. (5.1). Using the notation introduced in Eq. (4.8), we can write h as

$$h=\sum_k \xi(k)(\tilde{Z}_k^\dagger \tilde{Z}_k + Z_k^\dagger Z_k) + \langle\langle h_0 \rangle\rangle + (h-h_0)\ , \tag{6.1}$$

where the first and second terms are the Hamiltonian within the mean-field theory and the last one is the fluctuation therefrom. Since $\Delta q_p = 1$, F_k becomes independent of k, as seen from Eqs. (3.6). From Eqs. (3.25) and (3.26), it is given by the following gap equation, (when $u=0$),

$$1=(s/2)\sum_k N^{-1}/(\Delta E_k{}^2+F^2)^{1/2}\ . \tag{6.2}$$

The energy of the particle or the hole becomes

$$\xi(k)=(\Delta E_k^2+F^2)^{1/2}\ , \tag{6.3}$$

while the fluctuation $(h-h_0)$ is given by

$$(h-h_0)=-s\sum_{k,k',p} N^{-1}a^\dagger_{k+p/2,\alpha}a^\dagger_{-k+p/2,\beta}a_{-k'+p/2,\beta}a_{k'+p/2,\alpha}+s\sum_{k,k'} N^{-1}f_k(a^\dagger_{k'\alpha}a^\dagger_{-k'\beta}+a_{-k'\beta}a_{k'\alpha}-f_{k'})\ , \tag{6.4}$$

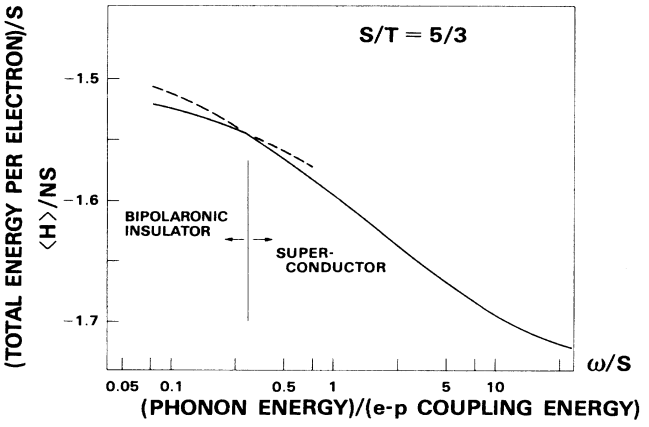

FIG. 5. The total energy per electron, $\langle H\rangle/NS$ as a function of ω/S calculated by Eq. (4.15). $S/T=5/3$, $U=0$.

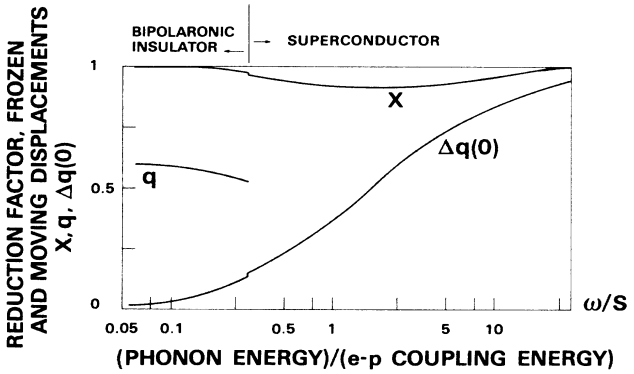

FIG. 6. The reduction factor X, the frozen and moving displacements, q and $\Delta q(0)$, as a function of ω/S. $S/T=5/3$, $U=0$.

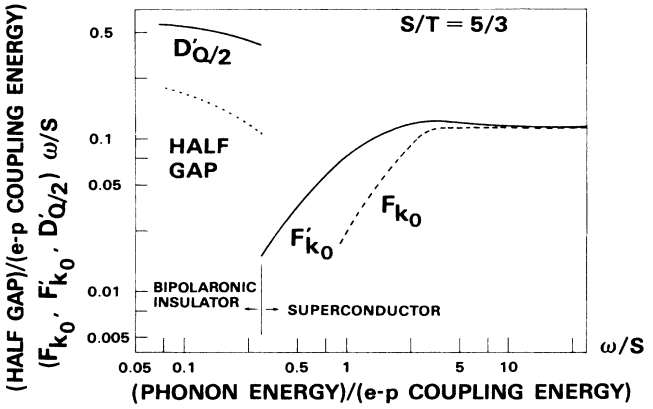

FIG. 7. Half of the energy gap, $(D'_{Q/2}, F'_{k_0}, F_{k_0})\omega/S$ and the true half gap (dotted line) as a function of ω/S. $S/T=5/3$. $U=0$.

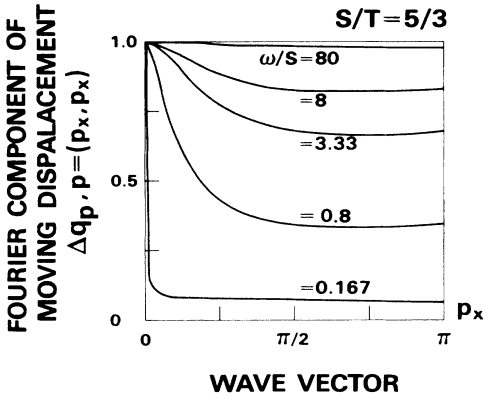

FIG. 8. The Fourier component Δq_p as a function of p and ω/S. $U=0$. $S/T=5/3$. $p=(p_x,p_x)$.

where $f_k=F/2\xi(k)$. What we will now calculate is the lowest energy of the particle-hole pair creation above the ground state given by the mean-field theory. Hence we introduce the pair creation operator ($\equiv\rho^\dagger_{kp}$) as

$$\rho^\dagger_{kp}=\tilde{Z}^\dagger_{k+p/2}Z^\dagger_{-k+p/2}\ ,$$

where k and p correspond to the momenta of the relative motion and the center-of-mass motion of this pair, respectively. According to the spirit of RPA, we rewrite (h-h_0) in Eqs. (6.1) and (6.4) in terms of $\tilde{Z}_k$ and Z_k and take up to the second order with respect to ρ_{kp}'s. This calculation is somewhat lengthy, but it is straightforward. We also rewrite the first term of Eq. (6.1) by using ρ_{kp} and finally get an effective Hamiltonian ($\equiv h_{\rm RPA}$) within the RPA as

$$\begin{aligned}h_{\rm RPA}=&\sum_{k,p}K(k,p)\rho^\dagger_{kp}\rho_{kp}-s\sum_{k,k'p}N^{-1}[\Lambda_-(k,p)\Lambda_-(k',p)+\Lambda_+(k,p)\Lambda_+(k',p)\\&+\Gamma_+(k,p)\Gamma_+(k',p)-\Gamma_-(k,p)\Gamma_-(k',p)]\rho^\dagger_{kp}\rho_{k'p}/2\\&-s\sum_{k,k',p}N^{-1}\{[\Gamma_+(k,p)+\Gamma_-(k,p)][\Gamma_+(k',p)+\Gamma_-(k',p)]\\&-[\Lambda_-(k,p)-\Lambda_+(k,p)][\Lambda_-(k',p)+\Lambda_+(k',p)]\}(\rho^\dagger_{kp}\rho^\dagger_{k',-p}+\rho_{k,-p}\rho_{k'p})/4\ ,\end{aligned}\tag{6.5}$$

$$K(k,p)\equiv\xi(k+p/2)+\xi(k-p/2)\ ,\tag{6.6}$$

$$\Lambda_\pm(k,p)\equiv\cos(\phi_{k+p/2}\pm\phi_{k-p/2}),\Gamma_\pm(k,p)=\sin(\phi_{k+p/2}\pm\phi_{k-p/2})\ ,\tag{6.7}$$

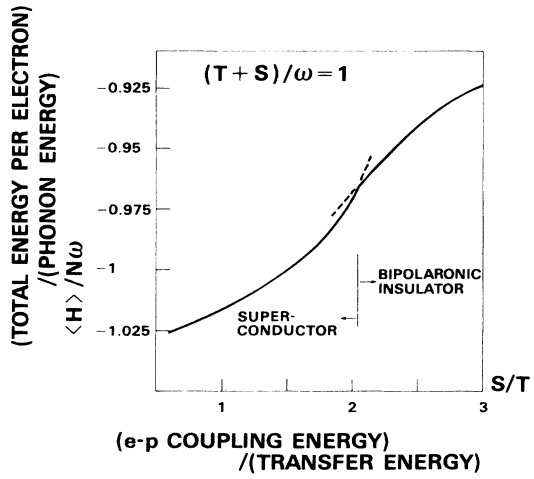

FIG. 9. The total energy per electron $\langle H\rangle/N\omega$ as a function of S/T, calculated by Eq. (4.15). $(T+S)/\omega=1$, $U=0$.

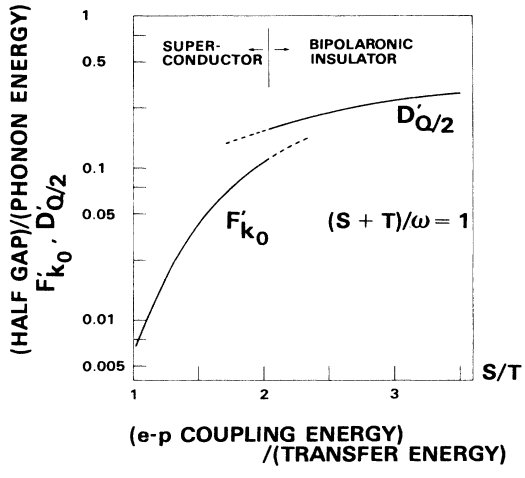

FIG. 10. Half of the energy gap, F'_{k_0} and $D'_{Q/2}$ as a function of S/T. $(T+S)/\omega=1$, $U=0$.

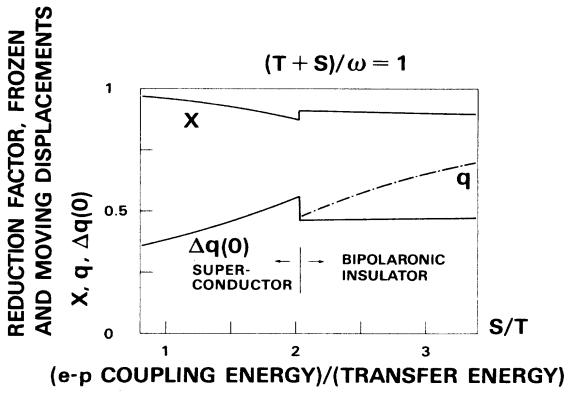

FIG. 11. The reduction factor X, the frozen and moving displacements, q and $\Delta q(0)$, as a function of S/T. $(T+S)/\omega=1$, $U=0$.

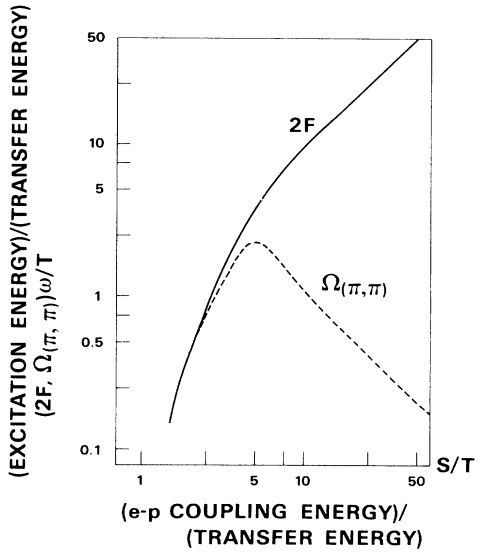

FIG. 13. The energy of the collective excitation $\Omega_{(\pi,\pi)}\omega/T$ and the gap energy $2F\omega/T$ as a function of S/T. $U=0$.

where the first term of Eq. (6.5) comes from the first term of Eq. (6.1), while the second and the third terms of Eq. (6.5) come from $(h\text{-}h_0)$. The second term gives the attraction between the particle and the hole, resulting in a bound state within the gap. The third term denotes the spontaneous creation and annihilation of pairs due to the fluctuation. Since our true ground state is such that many pairs are spontaneously created above the mean-field-theory ground state through this fluctuation, the corresponding true excitation operator $(\equiv\tau_p^\dagger)$ is also the linear combination of $\rho_{kp}^\dagger$ and $\rho_{k,-p}$, and it can be written as

$$\tau_p^\dagger=\sum_k[\mu_+(k,p)\rho_{kp}^\dagger-\gamma_p\mu_-(k,p)\rho_{k-p}]/(1-\gamma_p^2)^{1/2}\ . \tag{6.8}$$

Here $\mu_+(k,p)$ and $\mu_-(k,p)$ are the normalized wave functions that denote the internal motions of pairs and γ_p is the factor that denotes the strength of the spontaneous excitation. This is nothing but the generalized form of the Bogoliubov transformation. The energy of this excitation $(\equiv\Omega_p)$ is determined by the following equation of motion

$$\Omega_p\tau_p^\dagger=[h_{\mathrm{RPA}},\tau_p^\dagger]\ , \tag{6.9}$$

combined with the boson approximation for ρ_{kp}:

$$[\rho_{kp},\rho_{k'p'}^\dagger]=\delta_{kk'}\delta_{pp'}\ . \tag{6.10}$$

The details of the calculation are shown in the Appendix A, and the numerical results are shown in Figs. 12 and 13. In the case of small T, $T/S\gg1$, the problem becomes simple since we can use the second-order perturbation theory with respect to T, and can get an analytical solution based on the pseudomagnon approximation.[20,16] The details of this approximation are shown in Appendix B, and its result is as follows:

$$\Omega_p=[J^2(0)-J(p)^2]^{1/2}\ , \tag{6.11}$$

$$J(p)=16t^2s^{-1}\{g^2\cos(p_x)\cos(p_y)+[\cos(p_x)+\cos(p_y)]/2\}\ , \tag{6.12}$$

where p_x and p_y are the components of p.

As seen from Fig. 12, $\Omega_p=0$ at $p=0$, and it has a sound-wave-like dispersion in the region of small $|p|$. In the case of weak coupling $S/T\gg1$, as is well known, the sound velocity is almost equal to the Fermi velocity.[20] As S/T increases, however, the velocity gradually decreases, and in the strong coupling case; $S/T\gg1$, Ω_p becomes an order of magnitude smaller than $2F$. Moreover it has a rotonlike dispersion at around $p_x\sim\pi$, peculiar to the superfluid type state. According to the criterion due to Landau for the critical velocity of the persistent current, the energy gap relevant to the superfluidity or the superconductivity is $\Omega_{(\pi,\pi)}$ or $\Omega_{(\pi,0)}$ and not $2F$. As shown in Fig. 13, the two excitation energies, $\Omega_{(\pi,\pi)}$ and $2F$, are almost same if $S/T\lesssim3$. However, they become

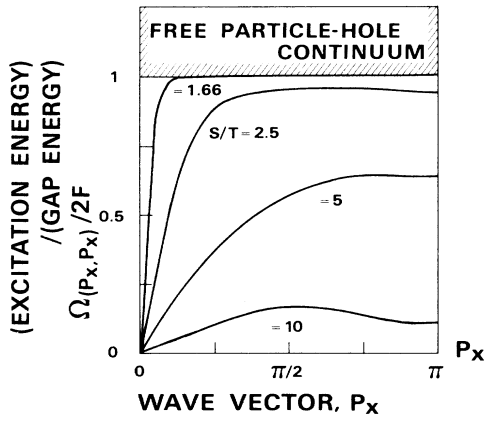

FIG. 12. The relative energy of the collective excitation in the gap of the SC state, $\Omega_p/2F$. $p=(p_x,p_x)$, $U=0$.

come quite different with each other, since $2F$ increases while $\Omega_{(\pi,\pi)}$ decreases as S/T increases. In the very limit of strong coupling, all electrons make singlet pairs (bipolarons), resulting in a Bose condensation. $2F$, in this case, corresponds to the pair breaking excitation, while $\Omega_{(\pi,\pi)}$ corresponds to the excitation that breaks only the coherence between pairs without changing its internal state. The results of our calculation show that this change from the weak limit to the strong one is continuous. The possible region of pairing, being limited only around the Fermi level in the case of weak coupling, gradually expands all over the energy band as the coupling increases. That is, the BCS-type state gradually changes to the superfluid-type state. This is consistent with the results by Pincus *et al.*,[15] Leggett,[21] and Nozières *et al.*[22] However, they did not explicitly show how the collective mode changes its nature as S/T increases.

It should be noted that the region of the aforementioned superfluid-type state is very small as marked in the phase diagram, since it appears in the SC region with $S/T \gtrsim 3$. Thus, we have clarified the interrelation between the BCS type state and the superfluid type state, as well as their competition with the bipolaronic insulator. That is, the strong coupling in the inverse-adiabatic limit results in the superfluid type state, while the strong coupling in the adiabatic limit results in the bipolaronic insulator, as summarized in the phase diagram.

VII. CONCLUSION AND DISCUSSION

We have thus clarified the competition between the SC-type order and the crystalline order of polarons in a two-dimensional system composed of N sites and N electrons, and the resultant phase diagram is given in the triangular coordinate space spanned by T, S, and ω. This triangle is shown to be divided into two regions; the SC region and the bipolaronic insulator region. In the adiabatic region near the TS line of the triangle, each electron becomes a large polaron with a thin phonon cloud, and as S/T increases its SC state changes discontinuously to the bipolaronic insulator with a frozen phonon. As the system approaches the ω vertex of the triangle, however, the polaron decreases its radius and the region of SC state expands in the phase diagram. It is also found, for the first time, that the mean-field-theory energy gap of the SC state for given S and T becomes maximum at the intermediate region, $\omega \sim T$.

The collective excitation within the energy gap of the SC state is also studied by RPA, and it is shown that the lowest excitation changes its nature continuously from the BCS-type pair breaking excitation to the superfluid type one as S/T increases.

Because of the mathematical complexities, we did not take the effects of intrasite Coulombic repulsion into account; however, this effect will be clarified in the near future. The reason why we have chosen the two-dimensional lattice is only to shorten the computation time, and hence an extension to the three-dimensional system is trivial.

Since Chakraverty[17] has conjectured about the possible ordered states of a many-polaron system, various theories have been published concerning the very strong e-ph coupling in metallic systems.[16,23] However, most of these theories do not take into account three main characteristics of the e-ph coupling; the possibility of the frozen displacement, the possible change of the polaron radius, and the residual interaction between the polaron and the new phonon. According to our theoretical results, all three of these parts are indispensable in order to cover the whole region of the T-S-ω triangle.

In the present calculation, we have fixed g in Eq. (2.19) at 0.35, in order to make the Fermi surface completely round. In the case of $g=0$, the Fermi surface becomes a square as denoted by the dashed lines in Fig. 3, and the bipolaronic insulator will be always more stable than the SC phase because of the perfect nesting of the Fermi surface. This situation will be almost same as that of the one-dimensional case which has already been clarified.[24] Hence, we can easily infer that the adiabatic phase boundary, denoted by C in Fig. 4, will move toward the T vertex as g decreases.

Since our theory is concerned only with the absolute zero of the temperature, the thermodynamic nature of the system is left unclarified. However, we can infer that the transition temperature T_c of the SC state is of the same order as that of $\Omega_{(\pi,\pi)}$. We are planning to extend our theory to the finite temperature region, by including the softening of the phonon as well as it possible anharmonicity.[19] Effects of the long-range Coulomb interaction on the excitation spectrum of the collective mode should also be studied in detail, but we leave this problem to a future study.

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APPENDIX A

In this appendix, we solve Eq. (6.9), using Eqs. (6.8) and (6.10). Substituting Eqs. (6.8) and (6.5) into Eq. (6.9), we get the equation for $\mu_{\pm}(k,p)$ as

$$\mu_{\pm}(k,p)=(K(k,p)_{\mp}\Omega_p)^{-1}sN^{-1/2}(\Lambda_-(k,p)\{[\Lambda_-(p)]_{\pm}-\gamma_p^{\pm 1}[\Lambda_-(p)]_{\mp}\} +\Gamma_+(k,p)\{[\Gamma_+(p)]_{\pm}+\gamma_p^{\pm 1}[\Gamma_+(p)]_{\mp}\})/2\ , \tag{A1}$$

where $[\cdots]_{\pm}$ is defined as

$$[\cdots]_{\pm} \equiv \sum_k N^{-1/2}\mu_{\pm}(k,p)(\cdots) . \tag{A2}$$

In this derivation we have neglected $\Gamma_-(k,p)$ and $\Lambda_+(k,p)$ in Eq. (6.5), assuming that $\mu_{\pm}(k,p)$ is an even function of k with no node. Equation (A1), multiplied by $\mu_{\pm}(k,p)(K(k,p)\mp\Omega_p)$ and integrated over k, gives (note that $\sum_k \mu_{\pm}(k,p)^2=1$),

$$[[K(p)]]_{\pm}\mp\Omega_p = s([\Lambda_-(p)]_{\pm}\{[\Lambda_-(p)]_{\pm}-\gamma_p^{\pm 1}[\Lambda_-(p)]_{\mp}\}+[\Gamma_+(p)]_{\pm}\{[\Gamma_+(p)]_{\pm}+\gamma_p^{\pm 1}[\Gamma_+(p)]_{\mp}\})/2 , \tag{A3}$$

where $[[\cdots]]_{\pm}$ is defined as

$$[[K(p)]]_{\pm} \equiv \sum_k N^{-1}\mu_{\pm}^2(k,p)K(k,p) . \tag{A4}$$

From Eq. (A3) we obtain

$$\gamma_p = (\{[I_+(p)+I_-(p)]^2-4O^2(p)\}^{1/2}-I_+(p)-I_-(p))/2O(p) , \tag{A5}$$

$$\Omega_p = (\{[I_+(p)+I_-(p)]^2-4O^2(p)\}^{1/2}+I_+(p)-I_-(p))/2 , \tag{A6}$$

where

$$I_{\pm}(p) \equiv [[K(p)]]_{\pm} - s\{[\Lambda_-(p)]_{\pm}^2+[\Gamma_+(p)]_{\pm}^2\}/2 , \tag{A7}$$

$$O(p) \equiv s\{[\Lambda_-(p)]_+[\Lambda_-(p)]_- - [\Gamma_+(p)]_+[\Gamma_+(p)]_-\}/2 . \tag{A8}$$

These equations for $\mu_{\pm}(k,p)$, γ_p, and Ω_p can be solved numerically, by making use of an iteration procedure. In the case of $p=0$, we can easily prove that $\gamma_0=-1$, $\Omega_0=0$, and $\mu_{\pm}(k,0) \propto K^{-1}(k,0)$, by using the gap equation for F; Eq. (6.2).

APPENDIX B

In this appendix, we calculate analytically the excitation energy Ω_p in the limit of $S/T \gg 1$, by making use of the pseudomagnon approximation.[16,20] In this limit all electrons make stable singlet pairs (bipolarons), and hence the excitation is concerned with the center-of-mass motion of the bipolaron with no change of its internal state. In this case the freedom of the system is only the presence or the absence of a bipolaron at each lattice site. It can be described by a pseudospin assigned to each site, where the up-spin state corresponds to the presence, and the down-spin one to the absence. Thus, we can rewrite h given by Eq. (5.1) as

$$h = -sN - \sum_{l,l'} 2t^2(l-l')s^{-1}\{[(0.5+S_l^z)(0.5-S_{l'}^z) + (0.5-S_l^z)(0.5+S_{l'}^z)] + 2[S_l^xS_{l'}^x+S_l^yS_{l'}^y]\} , \tag{B1}$$

where S_l^z, S_l^x, and S_l^y are the Pauli spin matrices. The first term of Eq. (B1) denotes the energy of the localized bipolarons. The first bracket $[\cdots]$ in the second term denotes the virtual transfer of a bipolaron through the second-order perturbation of $t(l-l')$, while the second bracket $[\cdots]$ denotes the real transfer. Since our system is composed of N sites and N electrons, there is no total pseudospin

$$\sum_l \langle S_l^z \rangle = 0 , \tag{B2}$$

where $\langle\cdots\rangle$ denotes the expectation value of .... In the SC state, the averaged pseudo-spin-density $\langle S_l^z\rangle$ is uniform and zero with no spatial order of spin, and hence we tilt the z axis of spin 90° in the zx plane, and transform S_l^z, S_l^x, and S_l^y into $\tilde{S}_l^z$, $\tilde{S}_l^x$, and $\tilde{S}_l^y$ as

$$\tilde{S}_l^x \equiv -S_l^z, \quad \tilde{S}_l^z \equiv S_l^x, \quad \tilde{S}_l^y \equiv S_l^y . \tag{B3}$$

By this transformation h is given as

$$h = -sN - N\sum_l t^2(l)s^{-1} + \sum_{l,l'} 4t^2(l-l')s^{-1} \times [-\tilde{S}_l^z\tilde{S}_{l'}^z+(\tilde{S}_l^+\tilde{S}_{l'}^+ + \tilde{S}_l^-\tilde{S}_{l'}^-)/2] , \tag{B4}$$

$$\tilde{S}_l^+ \equiv \tilde{S}_l^x + i\tilde{S}_l^y, \quad \tilde{S}_l^- \equiv \tilde{S}_l^x - i\tilde{S}_l^y . \tag{B5}$$

Within the linear pseudomagnon approximation after the Holstein-Primakoff transformation for $\tilde{S}_l^{\pm,z}$, we can replace pseudospin operators as

$$\tilde{S}_l^+ \to C_l, \quad \tilde{S}_l^- \to C_l^\dagger, \quad \tilde{S}_l^z \to (0.5-C_l^\dagger C_l) , \tag{B6}$$

where C_l and $C_l^\dagger$ are boson operators with the following commutation relation

$$[C_l, C_{l'}^\dagger] = \delta_{ll'} . \tag{B7}$$

Thus h can be rewritten as

$$H = -sN - 2N\sum_l t^2(l)s^{-1} + \sum_{l,l'} 4t^2(l-l')s^{-1} \times [C_l^\dagger C_l + (C_lC_{l'}+C_l^\dagger C_{l'}^\dagger)/2] . \tag{B8}$$

After the following Fourier transformation

$$C_p \equiv \sum_l N^{-1/2}C_l e^{-ip\cdot l} , \qquad J(p) \equiv \sum_l 4t^2(l)s^{-1}e^{-ip\cdot l} , \tag{B9}$$

we can diagonalize h by using the Bogoliubov transformation and we finally obtain

$$h = -sN - NJ(0) + \sum_k \Omega_p (\tau_p^\dagger \tau_p + \tfrac{1}{2}) , \tag{B10}$$

where

$$\Omega_p = (J^2(0) - J^2(p))^{1/2} , \tag{B11}$$

$$\tau_p^\dagger = (C_p^\dagger - \gamma_p C_{-p})/(1-\gamma_p{}^2)^{1/2} ,$$

$$\gamma_p = \{\mathrm{sgn}[J(p)/J(0)][J^2(0) - J^2(p)]^{1/2} - J(0)\}/J(p) . \tag{B12}$$

From Eq. (B9), $J(p)$ is given as shown in Eq. (6.12).

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