Charge-density wave with imperfect nesting and superconductivity

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(Received 23 June 1989; revised manuscript received 16 October 1989)

We study the effect of the existence of charge-density waves (CDW) on superconductivity within a mean-field approximation. When the band is slightly deformed to introduce the imperfect-nesting condition for the commensurate CDW, the metallic CDW states appear where a part of the Fermi surface is ungapped. We examine the phase diagram of the imperfect-nesting CDW states and the behavior of the superconducting critical temperature (T_c) on it. We find that the presence of the CDW always drives the T_c down.

I. INTRODUCTION

After the recent discovery of the 30-K superconductor $Ba_{1-x}K_xBiO_3$ (Ba-K-Bi-O),[1,2] bismuth-oxide-based superconductors have attracted much interest, copper-oxide-based superconductors have also. The copper-oxide-based systems such as $(La_{1-x}A_x)_2CuO_4$ (A=Sr, Ba, Ca) and $YBa_2Cu_3O_{6+x}$ exhibit a similar phase diagram and always have the insulating phase with magnetic ordered states in the vicinity of the superconducting (SC) phase. It could be considered that the existence of the magnetic order plays an important role for high-T_c materials. On the other hand, no magnetic order is observed in Ba-K-Bi-O and also in the parent compound $BaBiO_3$.[3] Since the discovery of Ba-K-Bi-O is an extension of the 13-K superconductor $BaPb_{1-x}Bi_xO_3$ (Ba-Pb-Bi-O),[4,5] and Ba-Pb-Bi-O has been extensively investigated from both of experimental and theoretical sides, it is significant to examine Ba-Pb-Bi-O for studying the origin of high T_c in bismuth-oxide-based systems.

In Ba-Pb-Bi-O a characteristic metal-insulator transition occurs at the Bi composition $x \simeq 0.35$ and superconductivity exists in the metallic phase. This system has the maximum SC critical temperature T_c at $x \simeq 0.25$. The band-structure calculation[6] for $BaBiO_3$ ($x=1$) indicates a metallic half-filled band, but experiments exhibit an insulating phase. In this case, due to the good nesting condition, the commensurate charge-density wave (CDW) is expected to be induced accompanying the breathing mode so that the system becomes insulating. Doping of Pb in $BaBiO_3$ acts to deviate the electron filling from the half-filled band condition. In the insulator region ($x \gtrsim 0.35$), the optical reflectivity measurement[7] shows a clear optical gap induced by the CDW. The Bi substitution gives no change for this CDW gap ($\simeq 2$ eV) when $x \gtrsim 0.7$ and suppresses the gap value with decreasing x when $x \lesssim 0.7$. Special emphasis should be put on the remarkable experiment that even in the metallic region ($x \lesssim 0.35$), the pseudogap, which indicates the presence of a CDW, is observed in the reflectivity spectra measurement.[8] We expect that the existence of the CDW plays an important role in the bismuth-oxide-based superconductors.

The purpose of this paper is to investigate the effect of the existence of a CDW on the standard BCS-type (Bardeen-Cooper-Schrieffer) superconductivity. The basic idea is simple as shown in the following: When the band is slightly deformed to introduce the imperfect-nesting condition for a CDW, the metallic phases in the CDW states can appear at a certain strength of electron-phonon coupling constant, where a part of the Fermi surface (FS) is ungapped. We are interested in the superconductivity which is expected to exist under this metallic CDW state. Along the same framework, Machida and Kato[9] discussed the possibility of an enhancement of T_c due to the presence of a CDW and Machida[10] proceeded to apply it to Ba-Pb-Bi-O. We will show, however, that such a large enhancement of T_c cannot be obtained when we consider the stability of the imperfect-nesting CDW. We examine the imperfect-nesting CDW states in detail and obtain the CDW phase diagram in the chemical potential and the CDW coupling-constant plane at the ground state. Assuming the SC coupling constant is much smaller than the CDW one, we study the behavior of the SC critical temperature T_c in the metallic CDW states.

We give the model Hamiltonian which describes the effect of the imperfect-nesting CDW on the superconductivity in Sec. II. In Sec. III we examine the CDW state with the imperfect nesting and study the superconductivity under the CDW states in Sec. IV. The last section is devoted to the conclusion.

II. FORMULATION

In order to consider the effect of the imperfect-nesting CDW on the superconductivity, we utilize the Peierls model for the CDW and the BCS model for superconductivity within a mean-field approximation introducing two order parameters W and Δ for CDW and superconductivity, respectively. The total Hamiltonian is described as the following:

$$H = H_0 + H_{\mathrm{CDW}} + H_{\mathrm{BCS}} , \tag{1}$$

$$H_0 = \sum_{k\sigma} (\varepsilon_k - \mu) c^{\dagger}_{k\sigma} c_{k\sigma} , \tag{2.1}$$

$$H_{\mathrm{CDW}} = -W \sum_{k\sigma} c^{\dagger}_{k+Q\sigma} c_{k\sigma} , \tag{2.2}$$

$$H_{\mathrm{BCS}} = -\Delta \sum_{k} (c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} + \mathrm{H.c.}) . \tag{2.3}$$

The self-consistent conditions for the two order parameters W and Δ are given by

$$W = u \sum_{k\sigma} \langle c^{\dagger}_{k+Q\sigma} c_{k\sigma} \rangle , \tag{3}$$

$$\Delta = g \sum_{k} \langle c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} \rangle , \tag{4}$$

where u and g are the CDW and SC coupling constants, respectively. In our model, the explicit Coulomb interaction term does not exist in H. If the Coulomb repulsion is properly included, it is necessary to discuss the symmetry of the SC order parameter.[11] For the simplicity of calculations we restrict ourselves to a two-dimensional (2D) square lattice. The nesting vector is fixed as $Q = (\pi, \pi)$, where the lattice constant is taken to be unit, because we consider the nearly half-filling case. The chemical potential μ is varied within the nearly half-filled band condition.

The model band structure ε_k in the 2D square lattice is represented by a tight-binding band, where we introduce the next-nearest-neighbor transfer t_1 as well as the nearest-neighbor one t_0 as the following:

$$\varepsilon_k - \mu = \gamma_k + \delta_k - \mu , \tag{5}$$

where

$$\gamma_k = -t_0(\cos k_x + \cos k_y) ,$$

$$\delta_k = -t_1 \cos k_x \cos k_y .$$

Here it should be noted that t_1 acts as the imperfect-nesting parameter and Q expresses the perfect-nesting condition in the just half-filled case when $t_1 = 0$. Hereafter the energy is normalized by t_0.

We first consider only the CDW state ($\Delta = 0$) with the imperfect nesting. After diagonalizing Eq. (1), we can easily obtain the CDW gap equation from Eq. (3),

$$1/u = \sum_{k\sigma} \frac{f(E_k^-) - f(E_k^+)}{(\gamma_k^2 + W^2)^{1/2}} , \tag{6}$$

$$E_k^{\pm} = \delta_k - \mu \pm (\gamma_k^2 + W)^{1/2} , \tag{7}$$

where $f(E)$ is the Fermi distribution function. In Eq. (6) the sum over k goes over the first Brillouin zone (BZ) of the CDW superlattice. E_k^+ and E_k^- represent the upper and lower band of quasiparticle energy spectra of the imperfect-nesting CDW state, respectively. Equation (6) determines a CDW gap W self-consistently for a given u.

Since various metallic phases are expected to appear due to the imperfect nesting, as seen in the next section, even when the CDW gap is open, we must compare the total energies among these phases. The total energy difference from the normal phase of this system is given by

$$\Delta E = \sum_{k\sigma} E_k^+ f(E_k^+) + \sum_{k\sigma} E_k^- f(E_k^-) + \frac{W^2}{2u} - \sum_{k\sigma} \varepsilon_k f(\varepsilon_k) , \tag{8}$$

where the third term expresses the energy of the lattice distortion. The most stable state among the solutions of Eq. (6) is determined by minimizing this total energy difference. Here we note that $\partial(\Delta E)/\partial W = 0$ gives the gap equation (6).

Next we consider the effect of the existence of the imperfect-nesting CDW on the BCS-type superconductivity, because the superconductivity can appear in the metallic CDW phase where the FS remains partially due to the imperfect nesting. Since the CDW gap is order of 1 eV and the SC gap is order of 10 meV in Ba-Pb-Bi-O, we can regard the SC order parameter as much smaller than the CDW one at $T = 0$. When we assume that $\Delta \ll W$, W is determined only by the CDW gap equation (6) independent of the SC order parameter Δ. The SC gap equation is given by

$$1/g = \tfrac{1}{4} \sum_{k} \left[\frac{1}{[(E_k^+)^2 + \Delta^2]^{1/2}} \tanh \left[\frac{[(E_k^+)^2 + \Delta^2]^{1/2}}{2T} \right] + \frac{1}{[(E_k^-)^2 + \Delta^2]^{1/2}} \tanh \left[\frac{[(E_k^-)^2 + \Delta^2]^{1/2}}{2T} \right] \right] . \tag{9}$$

We can determine the SC critical temperature T_c by putting $\Delta \to 0$ in Eq. (9),

$$1/g = \tfrac{1}{4} \sum_{k} \left[\frac{1}{E_k^+} \tanh \left[\frac{E_k^+}{2T_c} \right] + \frac{1}{E_k^-} \tanh \left[\frac{E_k^-}{2T_c} \right] \right] . \tag{10}$$

III. CDW STATE WITH THE IMPERFECT NESTING

In this section we discuss the CDW states with the imperfect nesting. In order to see the role of the imperfect-nesting parameter t_1, we show the dispersions E_k^+ and E_k^- given by Eq. (7) in Fig. 1. Since the nesting vector Q is fixed as (π, π), the CDW gap W opens on the nesting line $\cos k_x + \cos k_y = 0$, where the imperfect-nesting pa-

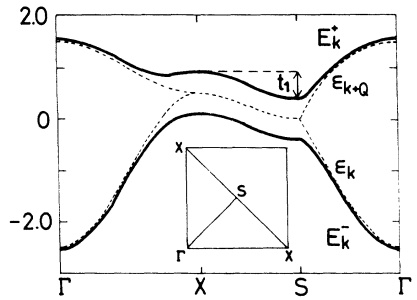

FIG. 1. Dispersion curves of E_k^+ and E_k^- in the CDW state (solid line), and ϵ_k and ϵ_{k+Q} in the normal state (dashed line) along the symmetry lines ($\Gamma XS\Gamma$) shown in the inset.

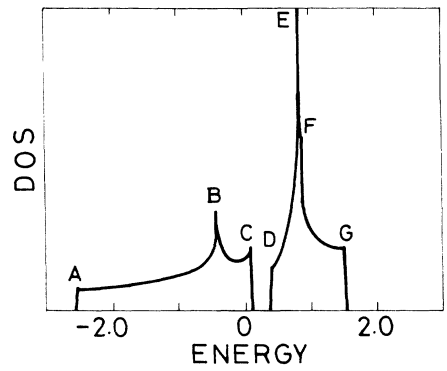

FIG. 3. Density of states for the dispersion E_k^+ and E_k^-. The properties of the van Hove singularities from A to G are summarized in Table I.

rameter t_1 gives the dispersion. Thus, we expect that metallic phases whose FS remains partially will appear for some values of μ while the CDW gap exists. We display three possible metallic phases, $M1$ (μ crosses only the lower band E_k^-), $M2$ (μ crosses only the upper band E_k^+), and $M3$ (μ crosses both the lower and upper bands), in Figs. 2(a)–2(c). The upper figures show the relative positions of μ and $E_k^\pm$ branches on the nesting line and the bold lines indicate the Fermi levels. The lower figures show the FS by the bold lines and the electron filling at the ground state by the shaded parts. For convenience the lower (upper) part from a diagonal line expresses the E^- (E^+) branch. The $M1$ and $M2$ phases have the partial FS near the X and S points, respectively. In the $M3$ phase, FS appears near both the X and S points. The density of states (DOS) corresponding to the dispersion in Fig. 1 is shown in Fig. 3 and the various singularities of DOS are summarized in Table I. We note that $E^+(F)$ corresponds to the local maximum of the E^+ band which is located at X point in Fig. 1. When $W < t_1/2$, the DOS of the E^+ band overlaps with the DOS of the E^- band.

We show the CDW gap W as a function of u obtained by the gap equation (6) in Fig. 4(a) when $\mu=0.02$ and Fig. 4(b) when $\mu=0.07$ at zero temperature in the case $t_1=0.1$. Three phases appear as the solutions of Eq. (6) when $\mu=0.02$; that is, the regions $0<W<0.02$, $0.02<W<0.08$, and $W>0.08$ correspond to the $M3$, $M1$, and insulating (I) phase, respectively. We compare the total energies given by Eq. (8) among them and show the stable state by the bold lines. The system undergoes the first-order phase transitions from the normal (N) to the $M1$ phase and to the I phase as u increases, and the

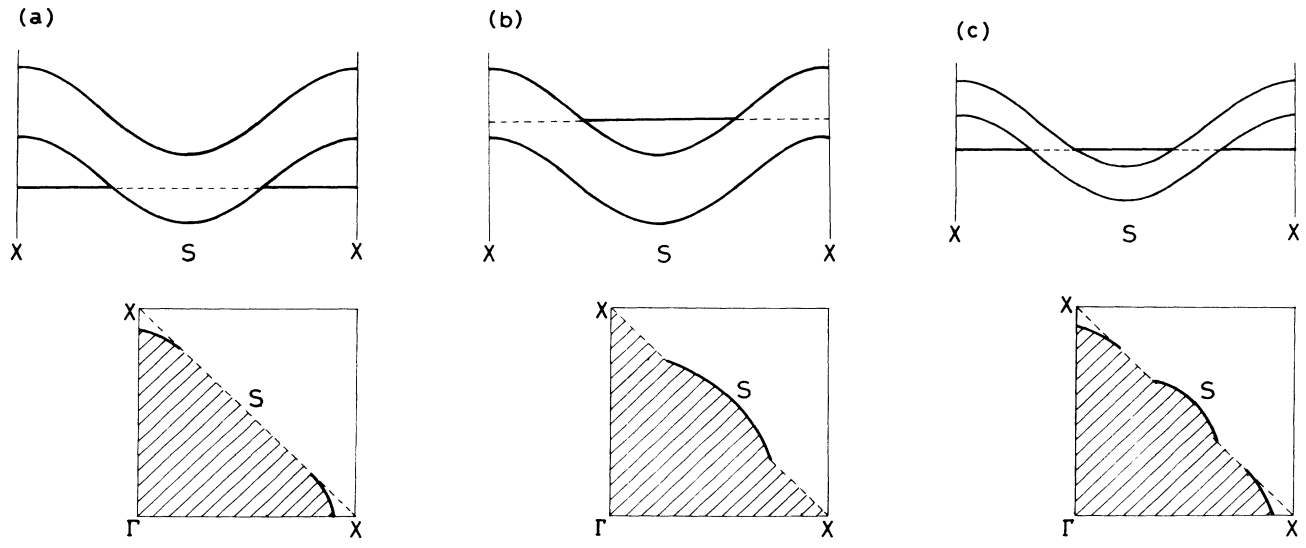

FIG. 2. Schematic indication of the three metallic CDW states: (a) $M1$ ($\mu<W$, $-W<\mu<t_1-W$), (b) $M2$ ($\mu>t_1-W$, $W<\mu<t_1+W$), and (c) $M3$ ($W<\mu<t_1-W$, $W<t_1/2$). The upper figures display the relative position between the Fermi level and the CDW gap along the nesting line XSX, and the lower figures show the electron filling in BZ by the shaded part where the FS is expressed by the bold lines. The lower (upper) part from a diagonal line in the lower figures expresses the E_k^- (E_k^+) branch for convenience.

TABLE I. The van Hove singularities in the DOS of the quasiparticle dispersions E_k^+ and E_k^-. The positions in energy and in BZ, the type and the analytic behavior of the singularities are listed in order. Here $x_c=\cos^{-1}[-1+Wt_1/(1-t_1^2)^{1/2}]$ and θ is a step function.

A:	$E^-(A)=-t_1-(4+W^2)^{1/2}$	at Γ: step	$\frac{(4+W^2)^{1/2}}{2+t_1(4+W^2)^{1/2}}\Theta(E-E^-(A))$
B:	$E^-(B)=-W^2$	at S: logarithmic	$\ln\lvert E-E^-(B)\rvert$
C:	$E^-(C)=t_1-W$	at X: step	$\frac{1}{t_1}\Theta(E^-(C)-E)$
D:	$E^+(D)=W$	at S: step	$\sqrt{W/t_1(2-Wt_1)}\Theta(E-E^+(D))$
E:	$E^+(E)=t_1+W^2\sqrt{1-t_1}$	at $(x_c,0)$: logarithmic	$\ln\lvert E-E^+(E)\rvert$
F:	$E^+(F)=t_1+W$	at X: step	$\frac{1}{t_1}\Theta(E^+(F)-E)$
G:	$E^+(G)=-t_1(4+W^2)^{1/2}$	at Γ: step	$\frac{(4+W^2)^{1/2}}{2-t_1(4+W^2)^{1/2}}\Theta(E^+(G)-E)$

$M3$ phase is unstable. In the case $\mu=0.07$ the system changes from the N to $M2$ phase by the first-order transition and from the $M2$ to I phase by the second-order transition as u increases.

We show the phase diagram in the μ-u plane at the ground state in the case $t_1=0.1$ in Fig. 5(a) where the dashed and solid lines indicate the first- and second-order transitions, respectively. For comparison the phase diagram for $t_1=0$ is shown in Fig. 5(b) where we see only the I and N phases with the first-order transition. This result is the computational fact, namely the transition in the case that $t_1=0$ is found to be always first order as far as we considered the region $0.001<u<1.5$. When the imperfect-nesting parameter t_1 exists, the two metallic phases $M1$ and $M2$, which have the partial FS, appear in addition to the N and I phases and the $M3$ phase does not appear in the phase diagram. We note that the electron filling is always just half-filled in the I phase. It should be mentioned that the transitions between the normal phase and other phases are of the first order except the special two points in the phase diagram indicated by the solid circles. At these two points the infinitesimal gap can be formed stably because μ is tangent to ε_k on the nesting line XSX at the X point when $\mu=t_1$ or the S point when $\mu=0$. In particular, when $\mu=t_1$ an infinitesimal gap can open at an infinitesimal u, because in this case μ

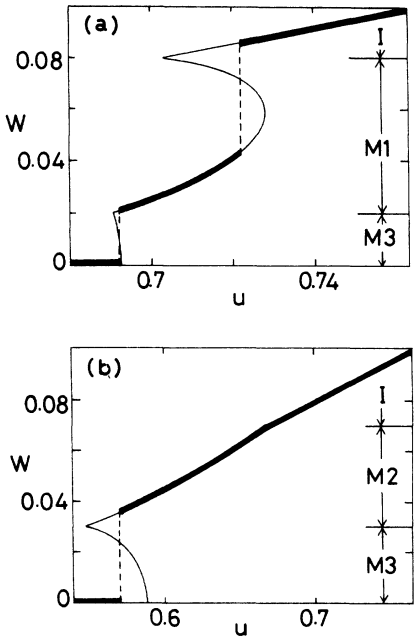

FIG. 4. CDW gap W as a function of u given by the gap equation (6) when (a) $\mu=0.02$ and (b) $\mu=0.07$ in the case that $t_1=0.1$. The bold lines indicate the stable states.

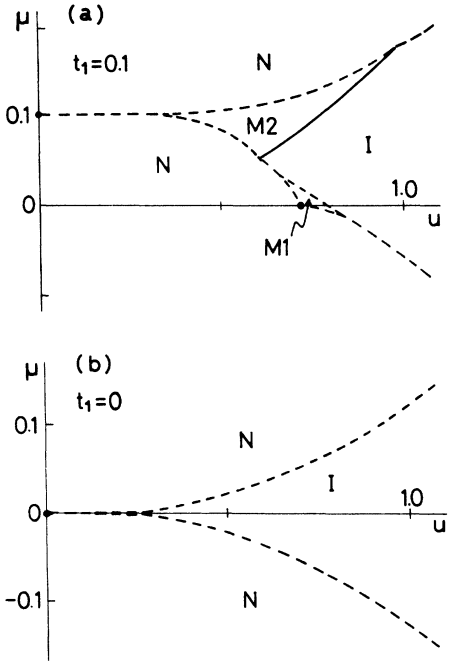

FIG. 5. The CDW phase diagram in the μ-u plane in the case that (a) $t_1=0.1$ and (b) $t_1=0$. The solid and dashed lines indicate the second- and first-order transitions, respectively. The solid circles in (a) denote the two special points where the transition between N and metallic CDW states is of the second order.

locates at the logarithmic singularity of DOS in the absence of a CDW, as in the case of the second-order transition point in Fig. 5(b) when $t_1=0$.

Finally we mention that the order of transition between the I phase and the two metallic phases changes with varying t_1. When we increase t_1, the transition between the $M1$ and I phases changes to the second order and the transition between the $M2$ and I phases changes to the first order corresponding to the variation of the magnitude of the singularity in DOS at the C point and D point, where the magnitude of the step of DOS decreases as $1/t_1$ and increases as $\sqrt{W/t_1(2-Wt_1)}$, respectively.

IV. EFFECT OF THE IMPERFECT-NESTING CDW ON THE SUPERCONDUCTIVITY

As seen in Sec. III, the metallic phases $M1$ and $M2$ appear in the CDW state with the imperfect nesting. Since the BCS-type superconductivity can exist in these metallic CDW phases, we study the behavior of the SC critical temperature T_c in these imperfect-nesting CDW states in this section.

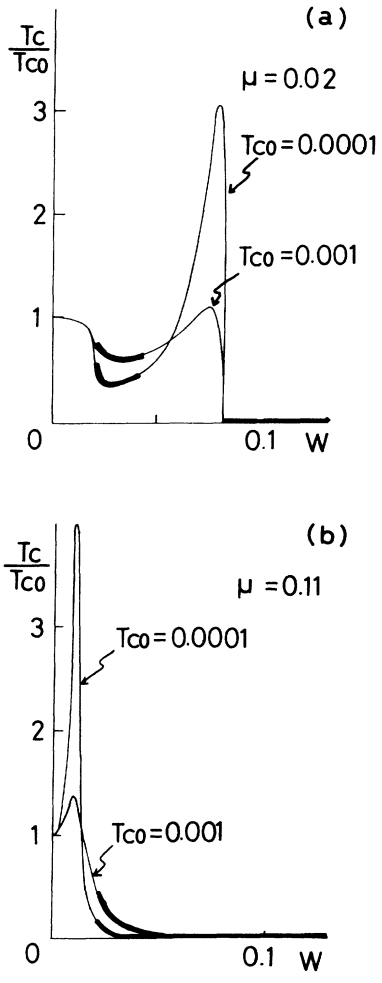

FIG. 6. Superconducting critical temperature T_c normalized by T_{c0} as a function of W when (a) $\mu=0.02$ and (b) $\mu=0.11$ in the case $t_1=0.1$. The bold lines represent the stable CDW states. (a) The stable state changes from N to $M1$ and $M1$ to I by the first-order transition as W increases. (b) The stable state changes from N to $M2$ by the first-order transition, and from $M2$ to I at $W=0.11$ by the second-order transition.

When we assume $\Delta \ll W$, T_c under the CDW gap W is given by Eq. (10). We show the calculated T_c as a function of W in Fig. 6(a) when $\mu=0.02$ and $t_1=0.1$, where T_c is normalized by $T_{c0}(\mu)$ which denotes the SC critical temperature in the absence of CDW, i.e.,

$$1/g=\tfrac{1}{2}\sum_k \frac{1}{\varepsilon_k}\tanh\left[\frac{\varepsilon_k}{2T_{c0}}\right].$$

As W increases, the CDW state changes from the N to the $M3$, $M1$, and I phases in order. We see that T_c has a peak near the boundary between the $M1$ and I phases and it tends to be enhanced at smaller T_{c0}. The peak of T_c, which is attributed to the magnitude of DOS at μ, results from the singularity at the C point corresponding to the band edge. This peak has been demonstrated already in the case $\mu=0$ by Machida and Kato.[9] As mentioned in Sec. III, however, we must consider the stability of the imperfect-nesting CDW because the first-order transition is an intrinsic feature in this system. The bold lines in Fig. 6(a) indicate the stable CDW gap corresponding to the solution in Fig. 4(a). We see that the CDW gap W, which gives the peak of T_c, is unstable. Next we show a similar result when $\mu=0.11$ in Fig. 6(b). The bold lines in the region $W<0.11$ and $W>0.11$ indicate the $M2$ and I phases, respectively. The system undergoes the first-order transition from the N to $M2$ phase, and the second-order transition from the $M2$ to I phase as increasing W. This peak of T_c which results from the logarithmic singularity of the E point at the Fermi level cannot exist in the stable state. We see that T_c in the stable CDW state does not exceed T_{c0} at both values of μ.

We examine the behavior of T_c on the CDW phase diagram when $t_1=0.1$ and show T_c as a function of μ at $u=0.7$ in Fig. 7(a). The bold and dashed lines indicate $T_c(\mu)/T_{c0}(\mu=t_1)$ and $T_{c0}(\mu)/T_{c0}(\mu=t_1)$, respectively. The $T_{c0}(\mu)$ has a maximum at $\mu=t_1$ because the logarithmic singularity in DOS is located at t_1 in the absence of CDW. We show in Fig. 7(b) the CDW gap W as a function of μ corresponding to Fig. 7(a). The bold and dashed lines denote the stable and unstable CDW gaps, respectively. When we decrease μ from the I phase, the system undergoes the first-order transition to the $M1$ phase where T_c is reduced to about a half of T_{c0}, and to the N phase further decreasing μ. Here the calculated T_c is indicated only in the region of $M1$, $M2$, and I, because the assumption $\Delta \ll W$ is broken in the N phase ($W=0$) when $\Delta\neq 0$. However, the transitions between N and other phases are always first order, so that the above assumption is satisfied for the $M1$, $M2$, and I phases. Inversely, increasing μ from the I phase, the system undergoes the second-order transition to the $M2$ phase at $W=0.08$. In the $M2$ phase near the I phase, T_c is very small and tends to enlarge rapidly as suppressing W. This abrupt enhancement of T_c is attributed to the logarithmic singularity of DOS at the E point near the Fermi level. The system, however, changes to the N phase be-

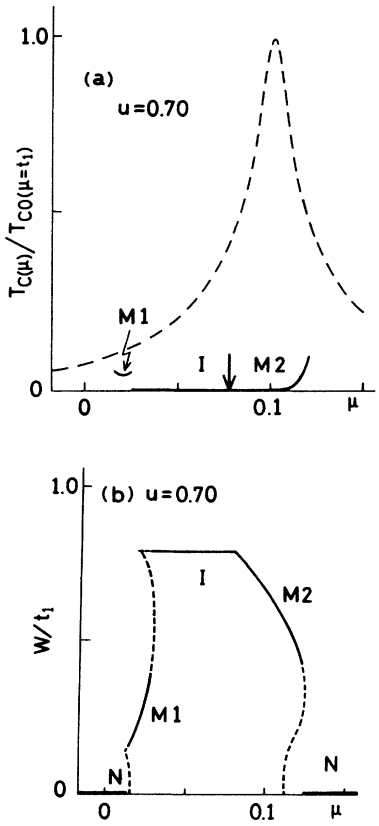

FIG. 7. (a) Superconducting critical temperature $T_c(\mu)$ (solid line) in $M1$ and $M2$ phases and $T_{c0}(\mu)$ (dashed line) normalized by $T_{c0}(\mu=t_1)$ as a function of μ when $u=0.7$. As increasing μ, the CDW stable state changes from N to $M1$, I, $M2$, and N in order. The arrow indicates the transition point between I and $M2$ phases. (b) The CDW gap W as a function of μ given by Eq. (6) when $u=0.7$. The solid and dashed lines indicate the stable and unstable solutions, respectively.

fore T_c exceeds T_{c0}. We conclude that the superconductivity can exist in the imperfect-nesting CDW state and that T_c never exceeds T_{c0} over the whole region of μ and u.

V. CONCLUSION

We have studied the effect of the existence of the imperfect-nesting CDW on the superconductivity in a 2D square lattice within a mean-field approximation. If the band is slightly deformed to introduce the imperfect-nesting condition for the commensurate CDW, the metallic CDW phases appear where a part of FS is ungapped. We examine the imperfect-nesting CDW states in detail in the μ-u plane and investigate the behavior of the superconducting critical temperature T_c in the metallic CDW phases $M1$ and $M2$ assuming that the CDW order parameter is much greater than the one of the superconductivity. Deviating the chemical potential μ from the I phase, the system undergoes the transition to the $M1$ and $M2$ phases and finally to the N phase. The abrupt enhancement of T_c is found near the boundary between the $M2$ and N phases due to the logarithmic singularity of DOS which is characteristic in a 2D system.

Machida and Kato demonstrated[9] that T_c is enhanced by the imperfect-nesting CDW along the same framework when $\mu=0$. The CDW gap, which gives the huge DOS at the Fermi level, however, cannot exist in the stable state because the first-order transition is the intrinsic feature when we restrict ourselves to the commensurate CDW. The SC critical temperature in the CDW states never exceed the one in the absence of CDW over the whole region of μ and u. This reduction of T_c in the CDW states is qualitatively similar to the result of Bilbro and McMillan,[12] which discussed the superconductivity and the martensitic transformation in $A15$ compounds. Machida and Kato also argued the relationship between the commensurate spin-density wave (SDW) with imperfect nesting and the superconductivity in various symmetries at finite temperatures.[13,14] We note that their phase diagram, obtained by assuming second-order transitions, will soon break down when we deviate from the region they considered, that is, $\mu=0$ and the SDW order parameter is much smaller than the imperfect-nesting parameter t_1.

Finally, let us try to briefly discuss the comparison between our results and the real system of Ba-Pb-Bi-O. In the metallic state, we have two stable phases $M1$ and $M2$ where FS remains partially with the CDW gap W. When the superconductivity appears, this CDW gap is considered to correspond to the pseudogap observed in Ba-Pb-Bi-O. Our argument cannot apply directly to the problem of Ba-Pb-Bi-O, however, because we treat the system as the grand canonical ensemble with an infinite reservoir and the insulating phase is always the half-filled case. Then, in our treatment, the system soon exhibits the transition to the metallic CDW phases when the electron filling deviates from the half-filling case. This is different from the case for Ba-Pb-Bi-O. For the quantitative comparison with the real system of Ba-Pb-Bi-O, it is necessary to treat it as a canonical ensemble where the chemical potential is determined self-consistently to fix the particle number. Therefore, we suppose that the incommensurate CDW plays an important role in the real system. The investigation for the incommensurate CDW will be reported in future.

ACKNOWLEDGMENTS

One of the authors (M.F.) thanks Dr. K. Machida for stimulating discussions in the early stage of this work.

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