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Superconductivity transition temperature enhancement due to Peierls instability

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The superconducting transition temperature (T_c) is theoretically shown to rise as a result of the presence of the Peierls instability within a simple incomplete-nesting model in two dimensions. It is demonstrated that T_c can exceed by an order of magnitude that in the absence of the Peierls transition under certain conditions. The implication of this is discussed for the high-T_c superconductors $La_{2-x}M_xCuO_4$.

Much attention has been focused on layered perovskite materials since Bednorz and Müller[1] indicated the possibility of raising the superconducting transition temperature (T_c) in La-Ba-Cu-O systems, and subsequently Uchida *et al.*[2] identified the structure of these systems. There have already accumulated many experimental[3-10] and theoretical[11-18] works, the number of which is rapidly increasing.

Key experimental findings are summarized as follows. (i) The reference system La_2CuO_4 exhibits a structural transition from a tetragonal (high-temperature) to an orthorhombic (low-temperature) phase at 520 K, accompanied by a metal-insulator transition. (ii) Dilute Sr or Ba doping as low as $x=0.05$ in $La_{2-x}(Ba,Sr)_xCuO_4$ induces superconductivity[3] and T_c reaches a maximum at around $x=0.15$. (iii) Two-dimensionality (2D) of the crystalline and band structures is important to enhance T_c as evidenced by a systematic study[4] of the lattice-constant changes in the pseudoternary compound $La_{2-x}(Sr,Ba,Ca)_xCuO_4$. (iv) The substantial orthorhombic component in x-ray measurements[5] persists up to $x\cong 0.34$ in $La_{2-x}Ca_xCuO_4$, and a system with the orthorhombic structure even at room temperature exhibits superconductivity.[5] As quoted by Weber,[14] Fleming, Batlogg, Cava, and Rietman[10] observe an orthorhombic distortion in many superconducting samples even below T_c. [However, Jorgensen *et al.*[9] observe no structural transition for $x(\mathrm{Ba})=0.15$].

The calculated electronic band structure[11-13] for the undistorted tetragonal phase at $x=0$ is extremely simple and essentially 2D with half filling near the Fermi surface (FS) reflecting the layered crystal structure. The nearly perfect nesting feature is evident and responsible for the tetragonal-orthorhombic transformation associated with the FS-instability-derived metal-insulator transition.[9] Dilute doping of Ba or Sr lowers the Fermi level away from the half filling, deteriorating the nearly perfect nesting situation. Although the degree of incompleteness in nesting is difficult to estimate quantitatively at the present stage, we can expect a certain nesting situation to be preserved in the dilute doping region as in Refs. 16 and 17.

The purpose of the present paper is to show the T_c enhancement due to the Peierls transition or charge-density wave (CDW) induced by the FS instability within a BCS framework. This is contrary to a general belief that the CDW simply kills superconductivity by opening up the Peierls gap at the FS. This is not always true. Needless to say if the nesting is complete, superconductivity never occurs via a second-order phase transition. However, if the nesting is incomplete as often happens in real materials, then under certain conditions T_c can be substantially enhanced as we will demonstrate below. Physically it is easy to see this: Near the boundary between the Peierls gapped and ungapped regions on the FS, the gap-edge singularities with diverging density of states (DOS) *always* just cross the Fermi level. This increases the effective DOS near the FS within the Debye-cutoff-energy shell region and leads to T_c enhancement in some cases. Such a boundary region on the FS can exist whenever the nesting for charge- and spin-density-wave formation is incomplete.

We start with the tight-binding Hamiltonian including the nearest- (t_0) and next- (t_1) nearest-neighbor transfer integrals on a 2D square lattice (lattice spacing of 1) (as we will see in the end, the T_c enhancement is not confined to strictly 2D and is also expected to occur in 3D.) We use a mean-field approximation to treat the CDW order parameter W and the superconductivity gap parameter Δ on an equal footing; then the total mean-field Hamiltonian is given by

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

where

$$H_0=\sum_{k,\sigma}\varepsilon(k)C^\dagger_{k\sigma}C_{k\sigma} ,$$
$$H_{\mathrm{CDW}}=W\sum_{k,\sigma}(C^\dagger_{k+Q,\sigma}C_{k\sigma}+\mathrm{H.c.}) ,$$
$$H_{\mathrm{BCS}}=\Delta\sum_{k}(C^\dagger_{k\uparrow}C^\dagger_{-k\downarrow}+\mathrm{H.c.}) ,$$

with the self-consistent equations

$$W=-u\sum_{k,\sigma}\langle C^\dagger_{k+Q,\sigma}C_{k\sigma}\rangle ,$$
$$\Delta=-g\sum_{k}\langle C^\dagger_{k\uparrow}C^\dagger_{-k\downarrow}\rangle , \tag{2}$$

where $\varepsilon(k)=\gamma_k+\delta_k$, $\gamma_k=-t_0(\cos k_x+\cos k_y)$, and $\delta_k=-t_1\cos k_x\cos k_y$. The nesting vector $\mathbf{Q}=(\pi,\pi)$. The chemical potential is fixed to be zero, thus we are considering an electron filling of slightly less than half. (See Fig. 1 for the FS of the undistorted phase.) We assume two independent attractive interactions u and g coming from appropriate electron-phonon couplings as in other works.[19]

It is easy to diagonalize (1). We obtain the coupled self-consistent equations from (2),

$$1 = gT\sum_{\omega_n}\sum_k (\omega_n^2+\gamma_k^2+\delta_k^2+\Delta^2+W^2)/D(\omega_n) \ , \quad 1 = uT\sum_{\omega_n}\sum_k (\omega_n^2+\gamma_k^2-\delta_k^2+W^2+\Delta^2)/D(\omega_n) \ , \tag{3}$$

$$D(\omega_n) = (\omega_n^2+\gamma k^2+\delta_k^2+W^2)^2 - 4\delta_k^2(\gamma_k^2+W^2) \ , \tag{4}$$

which completely determine W and Δ once the system's parameters are chosen.

We obtain the equation for T_c by putting $\Delta \rightarrow 0$ in (3) and (4) as

$$\frac{1}{g} = T_c \sum_{\omega_n}\sum_k \frac{\omega_n^2+\gamma_k^2+\delta_k^2+W^2}{[\omega_n^2+(\delta_k+\sqrt{\gamma_k^2+W^2})^2][\omega_n^2+(\delta_k-\sqrt{\gamma_k^2+W^2})^2]} \ . \tag{5}$$

This yields T_c as a function of a given W or implicitly the Peierls transition temperature (T_P) for t_0, t_1, and the Debye cutoff parameter ω_D chosen.

Before going into detailed calculations we briefly sketch the FS in the CDW phase: From the inspection of the quasiparticle spectrum, $E_k^2 = (\delta_k \pm \sqrt{\gamma_k^2+W^2})^2$, formed by the CDW, it is easy to see the new FS as shown in Fig. 1. The CDW gap tends to make the original rounded FS square up; more precisely, the CDW induces the gaps at around the point B, $(k_x,k_y) = (\pi/2,\pi/2)$, and its equivalent points [henceforth we only consider the Brillouin zone sectioned by the triangle: (0,0), $(\pi,0)$ and $(\pi/2,\pi/2)$]. On the straight line AB the CDW gap appears and simultaneously the remaining ungapped FS (denoted by the dotted curve AC) moves toward the X point $(\pi,0)$, where the position of C is given by

$$k_x(C) = \cos^{-1}\left[\frac{\sqrt{t_1^2(t_0^2+W^2)-t_0^2W^2-t_0^2}}{t_0^2-t_1^2}\right], \ k_y(C) = 0 \ .$$

When $W > W_{\rm cr} = t_1$, the point A coincides with X; thus the FS disappears and the system becomes insulator. There is no way to have superconductivity in this case. When $W < W_{\rm cr}$, there always exists such a point A whose position is $k_x(A) = \pi/2 + \sin^{-1}\sqrt{W/t_1}$ and $k_y(A) = \pi/2 - \sin^{-1}\sqrt{W/t_1}$. This is the very point on which the CDW gap-edge singularity is exactly situated at the Fermi level.

The results of the numerical computations of (5) are displayed in Figs. 2 and 3, where T_{c0} is the superconducting transition temperature in the absence of the CDW ($W=0$). Although we have not exhausted all possible parameter space to seek the maximum enhancement as yet, it was easy to find large-T_c-enhancement cases where the enhancement factor increases by an order of magnitude by optimizing the parameters within physically reasonable values. It should be noted from Fig. 2 that T_c is depressed in small-W regions where the decrease on the FS area is effective and as the enhancement increases the initial depression of T_c/T_{c0} also increases. Figure 3 shows the trace of the T_c-enhancement maxima as a function of t_1

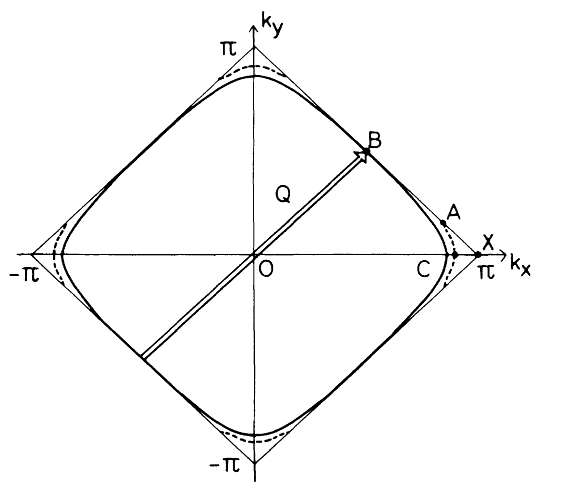

FIG. 1. The Fermi surface (thick curve: $t_0/2\pi T_{c0} = 5000$, $t_1/2\pi T_{c0} = 500$, and $W/2\pi T_{c0} = 400$) and the nesting vector $\mathbf{Q} = (\pi,\pi)$ (arrow). The square denotes the Fermi surface in the half-filled case ($t_1 = 0$). The dotted curves indicate the Fermi surface in the CDW state where the Periels gap opens on the line AB.

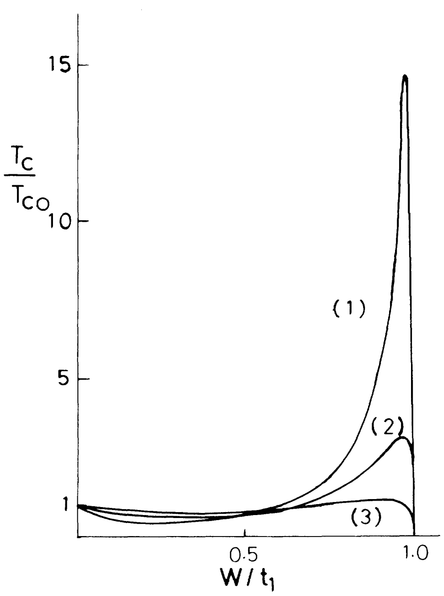

FIG. 2. Changes of the superconducting transition temperature: T_c relative to that in the absence of the Peierls transition T_{c0} as a function of W/t_1 for selected values of the parameters. (1) $t_0/2\pi T_c0 = 10000$, $t_1/2\pi T_{c0} = 1000$, and $\omega_D/2\pi T_{c0} = 300$. (2) 1000, 100, and 300. (3) 100, 10, and 30.

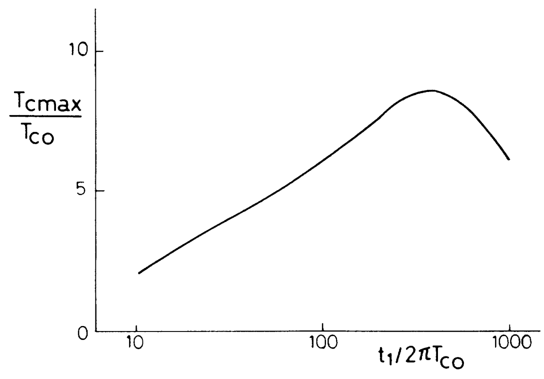

FIG. 3. Trace of the enhancement maximum T_{cmax}/T_{c0} as a function of $t_1/2\pi T_{c0}$, where $t_0/2\pi T_{c0}=5000$ and $\omega_D/2\pi T_{c0}=300$ are fixed.

under a fixed $t_0/2\pi T_{c0}$ ($=5000$). Again we see that the enhancement occurs over a rather large parameter space, not just at the accidental coincidence of some parameter values.

As is seen from Fig. 1 we have several conflicting factors which raise T_c; namely, (a) as W increases, the point A moves toward X and, simultaneously, C moves toward X. Since X corresponds to the saddle point in the equal-energy surface characterized by the logarithmic van Hove singularity (this is only true for the 2D system), the system gains additionally a large DOS at around X by the confluence of the two singularities. (b) On the other hand, the increment of W leads to the shrinkage of the FS area, losing the DOS. Therefore T_c/T_{c0} tends to vanish ultimately at $W\rightarrow W_{cr}$ ($\equiv t_1$) as shown in Fig. 2.

According to the present theory, to attain maximum T_c enhancement in $La_{2-x}M_xCuO_4$ and related materials it is advisable to tune the Fermi level, the Peierls temperature (T_P or W), and the band parameters (t_0 and t_1) to optimize these parameters by doping and pressure. We do not attempt to evaluate a realistic maximum T_c value because there are several unknown parameters involved. We believe, however, that we could explain a high T_c within the range of ~ 100 K, which is the maximum observed so far,[8] if we take, for example, $T_{c0}\simeq 13$ K from the other perovskite material $BaPb_{1-x}Bi_xO_3$. Neither exotic mechanisms[15,17] nor an anomalously large electron-phonon coupling[14] are needed.

We have demonstrated that contrary to a general belief that the Peierls instability suppresses superconductivity, it can indeed raise the superconducting transition temperature T_c by producing a coincidence of the CDW gap-edge singularity with the Fermi level. This situation always occurs somewhere on the Fermi surface whenever the nesting for the density wave is incomplete even in the three-dimensional band. The two-dimensional case more effectively gains a high density of states at the Fermi level by the confluence of the two singularities as mentioned above. It should be stressed that the present T_c enhancement does not rely solely on a special feature of the logarithmic van Hove singularity, which is quickly diminished as we take into account the interlayer coupling, characteristic in the 2D band structure with nearly half filling.

Finally we point out that we can show a similar T_c enhancement in the case[20] where anisotropic superconductivity with odd or even parity and the spin-density wave compete.

Note added in proof. A similar argument of the T_c enhancement is done by Yu. V. Kopaev and A. I. Rusinov, Phys. Lett. **121A**, 300 (1987).

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