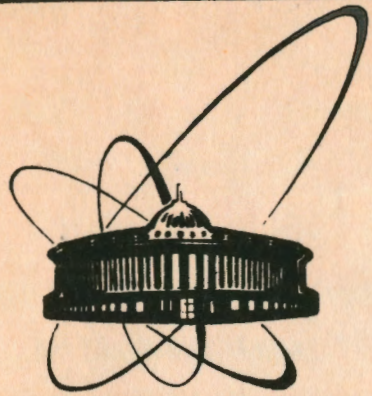

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Chan Minh Tien, N.M.Plakida

ELECTRON-PHONON MECHANISM OF SUPERCONDUCTIVITY IN THE TWO-BAND EMERY MODEL

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Чан Минь Тиен, Плакида Н.М. E17-92-55

Электрон-фононный механизм
сверхпроводимости в двухзонной модели Эмери

Рассматривается электрон-фононный механизм сверхпроводимости в двухзонной модели Эмери на квадратной решетке. На основе уравнений движения получена самосогласованная система уравнений для матричной электронной функции Грина. Вычислена зависимость температуры сверхпроводящего перехода Tc от концентрации дырок. Показано, что благодаря исключению двукратно занятых состояний на узлах меди максимальное значение Tc достигается при концентрации дырок $n \simeq 0.8$ и $n \simeq 2.3$, которые соответствуют появлению особенностей Ван Хова в медной и кислородной зонах, соответственно.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1992

Chan Minh Tien, Plakida N.M. E17-92-55

Electron-Phonon Mechanism
of Superconductivity in the Two-Band Emery Model

The electron-phonon mechanism of superconducting pairing in the two-band Emery model on a square lattice is considered. On the basis of the equation of motion the self-consistent system of equations for the matrix electron Green function is obtained. The dependence of the superconducting transition temperature Tc on the concentration of holes is calculated. It is shown that due to the exclusion of double occupancy of copper sites the maximum Tc occurs at the concentrations of holes $n \simeq 0.8$ and $n \simeq 2.3$, which correspond to the Van Hove singularities in copper and oxygen band, respectively.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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I Introduction

The crucial characteristics of high-temperature superconductors (HTSC) are the strong electron correlation [1] and the pronounced two-dimensional structure [2]. In order to study these properties, various models have been proposed: the one-band Hubbard model [3], the t-J model [4], the Emery model [5] and others. However, the numerical calculations in the one-band Hubbard [6] and Emery model [7] have shown that superconducting correlations are not found. At the same time, the observed large isotope shift at certain concentration of doping holes [8, 9], some anomalies in the phonon spectra and in the structural instability of oxide materials [10, 11] show the important role of phonons in the formation of Cooper pairs in HTSC. This allows one to propose the electron-phonon pairing mechanism in the system with strong electron correlation as one of the possible superconducting mechanism in HTSC.

In the present paper, we consider the Emery model with the electron-phonon coupling. After discussing the model in the next Sect., we obtain the self-consistent equations of the Green function in Sect.3. The equation for the superconducting temperature is obtained in Sect.4. The numerical results and discussions are presented in Sect.5.

II Model Hamiltonian

Electron-phonon coupling in the CuO_2 plane with strong electron correlations can be described by the following Hamiltonian:

$$
\begin{aligned}
H &= H_0 + H_{int} + H_{ph} \\
H_0 &= (\epsilon_d - \mu)\sum_{f\sigma} X_f^{\sigma\sigma} + (\epsilon_p - \mu)\sum_{f\sigma}\Phi_{f\sigma}^\dagger\Phi_{f\sigma} + \sum_{ff'\sigma} V_{ff'}(X_f^{\sigma 0}\Phi_{f'\sigma} + h.c) \\
H_{int} &= g_d\sum_{f\sigma} X_f^{\sigma\sigma}u_f + g_p\sum_{f\sigma}\Phi_{f\sigma}^\dagger\Phi_{f\sigma}u_f \\
H_{ph} &= \sum_f(\frac{p_f^2}{2M} + \frac{1}{2}Ku_f^2)
\end{aligned}
$$

where $X_f^{\sigma 0} = d_{f\sigma}^\dagger(1 - n_{f\bar\sigma}^d)$, $X_f^{\sigma\sigma} = n_{f\sigma}^d(1 - n_{f\bar\sigma}^d)$ are the Hubbard operators acting in the subspace of singly occupied copper sites, $\bar\sigma = -\sigma$. $\epsilon_d(\epsilon_p)$ are the energies of the Cu(O) holes. $\Phi_{f\sigma}^\dagger(\Phi_{f\sigma})$ are the creation (annihilation) operators for the b_{1g} symmetry combination of four oxygen orbitals (with respect to a given Cu ion)(see e.g [4]). The function $V_{ff'} = \frac{2}{N}t_{pd}\sum_k e^{ik(f-f')}\gamma_k$, where N is the number of copper sites, $\gamma_k = \sqrt{\sin^2\frac{1}{2}k_x + \sin^2\frac{1}{2}k_y}$, describes hybridization between copper and oxygen holes in f,f' unit cells of the CuO_2 plane; μ is the chemical potential which has to be found from the following equation for the concentration n:

$$n = \frac{1}{N}\sum_{f\sigma}(< X_f^{\sigma\sigma} > + < \Phi_{f\sigma}^\dagger\Phi_{f\sigma} >) \qquad (1)$$

H_0 is obtained from the Emery model in the limit $U_d \to \infty$ which eliminates the upper Hubbard sub-band corresponding to the states with doubly occupied copper sites (see e.g. [12])

H_{int} describes the electron-phonon coupling with the constants g_d and g_p for the Cu and O holes, respectively; H_{ph} is the phonon Hamiltonian where p_f and u_f are the momentum and coordinate operators, respectively, of the ions with mass M and the force constant K($\equiv M\omega_0^2$) in the lattice site f.

III Self-consistent equations for the electron Green function

We define the 4-component Nambu operators $\Psi_{f\sigma}$ and $\Psi_{f\sigma}^\dagger$ where, e.g.,

$$\Psi_{f\sigma}^\dagger = (\ X_f^{\sigma 0}\ ,\ \Phi_{f\sigma}^\dagger\ ,\ X_f^{0\bar\sigma}\ ,\ \Phi_{f\bar\sigma}\ )$$

and introduce the two-time Green function for holes

$$G_{ff'}(t - t') = << \Psi_{f\sigma}(t) \mid \Psi_{f'\sigma}^\dagger(t') >>$$

and for phonons

$$D_{ff'}(t - t') = << u_f(t) \mid u_{f'}(t') >>$$

After the Fourier transformation for the equation of motion for $G_{ff'}(t - t')$, we obtain the following equation:

$$
\begin{aligned}
\omega G_{ff'}(\omega) &= \hat N \times \tau_0 + (\hat\epsilon \times \tau_3)G_{ff'}(\omega) + \\
&+ \sum_i V_{fi} << \begin{pmatrix} X_f^{\bar\sigma\sigma}\Phi_{i\sigma} + (1 - n_{f\sigma}^d)\Phi_{i\sigma} \\ X_i^{0\sigma} \\ -\Phi_{i\bar\sigma}^\dagger X_f^{\bar\sigma\sigma} - (1 - n_{f\bar\sigma}^d)\Phi_{i\bar\sigma}^\dagger \\ -X_i^{\bar\sigma 0} \end{pmatrix} \mid \Psi_{f'\sigma}^\dagger >>_\omega + \qquad (2) \\
&+ (\hat g \times \tau_3) << \Psi_{f\sigma}u_f \mid \Psi_{f'\sigma}^\dagger >>_\omega .
\end{aligned}
$$

where

$$\hat{N} = \begin{pmatrix} 1 - n^d/2 & 0 \\ 0 & 1 \end{pmatrix} \ , \ \hat{\epsilon} = \begin{pmatrix} \epsilon_d - \mu & 0 \\ 0 & \epsilon_p - \mu \end{pmatrix} \ , \ \hat{g} = \begin{pmatrix} g_d & 0 \\ 0 & g_p \end{pmatrix}$$

τ_i $(i = 0, 1, 2.3)$ are the Pauli matrices and the symbol $A \times B$ denotes the direct product for matrices A and B.

Here, we suppose that the system is in the paramagnetic state i,e.:

$$< n^d_{f\uparrow} >=< n^d_{f\downarrow} >= n^d/2$$
$$< X^{\sigma\bar{\sigma}}_f >=< d^\dagger_{f\sigma} d_{f\bar{\sigma}} >= 0$$

In order to decouple the sequence of Green function equations, the following approximations of the Hubbard-I type have been used:

$$<< X^{\bar{\sigma}\sigma}_f \Phi_{i\sigma} \mid \Psi^\dagger_{f'\sigma} >> \simeq < X^{\bar{\sigma}\sigma}_f >< << \Phi_{i\sigma} \mid \Psi^\dagger_{f'\sigma} >> \simeq 0 \qquad (3)$$
$$<< (1 - n^d_{f\bar{\sigma}})\Phi_{i\sigma} \mid \Psi^\dagger_{f'\sigma} >> \simeq (1 - n^d/2) << \Phi_{i\sigma} \mid \Psi^\dagger_{f'\sigma} >>$$

Substituting the approximations (3) into (2) one obtains

$$\omega G_{ff'}(\omega) = \hat{N} \times \tau_0 + (\hat{\epsilon} \times \tau_3) G_{ff'}(\omega) +$$
$$+((\hat{N}\tau_1) \times \tau_3) \sum_i V_{fi} G_{if'}(\omega) + (\hat{g} \times \tau_3) << \Psi_{f\sigma} u_f \mid \Psi^\dagger_{f'\sigma} >>_\omega \qquad (4)$$

By differentiating the Green function $<< \Psi_{f\sigma} u_f \mid \Psi^\dagger_{f'\sigma}(t') >>_\omega$ over the second time t', one obtains in the same approximation as above the following equation:

$$<< \Psi_{f\sigma} u_f \mid \Psi^\dagger_{f'\sigma} >>_\omega \omega =<< \Psi_{f\sigma} u_f \mid \Psi^\dagger_{f'\sigma} >>_\omega (\hat{\epsilon} \times \tau_3) +$$

$$+ \sum_j << \Psi_{f\sigma} u_f \mid \Psi^\dagger_{j\sigma} >>_\omega V_{jf'}((\hat{N}\tau_1) \times \tau_3) + \qquad (5)$$
$$+ << \Psi_{f\sigma} u_f \mid \Psi^\dagger_{f'\sigma} u_{f'} >>_\omega (\hat{g} \times \tau_3)$$

In the q-representation the system of Eqs. (4)-(5) can be written in the form:

$$G(q,\omega) = G_0(q,\omega) + G_0(q,\omega) T(q,\omega) G_0(q,\omega) \qquad (6)$$

where

$$G_0^{-1}(q,\omega) = \begin{pmatrix} \mathcal{G}^{-1}(q,\omega) & 0 \\ 0 & -\mathcal{G}^{-1}(q,-\omega) \end{pmatrix} \qquad (7)$$

$$\mathcal{G}^{-1}(q,\omega) = \begin{pmatrix} \frac{1}{1-n^d/2}(\omega - \epsilon_d + \mu) & -2t_{pd}\gamma_q \\ -2t_{pd}\gamma_q & \omega - \epsilon_p + \mu \end{pmatrix}$$

The scattering matrix $T(q,\omega)$ is defined by:

$$T(q,\omega) = (\hat{g} \times \tau_3)(\hat{N}^{-1} \times \tau_0) \sum_{ij} << \Psi_{i\sigma} u_i \mid \Psi^\dagger_{j\sigma} u_j >>_\omega \cdot$$
$$\cdot (\hat{N}^{-1} \times \tau_0)(\hat{g} \times \tau_3) e^{-iq(i-j)}$$

Eq.(6) can be written also as the Dyson equation:

$$G^{-1}(q,\omega) = G_0^{-1}(q,\omega) - \Sigma(q,\omega) \qquad (8)$$

where $\Sigma(q,\omega)$ is the self-energy operator which is defined by the scattering matrix by the equation:

$$T(q,\omega) = \Sigma(q,\omega) + \Sigma(q,\omega) G_0(q,\omega) T(q,\omega)$$

In the Migdal approximation one can neglect vertex corrections to the electron-phonon coupling and obtain the following expression for the self-energy operator:

$$\Sigma(q,\omega) = (\hat{g} \times \tau_3)(\hat{N}^{-1} \times \tau_0)\frac{1}{2\pi^2}\iint_{-\infty}^{\infty}\frac{d\nu d\nu'}{\omega - \nu - \nu'}\,(th\frac{\nu}{2T} + cth\frac{\nu'}{2T}) \times \quad (9)$$

$$\times\frac{1}{N}\sum_p ImD(q-p,\nu'+i\delta)\; ImG(p,\nu+i\delta)\;(\hat{N}^{-1}\times\tau_0)(\hat{g}\times\tau_3)$$

Here we used the spectral representation for the correlation function and the following approximation:

$$< \Psi_{i\sigma}(t)u_i(t)\Psi^{\dagger}_{j\sigma}u_j > \approx < \Psi_{i\sigma}(t)\Psi^{\dagger}_{j\sigma} >< u_i(t)u_j >$$

In this way, we have obtained the self-consistent system of Eqs.(7)-(9) with the equation for the chemical potential (1)

IV Equation for the superconducting transition temperature

In the well known procedure used in the theory of weak coupling (see e.g. [13]) we propose the most simple approximation for the electron Green function

$$G^{-1}(q,\omega) = \begin{pmatrix} \mathcal{G}^{-1}(q,\omega) & \hat{\Delta}(\omega) \\ \hat{\Delta}^{\dagger}(-\omega) & -\mathcal{G}^{-1}(q,-\omega) \end{pmatrix}$$

where

$$\hat{\Delta}(\omega) = \begin{pmatrix} \Delta_1(\omega) & \Delta_3(\omega) \\ -\Delta_3(-\omega) & \Delta_2(\omega) \end{pmatrix}$$

is the matrix gap function.

In this way, from Eqs.(7)-(9) we obtain the linear equation for the matrix gap function in the weak coupling approximation:

$$\hat{\Delta}(\omega) = \theta(\omega_0 - \mid \omega \mid)\frac{\hat{g}}{2K}\int_{-\omega_0}^{\omega_0} d\nu\; th\frac{\nu}{2T}\;\hat{N}^{-1}\;\frac{1}{\pi}\times$$

$$\times\; Im\;\frac{1}{N}\sum_q \mathcal{G}(q,\nu+i\delta)\hat{\Delta}(\nu)\mathcal{G}(q,-\nu-i\delta)\;\hat{N}^{-1}\hat{g} \quad (10)$$

Here was used the local approximation for the phonon Green function: $D^{-1}(q,\omega) \equiv D^{-1}(\omega) = M\omega^2 - K$.

Now the superconducting transition temperature can be obtained from the matrix Eq.(10) by solving the linear system of equations for the matrix elements Δ_1,Δ_2,Δ_3.

V Numerical results and discussion

Consider the numerical solution of Eq.(10) by taking into account the equation of the chemical potential (1) which in the normal state has the following form:

$$\frac{n^d}{1-n^d/2} = 2\int_{-\infty}^{\infty} d\epsilon\; f(\epsilon)\; N_d(\epsilon) \quad (11)$$

$$n^p = 2\int_{-\infty}^{\infty} d\epsilon\; f(\epsilon)\; N_p(\epsilon) \quad (12)$$

$$n^d + n^p = n \quad (13)$$

where $f(\epsilon) = \left(\exp((\epsilon-\mu)/T)+1\right)^{-1}$ is the Fermi factor, $N_d(\epsilon) = N(\epsilon) \mid \epsilon - \epsilon_p \mid$, $N_p(\epsilon) = N(\epsilon) \mid \epsilon - \epsilon_d \mid$ and $N(\epsilon) = \frac{1}{N}\sum_q \delta((\epsilon-\epsilon_d)(\epsilon-\epsilon_p) - 4t_{pd}^2(1-n^d/2)\gamma_q^2)$.

Eqs.(11)-(13) are the self-consistent equations to determine the filling of the copper band n^d, the bonding oxygen band n^p, and the chem-

ical potential μ. As the values in the right-hand sides of Eqs.(11) and (12) do not exceed two, the maximal filling of the oxygen band is two while a filling of the copper band is always less or equal to one, i.e. $0 \leq n^d \leq 1$. This is due to the proper account (through the Hubbard operators) of the statistics for carriers in the copper band. Fig.1 shows the filling of the copper and oxygen band versus the concentration n at temperature T=0 for $\epsilon_p \equiv \epsilon = 2$. Here, we measure energy in units of t_{pd} and set $\epsilon_d = 0$. Fig.1 clearly shows, that for $n \geq 1.3$ the holes go mainly onto the oxygen band while the filling of the copper band is nearly constant and equals $n^d \approx 1$. In this region the holes of the oxygen band play a dominant role in the Cooper pair formation while in the region $0 \leq n \leq 1.3$ the holes in the copper band are important. In this case, the system has no electron-hole symmetry. On the contrary, in the usual two-band Fermi system, where the electron correlation is absent, the system has the electron-hole symmetry (see Fig.1). Fig.2 shows the dependence of the superconducting transition temperature Tc on the concentration n for $\epsilon = 2$, $\omega_0 = 0.5$, $\bar{g}_d = \bar{g}_p = 0.5$ (where $g = \bar{g}\sqrt{2M\omega_0}$) in two cases: for the Emery model and for the usual two-band Fermi system. For the Fermi system Tc(n) is symmetrical around n=2 while for the Emery model Tc(n) does not possess this symmetry. Fig.3 shows the Tc(n) dependence for several values of the electron-phonon coupling constant g_d, g_p. One clearly sees that in the region $0 \leq n \leq 1.3$ the electron-phonon coupling onto the copper sites dominates in the superconducting state formation while in the region $1.3 \leq n \leq 3$ the electron-phonon coupling onto the oxygen sites is important. In both regions Tc attains the maximal value near the Van-Hove singularity in the quasiparticle spectrum.

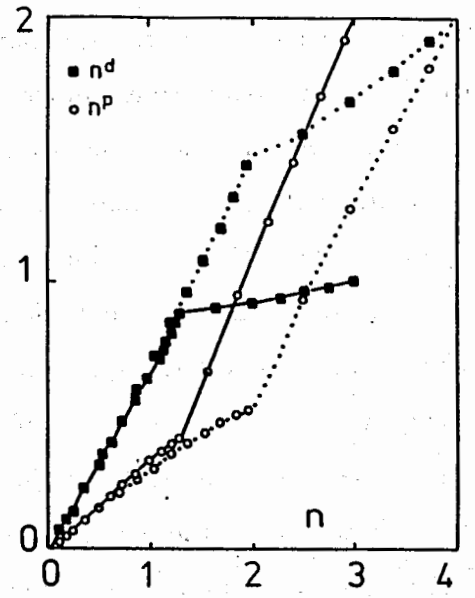

Fig.1 The dependence of the filling for copper and oxygen bands on the charge carriers concentration for the Emery model (solid line) and for the usual two-band Fermi system (dashed line). $\epsilon = 2$

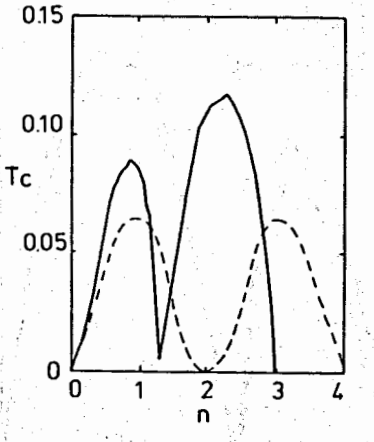

Fig.2 The dependence of the superconducting transition temperature on the charge carriers concentration for Emery model (solid line) and for the usual two-band Fermi system (dashed line). $\epsilon = 2$, $\bar{g}_d = \bar{g}_p = 0.5$

In summary, we have considered the electron-phonon mechanism of superconducting pairing in the two-band Emery model. In comparison to the usual two-band Fermi system, where the electron correlations are neglected, we have found for the present model an about two times higher transition temperature Tc with its maximum shifted from the half-filling values, n=1 or n=3, to the lower hole densities, $n \approx 0.8$ (d-band) and $n \approx 2.3$ (p-band). The electron-phonon coupling at the copper sites and the oxygen sites play a dominant role in the copper band ($0 \leq n \leq 1.3$) and in the oxygen one ($1.3 \leq n \leq 3$), respectively.

Finite life-time effects both due to the electron-phonon and anti-ferromagnetic spin-fluctuation scattering are neglected here. We also neglect Coulomb repulsion of holes ($\mu^* = 0$). All these effects suppress

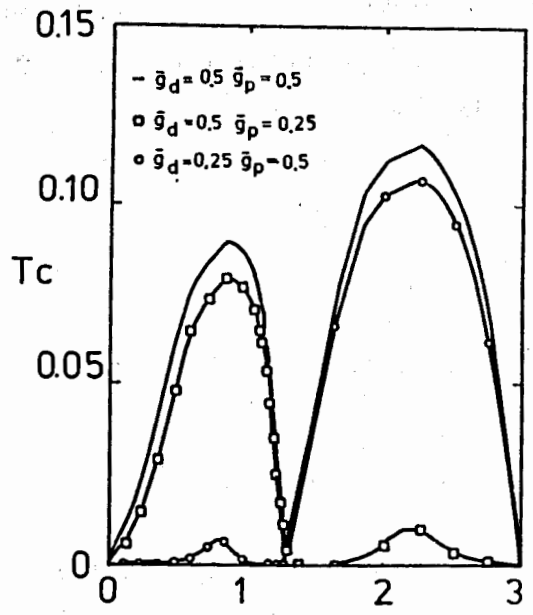

Fig.3 The dependence of the superconducting transition temperature on the charge carriers concentration. $\epsilon = 2$

Tc and should give a sharper Tc(n) dependence. We are planning to consider them as well as a more realistic phonon spectrum and non-local electron-phonon interaction in a separate study.

REFERENCES

[1] Fulde P. Physica C , v.153-155 (1990) , p.1769

[2] Pickett W.E. Rev.Mod.Phys. , v.61 (1989) , p.433

[3] Anderson P.W. Science , v.234 (1987) , p.1196

[4] Zhang F.C.,Rice T.M. Phys.Rev.B , v.37 (1988) , p.3759

[5] Emery V.J. Phys.Rev.Lett. , v.58 (1987) , p.2794

[6] Von der Linden W.,Morgenstern I.,de Raetd H. Phys.Rev.B , v.41 (1990) , p.4669

[7] Frick M.,et.al. Phys.Rev.B , v.42 (1990) , p.2665

[8] Crawford M.P.,et.al. Phys.Rev.B , v.41 (1990) , p.282

[9] Franck J.P.,et.al. Physica B , v.169 (1991) , p.697

[10] Pickett W.E.,et.al. Phys.Rev.Lett. , v.67 (1991) , p.228

[11] Pintschovins L. Advances in Solid State , v.30 (1990) , p.183

[12] Ihle D.,Kasner M. Phys.Rev.B , v.42 (1990) , p.4760

[13] Vonsovsky S.V.,Izymov Y.A.,Kurmaev E.Z. Superconductivity of Transition Metals. Springer, Heidelberg, 1982.

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