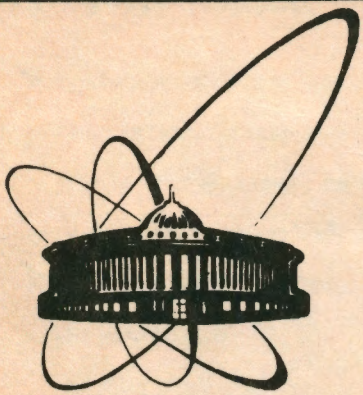

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ELECTRON-PHONON PAIRING IN THE HUBBARD MODEL

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1 Introduction

Recent experiments in oxide superconductors show a definite role of electron-phonon interactions in the pairing mechanism of carriers in conduction plains of CuO_2. For instance, an enhanced isotope effect $\alpha \geq 1/2$ was observed at definite carrier concentrations both in $La_{2-x}Sr_xCuO_4$ [1] and $Y_{1-x}Pr_xCu_3O_{7-y}$ [2]. Theoretical estimations also show strong electron-phonon interactions in oxide compounds [3, 4].

Strong electron correlations on Cu-sites lead to a charge–transfer gap in the electronic spectra which cannot be adequately described by a standard theory of Fermi-liquid. Hence, one should study the problem of pairing mechanism in a system near the metal–insulator transition with strong electron correlations. In the present paper, we consider a single band Hubbard model on a square lattice in the strong correlation limit $U \to \infty$ when double occupancy of states on the lattice sites at the average occupation number $n \leq 1$ is prohibited.

2 The model and equations for Green functions

To take into account strong anharmonic oxygen ion vibrations in oxide superconductors, we consider electron-phonon interactions within the framework of an anharmonic model [5]. The anharmonic model with strong correlations was proposed by K.A.Müller [6] and we consider here the model with a nonlocal electron-phonon interaction [7, 8].

In the strong correlation limit the Hamiltonian of the model [7, 8] written in terms of the Hubbard operators $X_j^{\sigma 0} = c_{i\sigma}^+(1-n_{i\bar{\sigma}})$, $X_j^{\sigma 0} = (X_j^{0\sigma})^+$, $\bar{\sigma} = -\sigma$

has the form

$$H = t\sum_{j\neq j'} X_j^{\sigma 0}X_{j'}^{0\sigma} - \mu\sum_{j,\sigma} X_j^{\sigma\sigma} + g\sum_i(\sum_\delta n_{i+\delta})S_i^x - \Omega\sum_i S_i^z \qquad (1)$$

where j and j' label lattice sites, δ runs over four oxygen sites within the CuO_4-plaquette denoted by the index i, σ is the fermion spin, t is the hopping matrix element, S_i^ν, $\nu \in \{x,y,z\}$ are the pseudospin operators, g denotes the coupling constant, $n_{j\sigma} = X_j^{\sigma\sigma} = X_j^{\sigma 0}X_j^{0\sigma}$ and $n_j = \sum_\sigma n_{j\sigma}$, the energy of pseudospin oscillations characterized by frequency Ω, μ is the chemical potential.

Let us introduce the two-component Nambu operators

$$X_i^\sigma = \begin{pmatrix} X_i^{0\sigma} \\ X_i^{+0\bar{\sigma}} \end{pmatrix}, X_j^{+\sigma} = (X_j^{\sigma 0}, X_j^{0\bar{\sigma}}) \qquad (2)$$

and define the two-time matrix Green function (GF)

$$G_{ij}^\sigma(t-t') = << X_i^\sigma(t), X_j^{+\sigma}(t') >>= \begin{pmatrix} << X_i^{0\sigma}(t), X_j^{+0\sigma}(t') >> & << X_i^{0\sigma}(t), X_j^{0\bar{\sigma}}(t') >> \\ << X_i^{+0\bar{\sigma}}(t), X_j^{+0\sigma}(t') >> & << X_i^{+0\bar{\sigma}}(t), X_j^{0\bar{\sigma}}(t') >> \end{pmatrix}, \qquad (3)$$

with normal diagonal matrix elements and anomalous nondiagonal ones. To calculate the GF, we employ the method of equation of motion for a dynamical variable $X_i^\sigma(t)$ in the Heisenberg representation. By differentiating Eg. (3) over time t, one gets in the ω-representation:

$$\omega\tau_0 G_{j,j'}(\omega) = \delta_{j,j'}Q\tau_0 + \sum_l (Qt_{jl} - \mu\delta_{l,j})\tau_3 G_{l,j'}(\omega) - g\sum_\delta << S_{j-\delta}^x X_j^\sigma | X_{j'}^{+\sigma} >>_\omega \qquad (4)$$

where τ_0, τ_3 is the Pauli matrix and $< X_i^{00} + X_i^{\sigma\sigma} >= (1 - < n_{j\bar{\sigma}} >) = (1 - n/2) = Q = 1 - < X_i^{\bar{\sigma},\bar{\sigma}} >$.

Strong electron correlations in (4) were considered in the Hubbard I approximation.

By differentiating the Green function $<< S_i^x X_j^{+\sigma}; X_{j'}^{+\sigma}(t') >>$ in Eq.(4) , over the second time t' and employing the same approximation we obtain the system of two equations. It can be solved in the form:

$$G(\mathbf{q},\omega) = G_0(\mathbf{q},\omega) + G_0(\mathbf{q},\omega)T(\mathbf{q},\omega)G_0(\mathbf{q},\omega), \qquad (5)$$

where we introduced the zero-order Green function in the q–representation:

$$G_0^{-1}(\mathbf{q};\omega) = \omega\tau_0 - (\epsilon_{\mathbf{q}} - \mu)\tau_3, \qquad (6)$$

with

$$\epsilon_{\mathbf{q}} = t(1-n/2)\gamma_{\mathbf{q}} = t(1-n/2)2(\cos q_x + \cos q_y) \qquad (7)$$

(the lattice constant $a = 1$)

$$T(\mathbf{q},\omega) = \frac{g^2\tau_3}{NQ}\sum_{j,i}\sum_{\delta\delta'} << S_{i-\delta}^x X_i^\sigma | S_{j-\delta'}^x X_j^{+\sigma} >>_\omega e^{-i\ \mathbf{q}\ (\mathbf{i-j})}\tau_3 \qquad (8)$$

is the scattering matrix. N is the number of lattice sites. By comparing Eq. (5) with the Dyson equation for the Green function $G(\mathbf{q},\omega)$:

$$G(\mathbf{q},\omega) = G_0(\mathbf{q},\omega) + G_0(\mathbf{q},\omega)\Sigma(\mathbf{q},\omega)G_0(\mathbf{q},\omega), \qquad (9)$$

one can obtain the equation for the self-energy operator

$$T(\mathbf{q},\omega) = \Sigma(\mathbf{q},\omega) + \Sigma(\mathbf{q},\omega)G_0(\mathbf{q},\omega)T(\mathbf{q},\omega). \qquad (10)$$

To obtain the self–energy operator Σ in the second order in electron–phonon coupling one can employ the approximation for the many particles time–dependent correlation function in the scattering matrix (8):

$$< S_l^x(t)X_i^\sigma(t)|S_{l'}^x X_j^{+\sigma} > \approx < S_l^x(t)S_{l'}^x >< X_i^\sigma(t)X_j^{+\sigma} >. \qquad (11)$$

Using this approximation which neglects vertex corrections, one can arrive at the equation:

$$\Sigma(\mathbf{q},\omega) \cong T(\mathbf{q},\omega) \cong \frac{g^2}{Q2\pi^2}\iint_{-\infty}^{\infty}\frac{dzdz'}{\omega-z-z'+i\epsilon}(th(\frac{z}{2T})+cth(\frac{z'}{2T}))\times \qquad (12)$$
$$\frac{1}{N}\sum_{\mathbf{p}}\gamma^2(\mathbf{q}\text{-}\mathbf{p})ImD(\mathbf{q}\text{-}\mathbf{p},z'+i\delta)\tau_3 ImG(\mathbf{p},z+i\delta)\tau_3,$$

where the pseudospin GF for anharmonic vibrations was introduced:

$$D_{ij}(t-t') = <<S_i^x(t),S_j^x(t')>> = \sum_{\mathbf{q}} e^{i\,\mathbf{q}(\mathbf{i}\text{-}\mathbf{j})}\frac{1}{2\pi}\int_{-\infty}^{\infty} D(\mathbf{q},\omega)e^{i\omega(t-t')}d\omega. \qquad (13)$$

To solve Eq. (10) we neglect the renormolisation of the energy of pseudospin excitations and use the following approximation:

$$ImD(\mathbf{q},\omega+i\delta) \approx ImD(\omega+i\delta) = -\Omega < S^z > \pi\delta(\omega^2-\Omega^2)sgn(\omega). \qquad (14)$$

Therefore, we obtain a closed system of equations for the Green function (9) and the self-energy operator (12)

3 Superconducting transition temperature

By using the standard procedure one can obtain the Eliaschberg equations. Then, in the weak coupling approximation [9] we arrive at the linearized equation for the superconducting gap (at $T \le T_c$):

$$\Delta(\mathbf{q},\omega) = \frac{g^2<S>}{2\Omega}\int_{-\Omega}^{\Omega} d\omega th\frac{\omega}{2T}\frac{1}{N}(\frac{-1}{\pi})Im\sum_{\mathbf{p}}\frac{\gamma^2(\mathbf{p}\text{-}\mathbf{q})\Delta(\mathbf{p})}{\omega^2-(\epsilon_{\mathbf{p}}-\mu)^2}. \qquad (15)$$

To solve this equation we consider the following $\mathbf{q}$—dependent representation for the gap (see e.g. [10]):

$$\Delta(\mathbf{q}) = \Delta_{0s} + \Delta_{cs}\gamma_{\mathbf{q}} + \Delta_{cd}\xi_{\mathbf{q}} + \Delta_{sd}\chi_{\mathbf{q}},$$

where $\xi_{\mathbf{q}} = 2(\cos(q_x)-\cos(q_y))$, $\chi_{\mathbf{q}} = \sin(q_x)\sin(q)_y$. Multiplying Eq.(15) by γ_q, ξ_q, χ_q and averaging it over the directions of wave—vectors $\mathbf{q}$ and $\mathbf{p}$, we arrive at the system of equations:

$$\Delta_{0s}(\omega) = \theta(\Omega-|\omega|)\frac{g^2<S^z>}{2\Omega}\int_{-\Omega}^{\Omega}\frac{dz}{z}4N(\mu+z)th(\frac{z}{2T})\Delta_{0s}(z), \qquad (16)$$

$$\Delta_{sd} = \theta(\Omega-|\omega|)\frac{g^2<S^z>}{2\Omega}\int_{-\Omega}^{\Omega}\frac{dz}{z}E(\mu+z)th(\frac{z}{2T})\Delta_{sd}(z), \qquad (17)$$
$$\Delta_{cs} = \Delta_{cd} = 0,$$

where $N(\epsilon) = \frac{1}{N}\sum_{\mathbf{k}}\delta(\epsilon-\epsilon_{\mathbf{k}})$, $E(\epsilon) = \frac{1}{N}\sum_{\mathbf{k}}\delta(\epsilon-\epsilon_{\mathbf{k}})\chi_{\mathbf{k}}$, $< S^z > = \frac{1}{2}th(\frac{\Omega}{2T})$. It is interesting to point out that due to the symmetry of an electron–phonon interaction $\gamma^2(\mathbf{p}\text{-}\mathbf{q})$, the coupling constants for the extended s-wave Δ_{sd} and d–wave Δ_{cd} pairing vanish.

The chemical potential μ is defined from the equation

$$n = \frac{1}{N}\sum_{i\sigma} < X_i^{\sigma\sigma} > = \frac{1}{N}\sum_{i\sigma} < X_i^{\sigma 0}X_i^{0\sigma} > . \qquad (18)$$

Eqs. (7), (16), (17), (18) form a set of fully self-consistent equations for the superconductivity transition temperature T_c. To solve Eqs. (16), (17) we adopt a standard approximation:

$$\Delta_i(\omega) = \begin{cases} \Delta_i = const, & |\omega| < \Omega \\ 0, & |\omega| > \Omega \end{cases},$$

where $i = 0s, sd$, and write Eqs.(16), (17) and Eq.(18) in the form:

$$1 = \frac{g^2}{4\Omega}th(\frac{\Omega}{2T})\int_{-\Omega}^{\Omega}\frac{dz}{z}4N(z+\mu)th(\frac{z}{2T}), \qquad (19)$$

$$1 = \frac{g^2}{4\Omega}th(\frac{\Omega}{2T})\int_{-\Omega}^{\Omega}\frac{dz}{z}E(z+\mu)th(\frac{z}{2T}), \qquad (20)$$

$$\frac{n}{1-n/2} = \frac{1}{N}\sum_{\mathbf{q}}[1 - th(\frac{\epsilon_{\mathbf{q}} - \mu}{2T})]. \qquad (21)$$

These equations were solved numerically for the following set of parameters: $a)\Omega = 0.1, g = 0.5$ and $b)\Omega = 0.1, g = 0.3$. The energy scale is given by the hopping matrix element, $t = 1$. The results of calculation of $T_c(n)$ are presented in figures 1 and 2.

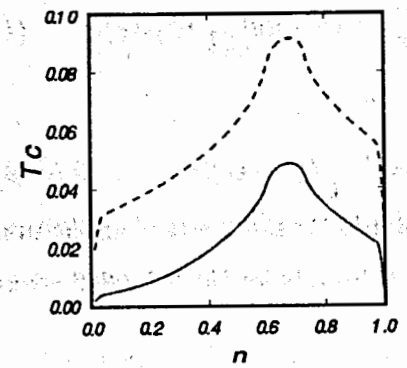

Figure 1. $T_c(n)$ dependence for the s–wave pairing for two parameter sets $a)\Omega = 0.1, g = 0.5$ (dashed line); $b)\Omega = 0.1, g = 0.3$ (solid line) .

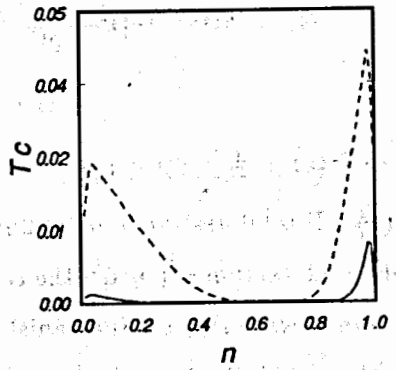

Figure 2. $T_c(n)$ dependence for the d–wave pairing for two parameter sets $a)\Omega = 0.1, g = 0.5$ (dashed line); $b)\Omega = 0.1, g = 0.3$ (solid line).

For the s-wave pairing $T_{cs}(n)$ in fig.1. has its maximal value at $\mu = 0$, $n \approx 0,66$ due to the van Hove singularity for the two—dimensional Brillouin zone (see e.g. [11], [12]). For the d-wave (b_{2g}) pairing T_{cd} on fig.2. due to the factor χ_q in the density of states has a different behavior in comparison with $T_{cs}(n)$. We see that the temperature calculated for the s-wave pairing is larger than in the d-wave pairing case.

In summary, the anharmonic electron–phonon model with strong correlation (1) was considered analytically and the dependence of superconducting transition temperature T_c on the electron concentration n was obtained. The nonlocal character of an electron–phonon interaction in the model results in a peculiar $T_c(n)$ dependence: T_c for the s-wave pairing has its maximal value at the van–Hove singularity, $\mu = 0$, $n \approx 0,66$, while $T_c = 0$ for the extended s–wave and d–wave (b_{1g} symmetry) pairing. For the d wave (b_{2g} symmetry) pairing $T_c(n)$ has its maximal value at low ($n \approx 0,1$) and high ($n \geq 0,95$) electron concentrations.

Our results for superconducting pairing in the strong correlation limit for the model (1) are in agreement with the off diagonal long range order which was found in [8], where the Hubbard model with the anharmonic electron–phonon coupling was investigated by the quantum Monte Carlo method.

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Электрон-фононное спаривание
в модели Хаббарда

Рассматривается система электронов с сильной корреляцией в рамках однозонной модели Хаббарда с сильно ангармоническим электрон-фононным взаимодействием. На основе метода функций Грина получена зависимость температуры сверхпроводящего перехода T_c от концентрации носителей n. Показано, что благодаря нелокальному характеру электрон-фононного взаимодействия в рассматриваемой модели, зависимость $T_c(n)$ определяется симметрией щели.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Electron-Phonon Pairing
in the Hubbard Model

A system of electrons with a strong correlations is considered within the framework of a single band Hubbard model with a strong anharmonic electron-phonon interaction. The dependence of superconducting transition temperature T_c on carrier concentrations n is obtained using the Green function technique. It is shown that due to the nonlocal character of the electron-phonon coupling in the model $T_c(n)$ strongly depends on the symmetry of the gap.

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

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