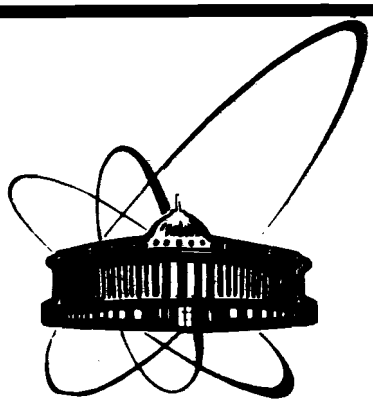

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ON THE THEORY OF SUPERCONDUCTIVITY IN A MODEL OF OXIDE METALS

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I. INTRODUCTION

Recently a large number of theoretical models has been proposed to explain the pairing mechanism in the new oxide high-T_c superconductors discovered by Bednorz and Muller [1]. These models may be divided into two classes: in the first one an electron-phonon mechanism is considered which has been proved in observing of a small isotope shift, and in the second class the pairing due to electronic correlation of exchange type is proposed (see, e.g. [2]). There is still increasing experimental evidence for large Coulomb correlation in 3d states of Cu^{2+} ions that strongly interact with 2p states of O^{2-} ions, which results in highly anisotropic electron bands. On the other hand, structural instability usually observed in perovskite-type compounds brings about a highly anharmonic lattice dynamics which may also enhance the superconducting transition temperature (see [3]). To develop a self-consistent theory of superconductivity in the new oxide compounds, all these specific properties of electrons and phonons should be taken into account. In the present paper, we propose for that aim a Green-function method within a simplified model of oxide metals.

2. A POLAR MODEL OF METAL

Due to a localized character of electron wave functions in 3d and 2p states in the new oxide superconductors the most appropriate method to calculate electron energy bands is the method of orthogonalized atomic orbitals developed by N.N.Bogolubov [4] in the polar model of metals originally proposed in [5].

For simplicity we consider a two-dimensional lattice in the basal plane of La_2CuO_4 (or $YBa_2Cu_3O_7$) with copper ions in the lattice sites $\vec{f} = n_1\vec{a}_x + n_2\vec{a}_y$ and oxygen ions at the lattice sites $\vec{g}_\alpha = \vec{f} + \vec{r}_\alpha$, where $2\vec{r}_{x,y} = \vec{a}_{x,y}$. By taking into account the crystal field effects we consider only one nondegenerate $d(x^2 - y^2)$ orbital with the atomic energy ϵ_p° and wave function $\Psi(\vec{f}, \vec{r})$ at lattice sites $\vec{f}$ and two p_x or p_y orbitals with the atomic energy ϵ_p° and wave functions $\phi_\alpha(\vec{g}_\alpha, \vec{r})$ at lattice sites $\vec{g}_x, \vec{g}_y$, respectively. By neglecting all overlap integrals except for the nearest-neighbour one for orthogonalized set of wave functions at the lattice sites $\vec{f}, \vec{g}_\alpha$ in the second order one gets:

$$\tilde{\Psi}(\vec{f},\vec{r}) = (1+\frac{3}{2}S^2)\,\Psi(\vec{f},\vec{r}) - \frac{1}{2}S\sum_{\pm\vec{r}_\alpha}\phi_\alpha(\vec{f}+\vec{r}_\alpha,\vec{r}) + \frac{3}{8}S^2\sum_{\pm\vec{a}_\alpha}\Psi(\vec{f}+\vec{a}_\alpha,\vec{r}), \quad (1)$$

$$\tilde{\phi}_\alpha(\vec{g}_\alpha,\vec{r}) = \phi_\alpha(\vec{g}_\alpha,\vec{r}) - \frac{1}{2}S[\Psi(\vec{f},\vec{r}) + \Psi(\vec{f}+\vec{a}_\alpha,\vec{r})] + \frac{3}{8}S^2\sum_{\pm\vec{r}_\beta}\{\phi_\beta(\vec{f}+\vec{r}_\beta) + \phi_\beta(\vec{f}+\vec{a}_\alpha+\vec{r}_\beta)\}, \quad (2)$$

where the overlap integral

$$S = \langle\Psi(\vec{f},\vec{r}) \mid \phi_\alpha(\vec{f}\pm\vec{r}_\alpha)\rangle \quad (3)$$

is considered to be a small parameter, $S \ll 1$.

Now by employing the orthogonalized one-particle set of wave functions (1), (2) the total Hamiltonian of the system $H = H_0 + V$ can be written in the second quantized form as

$$H = \sum_{ij\sigma} L_{ij}\, a^+_{i\sigma} a_{j\sigma} + \frac{1}{2}\sum_{ijk\ell\,\sigma\sigma'} V(ij|k\ell)\, a^+_{i\sigma} a^+_{j\sigma'} a_{k\sigma'} a_{\ell\sigma}, \quad (4)$$

where $L_{ij} = \{L_{fg}, L_{ff'}, L_{gg'}\}$ depends on the atomic energies $\epsilon_d^\circ, \epsilon_p^\circ$ and matrix elements of the one-particle part H_0 of the Hamiltonian, and the function $V(ij|k\ell)$ is described by matrix elements of the Coulomb interactions between electrons. Here $L_{fg} \sim S$ and $L_{ff'}$, $L_{gg'}$ are given by the renormalized energies ϵ_d and ϵ_p for $f = f'$ and $g = g'$ while for the next to nearest-neighbours they are given by matrix elements of S^2 order (for details see /6/). In the lowest order of S in (4) the generalized Hubbard Hamiltonian can be obtained as follows:

$$H = \sum_i \epsilon_i n_{i\sigma} + \sum_{i\neq j\,\sigma} t_{ij}\, a^+_{i\sigma} a_{j\sigma} + \frac{1}{2}\sum_{i\sigma} U_i n_{i\sigma} n_{i-\sigma} + \frac{1}{2}\sum_{i\neq j\,\sigma,\sigma'} V_{ij} n_{i\sigma} n_{j\sigma'}, \quad (5)$$

where $t_{ij} = t_{fg} \sim S$ and $U_i = (U_d, U_p)$, $V_{ij} = V_{fg}$ are of the zeroth order in S. To consider electron-phonon interaction, one should take into account lattice vibrations $\vec{u}_i$ by making the substitution $\vec{f} \to \vec{R}_f = \vec{f} + \vec{u}_f$, $\vec{g}_\alpha \to \vec{R}_{g\alpha} = \vec{g}_\alpha + \vec{u}_\alpha$ in (4) or (5). The Hamiltonian (4) or (5) can be generalized by considering other atomic orbitals, e.g. $d(3z^2-r^2)$ at copper sites $\vec{f}$ and p_z at oxygen sites g_α, or by taking into account a more complicated lattice structure in the case of $YBa_2Cu_3O_7$-type compounds. Since all the matrix elements in (4) are given by a small number of microscopic parameters, the Hamiltonian (4) or (5) can be used as a basis for calculations of electron energy bands, phonon spectra and for development of the theory of superconductivity in the oxide metals. By applying a perturbation theory in the operator form small S in eqs. (4) or (5) as proposed by N.N.Bogolubov /4/, one can obtain some effective Hamiltonians of the Heisenberg type with an exchange integral $J \sim t^2/U$ (see /2/). Some results of these calculations are presented in /6/.

3. GREEN FUNCTIONS

To consider the electronic band structure and superconductivity in the system described by the model Hamiltonian (4) of (5), we introduce the matrix Green function

$$G_{ij}(t-t') = \langle\langle \Psi_{i\sigma}(t) ; \Psi^+_{j\sigma}(t')\rangle\rangle. \quad (6)$$

Further we consider the model (5) with the electron-phonon interaction defined by the term $t^\mu_{ij} u^\mu_{ij}$ in the decomposition of the transfer integral $t(\vec{R}_i - \vec{R}_j)$ over ion displacements $u^\mu_{ij} = (\vec{u}_i - \vec{u}_j)_\mu$. By differentiating the Green function (6) with respect to time t and employing equations of motion for the Heisenberg operators one gets the following equation for the Fourier transform of the Green function:

$$(\omega\tau_0 - \epsilon_i\tau_3)\,G_{ij}(\omega) = \delta_{ij}\tau_0 + \sum_k t_{ik}\tau_3 G_{kj}(\omega) + \sum_k t^\mu_{ik}\tau_3 \langle\langle u^\mu_{ik}\Psi_{k\sigma} \mid \Psi^+_{j\sigma}\rangle\rangle_\omega + \sum_{k\sigma'} V^{\sigma\sigma'}_{ik}\langle\langle n_{k\sigma'}\Psi_{i\sigma} \mid \Psi^+_{j\sigma}\rangle\rangle_\omega, \quad (8)$$

where

$$\tau_0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},\ \tau_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\ V^{\sigma\sigma'}_{ik} = V_{ik}\tau_3 + \delta_{ik}U_i\begin{pmatrix}\delta_{-\sigma'\sigma} & 0\\ 0 & \delta_{\sigma'\sigma}\end{pmatrix}. \quad (9)$$

In the band limit ($t \gg U_i, V_{ik}$) the Coulomb interaction can be considered as a perturbation. For this we introduce an irreducible part (ir) of many-fermion operators as, e.g.,

$$(n_{k\sigma'}a_{i\sigma})^{ir} = a^{+}_{k\sigma'}a_{k\sigma'}a_{i\sigma} - \tag{10}$$

$$- \{ \langle n_{k\sigma'} \rangle a_{i\sigma} - \delta_{\sigma'\sigma} \langle a^{+}_{k\sigma} a_{i\sigma} \rangle a_{k\sigma} + \delta_{-\sigma'\sigma} \langle a_{k-\sigma} a_{i\sigma} \rangle a^{+}_{k-\sigma} \},$$

where both the Hartree-Fock correlation functions as well as superconducting one are taken into account [8]. To obtain equations for the Green functions with the irreducible parts, e.g. $\Gamma(t-t') = \langle\langle A_{ir}(t); \Psi^{+}_{j\sigma}(t') \rangle\rangle$ we differentiate them with respect to the second time t' and employ the same-type decomposition as in eq. (10). After some algebra (see [8]) we can obtain the Dyson equation in the form:

$$G_{ij}(\omega)^{-1} = \{(\omega\tau_0 - \bar{\epsilon}_i\tau_3)\delta_{ij} - L_{ij}\tau_3 - \Sigma^{c}_{ij} - \Sigma_{ij}(\omega)\}, \tag{11}$$

where $\bar{\epsilon}_i = \epsilon_i + \sum_{k\sigma'} V_{ik} \langle n_{k\sigma'} \rangle$ and the self-energy operator in the mean field approximation is given by

$$\Sigma^{c}_{ij} = \tau_3 \{ -U_i \langle \Psi^{+}_{i-\sigma} \Psi_{i-\sigma} \rangle \delta_{ij} + V_{ij} \langle \Psi_{i\sigma} \Psi^{+}_{j\sigma} \rangle \} \tau_3 . \tag{12}$$

The contributions to it from electron-phonon and higher order terms of Coulomb interactions are described by

$$\Sigma_{ij}(\omega) = \sum_{k\ell} t^{\mu}_{ik} t^{\nu}_{j\ell} \tau_3 \langle\langle u^{\mu}_{ik} \Psi_{k\sigma} | u^{\nu}_{\ell j} \Psi^{+}_{\ell\sigma} \rangle\rangle_{\omega} + \tag{13}$$

$$+ \sum_{k\ell\sigma'\sigma''} V^{\sigma\sigma'}_{ik} V^{\sigma\sigma''}_{j\ell} \langle\langle (n_{k\sigma'}\Psi_{i\sigma})^{ir} | (\Psi^{+}_{j\sigma} n_{\ell\sigma''})^{ir} \rangle\rangle_{\omega} .$$

Some approximations for (13) will be discussed in the next section.

In the limit of strong Coulomb interaction, $t_{ij} \ll U_i$ an atomic limit should be considered as a zero-order approximation. In this case the Green functions for many-fermion operators of the Hubbard type, e.g. $\{a_{i\sigma}(1 - n_{i-\sigma}), a_{i\sigma} n_{i\sigma}\}$ should be introduced and equations of motion for them should be considered as given below:

$$[a_{i\sigma}(1-n_{i-\sigma}), H] = \epsilon_i a_{i\sigma}(1-n_{i-\sigma}) + \tag{14}$$

$$+ \sum_j t_{ij} \{ a_{i-\sigma} a^{+}_{i-\sigma} a_{j\sigma} + a^{+}_{i-\sigma} a_{i\sigma} a_{j-\sigma} + a_{i-\sigma} a_{i\sigma} a^{+}_{j-\sigma} \}.$$

One can see that due to the projection operator $(1 - n_{i-\sigma})$ there appears in the right-hand side of eq. (14) a kinematical interaction that is usually described by special vertices of the diagram technique (see, e.g. [10]). To obtain the lowest order contribution from this interaction, one should consider the simplest approximations of the Hubbard-I type [9]:

$$a_{i-\sigma} a^{+}_{i-\sigma} a_{j\sigma} \to \langle a_{i-\sigma} a^{+}_{i-\sigma} \rangle a_{j\sigma} - \langle a_{i-\sigma} a_{j\sigma} \rangle a^{+}_{i-\sigma} ,$$

$$a_{i-\sigma} a_{i\sigma} a^{+}_{j-\sigma} \to \langle a_{i-\sigma} a_{i\sigma} \rangle a^{+}_{j-\sigma} - \langle a_{i-\sigma} a^{+}_{j-\sigma} \rangle a_{i\sigma} .$$

Here we take into account both the types of anomalous correlation functions: at different lattice sites, $\langle a_{i-\sigma} a_{j\sigma} \rangle$, as well as at the same lattice site, $\langle a_{i-\sigma} a_{i\sigma} \rangle$. The latter has not been considered in [10] though they play an essential role, especially for finite U. As a result of these approximations, a closed system of equations for the Green function (6) is obtained. Here we present this system only for a simple Hubbard model with $\epsilon_i = \epsilon$, $U_i = U$, $V_{ij} = 0$ in (5) (for details see [11]):

$$[1 - g(\omega)\, t(\vec{q})]\, G(\vec{q}, \omega) = g(\omega) + \gamma(\omega)\Delta(\vec{q})\, F(\vec{q}, \omega), \tag{16}$$

$$[1 - g(-\omega)\, t(\vec{q})]\, F(\vec{q}, \omega) = -\gamma(-\omega) F^{*} - \gamma(-\omega)\Delta^{*}(\vec{q})\, G(\vec{q}, \omega),$$

where the $\vec{q}$ representation for the Green functions in (6) is given by

$$\langle\langle a_{i\sigma} | a^{+}_{j\sigma} \rangle\rangle_{\omega} \to G(\vec{q}, \omega), \quad \langle\langle a^{+}_{i-\sigma} | a^{+}_{j\sigma} \rangle\rangle_{\omega} \to F(\vec{q}, \omega).$$

The Green function in the atomic limit, $t_{ij} = 0$, is described by the equations:

$$g(\omega) = (1 - n/2)\, g_1(\omega) + (n/2)\, g_2(\omega), \quad \gamma(\omega) = g_1(\omega) - g_2(\omega),$$

$$g_1(\omega) = (\omega - \epsilon)^{-1}, \quad g_2(\omega) = (\omega - \epsilon - U)^{-1} .$$

$t(\vec{q})$ is the $\vec{q}$-representation for t_{ij}. The $\vec{q}$-dependent gap $\Delta(\vec{q})$ in (16) is defined by the equations

$$\Delta(\vec{q}) = \Delta + t(\vec{q})\, F, \tag{17}$$

$$\Delta = 2 \sum_j t_{ij} \langle a_{i\sigma} a_{j-\sigma} \rangle, \quad F = \langle a_{i-\sigma} a_{i\sigma} \rangle .$$

Here the parameters Δ and F obey the condition $(2\epsilon + U)F = 2\Delta$. Some results obtained from eq. (16), (17) will be considered in Sect. 5.

4. ELECTRON-PHONON INTERACTION

Let us consider the self-consistent equation for the Green function (11) provided the electron-phonon interaction in the self-energy operator (13) in the second order

$$\Sigma^{ph}_{ij}(\omega) = \int\int_{-\infty}^{\infty} \frac{d\omega_1 d\omega_2}{\omega - (\omega_1 + \omega_2)} \frac{1}{2}\left(\mathrm{th}\frac{\omega_1}{2T} + \mathrm{cth}\frac{\omega_2}{2T}\right) \times$$

$$\times \sum_{k\ell} t^{\mu}_{ik} t^{\nu}_{j\ell} \left[-\frac{1}{\pi}\mathrm{Im} \ll u^{\mu}_{ik} | u^{\nu}_{j\ell} \gg_{\omega_2} \right] \left[-\frac{1}{\pi}\mathrm{Im}\, r_3 G_{k\ell}(\omega_1 + i\delta) r_3 \right] \qquad (18)$$

is taken into account. The last term in (13) that describes Coulomb scattering in the second order in $V^{\sigma\sigma'}_{ik}$ can be obtained by applying the "mode-coupling" type approximations (for details see [8]):

$$\langle n_{k\sigma'}(t)\, \Psi_{i\sigma}(t)\, \Psi^{+}_{j\sigma}\, n_{\ell\sigma'} \rangle \to \langle n_{k\sigma'}(t)\, n_{\ell\sigma'} \rangle \langle \Psi_{i\sigma}(t)\, \Psi^{+}_{j\sigma} \rangle .$$

In these approximations one can take into account electron screening effects which are both due to the one-site excitations and charge transfer excitation for a two-atomic system with $i = (\vec{f}, g_{\alpha})$. To solve the obtained system of equations, one should introduce the $\vec{q}$ — representation for the Green function. As a result, well-known equations for the supperconducting gap can be obtained, where the effective electron-electron coupling is described by the phonon Green function in (18) (see [8]). As have been pointed out in [3], highly-anharmonic bond-bending-type vibrations for oxygen ions can produce strong coupling and high T_c, $T_c \sim 100$ K, for reasonable values of parameters in the model of oxide superconductor. Since other types of oxygen-ion harmonic vibrations have a high frequency, $\hbar\omega \sim 50 \div 70$ meV, they give a small contribution to the coupling constant, which results in a low value of T_c, $T_c \lesssim 40$ K [12].

5. KINEMATICAL INTERACTION

In the limit of strong Coulomb correlations, $U \gg t$, there is a possibility for attraction for holes in the lower part ($2/3 < n < 1$) or for electrons in the upper part ($1 < n < 4/3$) of the Hubbard bands, that can bring about the superconductivity at high T_c [10]. We consider here this mechanism and obtain equations for the gap and T_c from our system of equations (10), (17). By calculating the anomalous-type correlation functions in (17) from the Green functions in (16), one gets an equation [11]:

$$\Delta = -\frac{1}{N}\sum_{q} \frac{t(q) U \Delta}{2\epsilon + U} \left\{ \frac{E_1^2(\vec{q}) - \epsilon^2 - (2\epsilon + U)\, U(1 - n/2)}{E_1(\vec{q})\left[E_2^2(\vec{q}) - E_1^2(\vec{q})\right]} \mathrm{th}\frac{E_1(\vec{q})}{2T} + \right.$$

$$\left. + \frac{E_2^2(\vec{q}) - \epsilon^2 - (2\epsilon + U)\, U(1 - n/2)}{E_2(\vec{q})\left[E_1^2(\vec{q}) - E_2^2(\vec{q})\right]} \mathrm{th}\frac{E_2(\vec{q})}{2T} \right\}, \qquad (19)$$

where

$$E^2_{1,2}(\vec{q}) = \frac{1}{2}\left[\epsilon_1^2(\vec{q}) + \epsilon_2^2(\vec{q})\right] \pm \frac{1}{2}\left\{\left[\epsilon_1^2(\vec{q}) - \epsilon_2^2(\vec{q})\right]^2 - 4U^2\Delta^2(\vec{q})\right\}^{1/2},$$

$$\epsilon_{1,2}(q) = \epsilon + \frac{1}{2}\left[U + t(\vec{q})\right] \pm \frac{1}{2}\left\{(U + t(\vec{q}))^2 - (1 - \frac{n}{2})\, U t(\vec{q})\right\}^{1/2}. \qquad (20)$$

Here $\epsilon = -\mu$, where chemical potential μ can be found from the equation

$$n = \frac{1}{2}\sum_{\vec{q}\sigma} \langle n_{\vec{q}\sigma} \rangle . \qquad (21)$$

Equation (18) is greatly simplified in the limit $U \to \infty$ when $F = 2\Delta/(2\epsilon - U) \to 0$. For the lower Hubbard band, $n < 1$, one gets

$$\Delta = \frac{1}{N}\sum_{\vec{q}} \frac{\Delta(1 - n/2)\, t(\vec{q})}{E_2(\vec{q})} \mathrm{th}\frac{E_2(\vec{q})}{2T} . \qquad (22)$$

By solving the system of equations (21), (22) for a model density of electronic states which is constant in the band with a half-width W, one can obtain $\Delta(T)$ and T_c. In the logarithmic approximation we get [11]:

$$T_c = \frac{4\gamma}{\pi} W \sqrt{\frac{n(n-1)}{2}} \exp\left\{-\frac{2n}{3n-2}\right\} \qquad (23)$$

and $2\Delta(0)/T_c = 2\pi/\gamma \approx 3.5$ — the standard value for the weak coupling limit. Analogous results can be obtained for the upper band when $1 < n < 4/3$. They reveal the particle-hole symmetry of the problem with respect to the substitution:

$$n \to 2 - n, \quad t(\vec{q}) \to -t(\vec{q}), \quad \epsilon_{1,2}(\vec{q}) \to -\epsilon_{2,1}(\vec{q}) .$$

The results obtained here for the Hubbard model on the basis of equations for the Green functions (16), (17) are in qualitative agreement with the theory [10] developed on the basis of diagram technique. But we have only one $\vec{q}$-dependent gap function of the extended s-type $\Delta(\vec{q})$ (17), instead of two functions, Δ_1, Δ_2 that have been obtained in [10]. The n-dependence in the exponent in the formula for T_c (23) does not coincide with

that in [10] though we have the same value for the critical concentration of holes, $x_c = 1 - n_c = 1/3$ for suppressing T_c.

As shown originally in [10] and here proved by the equation of motion method for the Green functions, in the limit of strong Coulomb correlations, $U \gg t$, an additional attraction due to the kinematic interaction develops for holes ($2/3 < n < 1$) or particles ($1 < n < 2/3$), which results in high T_c (23). The Coulomb interaction V_{ij} in (5), as well as the electron-phonon contribution (18) and higher-order terms in U and V_{ij} (13) can be easily incorporated in the present approach. The influence of these contributions on T_c will be considered elsewhere.

In summary, a model of oxide metals developed in the present paper in the framework of the polar model [4] permits one, in principle, to calculate microscopically the model parameters. The Green function method [7], applied to the model, gives us a sufficiently simple method for deriving equations for the superconducting gap and T_c both in the band and atomic limits. On its basis different types of pairing mechanism can be considered and compared. The developed theory can be applied to the new superconductors of La_2CuO_4 and $YBa_2Cu_3O_7$ types. With their real crystal structure taken into account, one may in detail describe the observed properties of these high-T_c superconductors.

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К теории сверхпроводимости в модели оксидных металлов

Рассмотрена система сильносвязанных 3d- и 2p-электронов на основе полярной модели металла. С помощью метода функций Грина получены уравнения сверхпроводимости. Отмечено, что высокие T_c в оксидных металлах могут возникать за счет сильно ангармонических колебаний ионов кислорода, а также за счет кинематического притяжения электронов в случае сильных одноузельных кулоновских корреляций.

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On the Theory of Superconductivity in a Model of Oxide Metals

A tight-binding system of $3d^9$ and $2p^6$ electrons is considered in the framework of a polar model for metals. By applying the Green function method an equation for a superconducting gap is derived. It is pointed out that high-T_c in metal oxides can be caused by highly anharmonic oxygen vibrations and by kinematic attraction of electrons due to the strong single-site Coulomb correlations.

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

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