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Anisotropic Eliashberg Equations for Strongly Correlated Superconductors

Anizotropowe równania Eliashberga silnie skorelowanych nadprzewodników

1. INTRODUCTION

Shortly after the discovery of high T_c superconducting (HTS) oxides [1] with transition temperatures T_c around 100 K *much* exceeding the most optimistic estimation of T_c resulting from electron-phonon interaction [2] the hot discussion started about the applicability of BCS theory [3] and electron-phonon (EP) mechanism [4]. At the beginning of HTS era the electron-phonon mechanism has been completely dismissed mainly on the theoretical grounds. The subsequent experimental discoveries have shown that electron-phonon interaction, though perhaps not responsible alone for the superconductivity in these materials, does play an important role and should not be abandoned completely.

The issue of competing retarted electron-phonon and usually assumed nonretarded Coulomb interactions is valid also for materials with low and even more with elevated transition temperatures. The serious studies of the interplay between them started early on with work of Eliashberg [5], Anderson and Morel [6] and others [7].

The parent compounds of superconducting oxides are antiferromagnetic insulators with Neél ordering temperature T_N as high as 250 K in $LaCuO_4$.

By doping with Sr or Ba T_N decreases to zero. The neutron scattering studies show the persistence of sizeable antiferromagnetic correlations deep in the metallic state [8]. This points out that short range Coulomb interactions are important in the description of (at least) normal state properties of HTS, making the materials strongly correlated systems.

It is the purpose of this paper to derive Eliashberg type [10, 12, 13] equations valid for the strongly correlated superconductor with electron--phonon interaction. To this end we assume the validity of Migdal [11] theorem which means that we assume relatively weak electron-phonon interaction. The strong correlations described by the Hubbard model will be treated via slave boson method. The derived equations are strongly anisotropic and lead to the possibility of various types of symmetries of order parameter. The relative stability of various symmetries does depend on the carrier concentration and other parameters. Recently there appeared a number of studies [14–25] related to the presented here. Their conclusion can be generally summarised as showing the importance of electron-phonon interaction in proper description of various aspects of correlated superconductors.

Starting with the single band Hubbard Hamiltonian

$$H_t = \sum_{ij\sigma} t_{ij}^{\mathrm{def}} C_{i\sigma}^{+} C_{i\sigma} - \mu \Sigma_{i\sigma} C_{i\sigma}^{+} C_{i\sigma} + U \Sigma_i n_{i\uparrow} n_{i\downarrow} = \hat{H}_0 + \hat{U} \qquad (1)$$

we can introduce the interaction with lattice vibrations by observing that at nonzero temperature the actual positions $\{\vec{R}_i\}$ of ions differ from the equilibrium ones $\{\vec{R}_i^0\}$. Accordingly the hopping parameters $t_{ij}^{\mathrm{def}} \equiv t^{\mathrm{def}}(\vec{R}_i - \vec{R}_j) = t(\vec{R}_i^0 - \vec{R}_j^0 - \vec{u}_i + \vec{u}_j)$ do depend on the displacements $\vec{u}_i$ from equilibrium positions. Expanding t_{ij}^{def} up to linear order in $(\vec{u}_i - \vec{u}_j)$ and denoting $t_{ij} = t(\vec{R}_i^0 - \vec{R}_j^0)$ we get

$$\begin{aligned} H_0 &= \sum_{ij\sigma} t_{ij} C_{i\sigma}^{+} C_{j\sigma} - \mu \sum_{i\sigma} C_{i\sigma}^{+} C_{i\sigma} + \sum_{ijs\alpha\sigma} T_{ijs}^{\alpha} u_s^{\alpha} C_{i\sigma}^{+} C_{j\sigma} \\ &= H_e + H_{e-\mathrm{latt}} \,. \end{aligned} \qquad (2)$$

Here $T_{ijs}^{\alpha} = \frac{\partial t_{ij}}{\partial R_{ij}^{0\alpha}} \delta_{is} - \frac{\partial t_{ij}}{\partial R_{ij}^{0\alpha}} \delta_{js}$.

We supplement the above Hamiltonian with another piece describing the lattice

$$H_{\text{latt}} = \sum_i \frac{p_i^2}{2M_i} + \frac{1}{2}\sum_{ij}\sum_{\alpha\beta} \mathcal{D}_{ij}^{\alpha\beta} u_i^\alpha u_j^\beta .$$

Here P_i is the lattice momentum, M denotes ion mass, $\mathcal{D}_{ij}^{\alpha\beta}$–dynamical matrix. The quantised version of lattice Hamiltonian may be written in the form

$$H_{\text{latt}} = \sum_{\vec{q}\nu} \hbar\omega_{\vec{q}\nu} \left(a_{\vec{q}\nu}^+ a_{\vec{q}\nu} + \frac{1}{2} \right) . \tag{3}$$

Writing the displacement operator u_i^α in terms of phonon–creation and annihilation operators $a_{q\nu}^+$, $a_{q\nu}$ we get

$$H_{\text{el-ph}} = \frac{1}{\sqrt{N}} \sum_{\vec{q}\nu}\sum_{ij\sigma} T'_{ij}(\vec{q}\nu) g_{\vec{q}\nu}^0 (a_{\vec{q}\nu} + a_{-\vec{q}\nu}^+) C_{i\sigma}^+ C_{j\sigma} . \tag{4}$$

Here

$$g_{\vec{q}\nu}^0 = \left(\frac{\hbar}{2M\omega_{\vec{q}\nu}} \right)^{1/2} ;$$

$$T'_{ij}(\vec{q},\lambda) = \sum_\alpha e_\nu^\alpha(\vec{q}) \frac{\partial t_{ij}}{\partial R_{ij}^\alpha} \left(e^{i\vec{q}\vec{R}_i} - e^{i\vec{q}\vec{R}_j} \right) \tag{5}$$

$e_\nu^\alpha(\vec{q})$ is the α–th component of the phonon–polarisation vector, ν denotes the phonon branch.

Thus the complete Hamiltonian describing electrons, phonons and electron-phonon interaction in presence of correlations consists of terms (2), (3) and (4) supplemented with the Hubbard term $\hat{U}$. Now the point is that for large U values the states corresponding to doubly occupied sites are pushed to high energies. In the limit $U = \infty$ they are unimportant at all and we expect the sites to be singly occupied or empty. Thus in general the condition quantifying this limit is $n_i = \sum_\sigma C_{i\sigma}^+ C_{i\sigma} \leqslant 1$.

The idea of slave bosons is to represent the physical electron in the $U = \infty$ limit by the fictitious fermion, described by the operators $\tilde{C}_{i\sigma}^+(\tilde{C}_{i\sigma})$ and an auxiliary boson $b_i^+(b_i)$. The condition of no double occupancy of a site can now be expressed in formally exact form

$$Q_i = \sum_\sigma \tilde{C}_{i\sigma}^+ \tilde{C}_{i\sigma} + b_i^+ b_i = 1 . \tag{6}$$

To keep track of the constraint one usually introduces a set of Langrange multipliers λ_i and adds to the Hamiltonian a term $\sum_i \lambda_i (Q_i - 1)$, neglecting at the same time the term proportional to U.

The model can thus be written as

$$\begin{aligned}\tilde{H} &= \sum_{ij\sigma} t_{ij}\tilde{C}^{+}_{i\sigma}\tilde{C}_{j\sigma}b_i b^{+}_j - \mu\sum_{i\sigma} C^{+}_{i\sigma}C_{i\sigma} + \sum_i \lambda_i\left(\sum_\sigma \tilde{C}^{+}_{i\sigma}\tilde{C}_{i\sigma} + b^{+}_i b_i - 1\right) + \\ &+ \sum_{ij\sigma}\frac{1}{\sqrt{N}}\sum_{\vec{q}\nu} T'_{ij}(\vec{q},\nu)g^0_\nu(\vec{q})(a_{\vec{q}\nu} + a^{+}_{-\vec{q}\nu})\tilde{C}^{+}_{i\sigma}\tilde{C}_{j\sigma}\, b_i b^{+}_j + \\ &+ \sum_{\vec{q}\nu}\hbar\omega_{\vec{q}\nu}(n_{\vec{q}\nu} + 1/2)\,.\end{aligned} \tag{7}$$

In the following we shall use mean field type of approximation to treat the strong correlations and their influence on the electron and phonon spectra.

2. MEAN FIELD TREATMENT

In this approach one assumes $\lambda_i = \lambda$ and treats boson operators as c–numbers with

$$\langle b_i\rangle = \langle b^{+}_j\rangle = r^{1/2} \tag{8}$$

Minimalisation of the energy $E = \langle\tilde{H}\rangle$ with respect to r and λ leads to the equations

$$r = 1 - \frac{1}{N}\sum_{i\sigma}\langle\tilde{C}^{+}_{i\sigma}\tilde{C}_{j\sigma}\rangle\,; \tag{9a}$$

$$\lambda = -\sum_{ij\sigma} t_{ij}\langle\tilde{C}^{+}_{i\sigma}\tilde{C}_{j\sigma}\rangle - \sum_{ij\sigma}\frac{1}{N}\sum_{q\nu} T'_{ij}(\vec{q}\nu)\, g^0_\nu(\vec{q})\langle(a_{\vec{q}\nu} + a^{+}_{-\vec{q}\nu})\tilde{C}^{+}_{i\sigma}\tilde{C}_{j\sigma}\rangle\,. \tag{9b}$$

Expectation values in (9) can be easily obtained from corresponding propagators by means of their spectral representation. To do this we use hamiltonian (7) with boson operators replaced as in (8). Explicitly we have in Fourier space

$$\begin{aligned}H &= \sum_{\vec{k}\sigma}(r\epsilon_{\vec{k}} - \mu + \lambda)\tilde{C}^{+}_{\vec{k}\sigma}\tilde{C}_{\vec{k}\sigma} + N\lambda(r-1) + \\ &+ \frac{1}{\sqrt{N}}\sum_{\vec{k}\vec{q}\sigma\nu} M_{\vec{k}\vec{q}\nu}(a_{\vec{q}\nu} + a^{+}_{-\vec{q}\nu})\tilde{C}^{+}_{\vec{k}+\vec{q}\sigma}\tilde{C}_{\vec{k}\sigma} \\ &+ \sum_{\vec{q}\nu}\hbar\omega_{\vec{q}\nu}(n_{\vec{q}\nu} + 1/2)\end{aligned} \tag{10}$$

where

$$M_{\vec{k}\vec{q}\nu} = r \sum_{\alpha} g^0_{\nu}(\vec{q}) e^{\alpha}_{\nu}(\vec{q})\, i\frac{Q}{a}\left(\frac{\partial \varepsilon_{\vec{k}}}{\partial k_{\alpha}} - \frac{\partial \varepsilon_{\vec{k}+\vec{q}}}{\partial k_{\alpha}}\right). \tag{11}$$

Q is the parameter describing the relative change of t_{ij} with small changes of distance between $\vec{R}^0_i$ and $\vec{R}^0_j$ and a is lattice constant. Note that $M^*_{\vec{k}\vec{q}\vec{\nu}} = -M_{\vec{k}\vec{q}\nu}$. In the following we shall assume that electrons couple to longitudinal phonons only and neglect the subscript ν. There are two changes to the spectrum of electrons in the mean field approximation for slave bosons. First is the band narrowing described by r^2 and its shift described by λ. The spectrum of noninteracting fermions in the mean field is given by $(r^2\epsilon_{\vec{k}} - \mu + \lambda)$ instead of $(\epsilon_{\vec{k}} - \mu)$ of original electrons (i.e. for $U = 0$). For the half filled band $n = 1$ the system is localised ($r = 0$).

To properly describe the superconducting state in the system at hand one has to work in site representation. The important point is that in considered $U = \infty$ limit the double occupation of a given site is strictly forbidden. This means *inter alia* that correlation functions $\langle c_{i\uparrow} c_{j\downarrow}\rangle$ describing superconducting pairs vanish exactly for $i = j$, i.e. the on–site pairing is forbidden. On the other hand the correlations of the type $\langle c^+_{i\sigma} c_{i\sigma}\rangle$ measure the average number of carriers at site i, and are allowed to enter into formula. This important fact has first been noted by Zieliński and coworkers [14, 18] and leads, as we shall see, to severe changes in the form of Eliashberg equations.

To derive Eliashberg equations we use the matrix formulation of the theory [12, 13]. One defines frequency dependent matrix Green's function in site representation

$$\hat{G}_{ij}(\omega) = \begin{pmatrix} \ll C_{i\uparrow}|C^+_{j\uparrow} \gg_{\omega}, & \ll C_{i\uparrow}|C_{j\downarrow} \gg_{\omega} \\ \ll C^+_{i\downarrow}|C^+_{j\uparrow} \gg_{\omega}, & \ll C^+_{i\downarrow}|C_{j\downarrow} \gg_{\omega} \end{pmatrix} \tag{12}$$

and writes the equation of motion for it. Following standard procedure [12] we obtain

$$\sum_{l}\{[\omega\hat{\tau}_0 + (\mu - \lambda)\hat{\tau}_3]\,\delta_{il} - r^2 t_{il}\hat{\tau}_3 - \widehat{M}_{il}(\omega)\}\hat{G}_{ij}(\omega) = \delta_{ij}\hat{\tau}_0\,. \tag{13}$$

Here $\hat{\tau}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\hat{\tau}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\hat{\tau}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are Pauli matrices and $\widehat{M}_{il}$ denotes the matrix self–energy, which in the present case is given by (from now on we omit the sign $\sim$ on fermion operators)

$$\widehat{M}_{ij}(\omega) = \sum_{i'j'} \sum_{\alpha\alpha' ss'} r^4 T^{\alpha}_{ij's} T^{\alpha'}_{i'js'} \tag{14}$$

$$\begin{pmatrix} \ll u_s^{\alpha} C_{j'\uparrow} | u_{s'}^{\alpha'} C_{i'\uparrow}^{+} \gg_{\omega}, & \ll u_s^{\alpha} C_{j'\uparrow} | u_{s'}^{\alpha'} C_{i'\downarrow}^{+} \gg_{\omega} \\ \ll u_s^{\alpha} C_{j'\downarrow}^{+} | u_{s'}^{\alpha'} C_{i'\uparrow}^{+} \gg_{\omega}, & \ll u_s^{\alpha} C_{j'\downarrow}^{+} | u_{s'}^{\alpha'} C_{i'\downarrow} \gg_{\omega} \end{pmatrix}.$$

Beyond mean-field approximation for slave bosons there are also other contributions from two and three particle scattering events: fermion–phonon, fermion–boson and mixed fermion–phonon–slave boson.

Making use of spectral representation and approximating the resulting correlation functions in the formula for $\widehat{M}_{ij}(\omega)$ *via* correlators which can be calculated from electron and phonon Green's functions we get a self-consistent equations for self–energy. The next important step on the way of derivation of Eliashberg equations is Fourier transformation. The important issue is the following. The normal part of self–energy is proportional to the correlator $\langle C_{j'\uparrow} C_{i'\downarrow}^{+} \rangle$ and all possible values of i', j' are allowed. Contrary to that the anomalous part depends on $< C_{j'\uparrow} C_{i'\downarrow} >$ and only values $i' \neq j'$ are allowed. The point is that for $i' = j'$ the correlator describes the amplitude for two electrons with opposite spins to be placed on the same site (on–site pair). In the $U = \infty$ limit, we are considering here, this is forbidden and only values of $i' \neq j'$ are allowed. This together with the experimental information on the short correlation length justifies the assumption that i', j' are nearest neighbours sites. From the theoretical point of view we have a possibility to study the properties of the system in dependence on the spatial extent of the pairs.

The Fourier transform of $\hat{M}_{ij}$ is denoted by $\hat{\Sigma}_k(\omega)$. To proceed, we expand matrix self–energy $\hat{\Sigma}_k(\omega)$ as

$$\hat{\Sigma}_k(\omega) = \omega[1 - Z_k(\omega)]\hat{\tau}_0 + \phi_k(\omega)\hat{\tau}_1 + \chi_k(\omega)\hat{\tau}_3 \tag{15}$$

and write down the equations for various parts of it. We get the real frequency axis Eliashberg equations in the form

$$\begin{aligned} \omega[1 - Z_{\vec{k}}(\omega)] &= \frac{1}{2}\int d\omega_1 \int d\omega_2 \frac{th\frac{\beta\omega_1}{2} + cth\frac{\beta\omega_2}{2}}{\omega - \omega_1 - \omega_2} \frac{1}{N}\sum_{\vec{k}'} K_{\vec{k}\vec{k}'}(\omega_2) \cdot \\ &\quad (-\frac{1}{\pi}) \operatorname{Im} \frac{\omega_1 Z_{\vec{k}'}(\omega_1)}{D_{\vec{k}'}(\omega_1)} \\ \phi_{\vec{k}}(\omega) &= \frac{1}{2}\int d\omega_1 \int d\omega_2 \frac{th\frac{\beta\omega_1}{2} + cth\frac{\beta\omega_2}{2}}{\omega - \omega_1 - \omega_2} \frac{1}{N}\sum_{\vec{k}'} \bar{K}_{\vec{k}\vec{k}'}(\omega_2) \cdot \\ &\quad (-\frac{1}{\pi}) \operatorname{Im} \frac{-\phi_{\vec{k}'}(\omega_1)}{D_{\vec{k}'}(\omega_1)} \end{aligned} \tag{16}$$

$$\chi_{\vec{k}}(\omega) = \frac{1}{2}\int d\omega_1 \int d\omega_2 \frac{th\frac{\beta\omega_1}{2} + cth\frac{\beta\omega_2}{2}}{\omega - \omega_1 - \omega_2} \frac{1}{N}\sum_{\vec{k}'} K_{\vec{k}\vec{k}'}(\omega_2) \cdot$$
$$(-\frac{1}{\pi})\,\mathrm{Im}\frac{r^2\epsilon_{\vec{k}'} - \mu + \lambda + \chi_{\vec{k}'}(\omega_1)}{D_{\vec{k}'}(\omega_1)}$$

where we denoted $D_{\vec{k}'}(\omega_1) = [\omega_1 Z_{\vec{k}'}(\omega_1)]^2 - [\phi_{\vec{k}'}(\omega_1)]^2 - [r^2\epsilon_{\vec{k}'} - \mu + \lambda + \chi_{\vec{k}'}(\omega_1)]^2$ and

$$K_{\vec{k}\vec{k}'}(\omega_2) = \sum_{\nu} |M^{\nu}_{\vec{k},\vec{k}-\vec{k}'}|^2(-\frac{1}{\pi})\mathrm{Im} \ll \phi_{\vec{k}-\vec{k}',\nu}|\phi_{-\vec{k}+\vec{k}',\nu} \gg_{\omega_2+io}; \quad (17)$$

$$\tilde{K}_{\vec{k},\vec{k}'}(\omega_2) = \frac{1}{N}\sum_{\vec{q}\nu} |M^{\nu}_{\vec{k},\vec{q}}|^2(-\frac{1}{\pi}) \quad (18)$$
$$\mathrm{Im} \ll \phi_{\vec{q},\nu}|\phi_{-\vec{q}\nu} \gg_{\omega_2+io} \gamma(\vec{k} - \vec{q} - \vec{k}').$$

Equations (16) form a set of generalised Eliashberg equations. Note the modifications of these equations in comparison to standard ones [13]. Due to strong correlations not only the electron band energies have been modified (band narrowing r^2 and band shift λ) but also two different kernels $K_{\vec{k}\vec{k}'}(\omega)$ and $\tilde{K}_{\vec{k}\vec{k}'}(\omega)$ appear. This very important fact (first discovered by Zieliński and cowerkers [18]) makes Eliashberg equations anisotropic and has a strong influence on the structure of the theory. In the correlated system the mass renormalisation due to electron-phonon interaction is different from the pairing parameter. The first is calculated from the kernel $K_{\vec{k}\vec{k}'}(\omega)$, while the second from $\tilde{K}_{\vec{k}\vec{k}'}(\omega)$. As a result the anisotropy of the superconducting order parameter does not follow the anisotropy of the interaction but is in fact much more complicated as can be inferred from comparison of (17) and (18). Both parameters will enter the McMillan [13] type of the expression for the transition temperature.

The equation for $\chi_{\vec{k}}(\omega)$ is usually neglected. In the theory valid for strongly corelated superconductors with short coherence length it has to be taken into account as it leads to nontrivial modification of the relation between chemical potential μ and carrier concentration n. The factor $\gamma(\vec{k})$ entering the formula (18) is connected with the structure of the pairing field. It has the same $\vec{k}$ dependence as the band energies $\varepsilon(\vec{k})$ for pair electrons located at nearest neighbour sites. One of the interesting problems will be a systematic study of the dependence of superconducting properties of the system on spatial extent of pairs.

The study of these and other consequences of generalised Eliashberg equations will be presented elsewhere [25].

In conclusion we have presented the derivation of the Eliashberg equations for the system with strong electron-electron and electron-phonon interactions. The results show the importance of the correlations which make the superconducting order parameter very anisotropic.

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STRESZCZENIE

W artykule przedstawiono wyprowadzenie uogólnionych równań Eliashberga opisujących własności silnie skorelowanych nadprzewodników. Do opisu korelacji zastosowano technikę bozonów pomocniczych w granicy nieskończenie silnego odpychania na węźle. Uzyskane równania są anizotropowe. Własności stanu normalnego określone są za pomocą standardowego jądra całkowego, natomiast jądro całkowe równania opisującego nadprzewodnikowy parametr porządku jest silnie zmodyfikowane. Prowadzi to do konieczności odróżniania parametrów sprzężenia elektron-fonon w stanie normalnym i nadprzewodzącym. Oba parametry wejdą do wzorów na temperaturę przejścia układu w stan nadprzewodnictwa.