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Part S2 - Superconductivity 1: HTS - Theory

COUPLED STATES AND MANY ZONE EFFECTS IN PROBLEM OF HTSC IN CRYSTALS

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The new theoretical approach is considered for description of the coupled states of electron-phonon system. Many zones effects are taking into account.

1. INTRODUCTION

As a rule the theoretical study of superconductivity (SC) is based on the physical idea about pairing of electrons with the opposite spins $(s+s'=0)$ and momenta $(k+k'=0)$. Using this postulate the possibility of appearence of the coupled states in the electron (electron-phonon) system has been investigated. Such coupled states are responsible for superconductivity in the above mentioned system.

Here we demonstrate that the coupled states in the electron system appear, taking into account only interactions between quasiparticles of electron-phonon (e-ph.) system without any additional demands. Our calculations have also shown that hypothesis of electron pairing postulated in BCS theory is only approximate, i.e. electron states which have nonzero momenta $(k+k'\neq 0)$ and spins $(s+s'\neq 0)$ are also responsible for SC. Our method of calculation is working for both traditional SC and HTSC crystals.

2. RESULTS

In this short communication we present the general idea of our approach. The density of current in the system of electrons can be written as follows

$$\langle j'(x)\rangle = \langle j(x)\rangle_0 - \frac{e^2}{mc}\langle n(x)\rangle_0 + (high\ order)\ , \quad (1)$$

$$\langle n(x)\rangle_0 = \langle \Psi^+(x)\Psi(x)\rangle_0 =$$

$$\lim_{x'\to x,t'\to t-0}\left\{\delta(x-x') - i\left\langle -iT\Psi(x,t)\Psi^+(x',t')\right\rangle\right\} =$$

$$= V_0^{-1}\sum_k 1 - i\sum_{k,\omega} G(k,\omega) \quad (2)$$

$\Psi(x) = \sum_{k,\sigma,\nu} a^{\nu}_{k,\sigma}\varphi^{\nu}_{k,\sigma}$; $\varphi^{\nu}_{k,\sigma} = \varphi^{\nu}_k \chi_\sigma(s)$, where φ^{ν}_k is the Bloch function of crystal and $\chi_\sigma(s)$ describes the spin of electron in energy zone; $\left\langle -iT\Psi(x,t)\Psi^+(x',t')\right\rangle$ is the Green function, and $G(k,\omega)$ is it's Fourier components. The spectral features of electron system in the actual region of energy with taking into account of interaction the electrons are described by Fourier component of this function and for the simplest case of one electron zone crossing the Fermi energy level can be given by the following expression

$$\Phi(k_1,k_2,\omega)=\frac{f(k_1,k_2,\omega)\sum_{\sigma,\sigma'}\varphi(\sigma,\sigma')}{1-V\sum_q\frac{1-n_{k_1+q}-n_{k_2-q}}{\omega-\varepsilon_{k_1+q}-\varepsilon_{k_2-q}}},\quad(3)$$

$$V=\tilde{V_q}=V_q-2\sum_s\frac{|X_{s,q}|^2}{\Omega_{s,q}}\approx const.$$

n_k is the filling number of electrons; V is the Fourier component of effective electron-electron (e-e) interaction. If the constant of e-e interaction renormalized by e-ph interaction (Xsq) becomes negative ($V<0$) the arising of coupled states in the electron system is possible.

It is seen from Eq.(3) that for $k_1=k_2=0$ or $k_2=-k_1$ the denominator is reduced to well known expression describing the SC gap of crystal, but for other arbitrary meanings of momenta k_1 and k_2 the situation becomes significantly different.

Besides the numerator of Eq.(3) give rise to new possibilities. Here $f(k_1,k_2,\omega)$ is the some function depending on the frequency (ω) and momenta $k_1$and k_2 of electrons; the function $\varphi(\sigma,\sigma')$ (which is written for one band crossing the Fermi level) is expressed by number of delta-functions $\delta_{\sigma,\sigma'}$, namely

$$\varphi(\sigma,\sigma')=\delta_{\sigma\sigma}\delta_{\sigma'\sigma'}-\delta_{\sigma\sigma'}\delta_{\sigma\sigma'}$$

where σ,σ' are spines of first (σ) and second (σ') electrons respectively. One may see that two cases are possible:

a) if spins of electrons are parallel to each other ($\sigma=\sigma'$) then $\varphi(\sigma,\sigma')=0$;

b) if spins of pair of electrons are antiparallel to each other ($\sigma\neq\sigma'$) the second term in the right hand part (which is proportional to $\delta_{\sigma,\sigma'}$) disappear and therefore $\varphi(\sigma,\sigma')\neq 0$. It means that only states with the oppositely directed spins, namely singlet states ($\sigma+\sigma'=0$) in this simplest case, can contribute into coupled states of electron system. For more complex structure of crystal zones, in particular for layer Bi-based type of crystal, for example, the function $\varphi(\sigma,\sigma')$ in (3) will be more complicated. Indeed for this case we have to change $\varphi(\sigma\sigma')\Rightarrow\varphi^{\mu\nu}(\sigma\sigma');\ \varepsilon_k\Rightarrow\varepsilon_k^{\mu},\ n_k\Rightarrow n_k^{\mu}$ where μ,ν are the numbers of crystal electron zones. Therefore many new possibilities arise (to be published). In particular the co-existence of singlet and triplet states of electron system occurs. Naturally the mentioned features in the density of electron states will be displayed in the high order terms of the currnt density (1) too.

3. CONCLUSION

The new approach to the investigation of SC (HTSC) problem without of BCS postulation of electron pairing is proposed. The more general rules for coupled states responsible for SC effect are derived.