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On the Excitonic Mechanism of Superconductivity

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We study the possibility of arising excitonic phase with doping in CuO-planes. The properties of the strongly interacting electron-exciton system are concerned. We also discuss the linear temperature dependence of the resistivity and the possibility of the nonphonon superconductivity of this system.

1. Introduction

The CuO-plane band structure of the copper-oxide compounds is believed to consist of three bands. Two of these bands are the narrow Hubbard subbands of copper atoms, being the lower and upper bands. The middle band has an oxygen origin and is a broad band. The effective mass of particles in this band is nearly of a few bare electron masses. For zero doping, the lower and middle bands are filled completely and the upper band is empty. Doping creates holes at the top of the middle (oxygen) band. With respect to the top of the oxygen band the lower copper subband lies much lower than the upper copper subband. For this reason, the lower copper subband can be ignored. Therefore we can regard the band structure consisting of only two bands, namely, the upper copper subband and the oxygen band. The gap between these two bands is about 2-3 ev. The binding energy of exciton (or the bound state of the electron and hole) is approximately the same. Thus the excitonic mechanism can be regarded as a possible candidate for the mechanism of high T_c superconductivity [1-4].

The two-band model of a semiconductor is used to study the transition from semiconductor into the excitonic insulator phase. This transition must occur provided the value of the semiconductor gap E_g is less than the excitonic binding energy E_c. The nature of this transition can be qualitatively understood by means of the following consideration. The creation of electron - hole pair requires the energy E_g but when an electron and a hole form an exciton, the energy E_c releases. This energy is greater than E_g. Therefore it is favorable energetically to create an exciton from the vacuum. That is why the ground state should have the excitonic phase. The properties of the excitonic phase were discussed in the number of the works [5-8].

We shall regard the semiconductor having the gap E_g more than E_c . The transition to the excitonic phase is impossible in those systems if doping is absent. The influence of doping is considered in this work. Let us suppose that the exciton is created from the vacuum by the external influence in the system with a small doping. This exciton will attract to a dopant electron. This attraction is sufficient to form a bounding state (the existence of ion H^- supports this assumption). For this case if the energy E_g being necessary to create the exciton is less than the evolving energy $E_c + J$ (where J is the binding energy of the electron - exciton bound state), the creation of excitons from the vacuum is possible. Thus it can be supposed that in the system with $E_g - E_c < J$ the Fermi - liquid of dopant electrons is strongly interacting with the excitonic phase have been created from the vacuum . The qualitative considerations given above are correct if the radius of the exciton - electron bound state is much more than the excitonic radius. This condition is fulfilled if the excitonic binding energy E_c is essentially more than the exciton-electron binding energy J. (Note that the ionization energy J of ion H^-, being much smaller than the atom H binding energy, is about 0.75 ev [9]). Thus it can be supposed that in the system with $E_g - E_c < J$, at any rate for rather small density of doping electrons, excitons are created from the vacuum and the Fermi - liquid of these electrons interacts strongly with the excitonic phase. The conditions for the possibility of the existence of the excitonic phase are provided by the dopant electrons and the properties of this strongly interacting system are investigated in this work. The possibility of the excitonic creation and some results of this effect were regarded in [4].

2. The effective action

For the simplicity, the electron dispersion spectra of these two bands can be treated in the following form

$$\epsilon_1 = E_g/2 - \nabla^2/(2m_1)$$

$$\epsilon_2 = -E_g/2 + \nabla^2/(2m_2) \qquad (1)$$

We suppose that doping creates charge carriers in the upper band having a light mass . Note that in this picture we invert the hole and electron bands. The functional integral representation of a statistical sum of the system can be written in the form:

$$Z = \int \exp(iS) D\overline{\Psi} D\Psi \qquad \mathbf{(2)}$$

$$S = \int dtd\mathbf{r} \sum_\alpha \overline{\Psi}^{(\alpha)}_{\mathbf{r},t}[i\partial_t - \epsilon_\alpha(-i\nabla) + \mu]\Psi^{(\alpha)}_{\mathbf{r},t} -$$

$$-\frac{1}{2}\int dtd\mathbf{r}d\mathbf{r}' \sum_{\alpha,\beta} \mid \Psi^{(\alpha)}_{\mathbf{r},t} \mid^2 V_{\mathbf{r}-\mathbf{r}'} \mid \Psi^{(\beta)}_{\mathbf{r}',t} \mid^2 \qquad (3)$$

$V_\mathbf{r} = e^2/(r\epsilon_0)$ is the potential of the Coulomb interaction, ϵ_0 is the static dielectric susceptibility, $\Psi_\alpha(\mathbf{x}, t)$ is Grassman fields of electrons, μ is the electrons chemical potential, α is band index $\alpha = 1, 2$. The spin indexes are omitted, the account of them is not difficult.

Since we want to get the effective action for dopant electron, we should integrate over Ψ_α - fields with the scale variation much smaller then the average distance between dopant electron. After this integration we obtain the effective action rewriting in terms of new slow electrons field χ and new excitonic field Φ which descries the collective properties of electrons and holes [10].

$$S_{eff} = S_{el} + S_{ex} + S_{int} \qquad \mathbf{(4)}$$

$$S_{el} = \int dtd\mathbf{r}\overline{\chi}_{\mathbf{r},t}[i\partial_t + \nabla^2/(2m_1) + \mu]\chi_{\mathbf{r},t} -$$

$$-\frac{1}{2}\int dtd\mathbf{r}d\mathbf{r}' \mid \chi_{\mathbf{r},t} \mid^2 V_{\mathbf{r}-\mathbf{r}'} \mid \chi_{\mathbf{r}',t} \mid^2$$

$$S_{ex} = \int dtd\mathbf{r}\overline{\Phi}_{\mathbf{r},t}[i\partial_t - (E_g - E_c) +$$

$$+\nabla^2/(2M) - f/2 \mid \Phi_{\mathbf{r},t} \mid^2]\Phi_{\mathbf{r},t}$$

$$S_{int} = -\gamma \int dtd\mathbf{r} \mid \chi_{\mathbf{r},t} \mid^2 \mid \Phi_{\mathbf{r},t} \mid^2 \qquad \mathbf{(5)}$$

where $M = m_1 + m_2$ is the excitonic mass, $m^* = m_1 m_2/(m_1 + m_2)$, f and γ are the electron - electron and electron - exciton interacting constants respectively. We shell assume that the electron - electron interaction is repulsion due to Pauli repulsion between electrons [7,8] and the electron - exciton interaction is attraction due to dipole-charge interaction [10].

3. The conditions necessary for arising the excitonic phase

Now we shall investigate the effective action of exciton-electron system (5) to determine the conditions necessary for arising the excitonic phase in the ground state of the system. Note that the coupling constants of the attractive electron-exciton and the repulsive exciton-exciton interactions should be renormalized. Since the electron - exciton coupling constant is attractive, it can result in the creation of the bounding state of electron and exciton if there is only two of these particles. Moreover, the exciton and the bound state of it with the electron can be created if the condition $E_g < E_c + J$ is valid. In this case the scattering amplitude of exciton and electron may have a pole if we do not take into account the many particle effects. However, if the average distance between the dopant electrons is less than the radius of the bound state the bound states are destroyed but the strong correlation effects may result in arising the excitonic phase. It is that interesting for us in this work. To take into account the strong correlation effects, we renormalize the attractive coupling constant of the electron - exciton interaction. This renormalization can be performed by the summation of the ladder diagrams. The consequence of these diagrams is selected in the case of the small excitonic densities and under the condition $\ln(E_c/\epsilon_F) \ll 1$, where ϵ_F is the Fermi energy of the dopant electrons.

It should be noted that one link of the ladder diagrams has the discontinuity value via the integration over the large moments and this integration should be limited by the moments $k \sim a_B^{-1}$,where a_B is Bohr radius. The value of this link in 2D can be easily calculated and in the logarithmic approximation is $1/(2\pi)m_{red}\gamma^2 \ln(E_c/\Omega)$, where $\Omega = max(E_g - E_c, \epsilon_F, \mu_{ex})$, $m_{red} = m_1 M/(m_1+M)$ and μ_{ex} is the chemical potential of the excitons. At the beginning of the excitonic creation, when the excitonic density is very small, the frequency $\Omega = max(E_g - E_c, \epsilon_F)$. The summation of the ladder diagrams gives

$$\Gamma = -\frac{|\gamma|}{1-(2\pi)^{-1}m_{red}|\gamma|\ln(E_c/\Omega)} \quad (6)$$

If there is only two particles, namely, exciton and electron the value Ω is the total energy of the exciton and electron. In this 2D case the expression (6) can have the pole for any value of γ. The value of Ω for which the denominator of (6) equals to zero is the value of the binding energy of electron and exciton and has the following form

$$J = E_c \exp(-\frac{2\pi}{m_{red}|\gamma|}) \quad (7)$$

We are interested in the situation when the electron liquid can be regarded as the system with the well defined Fermi surface. In this case the value of Ω should be more than the binding energy J. Using (7) it can be convenient to represent the renormalized exciton - electron vertex (6) in the form

$$\Gamma = -\frac{2\pi}{m_{red}\ln[\Omega/J]} \quad (8)$$

Note that in 2D case the renormalization of the exciton - exciton coupling constant is essential too. It is well known fact of the theory of 2D Bose-gas [11].

$$F \approx \frac{4\pi}{M\ln[E_c/\mu_{ex}]} \quad (9)$$

here μ_{ex} is the chemical potential of excitons, $\mu_{ex} \ll E_c$ if $n_0 a_B^2 \ll 1$.

To obtain the conditions necessary of arising the excitonic phase creation, the classical equation for the saddle - point trajectory of the excitonic field Φ should be written. It has the form

$$(i\partial_t - (E_g - E_c) + \nabla^2/(2M) - W)\Phi_{\mathbf{r},t} -$$
$$-F|\Phi_{\mathbf{r},t}|^2\Phi_{\mathbf{r},t} = 0 \quad (10)$$

The possibility of time independent and spatially homogeneous solution of the equation (10) is valid if the following condition is satisfied

$$|W| > E_g - E_c \quad (11)$$

Calculating W in the logarithmic approximation, we can suppose that Γ defined by (6) does not depend on the external moment and energy, since they are less than p_F and ϵ_F respectively and the value of the denominator in the expression (6) is not very sensitive to it. More precisely calculations can be done too. In this approximation W can be expressed in the form

$$W = \Gamma n_{el} \quad (12)$$

where Γ is defined by (8), n_{el} is the density of the dopant electrons. It should be noted that in the case of the developed excitonic phase when $\epsilon_F \ll \mu_{ex}$ the value Ω in (8) is proportional to μ_{ex} and does not depend on the external moment and energy. The density of the excitonic phase can be obtained from the following equation

$$n_0 F = -(E_g - E_c) - W \quad (13)$$

The investigation of (11) and (13) shows that the excitonic phase exists in the ground state of the system only when $E_g - E_c < J$ and when $\epsilon_F < \epsilon_F^{max} \sim J$; and the largest value of the excitonic density $n_0^{max} \sim J m_{red}\ln(E_c/J)$ and $\mu_{ex} = n_0 F$.

4. Properties of the electron liquid

The effective action (5) describes the electron liquid of the dopant electrons interacting with excitons created from the vacuum. To investigate the properties of the electron liquid let us suppose that the density of the excitonic phase is small. In this case the effective electron-exciton coupling constant is small and the calculations can be performed in the framework of the simple variant of the perturbation theory. The self - energy part of the electron Green function can be shown to be proportional to the temperature T. It can be represented by integral of electron and excitonic Green functions, were excitonic Green function is a sum of four Bose - gas functions [12]. This sum can be represented in the form

$$S(p) = \frac{2E_0(\mathbf{p})}{\omega^2 - E(\mathbf{p})^2 + i\delta} \quad (14)$$

where

$$E^2(\mathbf{p}) = E_0^2(\mathbf{p}) + 2E_0(\mathbf{p})\mu_{ex},$$

$$E_0(\mathbf{p}) = \mathbf{p}^2/(2M) \quad (15)$$

The sound character of the excitonic spectra is valid for the small moments $k \ll \sqrt{2M\mu_{ex}}$ and the sound velocity is $c = \sqrt{\mu_{ex}/M}$. For the large moments $k \gg \sqrt{2M\mu_{ex}}$ this spectra is $k^2/(2M)$. The expression of the electron self-energy part Σ_{el} for the nonzero temperature is

$$\Sigma_{el}(p) = -T\sum_{\omega}\int \frac{d\mathbf{p}}{(2\pi)^2} S(p-p')G_{el}(p') \quad (16)$$

Calculating integral (16) we have

$$Im\Sigma_{el} = \frac{T\Gamma^2 n_0 m_1 M}{\pi p_F\sqrt{2M\mu_{ex}}} \quad (17)$$

Thus the imaginary part of Σ_{el} is proportional to T and thus the resistivity in the normal state is proportional to too.

The interaction between two electrons can occur as the exchange by the exciton which is out of the Bose-condensate. This interaction is attractive. For this reason, the transition of the electron liquid into the superconductive state can be possible. For calculating the temperature of the superconducting transition the excitonic spectra can be regarded in the sound form. Using the ordinary BCS approximation, we can obtain the following expression for T_c.

$$T_c = \mu_{ex}\exp\left(-\frac{1}{m_1\lambda}\right) \quad (18)$$

where

$$\lambda = \frac{\Gamma^2 n_0}{\mu_{ex}} \quad (19)$$

Note that we neglect the possibility of the more complicated spin structure of the excitonic ground state. This problem is of importance and it should be investigated in the future work in detail.

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