

Excitonic Instability and Origin of the Mid-Gap States

Michael N. Kiselev

Department of Superconductivity and Solid State Physics, Kurchatov Institute, 123182 Moscow, Russia

In the framework of the two-band model of a doped semiconductor the self-consistent equations describing the transition into the excitonic insulator state are obtained for the 2D case. It is found that due to the exciton-electron interactions the excitonic phase may arise with doping in a semiconductor stable initially with respect to excitonic transition in the absence of doping. The effects of the strong interactions between electron (hole) Fermi-liquid (FL) and excitonic subsystems can lead to the appearance of the states lying in the middle of the insulating gap.

Let us consider a two-band model of a doped semiconductor. On the one hand this model allows us to describe the properties of a copper-oxide superconductors if we have a $Cu-O$ model with bands formed by the hybridized $Cu-d_{x^2-y^2}$ and $O-p_{x,y}$ orbitals [1,2]. On the other hand the two-band model has been used for studying the transition from the semiconductor state into the Excitonic Insulator State (EIS) [3,4]. In this case one considers that the Excitonic Transition (ET) arises only if the band gap E_g is smaller than the binding energy E_c of an exciton. The doping effectively decreases the exciton binding energy and, therefore, it destroys EIS.

The method based on the three-body scattering approach to studying the influence of a proximity to ET on the properties of the doping electron FL has been proposed in [2]. The alternative method based on the solution of the Bethe-Salpeter equation for electron-exciton scattering has been developed in Ref.[4]. It was found there that if $E_c < E_g < E_c + J$ (J is the binding energy of an exciton with an electron) the creation of an exciton from the vacuum would be favorable from the energy standpoint. The exciton creation process will be stabilized by the repulsion of excitons [3]. These arguments make it possible the estimation for the equilibrium exciton density in 2D and 3D cases. In the present work we intend to study the influence of an exciton subsystem on the doping electron FL properties in the framework of the method [4].

Following [3,4], let us consider the two-band model of a doped semiconductor with the electron dispersion relation ε_1 and hole dispersion relation

ε_2 in 2D case.

$$\varepsilon_i = \pm E_g/2 \pm p^2/(2m_i) \quad i = 1, 2 \quad (1)$$

The Hamiltonian of interaction in terms of electron density operator $\rho(\mathbf{x}) = \sum_i \Psi_i^\dagger(\mathbf{x})\Psi_i(\mathbf{x})$ is

$$H_{int} = \frac{1}{2} \int d\mathbf{x}d\mathbf{y} \rho(\mathbf{x}) \frac{e^2}{|\mathbf{x} - \mathbf{y}|} \rho(\mathbf{y}) \quad (2)$$

Without any loss of generality we will consider the case of doping into the upper band and $m_2 > m_1$. The path integral representation of partition function Z of the system in terms of slow electron field χ and excitonic field Φ describing the collective properties of electrons and holes [4] has the form:

$$Z = \int \exp(S_{el} + S_{ex} + S_{int}) D\bar{\chi} D\chi D\Phi^* D\Phi \quad (3)$$

$$S_{el} = \int_0^\beta d\tau \int d\mathbf{x} \bar{\chi} [-\partial_\tau + \nabla^2/(2m_1) + \mu] \chi - \frac{1}{2} \int_0^\beta d\tau \int d\mathbf{x}d\mathbf{y} |\chi_{\mathbf{x},\tau}|^2 V_{\mathbf{x}-\mathbf{y}}^{eff} |\chi_{\mathbf{y},\tau}|^2$$

$$S_{ex} = \int_0^\beta d\tau \int d\mathbf{x} \Phi^* [-\partial_\tau - \lambda(\mathbf{x}) - \frac{f}{2} |\Phi|^2] \Phi$$

$$S_{int} = -\gamma \int_0^\beta d\tau \int d\mathbf{x} |\chi_{\mathbf{x},\tau}|^2 |\Phi_{\mathbf{x},\tau}|^2 \quad (4)$$

where $M = m_1 + m_2$ is the mass of exciton, V^{eff} is the effective Coulomb potential of doping electrons, f and γ are, respectively, the exciton-exciton and exciton-electron constants. Moreover, γ corresponds to the exciton-electron attraction [4]. The quantity $\lambda(\mathbf{x}) = E_g - E_c[1 -$

$A(p_F a_B)^2] - \nabla^2/(2M)$ is the exciton dispersion relation, a_B is the first Bohr radius of electron and the other notations have a standard form. The expression for λ incorporates the circumstance that for the doping densities $p_F a_B \ll 1$ the exciton binding energy falls linearly with increasing the electron density, $A \sim 1$.

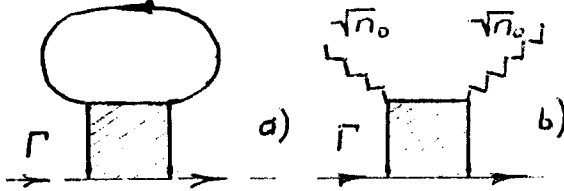


Fig. 1. Self-energy of excitons (a) and electrons (b)

The presence (or absence) of the excitonic condensate with the equilibrium density n_0 in the system at $T = 0$ is connected with the presence of time-independent spatially-homogeneous solution of classical equation for the saddle-point trajectory of field Φ :

$$(i\partial_t - \lambda(\mathbf{x}) - W - F |\Phi_{\mathbf{x},t}|^2)\Phi_{\mathbf{x},t} = 0 \quad (5)$$

where W is the self-energy Fig.1(a), $F \approx 4\pi/(M \ln[E_c/\mu_{ex}])$ is the renormalized vertex for the exciton-exciton interaction, and $\mu_{ex} = n_0 F$ is the exciton chemical potential. The condition $\mu_{ex} \ll E_c$ corresponds to the low density exciton gas $n_0 a_B^2 \ll 1$.

Let us consider Γ as a result of solution the Bethe-Salpeter equation for electron-exciton scattering.

$$\Gamma(P) = \gamma[1 - i\gamma \int \frac{d^3k}{(2\pi)^3} G(k)g(P-k)]^{-1} \quad (6)$$

where G and g are the Green's functions of electrons and excitons, respectively, $d^3k = dk d\epsilon$. On the Fermi surface the vertex Γ is a function only of the electron-exciton total energy. To take self-consistently into account the mutual influence of electron and exciton subsystems one should solve the system of equations (7) with Γ defined by relation (6), see Fig.1:

$$\begin{cases} -\lambda(\mathbf{k} = 0) + i \int \frac{d^3k}{(2\pi)^3} \Gamma(k)G(k) = n_0 F \\ \Sigma(k) = n_0 \Gamma(k) \end{cases} \quad (7)$$

where the Green's functions are defined self-consistently by

$$G = [\epsilon - \xi_{\mathbf{p}} - (\Sigma(\epsilon, \mathbf{p}) - \Sigma(0, \mathbf{p}_F) + i\delta \text{sgn} \xi_{\mathbf{p}})]^{-1}$$

$$g = 2E_0(\mathbf{P})[\omega^2 - E^2(\mathbf{P}) + i\delta]^{-1} \quad (8)$$

and the spectra are $E^2(\mathbf{P}) = E_0^2(\mathbf{P}) + 2\mu_{ex} E_0(\mathbf{P})$, $\xi_{\mathbf{p}} = (\mathbf{p}^2 - \mathbf{p}_F^2)/(2m_1)$, $E_0(\mathbf{P}) = \mathbf{P}^2/(2M)$.

Analysis of (6) and (7) shows that the equilibrium exciton density n_0 exists under the conditions $E_g - E_c < J$, $\epsilon_F < \epsilon_F^{max} = \alpha J$, $\alpha \sim 1$. In this case $n_0 \sim m_1 \epsilon_F^2/J$, $|\Sigma(0, \mathbf{p}_F)| \sim \epsilon_F$ and the effective electron mass on the Fermi-surface is $m^{eff}/m_1 = (1 - (\frac{\partial \Sigma}{\partial \epsilon})_{0, \mathbf{p}_F}) / (1 + (\frac{\partial \Sigma}{\partial \epsilon(\mathbf{p})})_{0, \mathbf{p}_F}) \gg 1$.

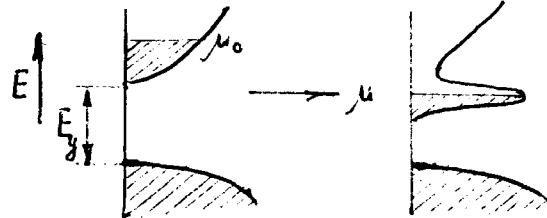


Fig. 2. Schematic change in the one-particle DOS due to the exciton-electron interaction

Let us consider the electron DOS

$$\nu(\epsilon) = -\frac{2}{\pi} \int \frac{d\mathbf{p}}{(2\pi)^2} \text{Im} G^R(\mathbf{p}, \epsilon) \quad (9)$$

The pinning of the chemical potential and the origin of states in the insulating gap (see Fig.2) are connected with the creation of the complex bound state of electron and excitons. The pseudo-gap that lies above the Fermi level ($\delta\epsilon \sim J$) corresponds to the increase of Γ (and Σ) near the threshold of the bound state formation. For the region in which an exciton condensate exists, the strong interaction between electron and exciton subsystems can lead to the marginal properties of the electron FL in the normal state. In addition, there is a possibility of nonphonon superconductivity for this liquid. A further analysis of the properties of such a system warrants a separate study.

This research was supported by the Russian Fund of Fundamental Research, Grant No 93-02-02538.

References

1. C.M. Varma, S. Schmütt-Rink and E. Abrahams. Solid State Commun., **62**, 681 (1987)
2. A.E.Ruckenstein and C.M.Varma. Physica C **185-189**, 134 (1991)
3. A.N.Kozlov and L.A.Maksimov. Sov. Phys. JETP **21**, 790 (1965), L.V.Keldysh and A.N.Kozlov. Sov. Phys. JETP **27**, 521 (1968)
4. V.S.Babichenko and M.N.Kiselev. J. Mos. Phys. Soc., **2**, 311 (1992), JETP Lett. **57**, 179 (1993), Physica C **209**, 133 (1993)