Doping-induced exciton transition

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In a semiconductor which is stable with respect to an exciton transition in the absence of doping, an exciton phase may arise upon doping because of an interaction of excitons with electrons.

The ground state of a semiconductor with a band gap E_g smaller than the binding energy of an electron and a hole (i.e., of an exciton), E_c, is known to be unstable with respect to a transition to a state of an exciton insulator.[1,2] In the present letter we adopt a two-band model of a doped semiconductor, and we assume $E_g > E_c$. In the absence of doping, the ground state of such a semiconductor is stable with respect to the formation of excitons. However, if we assume that the band gap is smaller than the sum of the exciton binding energy and the binding energy of an exciton with an electron, $E_g < E_c + J$ (J is the binding energy of an exciton with an electron), then the presence of even a single free electron in the system will make the creation of an exciton from vacuum favorable from the energy standpoint. A bound state of this exciton with the electron forms. This entity has a charge equal to the charge of the electron. If the repulsive interaction between excitons is sufficiently weak, this entity may cause the formation of yet another exciton. The entity may form a more complex bound state with this new exciton, and so forth. As a result, a large complex of a single electron and a large number of excitons may arise. The exciton creation process will be stabilized by the repulsion of excitons which occurs because an exciton, consisting of two Fermi particles, is not a Bose particle.[3,4] The qualitative arguments above are valid if the size of the exciton is small in comparison with the radius of the electron-exciton bound state. This condition is met if $J \ll E_c$ (for a negatively charged hydrogen ion H^-, the ionization potential is[5] $J \sim 0.75$ eV$\ll E_c$). Below we assume that J is indeed small in comparison with E_c.

In the present letter we analyze the conditions for the onset of an exciton condensate induced by doping. We discuss 2D and 3D systems. This model is of interest in connection with the problem of high-T_c superconductivity[6–8] and also for reaching an explanation of the superconducting properties of doped semiconductors.[9]

We consider a two-band model of a doped semiconductor with a hole dispersion relation $\epsilon_h(\mathbf{p})$ and an electron dispersion relation $\epsilon_e(\mathbf{p})$:

$$\epsilon_h(\mathbf{p}) = -E_g/2 - p^2/(2m_h), \quad \epsilon_e(\mathbf{p}) = E_g/2 + p^2/(2m_e). \tag{1}$$

We write the partition function of this system as the functional integral

$$Z = \int \exp(iS) d\bar{\Psi} D\Psi \tag{2}$$

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$$S=\int dt\sum_j\int d\mathrm{x}\bar{\Psi}_j(\mathrm{x},t)\{i\partial_t-\epsilon_j(-i\nabla)+\mu\}\Psi_j(\mathrm{x},t)$$

$$-1/2\int dt\sum_i\sum_j\int d\mathrm{x}d\mathrm{y}\bar{\Psi}E_i(\mathrm{x},t)\Psi_i(\mathrm{x},t)V_{\mathrm{x}-\mathrm{y}}\bar{\Psi}_j(\mathrm{y},t)\Psi_j(\mathrm{y},t),\qquad(3)$$

where S is the action of the system, Ψ are the Grassmann electron fields, i and j specify the bands (e and h), $V(\mathbf{r})=e^2/(\epsilon_0 r)$ is the Coulomb potential, ϵ_0 is the static dielectric constant of the semiconductor, and μ is the chemical potential of the electrons in the case of doping into the upper band.

We integrate (2) over all the fields Ψ_h and over those fields Ψ_e which vary over length scales smaller than the average distance between doping electrons. Introducing collective variables which describe the motion of the exciton as a whole, and which vary slowly at the exciton scales, we find the effective action for the system of doping electrons which are interacting with excitons produced from vacuum by the same interaction (the procedure for deriving the effective action is described in detail in Ref. 10):

$$S=S_0+S_{\mathrm{ex}}+S_{\mathrm{el}}+S_{\mathrm{el\text{-}ex}},$$

$$S_0=\sum_p\bar{a}(p)[\epsilon-\mathbf{p}^2/(2m_e)+\mu]a(p)+\sum_k B^*(k)[\omega-\lambda(\mathbf{k})]B(k),$$

$$S_{\mathrm{el}}=-\frac{1}{2}\sum_{qp}V_q^{\mathrm{eff}}\;\bar{a}(p_1)\bar{a}(p_2)a(p_2-q)a(p_1+q),$$

$$S_{\mathrm{ex}}=-\frac{f}{2}\sum_{qp}B^*(p_1)B^*(p_2)B(p_2-q)B(p_1+q),$$

$$S_{\mathrm{el\text{-}ex}}=-\sum_{qp}\gamma(\mathbf{q})\bar{a}(p_1+q)a(p_1)B^*(p_2-q)B(p_2).\qquad(4)$$

The fields a describe the electron subsystem, the fields B describe the exciton subsystem, $\lambda(\mathbf{k})=E_g-E_c[1-A(p_Fa_B)^d]+k^2/(2M)$ is the exciton dispersion relation in the case $\lambda_0=E_g-E_c>0$, $a_B=h^2\epsilon_o/(me^2)$ is the first Bohr radius of the electron, and p_F is the Fermi momentum. The expression for $\lambda(k)$ incorporates the circumstance that at doping densities $p_Fa_B\ll 1$ the exciton binding energy falls off linearly with increasing electron density. In this case the constant A is ~ 1. The quantity d is the dimensionality of the system, $M=m_e+m_h$ is the mass of the exciton, V_q^{eff} is the effective Coulomb potential of the doping electrons, and $\gamma(q)$ is the potential of interaction of the electrons with the excitons, which is an attractive potential:

$$\gamma(\mathbf{q})\sim-\int\frac{d^dk}{(2\pi)^d}(\mathbf{kd})(\mathbf{k}-\mathbf{q},\mathbf{d})V(\mathbf{k})V(\mathbf{k}-\mathbf{q})\frac{e^2}{\mathbf{k}^2/(2m^*)+E_c-E_c^{\mathrm{I}}}.\qquad(5)$$

Here $m^*=m_eM/(m_e+M)$, and $|\mathbf{d}|\sim ea_B$ is the matrix element of the dipole moment of a transition from the ground state to the first excited state of the exciton. Since $\gamma(\mathbf{q})$

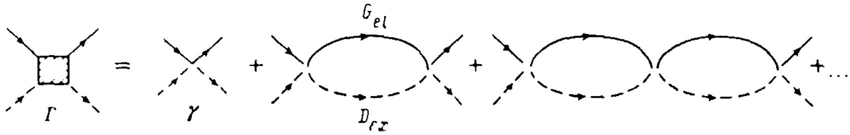

FIG. 1.

depends only weakly on the momentum at $qa_B \lesssim 1$, we will ignore the q dependence of γ below. The amplitude for the scattering of excitons by each other, f, is determined by the repulsion of excitons at short range; it is[3,4]

$$f=2(2\pi)^{-2d}\int d\mathbf{k}d\mathbf{p}[\Psi_0^3(\mathbf{p})V_\mathbf{k}\Psi_0(\mathbf{p}+\mathbf{k})-\Psi_0^2(\mathbf{p})V_\mathbf{k}\Psi_0^2(\mathbf{p}+\mathbf{k})]\sim E_c a_B^d, \qquad (6)$$

where Ψ_0 is the wave function of the ground state of a hydrogen-like atom.

If the derivation of action (4) is to be valid, we must assume that the density of the exciton system is small: $n_{\mathrm{ex}}a_B^d \ll 1$. We assume that the strength of the attraction between electrons and excitons is sufficient for the formation of a bound state even at $d=3$. In this case the vertex of the electron–exciton interaction, γ, is greatly renormalized, and the overall vertex is determined by a sequence of ladder diagrams (Fig. 1). Summing these diagrams, we find

$$\Gamma(P)=\frac{\gamma}{1-\gamma\Pi_{\mathrm{el-ex}}(P)}, \qquad (7)$$

where $\Pi_{\mathrm{el-ex}}$ is expressed in terms of the electron Green's function G_{el} and the exciton Green's function D_{ex} by

$$\Pi_{el-ex}(P)=i\int\frac{d^{d+1}k}{(2\pi)^{d+1}}G_{\mathrm{el}}(k)D_{\mathrm{ex}}(P-k). \qquad (8)$$

The integral in (8) diverges at large momentum, and the integration must be cut off at momenta $k\sim 1/a_B$, since the effective radius of the potential γ is on the order of a_B.

In general, the exciton–exciton interaction vertex f is also renormalized, and it must be replaced by the complete amplitude for the scattering of an exciton by an exciton, F. The amplitude F is determined by a sum of ladder diagrams if the exciton density is small, $n_{\mathrm{ex}}a_B^d \ll 1$. The renormalization of the exciton–exciton vertex is important only at $d=2$.

As a result of the renormalizations, the electron–exciton interaction vertex γ must be replaced by Γ, and the exciton–exciton interaction vertex f by F, in the effective action for the electron–exciton system, (4).

Let us consider the classical equation of motion for the exciton fields B, which determines a saddle trajectory for these fields:

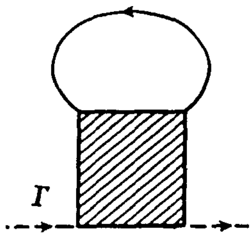

FIG. 2.

$$\left(i\partial_t-\lambda(0)+\frac{\nabla^2}{2M}-\Sigma\right)B(\mathbf{r},t)-F|B(\mathbf{r},t)|^2B(\mathbf{r},t)=0. \tag{9}$$

The quantity Σ in this equation is represented by the diagram in Fig. 2. A nonzero, static, homogeneous solution of Eq. (9), which determines an equilibrium exciton density, exists if

$$\lambda(0)+\Sigma<0. \tag{10}$$

In this case the equilibrium exciton density n_0 is given by

$$n_0=-\frac{\lambda(0)+\Sigma}{F}. \tag{11}$$

Let us consider the case $d=2$. Calculating $\Pi_{\text{el-ex}}(P)$, we find

$$\Pi_{\text{el-ex}}=-\frac{m^*}{2\pi}\ln[E_c/\max\{p_0^2/(2m^*),\lambda_0\}], \tag{12}$$

where $p_0=\max\{p_F,(\mu_{\text{ex}}M)^{1/2}\}$, and $\mu_{\text{ex}}=n_0F$ is the chemical potential of the excitons under the condition that a condensate exists. The expression for the renormalized electron–exciton vertex is

$$\Gamma(P)=-\frac{2\pi}{m^*\ln[\max\{p_0^2/(2m^*),\lambda_0\}/J]}, \tag{13}$$

where $J=E_c\exp\{-(2\pi/m^*|\gamma|)\}\ll E_c$, is the binding energy of an electron with an exciton. The renormalized amplitude for the scattering of an exciton by an exciton, F, which is determined by a sum of ladder diagrams, can be written as follows in the $d=2$ case:[11]

$$F=\frac{f}{1+f\frac{M}{4\pi}\ln[E_c/\mu_{\text{ex}}]}\approx\frac{4\pi}{M\ln[E_c/\mu_{\text{ex}}]}. \tag{14}$$

The expression for Σ (Fig. 2) takes its simplest form at $p_0>p_F$. As we show below, this condition holds in the region of maximum density of the condensate:

$$\Sigma=\Gamma n_{\text{el}}, \tag{15}$$

where n_{el} is the density of doping electrons. The expression for Σ at $p_0 \sim p_F$ is not as simple, but there is no qualitative change in the picture.

Analysis of inequality (10) shows that the equilibrium exciton density n_0 exists under the condition $\epsilon_F < \epsilon_F^{max} \sim J$ only for $\lambda_0 < J$. In this case the maximum exciton density n_0 is, in order of magnitude, $n_0 \sim m^* J \ln\{E_c/J\}$. In this case we have $\mu_{ex} \sim m^* J/M$ and $p_o \sim (m^* J)^{1/2}$.

Under the condition $\epsilon_F \ll J$ the system is unstable with respect to the formation of bound states of electrons and excitons, and it cannot be thought of as consisting of two homogeneous interacting subsystems.

In the $d=3$ case, the renormalized vertex of the electron–exciton interaction is

$$\Gamma(P) = -\frac{2\pi^2}{(2m^*)^{3/2}[\sqrt{\max\{p_0^2/(2m^*),\lambda_0\}} - \sqrt{J}]}, \tag{16}$$

where $J = (4/\pi^2)[1 - (\pi^2 a_B/m^* |\gamma|)]^2 E_c \ll E_c$ is the binding energy of an electron and an exciton. A bound state exists if $m^* |\gamma|/(\pi^2 a_B) > 1$. If the system is to be stable, the denominator in (16) must be positive.

Inequality (10), which is the condition for the existence of an exciton condensate, holds at doping densities for which we have $\epsilon_F^{min} < \epsilon_F < \epsilon_F^{max} \ll E_c$ and $\epsilon_F^{min} = \max\{J,\lambda_0\}$. In this case the equilibrium exciton density found from the solution of Eq. (11) is, in order of magnitude, $n_0 \sim (m^*/M)^{1/3} \epsilon_F/f$.

A large scattering amplitude Γ, which makes an exciton phase possible, may result from a scattering by both a resonant level ($J \ll E_c$) and a shallow quasiresonant level. The resulting densities of the exciton phase satisfy the condition $n_0 a_B^d \ll 1$ in both the $d=2$ and $d=3$ cases.

In the region in which an exciton condensate exists, the electron–exciton system constitutes an electron liquid which is interacting strongly with an exciton subsystem. As a result, there is a strong effect on the properties of the electron Fermi liquid in the normal state, and there is the possibility of a nonphonon superconductivity for this liquid. A further analysis of the properties (including superconducting properties) of such a system warrants a separate study.

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