Bound state of an exciton at a slightly attracting defect in a semiconductor with a degenerate valence band

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(Submitted 24 June 1988)
Pis'ma Zh. Eksp. Teor. Fiz. **48**, No. 4, 202–205 (25 August 1988)

In the absence of undulating constant-energy surfaces a bound exciton state is found to be present at any attracting defect in a semiconductor with a degenerate valence band.

Analysis of the formation of the bound state of an exciton at a defect usually reduces to the analysis of the localization of a particle whose mass is equal to the translational mass of an exciton in a potential well. The bound state in this case occurs only if the power of the well is greater than a certain threshold value. Defects with a power level lower than the threshold power have no bound state. We will show here that this conclusion does not apply to semiconductors with a degenerate valence band. We will also show that in the isotropic approximation any defect that attracts an exciton, however slightly, forms a bound state.

The Hamiltonian of an exciton in a semiconductor with a degenerate valence band is

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_L(\mathbf{p}_h) + \frac{\mathbf{p}_e^2}{2m_e} - \frac{e^2}{\kappa|\mathbf{r}_e - \mathbf{r}_h|}, \qquad (1)$$

where $\mathbf{r}_e$, $\mathbf{p}_e$ and $\mathbf{r}_h$, $\mathbf{p}_h$ are the coordinates and momenta of an electron and a hole, respectively; m_e is the electron mass, κ is the dielectric constant, and $\mathcal{H}_L$ is the Luttinger Hamiltonian

$$\hat{\mathcal{H}}_L(p) = \frac{\mathbf{p}^2}{2m_h}\hat{\Lambda}_h(\mathbf{p}) + \frac{\mathbf{p}^2}{2m_l}\hat{\Lambda}_l(\mathbf{p}), \qquad (2)$$

where m_h and m_l are the masses of the heavy and light holes, and $\hat{\Lambda}_h(p) = 9/8 - (\mathbf{p}\hat{\mathbf{J}})^2/2\mathbf{p}^2$ and $\hat{\Lambda}_l = 1 - \hat{\Lambda}_h$ are the operators of the projection onto the states of the heavy and light holes, respectively: $\hat{\mathbf{J}}$ is the spin angular momentum operator with a spin 3/2 (Ref. 1).

In the Hamiltonian (1) the variables are not distinguished, so the motion of the exciton as a whole cannot be separated from the relative motion of an electron and hole in it. Such a division is, however, possible at large momenta of the translational motion $\vec{\mathcal{P}}$, such that $\mathcal{P}^2/2m_l \gg E_B$, where $E_B = m_e e^4/2\hbar^2\kappa^2$. The last condition means that the splitting of the excitonic Mranches associated with the heavy hole is much greater than the binding energy E_B of an exciton (we assume $m_h \gg m_e \sim m_l$). The dispersion relation of a "heavy" exciton in this case is[2]

$$\epsilon(\mathcal{P}) = \frac{\mathcal{P}^2}{2m_h} + \frac{4E_B^2 m_e}{\mathcal{P}^2} - E_B, \qquad (3)$$

and the corresponding wave functions are

$$\Psi_{\vec{\mathcal{P}},\mu}(r,R) = \varphi_0(r)F_{\vec{\mathcal{P}},\mu}(\mathbf{R}) \qquad (4)$$

$$F_{\vec{\mathcal{P}},\mu}(\mathbf{R}) = e^{i\vec{\mathcal{P}}R/\hbar}\chi_\mu(\vec{\mathcal{P}}), \qquad (5)$$

where $\mathbf{R} = (m_e\mathbf{r}_e + m_h\mathbf{r}_h)/(m_e + m_h)$, $\mathbf{r} = \mathbf{r}_e - \mathbf{r}_h$, φ_0 is the hydrogen-like function of the ground state, and $\chi_\mu(\vec{\mathcal{P}})$ is the eigenfunction of the operator $(\hat{\mathbf{J}}\vec{\mathcal{P}})/\mathcal{P}$: $(\hat{\mathbf{J}}\vec{\mathcal{P}})/\mathcal{P}\chi_\mu(\vec{\mathcal{P}}) = \mu\chi_\mu(\vec{\mathcal{P}})$, where the μ subscript in (4) has the values $\pm 3/2$.

Using the same approximation, we find an effective Schrödinger equation which describes the motion of an exciton in the field of a defect. To be specific, we will assume that the potential of the defect affects only the hole. We can then write this equation in the form

$$(\epsilon(\mathscr{P})\hat{\Lambda}_h(\vec{\mathscr{P}}) + \frac{\mathscr{P}^2}{2m_l}\hat{\Lambda}_l(\mathscr{P}))F(\mathbf{R}) + V(\mathbf{R})F(\mathbf{R}) = EF(\mathbf{R}) . \tag{6}$$

We will seek its solution in the form

$$F(\mathbf{R}) = \sum_{\mathscr{P},\mu=\pm 3/2} A_{\vec{\mathscr{P}},\mu} F_{\vec{\mathscr{P}},\mu}(\mathbf{R}) . \tag{7}$$

Because of the condition $(2m_lE_B)^{1/2}$, we can ignore the "light"-exciton component which corresponds to $\mu = \pm 1/2$. Assuming that the radius of the potential $V(\mathbf{R})$ is much smaller than the wave function $F(\mathbf{R})$, we find the following expression for the coefficients $A_{\vec{\mathscr{P}},\mu}$:

$$A_{\vec{\mathscr{P}},\mu} = \frac{W(F(0)\chi_\mu(\vec{\mathscr{P}}))}{E-\epsilon(\vec{\mathscr{P}})} , \tag{8}$$

where $W = \int d^3rV(\mathbf{r})$. Substituting (8) into (7) and setting $R = 0$, we find an equation for the binding energy

$$1 = W\sum_{\vec{\mathscr{P}}} \frac{\hat{\Lambda}_h(\vec{\mathscr{P}})}{E-\epsilon(\mathscr{P})} . \tag{9}$$

We will show that this equation has a solution for any negative value of W, however small. The dispersion relation $\epsilon(\mathscr{P})$ has a minimum at $\mathscr{P} = \mathscr{P}_0 = (8E_B^2m_em_h)^{1/4}$. Near this minimum we have $\epsilon(\mathscr{P}) = \epsilon(\mathscr{P}_0) + 2/m_h\ (\mathscr{P} = \mathscr{P}_0)^2$. It is easy to reckon the energy E from $\epsilon(\mathscr{P}_0)$: $E = \epsilon(\mathscr{P}_0) = \Delta$. The contribution to the sum (9) from $\mathscr{P}_0$, which is approximately equal to $\mathscr{P}_0$, is proportional to $\Delta^{-1/2}$ and diverges as $\Delta \to 0$. As a result, we obtain the following expression for the binding energy

$$\Delta = \frac{W^2m_h\mathscr{P}_0^4}{32\pi^2\hbar^6} = \frac{W^2E_B^2m_h^2m_e}{4\pi^2\hbar^6} . \tag{10}$$

This expression is valid if the condition $\Delta \ll \epsilon_0 = E_B\ (2m_e/m_h)^{1/4}$, which allows us to restrict the analysis to momenta close to $\mathscr{P}_0$ in sum (9), is satisfied. The physical meaning of this result can easily be understood by calculating the state density of $\rho(\epsilon)$, which corresponds to dispersion relation (3). If ϵ is approximately equal to $\epsilon(\mathscr{P}_0)$, $\rho(\epsilon) \sim (\epsilon - \epsilon(\mathscr{P}_0))^{-1/2}$, i.e., it behaves the same way as it does in the case of a one-dimensional particle which obeys the quadratic dispersion relation. In the one-dimensional case, however, every attracting potential has a bound state.

The energy level (10) is fourfold degenerate. The corresponding normalized wave functions are

$$F_{\pm 3/2}(R) = \frac{1}{2\sqrt{\pi}}\left(\frac{2m_h\Delta}{\hbar^2}\right)^{1/4}\frac{\exp\left(-R\sqrt{\frac{m_h\Delta}{2\hbar^2}}\right)}{R}\left[2\left(1-\frac{3\hbar^2}{2(\mathcal{P}_0R)^2}\right)\sin\frac{\mathcal{P}_0R}{\hbar} + \frac{3\hbar}{\mathcal{P}_0R}\cos\frac{\mathcal{P}_0R}{\hbar}\right]\chi_{z,\pm 3/2}$$

$$F_{\pm 1/2}(R) = \frac{3}{2\sqrt{\pi}}(2m_h\Delta\hbar^2)^{1/4}\frac{\exp\left(-R\sqrt{\frac{m_h\Delta}{2\hbar^2}}\right)}{\mathcal{P}_0R^2}\times\left[\cos\frac{\mathcal{P}_0R}{\hbar} - \frac{\hbar}{\mathcal{P}_0R}\sin\frac{\mathcal{P}_0R}{\hbar}\right]\chi_{z,\pm 1/2}, \tag{11}$$

where $\chi_{z,\mu}$ are the eigenfunctions of the operator $\hat{\mathbf{J}}_z$ ($\hat{\mathbf{J}}_z\chi_{z,\mu} = \mu\chi_{z,\mu}$). The functions $F_\mu(R)$ are shown schematically in Fig. 1. The oscillator strength of the interband transition is the same for all states (11) and is proportional to

$$f = |\int d^3RF_\mu(R)|^2 = 9\sqrt{2}\pi^3\hbar^3(m_h\Delta)^{1/2}/\mathcal{P}_0^4. \tag{12}$$

It is useful to compare this quantity with f_0—the enormous oscillator strength of an exciton bound to a short-range defect with the same binding energy Δ but in nondegenerate bands[3]: $(f/f_0) = 9\pi^2/8)(\Delta/\epsilon_0)^2$. The rapidly oscillating function $F_\mu(R)$ accounts for the small value of this relation $(\Delta \ll e_0)$.

We considered the case in which only a hole interacts with the defect. The case in

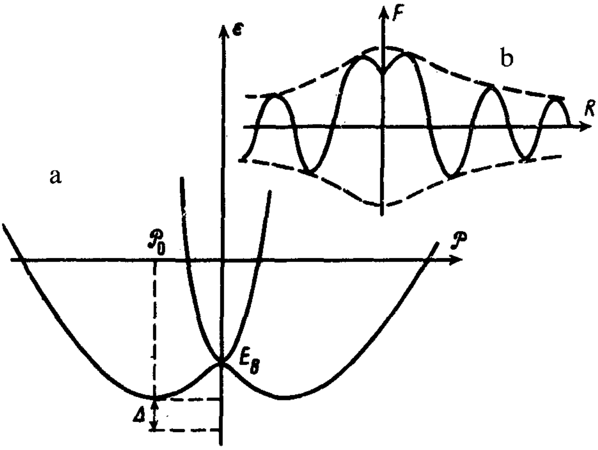

FIG. 1. (a) Energy position of the bound state of an exciton at a defect and (b) schematic representation of the relevant wave function.

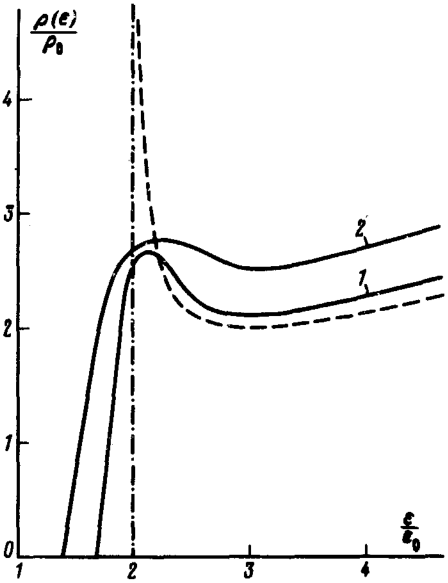

FIG. 2. Dimensionless state density $\rho(\epsilon)$ corresponding to dispersion relation (13) for the anisotropy parameter values $\Gamma_{\min} = (\gamma_1 - 2\gamma_3)\bar{m}_h/m_0 = 0.7$ and $\Gamma_{\max} = (\gamma_1 - 2\gamma_2)\bar{m}_h/m_0 = 1.4$—curve 1 and $\Gamma_{\min} = 0.5$, $\Gamma_{\max} = 1.4$—curve 2. Dashed curve—The state density in the absence of undulating (irregular) surfaces, $\Gamma_{\min} = \Gamma_{\max} = 1$.

which the potential of the defect acts on the electron can be analyzed in a similar way. The binding energy of the state corresponding to $\mu = \pm 3/2$ in this case is different from that of the state corresponding to $\mu = \pm 1/2$. For $\mu = \pm 3/2$ it is equal to $2\Delta m_e/m_h$ and for $\mu = \pm 1/2$ it is $9\sqrt{2}\pi^2\Delta m_e^{3/2}/m_h^{3/2}$.

Taking the corrugation of the valence band into account allows us to write dispersion relation (3) in the form[4]

$$\epsilon(\mathcal{P}) = \frac{4E_B^2 m_e}{\mathcal{P}^2} - E_B + \frac{\mathcal{P}^2}{2m_0}\left[\gamma_1 - \sqrt{4\gamma_2^2 + 12(\gamma_3^2 - \gamma_2^2)\frac{\mathcal{P}_x^2\mathcal{P}_y^2 + \mathcal{P}_y^2\mathcal{P}_z^2 + \mathcal{P}_z^2\mathcal{P}_x^2}{\mathcal{P}^4}}\right], \qquad (13)$$

where m_0 is the mass of the free electron, and γ_1, γ_2, and γ_3 are the Luttinger parameters[5] [relation (13) becomes relation (3) if $\gamma_2 = \gamma_3$. The position of the minimum $\epsilon(\vec{\mathcal{P}})$ in this case depends on the direction of the vector $\vec{\mathcal{P}}$, which accounts for the blurring of the structural feature in the state density $\rho(\epsilon)$. The results of a numerical calculation of $\rho(\epsilon)$ in units of $\rho_0 = \bar{m}_h^{3/2}\sqrt{2\epsilon_0}/2\pi^2\hbar^3$, where $(\bar{m}_h = 5m_0/(5\gamma_1 - 6\gamma_3 - 4\gamma_2))$, for two sets of parameters of the anisotropy are shown in Fig. 2. Taking the inhomogeneity into account, the bound state can occur only when the parameter $|W|$ is larger than a certain threshold value $|W_c| = \eta\hbar^3/E_B^{1/2}m_h^{5/4}m_e^{1/4}$, where the constant η depends on the anisotropy parameters. The values of η are 2.8

and 3.5, respectively, for the values of these parameters which correspond to curves 1 and 2 in Fig. 2.

We wish to thank B. L. Gel'mont, M. I. D'yakonov, A. S. Ioselevich, and A. L. Éfros for useful discussions.

[1] G. L. Bir and G. E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors*, Israel Program for Scientific Translations, Jerusalem; Wiley, New York, 1975.

[2] Al. L. Éfros and B. L. Gel'mont, Sol. State Commun. **49**, 883 (1984).

[3] É. I. Rashba and G. É. Gurgenishvili, Fiz. Tverd. Tela **4**, 1029 (1962) [Sov. Phys. Solid State **4**, 759 (1962)].

[4] B. L. Gel'mont, S. B. Sultanov, and Al. L. Éfros, Fiz. Tekh. Poluprovodn. **18**, 2214 (1984) [Sov. Phys. Semicond. **18**, 1380 (1984)].

[5] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).

Translated by S. J. Amoretty