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IMPURITIES IN NARROW-GAP QUANTUM DOTS

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The influence of a finite value of the energy gap on the electron-binding energy for an impurity atom and the size-quantization levels in a quantum dot are studied. The energy-gap finiteness lowers appreciably the size-quantization levels and exerts a smaller but more diversified effect on the binding energy. The results of calculations are presented graphically.

An energy spectrum of the impurity-bound (for definiteness, the donor-bound) electrons in narrow-bandgap semiconductors is defined by the Dirac equation similar to the one used in [1] to describe deep levels. In this study we consider a simplified (a two-band) Dirac model with equal and isotropic masses of electrons and holes [2]. A more exact three-band model of semiconductor, though offering a more precise description of electronic structure of a semiconductor of the diamond and zinc blende types, cannot provide radically new results but only complicates substantially the calculations.

The achievements of semiconductor technology made it possible to fabricate diverse semiconductor structures of nanometer size (nanostructures) where the charge-carrier transport is highly anisotropic (quantum wells, superlattices, quantum wires, and so on) [3]. We believe that of particular interest are the quantum dots, i.e., nanometer-sized inclusions of one semiconductor (with a narrower bandgap) in another. Owing to three-dimensional confinement, the quantum dots are, in effect, zero-dimensional and feature intriguing optical properties [4 - 6].

The energy of charge carriers in the quantum dots depends only slightly on the dot shape (spherical, cubical, cylindrical, etc.); therefore, for the sake of simplicity, we assume that the quantum dot is a sphere of radius R. The binding energy of donor electrons in nanostructures depends critically on the impurity-atom position with respect to the dot boundary if the effective radius of donors is of the order of the dot size (see, e.g., [7]) and is maximum when the impurity atom is located at the dot center. In what follows we ignore

this dependence and consider an impurity atom that has the charge Ze and is located at the sphere center. A similar problem, although related to quantum dots composed of wide-bandgap semiconductors, was treated in [8]. Because of spherical symmetry of the Dirac equation, the calculation of electron-binding energy for a donor in a narrow-gap quantum dot is reduced to solving the set of equations [9]

$$\begin{cases} \frac{d\psi_1}{dr} - \frac{k}{r}\psi_1 + \frac{1}{\hbar s}(E - \Delta(r) - V(r))\psi_2 = 0 \\ \frac{d\psi_2}{dr} + \frac{k}{r}\psi_2 - \frac{1}{\hbar s}(E + \Delta(r) - V(r))\psi_1 = 0. \end{cases} \quad (1)$$

Here the half-width of the forbidden band $\Delta(r) = \Delta_1$ for $r < R$ and $\Delta(r) = \Delta_2$ for $r > R$; furthermore, the relation $\Delta_1/\Delta_2 = \delta < 1$ is valid. The impurity-center field is defined by the potential $V(r) = -Ze^2/\epsilon r$, where ϵ is the static dielectric constant, which we consider to be the same in both semiconductors. The quantity $\kappa = l(l+1) - j(j+1) - 1/4$ defines the dependence of the energy E on the orbital angular momentum quantum number l and total angular momentum quantum number j. The effective mass of charge carriers in each of the semiconductors is related to the energy gap $2\Delta(r)$ by the expression $\Delta_{1,2} = m_{1,2}s^2$, where s is the Kane's matrix element ("speed of light"). We count the energy from the midgap whose position is the same in both semiconductors.

A solution to system (1) can be written in the analytical form. In the cases of $r < R$ and $r > R$, the functions ψ_1 and ψ_2 are expressed in terms of degenerate hypergeometric functions of the first kind $F(a, c, \rho)$ (for $r < R$) and of the second kind, $G(a, c, \rho)$ (for $r > R$) (see, e.g., [10]) that depend on the energy E as a parameter. We obtain the eigensolutions of system (1) by imposing the continuity conditions on ψ_1 and ψ_2, i.e.,

$$\left.\frac{\psi_1}{\psi_2}\right|_{r=R-0} = \left.\frac{\psi_1}{\psi_2}\right|_{r=R+0}.$$

With the quantum-dot sizes of interest, i.e., for $R \le a_x$ (where a_x is the Bohr radius of a donor in the bulk of the first semiconductor), $E > \Delta_1$ because the contribution of the size-quantization effect to the energy is larger than the negative contribution from Coulomb interaction. In what follows, we restrict our consideration to the case $E < \Delta_2$ when the equation defining the energy levels is of the form

$$\sqrt{\frac{E/\Delta_1 - 1}{E/\Delta_1 + 1}}\,\frac{\mathrm{Im}\Phi}{\mathrm{Re}\Phi} = \Lambda, \quad (2)$$

where

$$\Lambda = -\frac{\sqrt{1 - \frac{E}{\Delta_2}}\,G(a_2, c, \rho_2) + \frac{(a_2 - c + 1)a_2}{\gamma - \kappa - a_2}G(a_2 + 1, c, \rho_2)}{\sqrt{1 + \frac{E}{\Delta_2}} - G(a_2, c, \rho_2) + \frac{(a_2 - c + 1)a_2}{\gamma - \kappa - a_2}G(a_2 + 1, c, \rho_2)},$$

$$\Phi = a_1 e^{i\theta - ipR} F(a_1 + 1, c, 2\frac{ipR}{\hbar s}),\ p = \sqrt{E^2 - \Delta_1^2},\ \gamma = \sqrt{\kappa^2 - \alpha^2},$$

$$\alpha = \frac{Ze^2}{\hbar s\epsilon},\ \xi = \frac{\alpha E}{p},\ a_2 = \gamma - \frac{\alpha E}{\lambda},\ c = 2\gamma + 1,\ \lambda = \sqrt{\Delta_2^2 - E^2}.$$

$$a_1 = \gamma + i\xi,\ \rho_2 = 2\frac{\lambda}{\hbar s}R,\ e^{2i\theta} = \frac{\gamma - i\xi}{-\kappa - i\frac{\Delta_1\xi}{E}}.$$

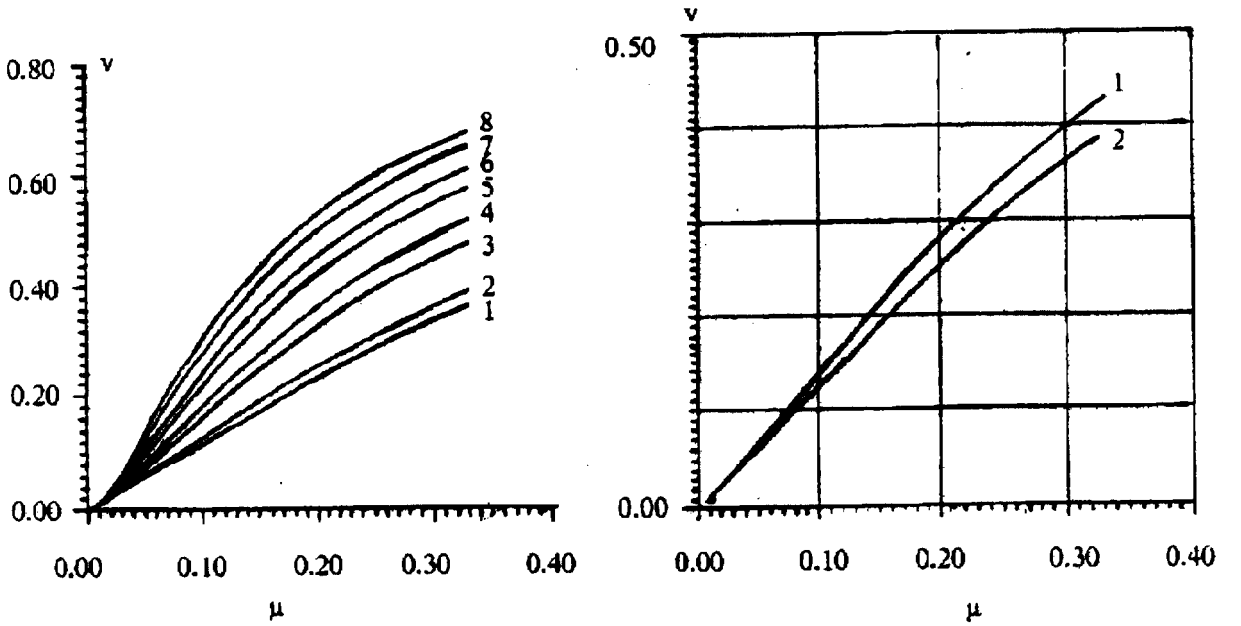

Fig. 1. The relative dimensionless energy v, of size-quantization levels as a function of the energy-gap width characterized by μ. (1) a level with $\kappa = -1$ and $n = 1$ (n is the number of the level in the order of increasing energy with κ kept constant); (2) $\kappa = 1$ and $n = 1$; (3) $\kappa = -1$ and $n = 2$; (4) $\kappa = 1$ and $n = 2$; (5) $\kappa = -1$ and $n = 3$; (6) $\kappa = 1$ and $n = 3$; (7) $\kappa = -1$ and $n = 4$; and (8) $\kappa = 1$ and $n = 4$.

Fig. 2. The splitting of the first excited level as a function of the energy-gap width μ. (1) $\kappa = 1$ and $n = 1$ and (2) $\kappa = -2$ and $n = 1$.

A quantity α (the "fine structure constant") defines the effect of finitiness of the energy gap on the electron-binding energy for donors and can reach values of 0.1 - 0.2 in certain semiconductors. Hereafter, for the sake of simplicity, we restrict ourselves to the case of $\delta = 0$, i.e., we consider a nanostructure with a narrow-bandgap semiconductor in contact with an insulator (or vacuum); under these conditions $\Lambda = 1$. In order to determine the electron-binding energy for a donor, we first evaluate a contribution of the size-quantization effect to the energy. If there is no impurity atom (i.e., $\alpha = 0$), equation (2) is reduced to

$$\mu\frac{\kappa}{|\kappa|}\sqrt{\lambda}\,J_{|\kappa-\frac{1}{2}|}(2\sqrt{\lambda(2+\lambda\mu^2)})+\sqrt{1+\mu^2\lambda}\,J_{|\kappa+\frac{1}{2}|}(2\sqrt{\lambda(2+\lambda\mu^2)})=0, \qquad (3)$$

where $\lambda = (E-\Delta_1)/\tilde{E}$, $\mu = \sqrt{\tilde{E}/\Delta_1}$, and $\tilde{E} = \frac{\hbar^2}{mR^2}$.

In the case of wide-bandgap semiconductors, i.e., for $\mu = 0$, the size-quantization levels are defined by the conventional equation [9]

$$J_{|\kappa+\frac{1}{2}|}(\sqrt{2\lambda}) = 0.$$

Allowance for finiteness of the energy-gap width leads to violation of the quadratic dependence of the energy on R^{-1}, which is characteristic of the case $\mu = 0$. As can be inferred from (3), the quantity $v = (\lambda_{\mu=0}-\lambda_\mu)/\lambda_{\mu=0}$ defining the relative lowering of the size-quantization level when the energy-gap finiteness is involved, depends on μ only. The results of numerical calculations are shown in Fig. 1.

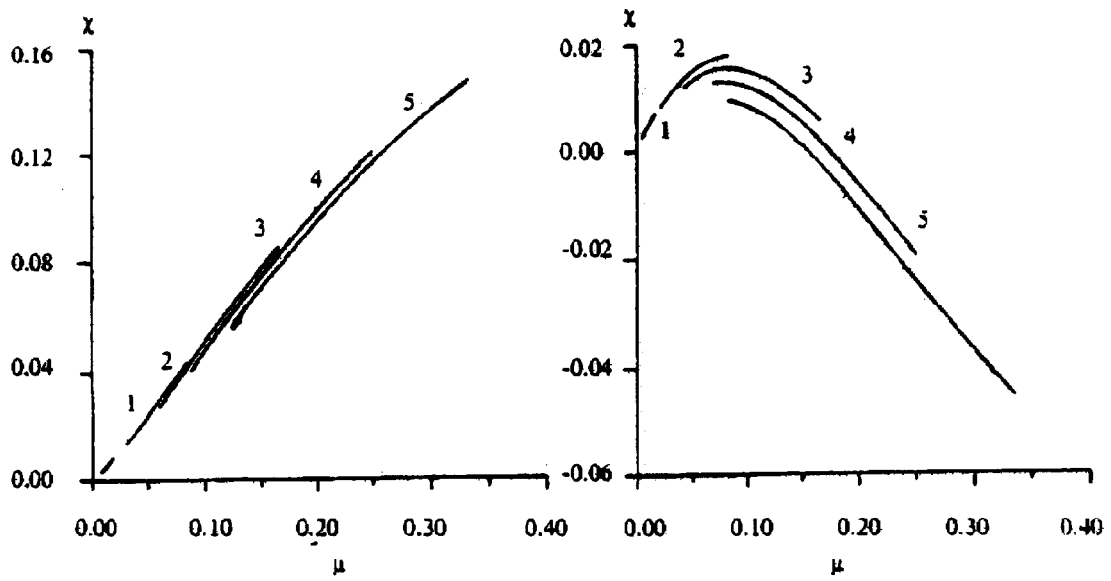

Fig. 3. The binding energy χ for the ground state ($\kappa = -1$ and $n = 1$) as a function of the energy-gap width μ. $\chi = (\tilde{\lambda}_\infty - \tilde{\lambda})/\tilde{\lambda}_\infty$, where $\tilde{\lambda} = \lambda_{\alpha=0} - \lambda_\alpha$ and $\tilde{\lambda}_\infty$ is the value of $\tilde{\lambda}$ in the limit of the infinite energy-gap width μ. (1) $\alpha = 0.01$; (2) $\alpha = 0.05$; (3) $\alpha = 0.1$; (4) $\alpha = 0.15$; and (5) $\alpha = 0.2$.

Fig. 4. The binding energy χ for the level with $\kappa = 1$ and $n = 1$ as a function of the energy-gap width μ. (1) $\alpha = 0.01$; (2) $\alpha = 0.05$; (3) $\alpha = 0.1$; (4) $\alpha = 0.15$; and (5) $\alpha = 0.2$.

The size-quantization levels are lowered as the parameter μ increases. The larger the size-quantization energy in the case of an infinitely wide gap, the more pronounced the relative effect of variation in the energy-gap width. With experimentally attainable values of μ (e.g.,

$\mu = 0.4$). the effect of finiteness of the energy gap is quite substantial ($0.35\lambda_{\mu=0}$) for the ground state. This effect also manifests itself in the splitting of the levels with the same values of l and degenerate with respect to κ for $\mu = 0$. Figure 2 illustrates this splitting for the first excited level. The magnitude of splitting is proportional to $\mu\lambda_{\mu=0}$. If there is an impurity center in the dot. then equation (2), which defines the energy levels for $\delta = 0$. is of the form

$$\sqrt{2+\lambda\mu^2}\mathrm{Re}\Phi - \mu\sqrt{\lambda}\mathrm{Im}\Phi = 0,$$

where

$$\Phi = \sqrt{\left(\gamma + i\frac{Z\alpha(1+\lambda\mu^2)}{\mu\sqrt{\lambda(2+\lambda\mu^2)}}\right)\left(-\kappa + i\frac{Z\alpha}{\mu\sqrt{\lambda(2+\lambda\mu^2)}}\right)}\, e^{-i\sqrt{\lambda(2+\lambda\mu^2)}}\times$$

$$\times F\left(\gamma + 1 + i\frac{Z\alpha(1+\lambda\mu^2)}{\mu\sqrt{\lambda(2+\lambda\mu^2)}}, 2\gamma+1, 2i\sqrt{\lambda(2+\lambda\mu^2)}\right).$$

The results of calculations for the ground state are shown in Fig. 3. The binding energy decreases with increasing α, i.e., with decreasing width of the energy gap. In the case of excited levels, the finite width of the energy gap results in more diversified effects of parameter α. Thus, the binding energy for the first excited state at $\kappa = 1$ increases with reasonably large α, as is evident from Fig. 4. However, it is pertinent to note that variation in the binding energy when the finiteness of the energy-gap width is included is less marked than a similar variation for the size-quantization levels (this difference amounts to the factor of 2.5 for the ground state).

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