lew mechanism of exciton self-localization in luasi-one-dimensional and quasi-two-dimensional ;emiconductors

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In quasi-one-dimensional and quasi-two-dimensional systems, the Coulomb attraction between bound electrons and holes in different planes or on different filaments leads to deformation of the lattice and the production of self-localized excitons with large translational mass, even in those cases when the interaction with the lattice of the free carriers is negligibly small.

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In quasi-one-dimensional and quasi-two-dimensional systems with states orresponding to spatially-separated electrons and holes, the Coulomb interctions of the quasiparticles with one another leads in a number of cases to the ppearance of spontaneous lattice deformation, is in a certain sense the analog f polaron effects. This deformation, however, can occur also under conditions hen the ordinary constants for the scattering of free quasiparticles by phonons re negligibly small, as will be assumed below.

To illustrate the foregoing we consider, just as in[1] large-radius excitons. he electron and hole that lie on different planes or strings, being attracted to ach other, deform the planes (filaments). The result is a gain in the Coulombteraction energy, and this can lead to localization of the exciton as a unit in ie produced deformation region. The deformation accompanying the exciton iotion then increases appreciably its translational mass.

We start from the strong-coupling approximation well known in the theory of irge-radius polarons[2] and assume, for simplicity, that the radius of the inernal motion of the exciton is small in comparison with the dimension of the eformation region. Then, in the static approximation, the system energy is iven by

$$F = \frac{\hbar^2}{2m} \int |\nabla\psi|^2 d\mathbf{r} - \frac{\partial E}{\partial d} \int d\mathbf{r}\, u(\mathbf{r}) |\psi(\mathbf{r})|^2 + \frac{1}{2} \sum_{\mathbf{k}} \omega_{\mathbf{k}}^2 |q_{\mathbf{k}}|^2, \qquad (1)$$

here $\psi(r)$ is the wave function of the motion of the center of gravity of the exiton, E is its internal energy in the undeformed crystal,[1] d is the distance etween the planes (filaments), $u(\mathbf{r})$ is the deformation-induced change of this istance, and m is the combined effective mass of the electron and hole. The ist term in (1) takes into account the energy of the static deformation of the ittice.

We express $u(\mathbf{r})$ in terms of the normal coordinates q_k, and then, minimizing with respect to q_k, obtain the connection between $u(\mathbf{r})$ and $|\psi(\mathbf{r})|^2$. Substitutig the obtained expression for $u(\mathbf{r})$ in (1), we obtain a functional that depends only on $\psi(\mathbf{r})$. The obtained functional coincides in form with that considered in[5], where it is shown that in the one-dimensional case the problem of minimization admits of an exact solution. To estimate the minimum in a two-dimensional system, it suffices to choose a simple form of the trial function $\psi(\mathbf{r})\exp(-\kappa|\mathbf{r}|)$. As a result, assuming a Debye spectrum, we obtain for a quasi-one-dimensional system ($E_1 = e^2/d\sqrt{\epsilon_{\parallel}\epsilon_{\perp}}$).

$$F_1 = -\frac{a^2 m}{2\hbar^2}, \tag{2}$$

and for a quasi-two-dimensional system ($E_2 = e^2/d\epsilon_{\parallel}$)

$$F_2 = \frac{\hbar^2\kappa^2}{2m} - \beta\kappa^2 \tag{3}$$

where

$$a = \frac{e^4}{2\pi d^4 \rho\epsilon_{\perp}\epsilon_{\parallel}}\left(\frac{1}{c_l^2} + \frac{1}{2c_t^2}\right), \tag{4}$$

$$\beta = \frac{e^4}{2\pi d^3 \epsilon_{\parallel}^2 \rho c_l^2}. \tag{5}$$

In expressions (4) and (5), ρ is the density of the medium, c_l and c_t are the velocities of the longitudinal and transverse sound, while $\epsilon_{\parallel}$ and $\epsilon_{\perp}$ are the principal values of the dielectric tensor. For quasi-one-dimensional systems, the homogeneous state is always unstable. For the parameters values

$$\epsilon_{\parallel}\epsilon_{\perp} = 100,\ \bar{c}^2 = c_l^2\left(1 + \frac{c_l^2}{2c_t^2}\right)^{-1} = 2\times 10^9\ \text{cm}^2/\text{sec}^2,\ d = 6\text{Å},$$

we obtain for the dimension of the deformed region $2\kappa^{-1} = 2\hbar^2/\alpha m = 40$ Å $\gg \bar{x} = 8$ Å ($\bar{x}$ is the internal dimension of the exciton).[1] For the parameters considered above we have $|F_1| = 8\times 10^{-3}$ eV $\gtrsim \hbar\omega_0$, where ω_0 is the Debye frequency. Therefore, strictly speaking, some refinements of the estimates must be made within the framework of the intermediate-coupling approximation.

To find the translational mass of the new exciton plus deformation quasiparticle, we assume, just as in[3], that the exciton and the deformation move as a unit with velocity v. Taking into account in (1) additionally the kinetic energy of the lattice motion $T = (1/2)\sum_k |\dot{q}_k|^2$, we get

$$m^* = m + \frac{e^4\kappa^3}{4\pi d^2 \epsilon_{\parallel}\epsilon_{\perp}\rho c_l^4}\left[3 + \frac{c_l^4}{2c_t^4}\right]\ln\frac{1}{\kappa d}. \tag{6}$$

For the considered parameters $m^* \approx 200 m_e$, and increases strongly with decreasing dimension of the deformation region (m_e is the electron mass). For a quasi-two-dimensional system, as seen from (3), consequently, the "localized" state of the exciton in the considered region is produced only at $\beta > \hbar^2/2m$. Inasmuch as in this case the gain of energy in the deformed state increases monotonically with decreasing dimension of the deformed region, the equilibrium alue $\kappa \gtrsim 1/\bar{x}$ cannot be obtained within the framework of the employed approach, here it is assumed $\kappa\bar{x} \ll 1$. As seen from (3) and (5), the condition for the onet of deformation is of the form $e^2 m/\pi d^3 \epsilon_{\parallel}^2 c_l^2 \rho \hbar^2$, and this condition is satisfied, or example, when $\epsilon_{\parallel} = 3$, $m = 2m_e$, $d = 8$ Å, $c_l = 0.7 \times 10^5$ cm/sec, and $\rho = 1$ g/m^3.

We note in conclusion that the lattice-deformation effect produced by the electron-hole attraction in the systems considered here can stimulate the onset of nstability of the homogeneous state of electrons and holes, and in particular, ead to stabilization of the electron-hole drops. In addition, in a semiconductor ith a narrow forbidden band this effect can, generally speaking, lead to intability of the ground state of the semiconductor relative to the spontaneous roduction of self-localized excitons or clusters (drops). These effects of selfocalization and increase of the translational mass of the excitons are important lso in systems of the indicated type when the phenomena discussed in[1,4] are onsidered (exciton insulator, electron-hole drops, exciton superfluidity, etc.).

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