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SEMICONDUCTOR STRUCTURES, LOW-DIMENSIONAL SYSTEMS, AND QUANTUM PHENOMENA

Wannier–Mott Excitons in Semiconductors with a Superlattice

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Abstract—The effect of the motion of a Wannier–Mott exciton in semiconductors with a superlattice formed by heterojunctions on the exciton binding energy and wave function is analyzed. This effect arises as a result of the fact that the dispersion laws of the electron and hole that form an exciton in a superlattice differ from the quadratic law. The investigated one-dimensional superlattice consists of alternating semiconductor layers with different energy positions of the conduction and valence bands, i.e., with one-dimensional wells and barriers. The exciton state in a superlattice consisting of quantum dots is analyzed. It is demonstrated that the closer the electron and hole effective masses, the greater the dependence of the binding energy on the exciton quasi-momentum. The possibility of replacing the tunneling excitation transfer between superlattice cells with the dipole–dipole one at certain exciton quasi-wave vector values is investigated.

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1. INTRODUCTION

This study is aimed at elucidation of the effect of motion of the Wannier–Mott exciton center of inertia in semiconductors with a superlattice (SL) formed by heterojunctions on the exciton binding energy and wave function. Consideration of this effect arises because the dispersion laws of the electron and hole that form an exciton in the SL are significantly different from quadratic law. First, we consider a one-dimensional (1D) SL consisting of alternating semiconductor layers with different energy positions of the conduction and valence bands, i.e., with one-dimensional wells and barriers. Then, we generalize our analysis to a three-dimensional (3D) SL consisting of quantum dots (QDs). We demonstrate that the binding energy and structure of the exciton strongly depend on its motion as a whole.

2. LAYERED SUPERLATTICE

Here, we discuss a semiconductor structure consisting of alternating semiconductor layers with different band gaps, which form a periodic sequence of potential wells and barriers for electrons and holes. Hereinafter, we investigate a SL with barriers that are high enough to limit the consideration to the amplitudes of tunneling between only the nearest potential wells for both holes and electrons.

We seek the exciton wave function in the form[1]

$$\Psi(x_e, \boldsymbol{\rho}_e; x_h, \boldsymbol{\rho}_h) = \sum_{n_e, n_h} \Phi(n_e, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h) w_e(x_e - an_e) w_h(x_h - an_h). \quad (1)$$

Here, x_e and x_h are the electron and hole coordinates along the SL axis, respectively; a is the SL period; $\boldsymbol{\rho}_e$ and $\boldsymbol{\rho}_h$ are the electron and hole coordinates in the SL-layer plane; $w_e(x_e - an_e)$ and $w_h(x_h - an_h)$ are the Wannier functions [1] of an electron and a hole localized in layers with numbers n_e and n_h, respectively; and $\Phi(n_e, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h)$ is the envelope function describing the relative motion of an electron and a hole in an exciton and its motion as a whole.

We assume the motion of an electron and a hole along the SL layers to be free and described by respective the effective masses m_e and m_h.[2]

In the nearest neighbor approximation, the equation for the envelope function acquires the form

$$\left[-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial\boldsymbol{\rho}_e^2} - \frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial\boldsymbol{\rho}_h^2} - V(\boldsymbol{\rho}_e - \boldsymbol{\rho}_h, n_e - n_h)\right] \times \Phi(n_e, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h) + \frac{J_e}{2}[2\Phi(n_e, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h) - \Phi(n_e + 1, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h) - \Phi(n_e - 1, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h)] + \frac{J_h}{2}[2\Phi(n_e, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h) - \Phi(n_e, \boldsymbol{\rho}_e; n_h + 1, \boldsymbol{\rho}_h) - \Phi(n_e, \boldsymbol{\rho}_e; n_h - 1, \boldsymbol{\rho}_h)] = (E - E_G)\Phi(n_e, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h). \quad (2)$$

Here, J_e and J_h are the electron and hole resonance integrals, which relate the neighboring wells and E_G is the energy gap. The energy scale was chosen so that in the absence of interaction the energies of an electron and a hole with zero quasimomenta were equal to E_G

[1] For the sake of briefness, here we assume the hole wave function to be scalar.

[2] We note that these masses, especially the hole mass, may depend on the thickness of the quantum wells that form the SL.

and zero, respectively.[3] The potential describing the Coulomb attraction between an electron in the well with the number n_e and the in-plane coordinate $\boldsymbol{\rho}_e$ and a hole in the well with the number n_h and the in-plane coordinate $\boldsymbol{\rho}_h$ is

$$V(\boldsymbol{\rho}_e - \boldsymbol{\rho}_h, n_e - n_h) = -\frac{e^2}{\epsilon}\int\int dx_e dx_h \times \frac{1}{\sqrt{(x_e - x_h)^2 + (\boldsymbol{\rho}_e - \boldsymbol{\rho}_h)^2}} w_e(x_e - an_e)^2 w_h(x_h - an_h)^2. \quad (3)$$

For the sake of briefness, here we disregard variations in the permittivity ϵ from layer to layer[4] because of their relative smallness in heterostructures based on III–IV compounds.

Obviously, at distances smaller than or comparable to the thickness of the quantum wells that form the SL, the amplitude of this potential is smaller than that of the Coulomb potential due to smearing of the electron and hole charges, which is described in expression (3) by the squared Wannier function.

By virtue of the translational invariance of Eq. (2) in the SL plane, we can, as usual, separate the coordinates of the center of mass and the relative motion

$$\mathbf{R} = \frac{m_e\boldsymbol{\rho}_e + m_h\boldsymbol{\rho}_h}{m_e + m_h} \quad \text{and} \quad \boldsymbol{\rho} = \boldsymbol{\rho}_e - \boldsymbol{\rho}_h.$$

Then, the envelope function acquires the form

$$\Phi(n_e, \boldsymbol{\rho}_e; n_h, \boldsymbol{\rho}_h) = e^{i\mathbf{PR}}\varphi(n_e, n_h; \boldsymbol{\rho}). \quad (4)$$

By virtue of the periodicity of the SL, the equation for the envelope is invariant relative to an identical shift in the site numbers for an electron and a hole by an integer number of periods N

$$\{n_e; n_h\} \longrightarrow \{n_e + N, n_h + N\}. \quad (5)$$

It is convenient to seek the envelope in the form

$$\varphi(n_e, n_h; \boldsymbol{\rho}) = e^{i[Q/2 - \gamma(Q)]n_e + i[Q/2 + \gamma(Q)]n_h}\chi_Q(n; \boldsymbol{\rho}), \quad (6)$$

where $n = n_e - n_h$.

Upon translation (5), the wave function (6), as it should, acquires the phase factor e^{iQN}. Thus, parameter Q plays the role of dimensionless quasi-momentum of the center of mass of the exciton in the SL-axis direction and lies between $-\pi$ and π. The $\gamma(Q)$ phase should be selected so that the obtained equation for the function $\chi_Q(n_e - n_h; \boldsymbol{\rho})$ is dependent only on the difference $n_e - n_h$. Substituting function (6) into Eq. (2), we see that we should choose

$$\gamma(Q) = \arctan\left(\frac{J_e - J_h}{j_e + J_h}\tan\frac{Q}{2}\right).$$

Substituting this into Eq. (2), we obtain the following equation for the function $\chi_Q(n; \boldsymbol{\rho})$ describing an exciton in the system of relative coordinates of an electron and a hole:[5]

$$\left[-\frac{1}{2m_r}\frac{\partial^2}{\partial\boldsymbol{\rho}^2} - V(\boldsymbol{\rho}, n)\right]\chi_Q(n; \boldsymbol{\rho}) + \frac{J(Q; J_e, J_h)}{2} \times [2\chi_Q(n; \boldsymbol{\rho}) - \chi_Q(n+1; \boldsymbol{\rho}) - \chi_Q(n-1; \boldsymbol{\rho})] = \left[E - E_G - \frac{\mathbf{P}^2}{2(m_e - m_h)} - K(Q; J_e, J_h)\right]\chi_Q(n; \boldsymbol{\rho}). \quad (7)$$

Here, the resonance integral

$$J(Q; J_e, J_h) = \sqrt{(J_e + J_h)^2 - 2J_eJ_h(1 - \cos Q)} \quad (8)$$

describes the relative motion in the electron–hole pair with the quasi-momentum Q/a along the SL axis. The kinetic energy of the electron–hole pair with the quasi-momentum Q/a of the center of mass along the SL axis is

$$K(Q; J_e, J_h) = J_e + J_h - \sqrt{(J_e + J_h)^2 - 2J_eJ_h(1 - \cos Q)}. \quad (9)$$

The kinetic energy of motion of the center of mass in the plane of SL layers with momentum $\mathbf{P}$ is, as usual, $P^2/2(m_e + m_h)$ and $m_r = \frac{m_em_h}{m_e + m_h}$ is the reduced mass in the layer plane.

First, let us discuss expression (9) for the kinetic energy of exciton motion along the SL axis. At small Q values, we obtain

$$K(Q; J_{[e}, J_h) \approx \frac{1}{2}\frac{J_eJ_h}{2J_e + J_h}a^2\left(\frac{Q}{a}\right)^2. \quad (10)$$

It is worth noting that, in the nearest neighbor approximation, the kinetic energy of motion of an electron (hole) with the quasi-momentum q/a along the SL axis is

$$K_{e(h)}(q) = J_{e(h)}[1 - \cos(q)].$$

Therefore, the components of the electron and hole effective masses along the SL axis near the bottom of the miniband ($|q| \ll \pi$) are

$$m_e^{\parallel} = 1/J_ea^2, \quad m_h^{\parallel} = 1/J_ha^2.$$

[3] Naturally, the value depends on the quantum-well width and barrier thickness and height.

[4] The effect of the difference between permittivities on the exciton binding energy in thin films was studied in [2, 3].

[5] Hereinafter Planck's constant is assumed to be $\hbar = 1$.

Thus, the kinetic energy of exciton motion along the SL axis at small momenta (10) acquires the rather natural form

$$K(Q; J_e, J_h) \approx \frac{1}{2}\frac{1}{m_e^{\parallel} + m_h^{\parallel}}\left(\frac{Q}{a}\right)^2, \qquad (11)$$

which involves the resulting electron and hole mass.

At the boundary of the SL Brillouin zone ($Q = \pm\pi$), we have

$$K(Q; J_e, J_h) = J_e + J_h - |J_e - J_h|,$$

i.e.,

$$K(Q; J_e, J_h) = 2\min\{J_e, J_h\} = \frac{2}{a^2}\min\left\{\frac{1}{m_e^{\parallel}}, \frac{1}{m_h^{\parallel}}\right\}.$$

Thus, it is the heavy particle that determines exciton motion along the SL axis at all values of the quasi-momentum Q/a, which is completely natural. It is also natural that at $J_h \ll J_e$ the exponent in wave function (6) with regard to the expression for $\gamma(Q)$ transforms into e^{iQn_h}, which corresponds to coincidence of the coordinate of the center of inertia with the coordinate of the heavy particle, i.e., hole. If $J_h = J_e$, i.e., the components of the electron and hole masses along the SL axis are equal, then $\gamma(Q) = 0$ and the exponent $e^{iQ(n_h + n_h)/2}$ corresponds to the coordinate of the center of inertia at the same distance from both of them.

Now, let us pass to resonance integral (8) which describes the relative motion of an electron and a hole along the SL axis in the exciton. At $Q = 0$, we have

$$J(0; J_e, J_h) = J_e + J_h,$$

or, with (11) taken into account,

$$J(0; J_e, J_h) = \left(\frac{1}{m_e^{\parallel}} + \frac{1}{m_h^{\parallel}}\right)\frac{1}{a^2}.$$

Thus, at $Q = 0$, the relative motion along the SL axis is determined by the longitudinal component of the reduced mass. As the momentum of the center of mass is increased, the resonance integral decreases and at $Q = \pm\pi$,

$$J(\pm\pi; J_e, J_h) = \left|\frac{1}{m_e^{\parallel}} - \frac{1}{m_h^{\parallel}}\right|\frac{1}{a^2}.$$

If the resonance integrals and, consequently, the electron and hole masses are similar, then the relative motion along the SL axis becomes difficult. In the limit of equal masses,[6] both the electron and hole of the exciton appear localized, each in its own SL well. The dependence of the resonance integral $J(Q)$ in units of J_e on the quasi-momentum for three values of the ratio J_h/J_e is presented in Fig. 1.

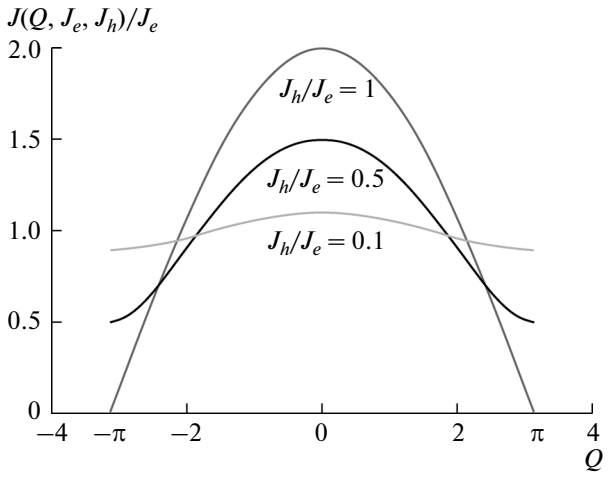

Fig. 1. Dependence of the resonance integral $J(Q; J_e, J_h)$ in units of J_e on the quasi-momentum for three values of the J_h/J_e ratio.

3. EXCITON BINDING ENERGY IN A LAYERED SUPERLATTICE

The exciton binding energy is determined as the eigenvalue of the Hamiltonian

$$\langle n|\hat{H}_{\text{exc}}|n'\rangle = \left[-\frac{1}{2m_r}\frac{\partial^2}{\partial\boldsymbol{\rho}^2} - V(\boldsymbol{\rho}, n)\right]\delta_{n,n'} + \frac{J(Q;J_e,J_h)}{2}(2\delta_{n,n'} - \delta_{n+1,n} - \delta_{n-1,n'}), \qquad (12)$$

where $\delta_{n,n'}$ is the Kronecker symbol. We should consider two limiting cases.

3.1. Exciton with Blocked Motion along the SL Axis ($J(Q; J_e, J_h) = 0$)

The eigenfunctions of Hamiltonian (12) at zero resonance integral $J(Q; J_e, J_h)$ have the form[7]

$$\chi^N_{Q,\nu}(n;\boldsymbol{\rho}) = \delta_{n,N}\psi_{\nu,N}(\boldsymbol{\rho}), \qquad (13)$$

where ν is the set of eigenvalues of the axial moment and number of the state and the eigenfrequencies E^N_ν depend on the number N of periods separating the electron and hole and playing the role of a quantum number. The wave functions $\psi_{\nu,N}(\boldsymbol{\rho})$ in (13) are the

[6] This is attainable in a structure where the barrier separating the wells is lower for holes than for electrons.

[7] It should be noted that set of functions (13) forms a complete system in the framework of the one-miniband approximation for electrons and holes:

$$\sum_{\nu,N}\chi^N_\nu(n;\boldsymbol{\rho})\chi^{-N}_\nu(n';\boldsymbol{\rho}') = \delta_{n,n'}\delta(\boldsymbol{\rho}-\boldsymbol{\rho}').$$

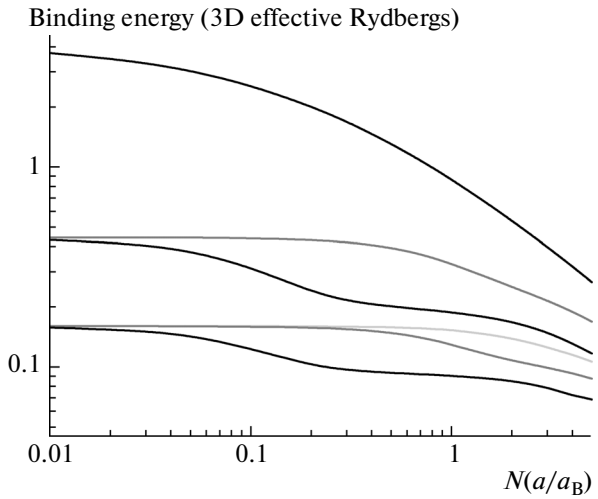

Fig. 2. Dependence of the binding energy of an exciton on the distance between the electron and hole of the exciton along the SL axis for the first three values of the angular momentum in the SL-layer plane [5].

eigenfunctions of the two-dimensional (2D) Hamiltonian

$$-\frac{1}{2m_r}\frac{\partial^2}{\partial\boldsymbol{\rho}^2} - V(\boldsymbol{\rho}, N),$$

which describe the excitons in the eigenstate with quantum numbers ν. In the limit of a very deep and narrow well, potential (3) can be replaced with

$$V(\boldsymbol{\rho}, N) = \frac{e^2}{\epsilon}\frac{1}{\sqrt{\boldsymbol{\rho}^2 + a^2N^2}}. \quad (14)$$

At $N = 0$, we deal with a 2D exciton, the binding energy of which at $N = 0$ is $4E_B$, where the Bohr energy of the 3D exciton is

$$E_B = \frac{e^4 m_r}{2\epsilon^2\hbar^2}.$$

The binding energies of the ground and excited states of the exciton are [4]

$$E_B/(s - 1/2)^2,$$

where $s = 1, 2, 3$ is the main quantum number ($s = 1$ corresponds to the ground state). Due to the well-known degeneracy of a system with Coulomb interaction at $N = 0$, the binding energy is independent of the angular momentum. We note that, in the general case of potential (3), this degeneracy is lifted [5].

Obviously, in this approximation, eigenfunction (13) and the eigenenergy of relative motion are independent of the momentum of the center of inertia, since we disregarded the term with $J(Q; J_e, J_h)$ in (12). The sequence of values $N = 0, 1, 2,...$corresponds to an exciton consisting of an electron and a hole in the same SL potential well ($N = 0$) and spatially indirect excitons in which the electron and hole are separated by one ($N = 1$), two ($N = 2$), etc. barriers. It is clear that the larger the N value, the lower the binding energy $E_{\nu, N}$ of the exciton.

Figure 2 shows the dependences of energies E_ν^N of several lower states of the exciton on the parameter $(a/a_B)N$ in the SL [5] in the limit of a very deep and narrow well, when the potential of the electron–hole interaction can be presented in form (14). It can be seen that at $N \neq 0$, the degeneracy by the angular momentum is lifted and the levels are split [5].

At nonzero values of the resonance integral $J(Q; J_e, J_h)$, the term nondiagonal in terms of n can be taken into account using perturbation theory, if the distances between the energy levels exceed its value. For highly excited exciton states and/or large N values, this is incorrect and the possible resonances of states should be taken into account.

3.2. "Three-Dimensional" Exciton $J(Q; J_e, J_h) \neq 0$

We assume that a three-dimensional (3D) exciton is an exciton with a wave function along the 1D SL axis that is much longer than its period. In this case, Hamiltonian (12) can be reduced to the continuum limit

$$\hat{H}_{exc} = -\frac{1}{2m_r}\frac{\partial^2}{\partial\boldsymbol{\rho}^2} - \frac{J(Q; J_e, J_h)a^2}{2}\frac{\partial^2}{\partial z^2} - V(\boldsymbol{\rho}, z). \quad (15)$$

In expression (12), we replaced the number n of the SL cell multiplied to the period a by the continuous coordinate z directed along the SL axis and the difference operator in the latter parenthesis of (12), with the second derivative in respect to z multiplied to the squared period. It can be seen from expression (15) that the value $M = 1/J(Q; J_e, J_h)a^2$ plays the role of a component of reduced mass along the SL axis. It differs from the reduced mass in the plane (as a rule, exceeds the latter).

The problem with the Coulomb bound state of a particle with anisotropic mass has a long history. It was considered in relation to the donor states in germanium and silicon, where the isoenergy surfaces for electrons are extended ellipsoids of revolution [4].

If the reduced mass along the SL axis far exceeds that along the layers, we can use the adiabatic approximation and obtain the energy of the exciton ground state with the lowest correction by the mass ratio, as was done in [4] for the donor states in Si and Ge,

$$E_0 = -4E_B[1 - 2.58(m_rJa^2)^{1/3}].$$

In the same approximation, the characteristic extent of the wave function along the SL axis is

$$\tilde{z} \sim a_B\left(\frac{m_rJa^2}{32}\right)^{1/3}.$$

The essence of the approximation used in [4] and reformulated for a exciton consists in the fact that the rapid relative motion forms a 2D exciton and slow motion along the SL axis is quantized in a triangular well formed by a 2D charge with the edge effect disregarded. The latter is applicable, since the length of localization along the SL axis is much smaller than the 2D exciton radius. On the other hand, the continuum approximation is valid if this length exceeds the SL period,

$$a \ll \tilde{z} \ll a_B/2,$$

or, with regard to the fact that for the ground state in the purely 2D case, $a_B^{2D} = a_B/2$ and $E_B^{2D} = 4E_B$ (index 2D indicates the 2D exciton),

$$\frac{a}{a_B^{2D}} \ll \frac{J}{8E_B^{2D}} \ll \left(\frac{a_B^{2D}}{a}\right)^2. \quad (16)$$

These conditions can be met only if the SL period is much smaller than the Bohr radius of the 2D exciton, $a/a_B^{2D} \ll 1$, and the ratio between the miniband width and the Bohr energy lies in a rather narrow range. We note that, although the dependence of the resonance integral J on a is of the power-law type, the exponential dependence of this integral on the height and thickness of the barrier separating the potential wells is the most important. Therefore, we consider the resonance integral as an independent parameter.

4. SUPERLATTICE COMPOSED OF QUANTUM DOTS

Now, let us briefly discuss the properties of excitons in a SL composed of quantum dots (QDs) using the one-miniband approximation once again. The wave function of the electron–hole pair should be presented in the form

$$\Psi(\mathbf{r}_e, \mathbf{r}_h) = \sum_{\mathbf{R}_e, \mathbf{R}_h} \Phi(\mathbf{R}_e, \mathbf{R}_h) w_e(\mathbf{r}_e - \mathbf{R}_e) w_h(\mathbf{r}_h - \mathbf{R}_h). \quad (17)$$

where $\mathbf{r}_e$ and $\mathbf{r}_h$ are the electron and hole coordinates, respectively; $\Phi(\mathbf{R}_e, \mathbf{R}_h)$ is the envelope function of the electron–hole pair; $\mathbf{R}_e$ and $\mathbf{R}_h$ are the coordinates of QD sites in the SL; and $w_e(\mathbf{r}_e - \mathbf{R}_e)$ and $w_h(\mathbf{r}_h - \mathbf{R}_h)$ are the Wannier functions.

For the sake of briefness, we limit consideration to a simple cubic or square (in the 2D structure) SL composed of QDs, taking into account tunneling amplitudes only between the nearest neighbors. Then, Eq. (2) for the envelope acquires the form

$$\begin{aligned}[-V(\mathbf{R}_e - \mathbf{R}_h)]\Phi(\mathbf{R}_e, \mathbf{R}_h) + \sum_i \frac{J_e}{2}[2\Phi(\mathbf{R}_e, \mathbf{R}_h) \\ - \Phi(\mathbf{R}_e + a\mathbf{e}_i, \mathbf{R}_h) - \Phi(\mathbf{R}_e - a\mathbf{e}_i, \mathbf{R}_h)] \\ + \sum_i \frac{J_h}{2}[2\Phi(\mathbf{R}_e, \mathbf{R}_h) - \Phi(\mathbf{R}_e, \mathbf{R}_h + a\mathbf{e}_i) \\ - \Phi(\mathbf{R}_e, \mathbf{R}_h - a\mathbf{e}_i)] = (E - E_G)\Phi(\mathbf{R}_e, \mathbf{R}_h).\end{aligned} \quad (18)$$

Here, $J_{e(h)}$ is, as previously, the electron (hole) resonance integrals, a is the SL period, and $\mathbf{e}_i$ are the unitary vectors along the SL axes ($i = x, y, z$ or $i = x, y$ for the 2D structure).

The Coulomb interaction potential is

$$\begin{aligned}V(\mathbf{R}_e - \mathbf{R}_h) = \frac{e^2}{\epsilon}\iint d\mathbf{r}_e d\mathbf{r}_h \frac{1}{|\mathbf{r}_e - \mathbf{r}_h|} \\ \times w_e(\mathbf{r}_e - \mathbf{R}_e)^2 w_h(\mathbf{r}_h - \mathbf{R}_h)^2.\end{aligned} \quad (19)$$

Similarly to (6), we present the envelope in the form

$$\begin{aligned}\Phi(\mathbf{R}_e, \mathbf{R}_h) = e^{i[\mathbf{Q}/2 - \gamma(\mathbf{Q})]\mathbf{R}_e + i[\mathbf{Q}/2 + \gamma(\mathbf{Q})]\mathbf{R}_h} \\ \times \chi_{\mathbf{Q}}(\mathbf{R}_e - \mathbf{R}_h)\end{aligned} \quad (20)$$

and arrive at the equation for the components of parameters $\gamma_i(\mathbf{Q})$, which ensure the dependence of the function $\chi_{\mathbf{Q}}(\mathbf{R}_e - \mathbf{R}_h)$ only on the difference between the site coordinates $\mathbf{R}_e - \mathbf{R}_h$:

$$\gamma_i(\mathbf{Q}) = \arctan\left(\frac{J_e - J_h}{J_e + J_h}\tan\frac{Q_i}{2}\right). \quad (21)$$

As in the 1D SL case, we obtain the equation for $\chi_{\mathbf{Q}}(\mathbf{R})$:

$$\begin{aligned}[-V(\mathbf{R})]\chi_{\mathbf{Q}}(\mathbf{R}) + \sum_i \frac{J_i(\mathbf{Q}; J_e, J_h)}{2} \\ \times [2\chi_{\mathbf{Q}}(\mathbf{R}) - \chi_{\mathbf{Q}}(\mathbf{R} + a\mathbf{e}_i) - \chi_{\mathbf{Q}}(\mathbf{R} - a\mathbf{e}_i)] \\ = [E - E_G - K(\mathbf{Q}; J_e, J_h)]\chi_{\mathbf{Q}}(\mathbf{R}).\end{aligned} \quad (22)$$

Here, the ith component of the resonance integral is

$$J_i(\mathbf{Q}; J_e, J_h) = \sqrt{(J_e + J_h)^2 - 2J_eJ_h(1 - \cos Q_i)}. \quad (23)$$

and the kinetic energy of motion of the center of energy of the exciton with quasi-momentum $\mathbf{Q}/a$ is

$$\begin{aligned}K(\mathbf{Q}; J_e, J_h) = 3(J_e + J_h) \\ -\sum_i \sqrt{(J_e + J_h)^2 - 2J_eJ_h(1 - \cos Q_i)}.\end{aligned} \quad (24)$$

At small $|\mathbf{Q}|$, the energy of motion of the center of mass of the exciton (23) is described by the quadratic dispersion law with the resulting electron and hole mass $(J_e^{-1} + J_h^{-1})a^{-2}$:

$$K(\mathbf{Q}; J_e, J_h) = \frac{\mathbf{Q}^2 a^2}{2(J_e^{-1} + J_h^{-1})}.$$

Regarding the components of integral (23), we should emphasize their dependence on the components of the vector of quasi-momentum of the center of mass, which becomes more pronounced at close J_e and J_h values. Therefore, the binding energy is sensitive both to the value of vector $\mathbf{Q}$ and to its direction, i.e., to the direction of motion of the exciton as a whole. For example, if $J_e = J_p$ and $Q_z = \pm\pi$, then $J_z(\mathbf{Q}; J_e, J_h) = 0$ and the SL transforms into a set of 2D SLs in the layers normal to the z axis and not related to one another by tunneling.

In the continuum approximation, when the difference operator in parentheses in the second term in (22) is replaced by the second derivative and $\mathbf{R}$ is considered as a continuous variable, Eq. (21) acquires the form of the ordinary Schrödinger equation with anisotropic effective mass

$$-\sum_i \frac{J_i(\mathbf{Q}; J_e, J_h)a^2}{2}\frac{\partial^2}{\partial R_i^2}\chi_{\mathbf{Q}}(\mathbf{R}) - V(\mathbf{R})\chi_{\mathbf{Q}}(\mathbf{R}) = [E - E_G - K(\mathbf{Q}; j_e, J_h)]\chi_{\mathbf{Q}}(\mathbf{R}). \quad (25)$$

It is noteworthy that the components of the effective mass

$$m_i^* = 1/J_i(\mathbf{Q}; J_e, J_h)a^2$$

depend on both the value and direction of the dimensionless quasi-momentum $\mathbf{Q}$ of the center of inertia of the exciton.

The continuum approximation is valid, in as far as the extent of the wave function $\chi_{\mathbf{Q}}(\mathbf{R})$ exceeds the SL period. In this case, the potential $V(\mathbf{R})$ can be replaced with $(e^2/\epsilon)(1/|\mathbf{R}|)$ and Eq. (25) can be made dimensionless by choosing as the unit length the smallest of the values

$$\frac{\epsilon J_i(\mathbf{Q}; J_e, J_h)a^2}{e^2} = \frac{\epsilon}{m_i^*(\mathbf{Q}; J_e, J_h)e^2},$$

which corresponds to the Bohr radius of a particle with reduced effective mass along the ith SL axis $m_i^*(Q; J_e, J_h)$. Obviously, the continuum approximation is valid at $\epsilon J_i(\mathbf{Q}; J_e, J_h)a^2/e^2 \gg a$ or $J_i(\mathbf{Q}; J_e, J_h) \gg e^2/\epsilon a$, i.e., if the smallest resonance integral is larger than the energy of the Coulomb interaction at a distance of one SL period. If, in one of the directions, the continuum approximation is inapplicable, the problem should be considered as in the case of a layered SL at a small resonance integral. If, in the 3D SL, the resonance integrals along two axes are small, then we deal with weakly coupled quantum wires. They are considered similarly to the analysis of the 2D system with sites from the quantum wires the exciton spectrum of which was described, e.g., in [6]. We note that the previous investigation is obviously generalized to second-order heterostructures where electrons and holes are spatially separated.

Now, let us discuss the possibility of the transformation of the thus far investigated Wannier–Mott exciton to the Frenkel exciton in a semiconductor SL.

For this purpose, the amplitude of excitation transfer from one SL site to another due to the dipole–dipole interaction should be larger than the tunneling one. The first of them is a value of about $\mu^2/\epsilon a^3$, where μ is the dipole moment of the exciton transition. Thus, the inequality

$$\frac{\mu^2}{\epsilon a^3} \gg J_i(\mathbf{Q}; J_e, J_h) \quad (26)$$

should be valid.

Thus, an interesting feature can arise in a semiconductor SL. If the resonance integrals of electrons and holes have the similar values, then in certain directions of quasi-momentum $\mathbf{Q}$ and at its values larger than a certain value, the key role in the transport will be played by the dipole–dipole interaction. Thus, the situation can be implemented in which the exciton is simultaneously of Frenkel and Wannier–Mott types.[8] Generally speaking, the same change in the transport mechanism can occur in a layered SL under a condition similar to (26).

5. CONCLUSIONS

It was shown that the resonance integral that determines the tunnel coupling of the Wannier–Mott exciton in neighboring SL cells depends on the quasi-momentum of the center of inertia of the exciton. The closer the resonance integrals of the electron and hole, the stronger this dependence is. Consequently, both the binding energy of the exciton and its wave functions in a semiconductor with a SL depend on the quasi-momentum of the center of inertia of the exciton.

In the continuum approximation, the exciton problem is reduced to the well-known problem of the Coulomb center for a particle with anisotropic mass solved by Kohn and Luttinger for donor states in germanium and silicon in 1955 [4]. The determined range of parameters in the limit of which the continuum approximation is applicable was shown to be rather narrow.

The properties of excitons in a semiconductor with a SL were briefly analyzed. It was demonstrated that

[8] Frenkel excitons in the SL of QDs were investigated in [7].

the continuum approximation is applicable if, which is natural, the Coulomb energy at a SL period is smaller than the width of the miniband for the exciton as a whole.

It was shown that, at similar electron and hole masses and an exciton quasi-momentum close to the Brillouin-zone boundary, the transport of the exciton from one site to another in the direction of this quasi-momentum should occur due to dipole–dipole interaction, as in the case of Frenkel excitons.

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