Energy structure of multiexcitons in quantum wires with a longitudinal confining potential

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The energy spectra of many-particle excitons in quantum wires with a longitudinal confining potential providing a confinement energy comparable with the characteristic energy of the Coulomb interaction of charge carriers are calculated. It has been found that, upon excitation of one of the charge carriers, the binding energy of a multiexciton decreases by a value several times greater than the confinement energy.

Key words: quantum wires with longitudinal confining potential; multiparticle excitons.

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1. Introduction

Recently, a technology for the growth of new quantum confined structures — quantum wires with a composition gradient along their growth axis — has been developed, which provides a longitudinal confining potential [1–5]. These systems open promising opportunities for a single photon emitter development [6–9].

A specific feature of these structures is that a slowly varying confining longitudinal potential leads to low confinement energies while providing a sufficiently strong localization of carriers so that the characteristic Coulomb interaction energy exceeds the interlevel distance. Therefore, in such structures, one can expect a strong coherence of charge carriers, and, consequently, a significant transformation of the energy spectrum of many-particle complexes due to the Coulomb interaction — the energy level splitting, changes in the level order, etc.

In addition, in these structures, the size quantization energies of heavy holes are close to the thermal energy kT for helium temperatures. Therefore, for optical applications, the question of the change in the binding energy of excitons upon the excitation of holes is quite important.

In this work, we calculate the energy spectra of many-particle exciton complexes in these structures and reveal features associated with a strong correlation of charge carriers.

2. Calculation method

We consider a cylindrical quantum wire $Al_xGa_{1-x}As/Al_{x_{max}}Ga_{1-x_{max}}As$ of length $2d$ and radius R (Fig. 1, *a*). The aluminum concentration x changes along the wire axis symmetrically in both directions from the smallest value x_{min} in the center of the wire to the largest value x_{max} at its ends (Fig. 1, *b*).

The energy spectrum of excitons was calculated in the parabolic approximation of the envelope function formalism [10]. We consider structures with $x_{max} < 0.45$. In these structures, the band edges are well described by a linear dependence on the Al concentration, and, accordingly, a change in the aluminum concentration along the wire axis leads to a similar change in the longitudinal potential [11]. The Coulomb interaction between carriers is considered using the matrix approach. The wave functions of noninteracting charge carriers that comprise the complex under consideration are used as the initial basis. The classification of states in the electron subsystem (i. e., in the absence of holes) and in the exciton is carried out according to the maximum value of the modulus of the expansion coefficient of the wave function of this state in terms of the basis wave functions of the problem without Coulomb interaction. The binding energy of a multiexciton is determined as the difference between its energy and the energy of the system of noninteracting charge carriers constituting the exciton.

3. Many-particle effects in the electronic subsystem

Figure 2, *a* shows the spectra of a two-electron system for a structure with a V-shaped dependence of the aluminum concentration along the wire axis, leading to a V-shaped longitudinal potential. The left side of the figure shows a two-electron spectrum calculated without considering the interaction between electrons. The energy is measured from the minimum value of the conduction band edge in the quantum wire. The right side of the figure shows the spectrum with considering the electron-electron interaction.

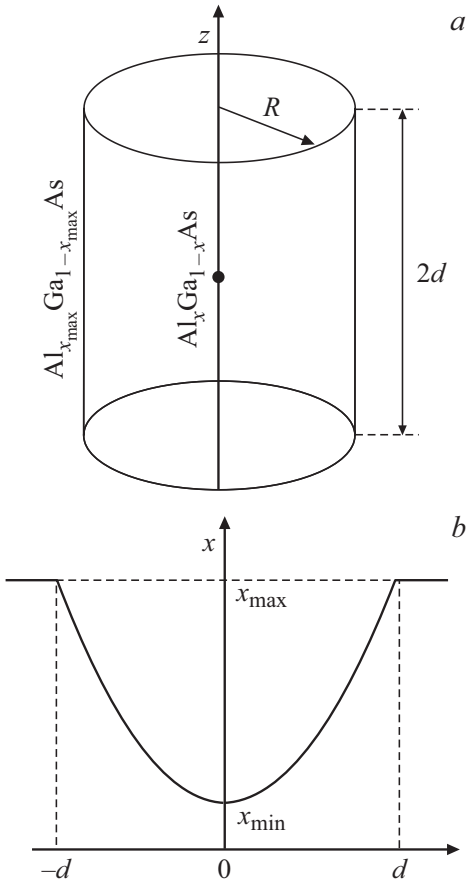

Figure 1. Schematic of the considered structure (a) and dependence (b) of the Al concentration on the coordinate along the quantum wire axis (z axis).

One can see that the electron-electron interaction qualitatively changes the spectrum. First, it results in a considerable shift of the „00“ ground level, so that the ground state becomes excited. The next level without electron-electron interaction corresponds to the „01“ configuration, when one electron is at the ground energy level, and the other is at the first excited one. This level is fourfold degenerate, corresponding to one singlet and three triplet states. When the interaction is turned on, a strong splitting into singlet and triplet levels occurs due to the exchange interaction. Moreover, this splitting exceeds the interlevel distance of the zero problem.

The fourth energy level of non-interacting electrons corresponds to configuration „11“ when both electrons are at the first excited level. We see that the energy of this level increases but by an amount less than the increase in the „00“ level.

Thus, we see that the electron-electron interaction leads to an increase in the energy of singlet states (total spin $S = 0$) and a decrease in the triplet states energy ($S = 1$). Moreover, these energy shifts are very significant — they are comparable and even exceed the distance between the energy levels of noninteracting electrons.

We also observe a tendency for energy shifts to decrease as the energy of the interacting electrons increases. The latter occurs in accordance with the oscillatory theorem — as the energy level number increases, the wave function becomes more complex and has more zeros, which leads to a decrease in the matrix elements of the Coulomb potential.

Figure 2, b shows the energy spectrum of two electrons in a quantum wire with a parabolic potential along the axis. Behavior similar to that of a V-shaped potential is observed, but a feature arises associated with the equidistance of single-particle energy levels.

The equidistance in the single-electron spectrum leads to additional degeneracy in the spectrum of two noninteracting electrons. For example, configurations „11“ and „02“ have the same energy. The Coulomb interaction lifts this degeneracy. Since only a singlet state is possible for configuration „11“, this level is split into three — two singlets and one triplet. Also, configurations „03“ and „12“ have the same energy. Here, singlet and triplet states correspond to each of the configurations. As a result, the Coulomb interaction leads to the splitting of this level into four levels — two singlets and two triplets.

4. Exciton complexes

Figure 3 shows the dependence of the exciton binding energy in a quantum wire with a parabolic potential on the energy level number of the heavy hole. As can be seen, the binding energy decreases as the hole passes from the ground state to the excited energy level. This decrease is considerable, more than twice the distance between the hole levels (0.57 meV). A further change in the binding energy with increasing hole energy occurs more smoothly.

This behavior is explained by the difference between the electron and hole wave functions and, accordingly, the charge distributions in the ground and excited states. Figure 4 shows the distribution of the square of the wave function modulus for various heavy hole energy levels along the z-axis passing through the center of the wire. In the ground state, the wave function has no zeros, and the charge density distribution is a peak located at the center of the well along z. In the first excited state, the wave function has one zero, and the charge density distribution changes qualitatively, representing two narrower peaks separated by a dip. Since the electron remains in the ground state, this leads to a significant decrease in the Coulomb interaction matrix elements and, accordingly, to an exciton binding energy decrease. With a further increase in the hole energy, the number of wave function zeros and, correspondingly, the number of peaks in the charge density distribution increase. However, this change is not as dramatic as in the case of the transition of a hole from the ground state to the first excited level. Therefore, the binding energy continues to decrease, but more slowly.

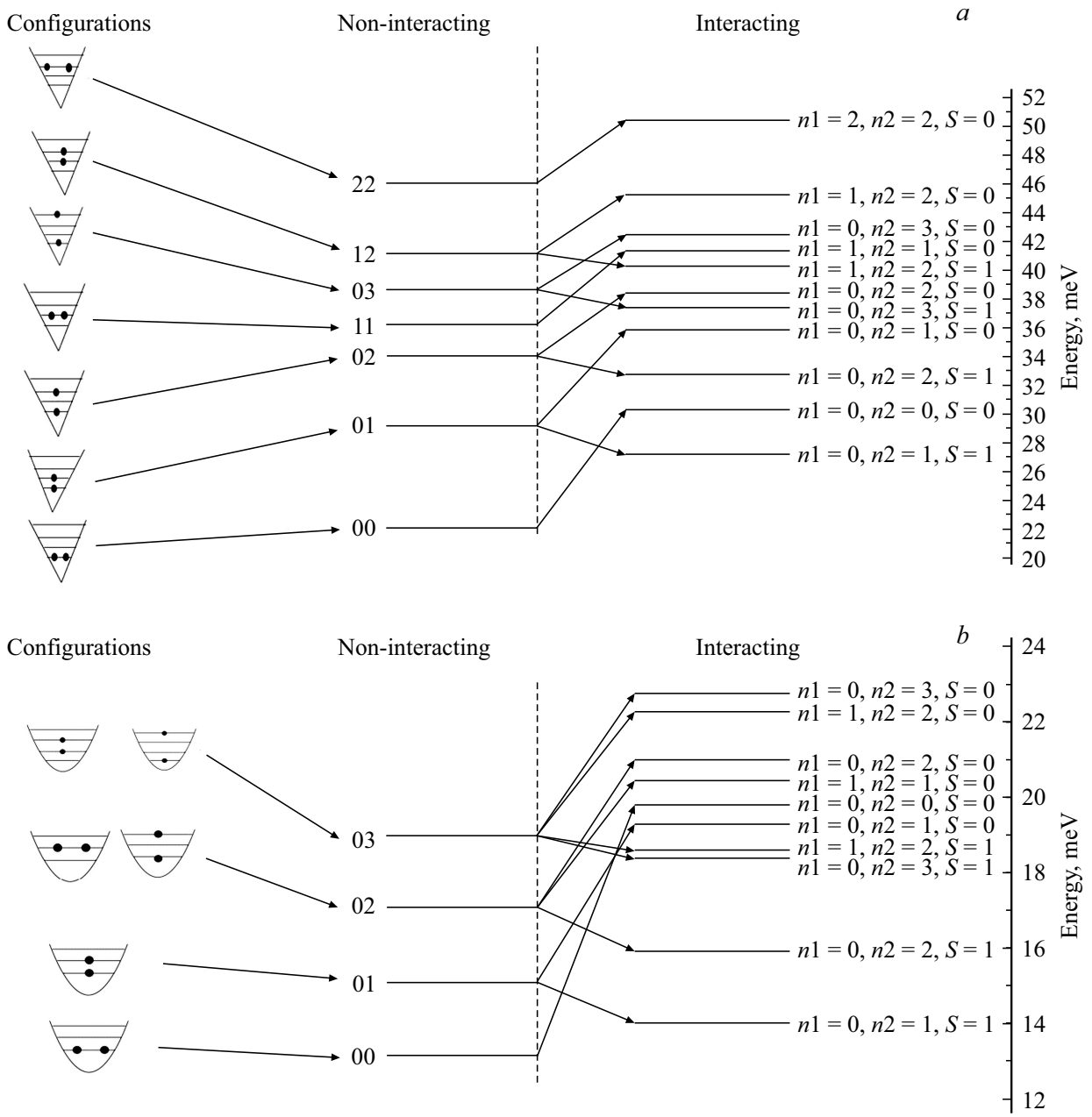

Figure 2. Energy spectrum of two electrons in a quantum wire $Al_xGa_{1-x}As/Al_{x_{max}}Ga_{1-x_{max}}As$ with length $2d = 275$ nm and radius $R = 10$ nm. The aluminum concentration x changes symmetrically from the minimum value $x_{min} = 0.2$ at the center of the wire to the maximum value $x_{max} = 0.4$ at its ends according to a linear (a) and parabolic (b) law.

We see similar behavior in multiparticle excitons. Figure 5 shows the energy levels of a trion consisting of two electrons and a heavy hole for „00n“ configurations, where two electrons are at the ground (0th) energy level and a hole is at the nth hole level. As can be seen, in the „000“ ground state, the Coulomb interaction leads to a decrease in the energy of the trion, which means that the attraction between the electrons and the hole prevails over the repulsion between the two electrons. Excitation of the hole to the first level, i. e. in configuration „001“, drastically reduces this shift. In other words, there is a considerable decrease in the binding energy of the trion (Fig. 6), which is almost four times the distance between the hole levels. When the hole is excited to higher levels, the change in the binding energy occurs more smoothly.

In addition, there is a transition from a situation with a predominance of attraction between electrons and a hole to a situation where repulsion between two electrons predominates. As can be seen, if the hole is below the third excited level, then the Coulomb interaction leads to a decrease in the exciton energy (the binding energy is negative), i. e. attraction prevails over repulsion. If the hole

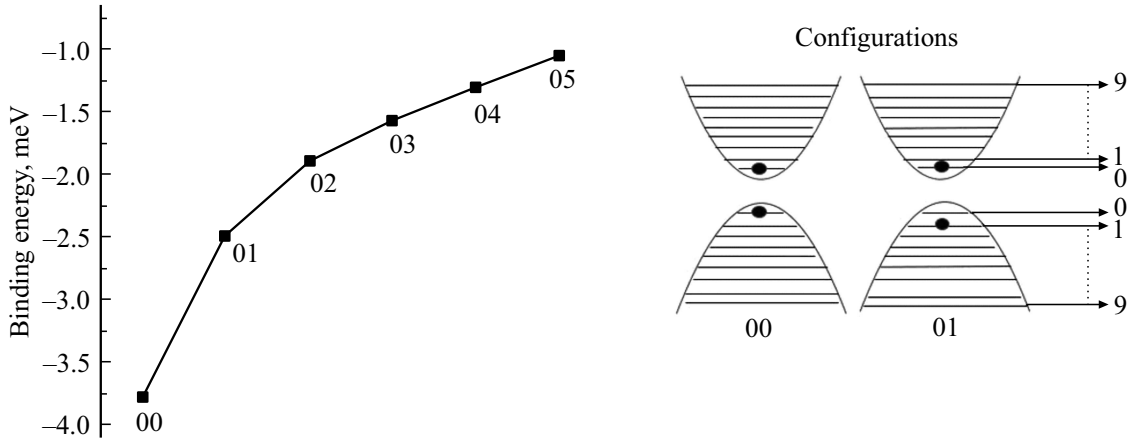

Figure 3. The binding energy of an exciton with a heavy hole for a quantum wire $Al_xGa_{1-x}As/Al_{x_{max}}Ga_{1-x_{max}}As$ with a length of $2d = 275$ nm and a radius $R = 10$ nm with a parabolic change in the aluminum concentration x from the minimum value $x_{min} = 0.2$ at the center of the wire to the maximum value $x_{max} = 0.4$ at its ends. The binding energies are shown for configurations „0n“, in which the electron is at the ground energy level ($n = 0$), and the hole is at the nth hole level.

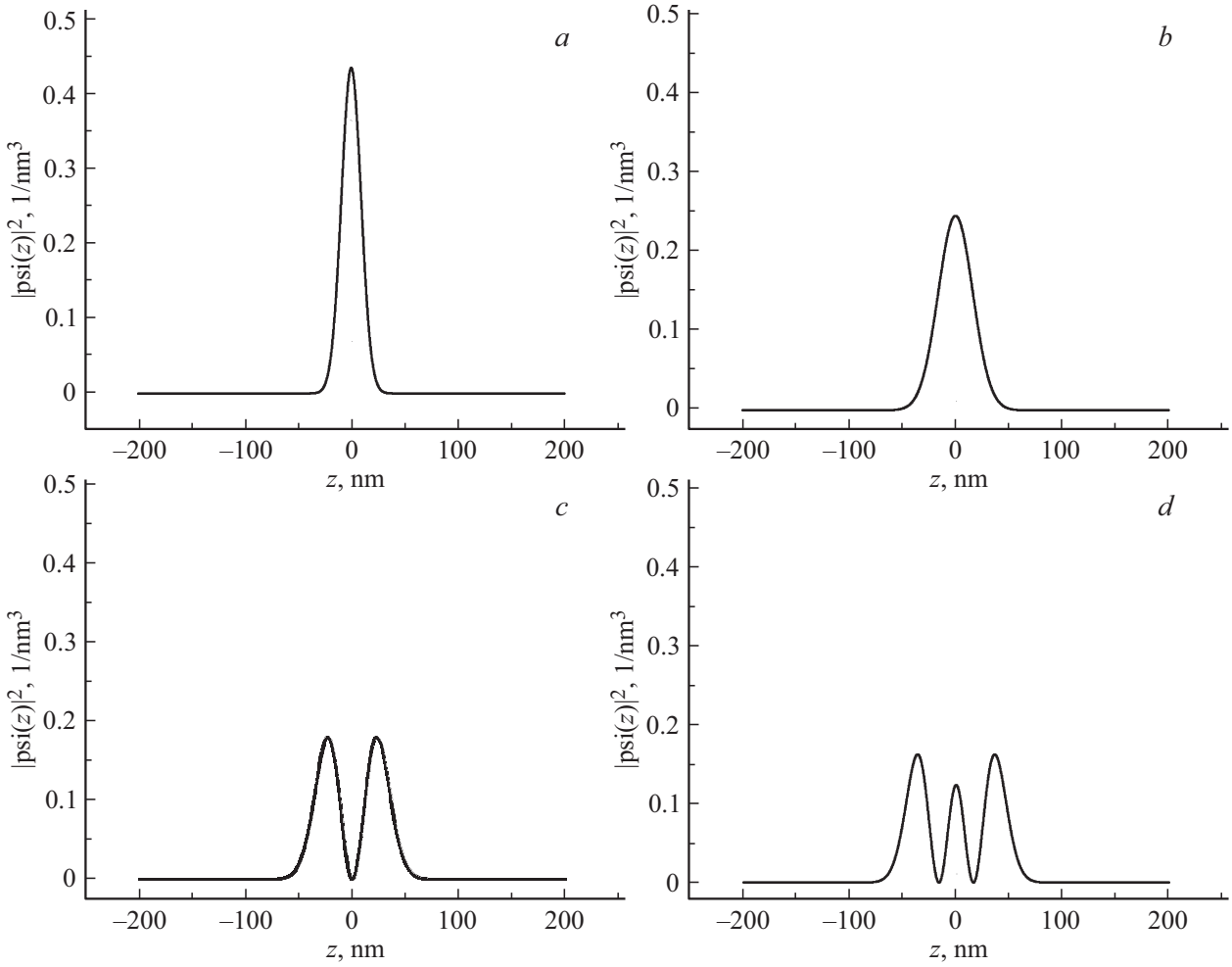

Figure 4. Distribution of the squared modulus of the single-particle wave function along the wire symmetry axis (z-axis): (a) for an electron in the ground state ($n = 0$); (b) for a heavy hole in the ground state; (c) for a heavy hole at the first excited level ($n = 1$); (d) for a heavy hole at the second excited energy level ($n = 2$). The origin of coordinates ($z = 0$) is at the center of the wire.

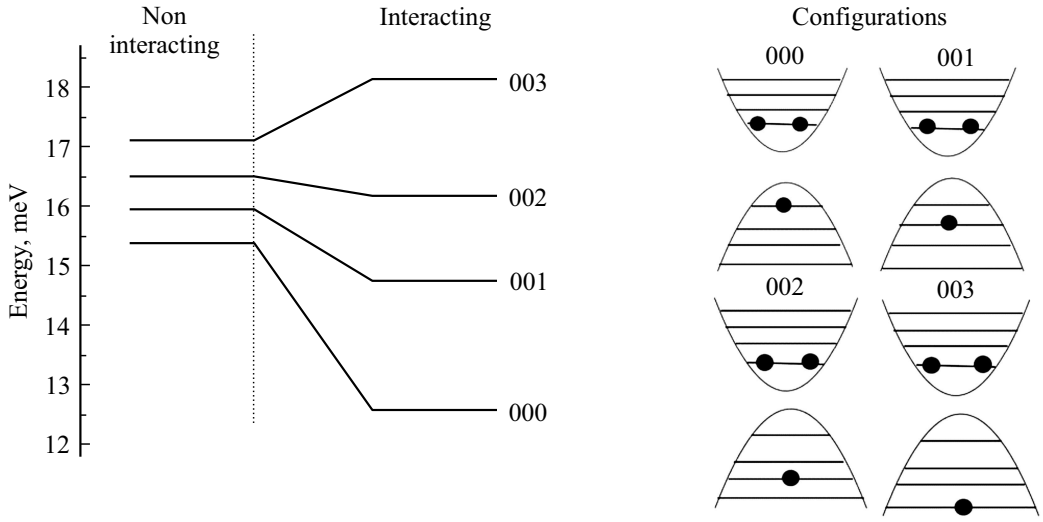

Figure 5. The energy levels of a trion consisting of two electrons and a heavy hole in a quantum wire with a longitudinal parabolic potential. The energy levels are shown for the „00n“ configurations, in which both electrons are at the ground (0th) level, and the hole is at the nth energy level.

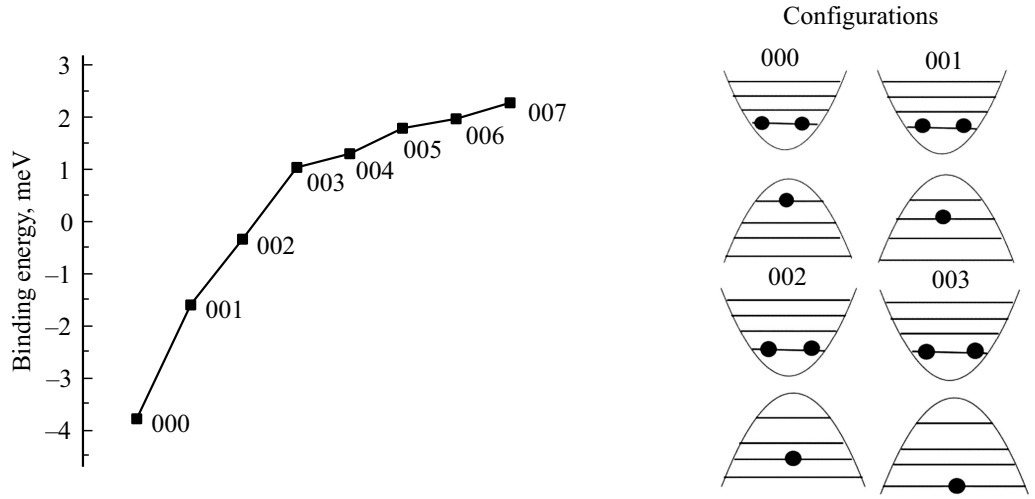

Figure 6. The binding energy of a trion, consisting of two electrons and a heavy hole, in a quantum wire with a longitudinal parabolic potential for „00n“ configurations, in which both electrons are at the ground (0th), and the hole is at the nth energy level.

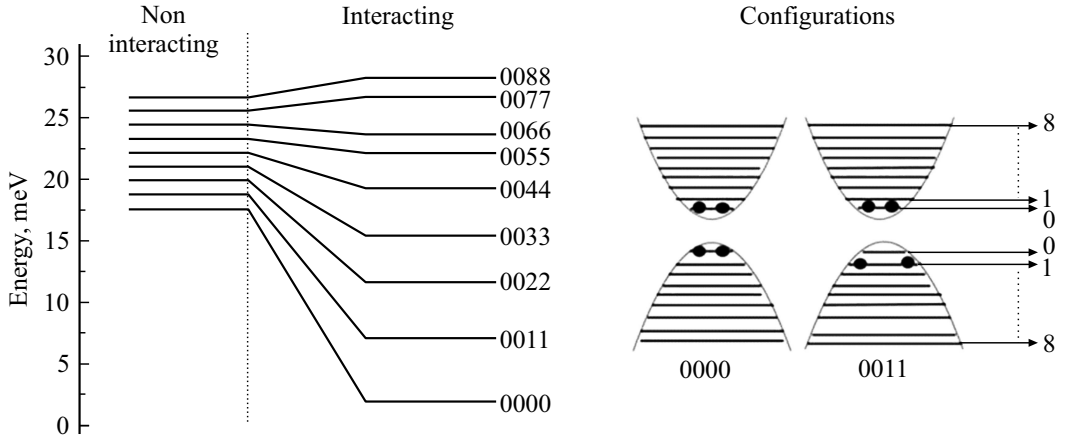

Figure 7. Energy levels of a four-particle exciton consisting of two electrons and two heavy holes. The energy levels of configurations „00nn“ are shown, in which both electrons are in the ground state ($n = 0$), and both holes are at the n-th hole energy level.

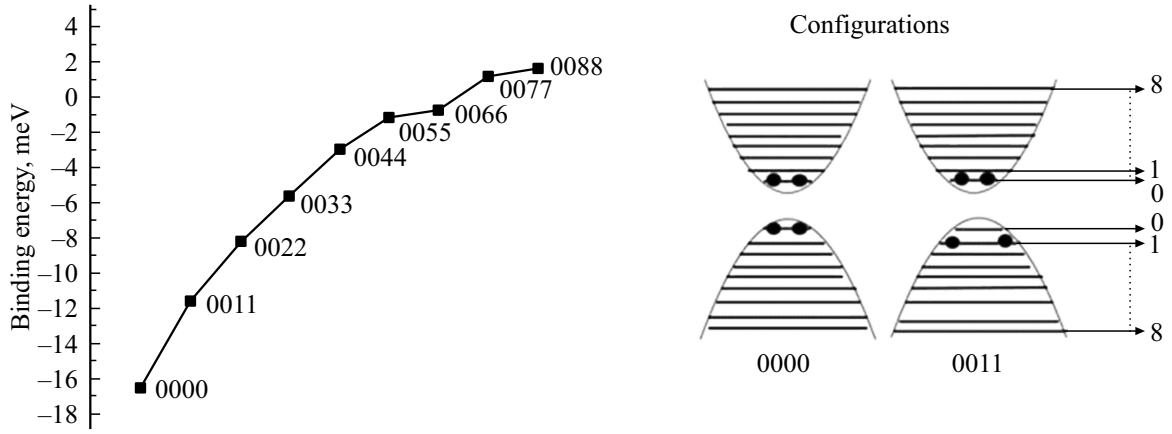

Figure 8. The binding energy of a four-particle exciton, consisting of two electrons and two heavy holes, for „00nn“ configurations, in which both electrons are in the ground state ($n = 0$), and both holes are at the n th hole energy level.

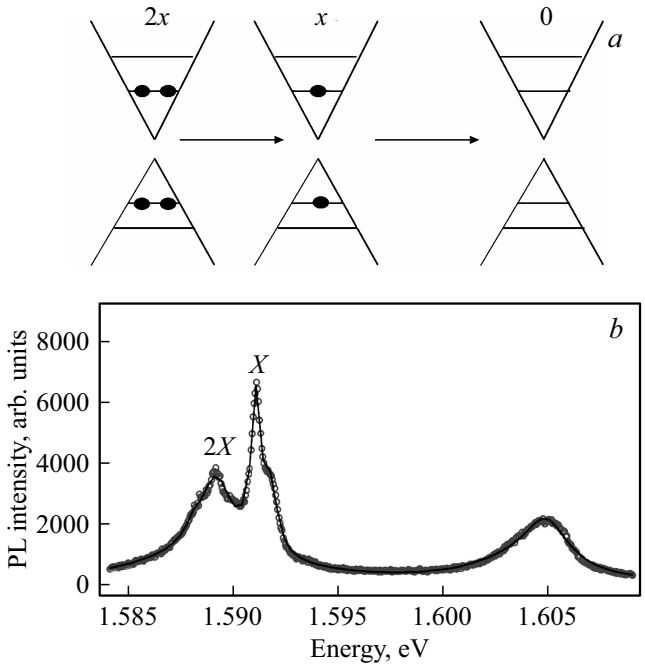

Figure 9. (a) Schematic of recombination of a four-particle exciton consisting of two electrons and two holes. (b) The photoluminescence spectrum of a quantum wire with a V-shaped potential measured experimentally in [12]. Data taken from [12] with the permission of the authors. The structure parameters are indicated in the caption to Figure 2.

occupies the third or higher level, the Coulomb interaction results in an increase in the total energy of the system, i. e. the repulsion of the two electrons dominates the attraction between the electrons and the hole.

Similar general trends in behavior are also observed in a four-particle exciton consisting of two electrons and two heavy holes. Figure 7 shows the energy levels of such a multiexciton in a quantum wire with a parabolic potential, corresponding to the „00nn“ configurations when both electrons are at the ground energy level, and both holes are at the nth hole level. Figure 8 shows the binding energy values of such a four-particle exciton. One can see that when holes pass to the first excited level, the binding energy decreases significantly, and when holes are excited to higher levels, the binding energy changes more weakly. A transition from configurations with predominant attraction to configurations with predominant repulsion is also visible.

5. Comparison with experimental data

We calculated the recombination energies of four-particle excitons for the structure experimentally studied in [12] with a V-shaped longitudinal potential. Figure 9a shows the recombination scheme. First, one electron-hole pair recombines ($2x \to x$), then another ($x \to 0$). In the photoluminescence spectrum, two lines should correspond to these two stages, and the line corresponding to the $2x \to x$ transition should be observed at a lower frequency than the $x \to 0$ line. The corresponding experimental photoluminescence spectrum, taken from [12], is shown in Figure 9, b. As can be seen, the $2X$ line corresponding to the $2x \to x$ transition is shifted relative to the X ($x \to 0$) line toward lower energies by about 7 meV. The calculated position of the $2X$ line also shifts relative to the X line towards lower frequency, with the shift amounting to 4.58 meV, which is quite close to the experimental value.

6. Conclusion

The energy spectra of charge carrier complexes in quantum wires with a longitudinal confining potential are calculated. The potential provides low confinement energies of charge carriers along with strong Coulomb interaction, so that the characteristic Coulomb interaction energy exceeds the interlevel distance in the spectrum of carriers.

It is found that when one of the charge carriers passes to an excited level, the binding energy of a multiexciton

decreases by a value several times greater than the confinement energy. This effect is due to a change in the degree of localization of the charge carrier in the excited state.

The comparison of calculated values of the exciton binding energy with the experimentally measured ones revealed good quantitative agreement between theoretical calculations and experimental data.

Conflict of interest

The authors declare that they have no conflict of interest.

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