Simple Estimation of \( X^- \) Trion Binding Energy in Semiconductor Quantum Wells

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A simple illustrative wave function with only three variational parameters is suggested to calculate the binding energy of negatively charged excitons (\( X^- \)) as a function of quantum well width. The results of calculations are in agreement with experimental data for GaAs, CdTe and ZnSe quantum wells, which differ considerably in exciton and trion binding energy. The normalized \( X^- \) binding energy is found to be nearly independent of electron-to-hole mass ratio for any quantum well heterostructure with conventional parameters. Its dependence on quantum well width follows an universal curve. The curve is described by a simple phenomenological equation.

I. INTRODUCTION

The first consideration of atomic-like three-body system is regarded to Bethe, by whom the attention to the hydrogen ion \( H^- \) has been attracted as early as 1929 [1]. The existence of negatively (\( eeh \)) and positively (\( ehh \)) charged excitons (trions) in semiconductors, being analog of the hydrogen ions, was predicted by Lampert in 1958 [2]. The investigation of three-body complexes has a fundamental importance, particularly in semiconductors, where there is a possibility to vary parameters in a wide spectrum. However, the experimental observation of trions in bulk semiconductors is rather difficult due to their small binding energies.

The interest to experiment and theory of trions has grown due to the progress in the semiconductor heterostructure fabrication. Theoretical calculations performed at the end of the 1980s [3] predicted a considerable (up to tenfold) increase of the trion binding energy in quantum well heterostructures compared with bulk semiconductors. The first experimental observation of negatively charged excitons (\( X^- \)) has been reported for CdTe-based quantum wells (QWs) by K. Kheng et al in 1993 [4]. The trions have also been observed in QWs based on GaAs and ZnSe semiconductors [5, 6, 7]. Nowadays, a large number of experimental data on \( X^- \) trion are available for various types of heterostructures with different parameters.

The main characteristic of the negatively (or positively) charged exciton is its binding energy, i.e. the energy required to separate the trion in a neutral exciton and an unbound electron (hole). The variation of the binding energy of \( X^- \) trion [8, 9, 10, 11] and, the similar system, \( D^- \) center [12, 13] with the QW width have been extensively studied theoretically. But, most of these calculations are limited to specific material systems. In order to achieve a better agreement with experimental data the problem is treated with a considerable number of fitting parameters. This makes it very difficult to compare trion binding energies in heterostructures based on different semiconductors, which differ in Coulomb energies.

The aim of this paper is to present a simple universal model, which allows to estimate the trion binding energy (\( E_B^T \)) in any semiconductor QW. In the following we show that the plausible value of the \( E_B^T \) at arbitrary QW width can be obtained using a simple trial wave function, which provides a vivid picture of the trion structure. The similar approach we used in Refs. [14, 15, 16] for the analysis of the singlet and triplet states of trions in ideal two-dimensional quantum wells and for the calculation of the trion ground state in heterostructures with spatially separated carriers.

In this paper we concentrate on the negatively charged exciton, which is caused by the reliable set of experimental data available. It is important to note, that, commonly, the effective mass of a hole is larger than that of an electron. So the \( X^- \) is constructed of one heavy particle only, which simplifies the theoretical consideration. The negatively charged trion can be analyzed with the infinitely heavy hole centered at the QW, while the electron-to-hole mass ratio, \( \sigma = m_e/m_h \), typically being in the range of 0.01 < \( \sigma \) < 1, taken as a perturbation parameter.

In section II the experimental data for the trion binding energy in heterostructures of different material systems are summarized and discussed. In section III a simple model of the trion with a heavy hole in an ideal QW is proposed and the binding energy dependence versus the effective well width is variationally calculated. The mass ratio dependencies of the exciton and the trion binding energies in the quantum well are considered in section IV. In section V the corrections to the trion binding energy due to QW imperfections are discussed.

II. EXPERIMENTAL RESULTS

Charged excitons in various heterostructures have been extensively studied during the last decade. Experimental data of the \( X^- \) trion binding energy (\( E_B^T \)) for ZnSe, CdTe and GaAs quantum wells of various widths (\( L_z \))
are collected in Table I and illustrated in Fig. I. One can clearly follow the increase of the trion binding energy by decreasing well width.

In spite of the variety of the experimental data, similarities between the trions in different semiconductors are expected. Indeed, considering the bulk trion in the frame of a simple model of a Coulomb potential with the effective masses, one can take the Bohr energy (i.e. exciton Rydberg), \( E_B = \frac{\mu e^2}{2\varepsilon a^2} \), and Bohr radius, \( a_B = \frac{\hbar^2\varepsilon}{\mu e^2} \), as scaling parameters. Here \( \mu = m_e m_h / (m_e + m_h) \) is the reduced mass of the electron \( m_e \) and the hole \( m_h \), \( \varepsilon \) is the permittivity, and \( e \) is the electron charge. The binding energy of the trion normalized by 3D Rydberg is nearly independent of the electron-to-hole mass ratio, \( \sigma = m_e / m_h \), and is \( E_B^T \approx 0.055 \) Rydberg for most of the semiconductors studied [3]. The same feature is valid for the ideally 2D trion, i.e. for the trion being strongly localized in the growth direction with the localization length much smaller than \( a_B \). In this case the trion binding energy is \( E_B^T \approx 0.48 \) Rydberg and also shows no dependence on the mass ratio (\( \sigma \)) and on the semiconductor material [2]. Therefore, it is rather natural to expect that the \( E_B^T \) does not strongly depend on \( \sigma \) in the case of finite width of a quantum well.

In order to compare experimental data for different materials collected in Table I we plotted them in Bohr units, \( E_B^T / \) Rydberg against \( L_z / a_B \), as shown in Fig. I. The following values of 3D exciton Rydberg \( E_B^T = 4.2, 10, 20 \) meV and 3D exciton Bohr radius \( a_B = 140, 67, 40 \) Å were taken for GaAs, CdTe and ZnSe respectively [25]. It can be seen that, in these units, all dependences can be well approximated by one universal curve. For example, a plausible estimation of the trion binding energy in quantum wells of a thickness more than \( a_B \) and less than \( 10a_B \) can be obtained with the simple fitting equation (shown in Fig. I), by a solid line:

\[
\frac{E_B^T}{\text{Rydberg}} \approx \frac{1}{3 \sqrt{L_z / a_B}}.
\]

It is the simplest fitting equation found to well approximate the experimental data. Of course, it cannot be used at the limiting cases \( L_z \to 0 \) and \( L_z \to \infty \). Nevertheless it gives plausible estimation of the trion binding energy for the wide range of \( L_z \) and can be very useful due to its simplicity.

The fact that the experimental results for different semiconductors coincide with the universal curve is remarkable. It signifies that the trion binding energy for each effective width of a QW is mainly scaled with Bohr units, and the influence of all other parameters, i.e. electron-to-hole mass ratio or band offsets, is rather weak.

III. TRION WITH INFINITELY HEAVY HOLE

In the previous section we showed that the experimental data of the trion binding energy versus the QW width are well approximated by the universal curve for all semiconductors, if the length and the energy scales are expressed in exciton units. In this section we obtain the universal dependence analytically. The requirement of the universality greatly simplifies the task, because one can leave only those parameters of the system, which can be directly expressed in exciton energies and quantum well widths. Moreover, in the next sections we show that the influence of other parameters has no much effect on the universal curve obtained in this section.

The simplification is the following. The trion is considered as a three-body Coulomb system, using the effective mass approximation. The reduced mass (\( \mu \)) and the permittivity (\( \varepsilon \)) are supposed to be isotropic and identical in the quantum well and in the barriers. The real potential of the quantum well is replaced by an ideal one with infinite barriers. The hole is taken to be much heavier than the electron, so the mass ratio \( \sigma = m_e / m_h \) is zero. In this case of only one heavy particle in the system, namely the hole, it occupies the center of the quantum well, where the adiabatic potential of the electrons reaches a minimum. It reduces the number of independent coordinates in the trion problem from 6 (the in-plane center-mass motion and the total angular mo-

### TABLE I: The original experimental data collected for various semiconductor materials. Note, that for correct comparison the binding energy of “isolated” trion, which is unperturbed by interaction with two-dimensional electron gas, must be taken into account [18, 29]. Therefore, we either select the data for undoped QWs or extrapolate the binding energies in doped structures to the low-concentration limit. In the latter case the initial values are given in brackets.

| Material | \( L_z, \) Å | \( E_B^T, \) meV |
|----------|--------------|----------------|
| ZnSe     | 29, 48, 50, 64, 67, 80, 95, 190, 200 | 8.9\(^a\), 6.6\(^a\), 5.8\(^a\), 5.2\(^a\), 5.3\(^a\), 4.4\(^a\), 4.0\(^a\), 1.4\(^a\), 2.5\(^b\) |
| CdTe     | 38, 50, 55, 80, 100, 120, 150, 260, 400, 500, 600 | 4.4\(^c\), 3.5\(^c\), 3.4\(^c\), 2.9\(^c\), 2.1\(^d\), 2.5\(^d\), 2.2\(^d\), 1.8\(^d\), 1.3\(^f\), 1.2\(^f\), 1.1\(^f\) |
| GaAs     | 80, 100, 200, 220, 250, 300 | 2.1\(^g\), 2.1\(^h\), 1.15\(^i\), 1.1\(^j\), 0.8\(^k\), 0.9\(^l\) |

\(^a\)Reference 26, \(^b\)Reference 28, \(^c\)Reference 24, \(^d\)Reference 24, \(^f\)Reference 24, \(^g\)Reference 24, \(^h\)Reference 26, \(^i\)Reference 18, \(^j\)Reference 31, \(^k\)Reference 18, \(^l\)Reference 31, \(^m\)Reference 24, \(^n\)Reference 24, \(^o\)Reference 18, \(^p\)Reference 31.
FIG. 1: The $X^-$ trion binding energy $E_B^T$ versus the QW width $L_z$ plotted for different semiconductors: ZnSe by circles, CdTe by triangles, and GaAs by stars. These data are also collected in Table 1.

(a) The experimental dependences are plotted in natural units, i.e. energy and length being expressed in [eV] and [Å], respectively.

(b) The experimental dependences are plotted in 3D exciton units.

The number of the terms in the Hamiltonian decreases in the case of any arbitrary quantum well to 5. The number of terms in the Hamiltonian decreases as well.

The Schrödinger equation for the trion in such a case is (hereafter we use 3D exciton units for the length and the energy):

$$[-\Delta_{\mathbf{r}_1} - \Delta_{\mathbf{r}_2} + (V_C(\mathbf{r}_1, \mathbf{r}_2) + V^{QW}(z_1) + V^{QW}(z_2)) + E_B^X + E_B^T - 2E_c^{QW}]\Psi_T(\mathbf{r}_1, \mathbf{r}_2) = 0.$$  (2)

Here $\mathbf{r}_1$ and $\mathbf{r}_2$ are three-dimensional vectors connecting the hole with the electrons, $z_1$ and $z_2$ are their projections on the growth direction. $V_C(\mathbf{r}_1, \mathbf{r}_2) = 2(1/R - 1/r_1 - 1/r_2)$ is a Coulomb potential of the system, where $R = |\mathbf{r}_1 - \mathbf{r}_2|$ is the distance between the electrons. $E_B^X$ and $E_B^T$ are the exciton and trion binding energies. $V^{QW}(z)$ is the quantum well potential, it is 0 if $|z| < L_z/2$ and $+\infty$ otherwise. $E_c^{QW}$ is the quantization energy of the free electron in the ground state of the quantum well:

$$E_c^{QW} = \frac{1}{1 + \sigma} \frac{\pi^2}{L_z^2} \left( \text{if } \sigma = 0, \ E_c^{QW} = \frac{\pi^2}{L_z^2} \right).$$  (3)

The equation (2) is solved by a variational method, when the energy in the ground state, calculated by a trial function with variational parameters, is minimized. The most critical point, effecting the accuracy of calculations, is the proper choice of the trial function, which should be simple and close to the real wave function. In order to obtain the trion binding energy one has to find the trion energy and subtract it from that of the exciton. Therefore, to minimize the mistake in the $E_B^T$ calculation, the exciton energy should be calculated in the same manner as the trion one. Consequently, the trion function should be based on the exciton function, transforming to the latter when one of the electrons is removed.

The simplest trial function for the exciton with only one variational parameter $(a)$, which gives plausible results for the exciton binding energy in the whole range of the quantum well widths, is:

$$\Psi_X(\mathbf{r}) = A \exp(-a r) Z_0(z, L_z),$$  (4)

Here $\mathbf{r}$ is 3D vector connecting the hole and electron, and $z$ is its projection on the growth direction. $A$, here and after, is a normalization factor of the corresponding wave function. The last multiplier, $Z_0(z, L_z)$, provides the additional localization of the electron in the growth direction due to the quantum well potential. It should be stressed that in-plane and in-growth motion of the electron in the function (4) is not separated, and the influence of the electron-hole interaction on the in-growth electron motion is substantially taken into account by the exponential multiplier. So, in contrast to the adiabatic case, where the excited states of the quantum well have to be included (see, for example, [10]), we can take $Z_0(z, L_z)$ as a function of the ground state:

$$Z_0(z, L_z) = \sqrt{\frac{2}{L_z}} \cos(\pi \frac{z}{L_z}), \quad \text{for } |z| \leq L_z/2,$$

$$Z_0(z, L_z) = 0, \quad \text{for } |z| > L_z/2.$$  (5)

Here $\mathbf{r}$ is 3D vector connecting the hole and electron, and $z$ is its projection on the growth direction. It is easy to see that function (4) turns into the exact wave function of the exciton in both limiting cases of an ideal 2D quantum well ($L_z \to 0$) and a 3D bulk semiconductor ($L_z \to \infty$). Besides the simplicity, the function (4) has one more benefit. It can be shown that the full kinetic energy of the electron in the case of any arbitrary quantum
well potential $V_{QW}(z)$ is:

$$E_{e}^{kin} = \langle \Delta r \rangle = \left\langle \frac{\partial}{\partial r} \Psi_{X}(r, z) \left| \frac{\partial}{\partial r} \Psi_{X}(r, z) \right\rangle + E_{QW}^{e} - \langle \Psi_{X} | V_{QW}^{e} | \Psi_{X} \rangle = a^{2} + E_{e}^{QW} - \langle V^{QW} \rangle .$$

Consequently, the quantization energy $E_{e}^{QW}$ and the mean value of the quantum well potential $V^{QW}$ in the Schrödinger equation can be eliminated analytically. In this case the mistakes arising from the application of numerically methods are avoided, which considerably simplifies the calculations. Consequently, the binding energy of the exciton ($E_{B}^{X}$) can be estimated by the formula:

$$E_{B}^{X} = -\min_{a}(a^{2} - \langle V_{C}(r) \rangle).$$

Here $V_{C}(r) = -2/r$ is a Coulomb potential between the electron and the hole. It should be noted, that the parameters of the quantum well are included in the mean value of the Coulomb potential through the last multiplier of the function $\Psi_{X}$. The first term in Eq. (7) also has a slight dependence on the quantum well structure if the exponent in the function $\Psi_{X}$ is replaced by any other radial function. The equalities similar to (8) are valid for all trial functions considered below.

The simplest trion function, based on the exciton function $\Psi_{X}$, is the 3-parameter Chandrasekhar-like one:

$$\Psi_{T}(r_{1}, r_{2}) = A(\exp(-a_{1}r_{1} - a_{2}r_{2}) + \exp(-a_{2}r_{1} - a_{1}r_{2}))(1 + cR)Z_{0}(z_{1}, L_{z})Z_{0}(z_{2}, L_{z}).$$

Here $a_{1}$, $a_{2}$, and $c$ are variational parameters. Analogously to the function $\Psi_{X}$, this function transforms into the appropriate Chandrasekhar’s one in the limiting cases of two and three dimensions:

$$\Psi_{T}(r_{1}, r_{2}) = A(\exp(-a_{1}r_{1} - a_{2}r_{2}) + \exp(-a_{2}r_{1} - a_{1}r_{2}))(1 + cR).$$

The relative mistake in the trion binding energy obtained with function (10) is known to be less than 10% both in the 2D and 3D cases. Therefore, we can expect that the estimations, given by (10) even in the intermediate cases of the finite-width quantum wells, are also not far from the exact values.

The calculated trion binding energy versus the quantum well width within the described approach is shown in the Fig. (1) (the dashed line pointed by $\sigma = 0$). The calculation is in very good agreement with the experimental data for wide quantum wells ($L_{z} \geq 2a_{B}$). However, in narrow ($L_{z} < 2a_{B}$) quantum wells the discrepancy becomes considerable. The possible reasons for this will be discussed in section V.

### IV. MASS RATIO EFFECT IN THE EXCITON AND TRION IN QW

It is known that the binding energy of $X^{-}$ trion, expressed in Bohr units, is nearly independent of electron-hole mass ratio $\sigma$ both for an ideal 2D quantum wells and for 3D bulk semiconductor. It is rather natural to expect that in the quantum well of arbitrary width the $X^{-}$ trion binding energy to be weakly dependent on $\sigma$. The results of calculation of the trion binding energy versus the mass ratio for a 250 Å-wide GaAs QW also confirm this assumption.

The correction to the trion binding energy due to nonzero mass ratio is supposed to be small. Therefore in what follows we will consider it as a perturbation and calculate in the adiabatic approximation. To simplify this calculation we start by analyzing the exciton and then expand the results to the trion case. In the case of the exciton with a very heavy hole, the particle wave functions are separated and the adiabatic approximation is applicable (for narrow quantum wells the influence of the in-plane electron motion on the in-growth hole localization is analyzed in [34]).

The Schrödinger equation for the hole motion in the growth direction is (in 3D exciton units):

$$\left( - \frac{\sigma}{1 + \sigma} \frac{\partial^{2}}{\partial z^{2}} + \left( V_{e}^{adiab}(z) + E_{B}^{X} - E_{h}^{QW} \right) \right) Z_{h}(z) = 0 .$$

Here $Z_{h}(z)$ is the wave function of the hole in growth direction. $V_{e}^{adiab}(z)$ is a sum of the averaged Coulomb potential of the electron and the quantum well. $E_{h}^{QW}$ is a quantization energy of the free hole in the ground state of the quantum well:

$$E_{h}^{QW} = \frac{\sigma}{1 + \sigma} \frac{\pi^{2}}{L_{z}^{2}} .$$

As mentioned in the previous section, the quantum well potential is taken to be ideal, with infinite barriers. It is easy to show that the hole with infinitely heavy mass ($\sigma = 0$) is located in the minimum of the adiabatic potential ($z = 0$). The binding energy of the exciton in such case is:

$$E_{B}^{X} = -V_{e}^{adiab}(0) .$$

As the mass ratio increases, the binding energy of the exciton decreases because, by the definition:

$$\langle Z_{h} | \frac{\partial^{2}}{\partial z^{2}} | Z_{h} \rangle \geq E_{h}^{QW} \geq V_{e}^{adiab}(0) .$$

Qualitatively, if the mass of the hole becomes smaller, its localization along $z$-direction increases until it achieves the width of the QW, and then stays unchanged. Therefore, the main factor defining the evolution of the exciton binding energy with the mass ratio is the hole localization in the growth direction due to the Coulomb attraction of the electron. The simplest wave function taking this into account is:

$$\Psi_{X}(r, z_{e}, z_{h}) = A \exp(-a r) Z_{0}(z_{e}, L_{z}) Z_{0}(z_{h}, bL_{z}) .$$
The exciton binding energy $E_X^\sigma$ is unrealistic heavy (between even the extreme curves ratio for few values of mass limit of the mass ratio $\sigma = m_e/m_h$). The curves with $\sigma = 1$ (squares) and $\sigma = 0.01$ (circles) are nearly coincide. The curve with $\sigma = 0$ (stars) is precisely approximated by the rescaled dependence with $\sigma = 1$ (diamonds), the coefficient being $\sqrt{2}$.

Here $r$ is the 3D distance between the particles, $a$ is the reciprocal radius of the exciton, $b \in [0,1]$ is the degree of hole localization. The value $b = 1$ means the function of the hole in the growth direction is nearly the same as that of the electron. The opposite case, $b = 0$, signifies that the hole is strongly localized in the center of the well corresponding to the case of an infinitely heavy hole.

The dependences $E_X^\sigma(L_z)$ are calculated by variational method with the trial function $\psi(14)$ for few values of mass ratio $\sigma = m_e/m_h$ (see Fig.2). The difference in energy between even the extreme curves $\sigma = 0$ and $\sigma = 1$ is rather small ($<10\%$) for all values of $L_z$. Moreover, it can be noticed that the curve corresponding to $\sigma = 0.01$ is closer to the curve for $\sigma = 1$ than $\sigma = 0$. For example, the curves $\sigma = 0.1$ and $\sigma = 1$ would not be distinguishable in the scale of the figure. It means, that the exciton binding energy does not depend on the mass ratio for $\sigma > 0.1$ and has an extremely weak dependence if $\sigma \in [0.1,0.01]$. A considerable increase of $E_B^\sigma$ takes place only if the hole is unrealistic heavy ($\sigma < 0.01$). Consequently, we can neglect the variation of the binding energy with the mass ratio for all experimental values of the latter.

This fact is easy to understand, if we consider the degree of the hole localization ($b$) in such cases (see Fig.3). It can be seen that even if the hole is rather heavy (for example, $\sigma = 0.1$) the value of the hole localization in the growth direction is nearly $b \sim 1$ for all $L_z$, whereas the limiting value $\sigma = 0$ corresponds to $b = 0$. It means that the exciton wave function $\psi(14)$ is nearly independent of the mass ratio for $\sigma > 0.1$. Consequently, due to Eq. (7), which is valid for function $\psi(14)$ as well, $E_B^\sigma$ appears also to have no dependence on $\sigma$ in the same value range.

Note, the curve with $\sigma = 0$ in Fig. 2 can easily be obtained from the curve with $\sigma = 1$ if the abscissa is multiplied by a coefficient $\sqrt{2}$. A small discrepancy between these curves takes place only for wide quantum wells, but even there, it is nearly negligible. This is a consequence of the fact, that the function $\psi(14)$ involves in an explicit form the electron and hole $z$-coordinates ($z_e$ and $z_h$) only through the functions $Z_0$. Indeed, for the case of:

$$Z_0(z,L) = \frac{1}{\sqrt{\pi L}} \exp\left(-\frac{z^2}{2L^2}\right), \quad (15)$$

it can exactly be shown, that the binding energy of the exciton, given by Eq. (4), is the same both for $b = 1$, $L \equiv L_z$ and $b \equiv 0$, $L \equiv \sqrt{2}L_z$:

$$E_B^\sigma(L_z,\sigma = 1) \equiv E_B^\sigma(\sqrt{2}L_z,\sigma = 0). \quad (16)$$

The equality (16) is valid even if the exponent in the exciton function (13) is replaced by any other radial function. However, if the function $Z_0$ differs from a Gaussian function, the equality (16) becomes not valid. Nevertheless, as can be seen in Fig. 2, it produces a good estimation of the binding energy of the light-hole exciton (i.e. with $\sigma = 1$) for a wide range of quantum well width values.

The obtained results for the exciton can be extended to the trion. It is known that the binding energy of the second electron in the trion is much smaller ($\sim 10$ times) than that of the first one. Therefore, the negatively charged trion, containing only one heavy particle, can be considered in a rather crude model as an electron bound to an unperturbed exciton via some effective central potential $V_{X}^{eff}(r)$. Here $r$ is the distance between the electron and the center of mass of the exciton, which is assumed to be unperturbed. In that way, the problem of the trion becomes very similar to the exciton one con-
Considered in this section earlier. Therefore, one can suppose that the only effect which causes an alteration of $E^T_B(L_z, \sigma)$ with $\sigma$ is the increase of the exciton localization in the growth direction due to the interaction with the additional electron. By analogy to Eq. (14), the dependence of the trion binding energy with a mass ratio $\sigma = 1$ can be obtained via rescaling the curve with $\sigma = 0$:

$$E^T_B(L_z, 1) \approx E^T_B(\sqrt{2}L_z, 0),$$  \hspace{1cm} (17)

where the latter is known from the previous section. Obviously, all possible dependences on the QW width of the trion binding energy are confined by these two extreme cases with $\sigma = 1$ and $\sigma = 0$, as are presented in Fig. 1b by the filled area. The obtained scattering of the binding energy is less than 20%, which is even smaller than the experimental data dispersion. Moreover, as for the exciton binding energy, the trion $E^T_B$ is expected to be about the same for $\sigma > 0.01$, allowing to take $\sigma = 1$ for any QW with realistic parameters. All these arguments prove the thesis, that the binding energy of $X^-$ trion is nearly independent of the mass ratio in most quantum well heterostructures.

It is worth to note that our considerations taken for GaAs-based QWs generally represent the results of previous numerical calculations [8, 9, 10, 11]. However, in contrast to them, in the present paper the theoretical results have been obtained with the use of only three fitting parameters, and an agreement is achieved for various semiconductor systems (i.e. for CdTe and ZnSe in addition to GaAs).

V. CORRECTIONS TO THE TRION BINDING ENERGY

In the previous sections the corrections to the trion binding energy, appearing from those parameters of QWs, which cannot be expressed in Bohr units, are neglected for simplification. The relatively small dispersion of the experimental data for $E^T_B$ in different semiconductors allows us to conclude that the scale of these corrections is at most in the range of 20% (see Fig. 1b). In this section we discuss possible corrections and evaluate their input in the trion binding energy.

**Correction due to lateral localization.** The largest difference between the calculation and the experiment is observed for narrow QWs (Fig. 1b). The reasonable explanation of this fact is that the trion binding energy increases due to in-plane localization at one-monolayer fluctuations of the QW width (see, for example, [22]). As the QW becomes narrower, these fluctuations, forming lateral islands, become more important. The energy alteration due to this effect strongly depends on the effective size of the islands, which are controlled by growth conditions and expected to be individual for each sample. The formation of lateral islands is confirmed by the broadening of the trion line in optical spectra being observed experimentally [18]. However, it is not clear up to now, why the results for different semiconductors are so similar.

**Polaron correction.** It has been assumed that the interaction between the particles is of Coulomb type, and the effective mass approximation has been used. However, the polaron correction is known to cause a considerable increase of the binding energy of $D^-$ center in narrow quantum wells due to reducing the distance between the electrons [12]. It might also explain the discrepancy of the experimental and the theoretical data for narrow quantum wells (see Fig. 1b). The polaron correction was also used in fitting the experimental data for the trion binding energy reported in Ref. 2. Nevertheless, it must be stressed, that the polaron correction for $X^-$ trion is expected to be nearly the same as for $D^-$ center. But the correction for the $D^-$ binding energy quickly saturates in wide quantum wells and remains quite significant there, whereas the discrepancy between the theory and experiment in Fig. 1b, is negligible small for wide quantum wells.

**Corrections due to anisotropy.** The next simplification, the reduced mass ($\mu$) and the permittivity ($\varepsilon$) have been taken to be isotropic and to have the same values in the quantum well and in barriers. It allows us to take the Bohr energy and the Bohr radius of the QW material as a system scale. It is clear that the role of the mass and permittivity anisotropy diminishes in the limit of two dimensions. Therefore, if the anisotropy is small enough to considerably change the bulk trion energy, then it can be neglected in finite quantum wells as well. The discontinuity of the permittivity across the interfaces causes image charges in the barrier areas [20, 21]. For the typical situation of smaller in the barriers compared to the value in the wells, the Coulomb interaction (i.e. binding energy) between particles is effectively increased. For example, the relative increase of the exciton binding energy in narrow GaAs quantum wells due to this effect is about 10-20% [22]. This value is comparable with the error of our estimations and cannot qualitatively change the results.

**Corrections caused by finite barriers.** The main effect of the quantum well potential is the localization of carriers in the structure growth direction. The binding energy of the trion depends more on the localization degree, than on the real shape of the quantum well potential. The simplest way to take it into account is to consider the real quantum well as an ideal one with infinite barriers and different effective widths for electrons ($L_e$) and holes ($L_h$), which is caused indeed by penetration of their wave functions in the barriers. These quantities should be treated as phenomenological parameters and, with a reasonable accuracy, can be taken so that the mean-square deviation of the particles in the growth direction remains the same in the ideal quantum well as in the real one. As has been shown above, a small relative inaccuracy in the effective well width does not lead
to a considerable change of the binding energy. For example, if the width is taken to be 10% larger the binding energy decreases at most by 4%, which is quite small compared with the uncertainty of experimental data. In wide quantum wells $L_h$ is nearly equal to $L_e$, and one can take $L_z \approx L_e \approx L_z$. In narrow QWs, these values can be considerably different $L_e \neq L_h$ due to the tails of wave functions penetrating into the barrier, which depend on the barrier specifics for the electron and the hole.

In most cases of narrow QWs $L_h < L_e$, which is easy to consider. Indeed, as $L_h$ decreases, the electron-hole interaction becomes stronger and the trion binding energy increases. The case $L_h \rightarrow 0$ is very similar to the case when $\sigma = 0$, considered in the section III. Therefore, in the frames of model considered, the simple estimation can be obtained:

$$E_B^T(L_e, L_e, 1) \leq E_B^T(L_e, L_e, \sigma) \leq E_B^T(L_e, L_h, \sigma) \leq E_B^T(L_e, L_h, 0) = E_B^T(L_e, L_e, 0) \quad (18)$$

where the relative difference between the boundaries does not exceed 20% (Fig. 1b). Moreover, the trion binding energy can be estimated more accurately. If $\sigma$ is not small enough to cause a considerable localization of the hole in the growth direction ($\sigma > 0.01$), one can take:

$$E_B^T(L_e, L_h, \sigma) \approx E_B^T(L_e, L_h, 1) \approx E_B^T(L_e^*, L_z^*, 0), \quad \text{where} \quad L_e^* = \sqrt{L_e^2 + L_h^2}. \quad (19)$$

In the same way, as it is shown for Eq. (16), the last equality can be rigorously proven, if the ground state functions of the electron and hole in the quantum well are Gaussian functions (18). However, the estimation (19) can still be used in very arbitrary quantum wells.

The opposite case, $L_h > L_e$, corresponding to a extremely shallow potential for the hole, becomes more complicated. In the extreme case of $L_e \rightarrow 0$ and $L_h \rightarrow \infty$ the hole is localized in the field of electrons only. In this limit, if $\sigma = 0$, the trion binding energy is equal to that of an ideally 2D case, because the hole is localized in the same plane as the electron. However, if $\sigma$ grows, the zero-point oscillations of the hole becomes important. In the case of the exciton, the adiabatic potential, produced by the electron in growth direction, is:

$$V_{\text{n} \text{adh}}(z) = -4 + 16|z|, \quad z \rightarrow 0. \quad (20)$$

Accordingly, it is easy to obtain, that the exciton binding energy quickly decreases with the increase of $\sigma$:

$$E_B^X(\sigma) \approx 4 - 6.5 \sigma^{1/3}, \quad \sigma \rightarrow 0. \quad (21)$$

The effect for the trion is even stronger. For example, if $\sigma$ becomes $\sim 1$, the binding energy of the $X^-$ trion decreases about one order of magnitude compared to $\sigma = 0$. This happens because, after averaging over the $z$-coordinate of the hole, the electron-hole interaction becomes weaker than the electron-electron one. Such situation is similar to the system with spatially separated carriers, so the effective distance between the carrier layers increases, as the mass of the hole becomes smaller.

**Corrections owing to a build-in electric field.** Special attention should be drawn, if the quantum well is not symmetric, and there is a spatial separation in the growth direction between the carriers. In such a case, it should be taken into account that the binding energy of the trion strongly reduces with the distance between the electron and hole layers. For example, if the splitting of the layers becomes $\sim a_B$, the binding energy of the $X^-$ trion decreases more than one order of magnitude (17). It is very possible, that the relatively low binding energy observed in the wide ZnSe quantum well (see Fig. 1b) is caused by a build-in electric field or a quantum well asymmetry leading to some spatial separation of the carriers.

Thus, it has been shown, that for the most of the quantum wells, the binding energy of the negatively charged trion can be easily estimated by means of the universal model containing only few parameters.

**VI. CONCLUSIONS**

The experimental values of the trion binding energy for various semiconductor quantum wells, being represented in corresponding exciton units, are found to be well approximated by an universal function. The theoretical estimations confirm that in a simplified Coulomb model the $X^-$ trion binding energy is nearly independent of the electron-to-hole mass ratio at any value of quantum well width. Consequently, for the sake of simplicity, calculations of the trion binding energy can be performed with infinite hole mass values. In narrow quantum wells the experimental data cannot be explained in the frame of an idealized model and additional factors should be involved in the consideration.

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