Self-consistent approach for the quantum confined Stark effect in shallow quantum wells

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A computationally efficient, self-consistent complex scaling approach to calculating characteristics of excitons in an external electric field in quantum wells is introduced. The method allows one to extract the exciton resonance position as well as the field-induced broadening for the exciton resonance. For the case of strong confinement the trial function is represented in factorized form. The corresponding coupled self-consistent equations, which include the effective complex potentials, are obtained. The method is applied to the shallow quantum well. It is shown that in this case the real part of the effective exciton potential is insensitive to changes of external electric field up to the ionization threshold, while the imaginary part has non-analytical field dependence and small for moderate electric fields. This allows one to express the exciton quasi-energy at some field through the renormalized expression for the zero-field bound state.

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I. INTRODUCTION

The quantum-confined Stark effect (QCSE) has attracted a lot of attention since its discovery[1,2] due to its diverse optoelectronics applications (see for example Ref.3). In quantum well (QW) structures with a layer thickness less than the effective exciton Bohr radius, an electron and a hole are forced to orbit closer to each other, and the binding energy of the electron-hole pair increases by a factor between two and three. This additional stability makes exciton resonances in QW's observable even at room temperatures. More important, these resonances are still observable in a uniform electric field perpendicular to the growth direction, which is as large as 50 times the classical ionization field for a three-dimensional exciton. The latter also produces a relatively large red shift in the absorption peak up to 2.5 times the binding energy of the exciton, while the width of the exciton resonance grows only moderately. Such a behavior is opposite to the properties of 3-d excitons or QW excitons in a field parallel to the plane of the QW.[1,2] The origin of this phenomenon stems from the fact that the electric field induced decay time for QW excitons is determined not by its binding energy (~ 10 meV in GaAs/AlGaAs quantum wells), but rather by the quantum well barriers' heights ($\sim 300 - 400$ meV).

Despite the fact that the QCSE was discovered almost 20 years ago and qualitatively is well understood, there is no complete quantitative solution for the problem so far. Usually, it is treated numerically with different degrees of approximation. The conventional approach consists in the separation of the problem into two consecutive steps. The first step in modelling QCSE is to omit the Coulomb interaction of an electron-hole pair and to find single particle resonance positions for an electron and a hole separately. In moderate fields (up to 10^5 V/cm) and non-shallow quantum wells (quantum wells with more than one discrete level inside) the lowest-lying resonances are so sharp that they are often approximately treated as bound states, neglecting the possibility of tunnelling. These simple methods include either an infinite well approximation,[2,4,5,6] where the effect of penetration of the electron (hole) wave functions under the barrier is taken into account by introducing an effective QW width,[2,6] or variational calculations for finite potential wells[4,7], which produce only the real part of the exciton quasi-energy. Within a weak-field regime, the Stark shift is a small second-order effect in the perturbation theory sense. The absolute value of a shift decreases with a decrease of the QW width. Achieving large shifts requires strong fields, where the perturbation theory fails. In this regime a significant broadening of the states appears due to the field induced tunnelling. Therefore, it is necessary to devise non-perturbative methods for the correct determination of the exciton resonance energies and tunnelling life-times in these systems in the presence of a strong field.

There are several ways of approaching this problem mathematically. The single-particle quasi-bound states in QW's in the presence of a uniform electric field have been studied with the help of the time-independent Schrödinger equation using Airy functions with real and complex arguments[8,9,10], stabilization technique[11,12,13], finite difference method[14] and complex coordinate method[15]. Another group of methods utilizes a dynamical approach[13,16,17] where the time evolution of a tunnelling wave packet is simulated by numerical integration of the time-dependent Schrödinger equation.

It is worth pointing out that all of the above mentioned calculations of decaying quasi-bound states are made in the single-particle approximation without consideration of the Coulomb attraction between the electron and the hole. Excitonic effects are incorporated at the next step of the calculations, which usually take into account only a real part

of the exciton binding energy shift, and are performed with the help of variational methods[2,5,7,18].

The goal of this paper is twofold. First, we develop an alternative method of studying QCSE that allows us to calculate both the position of the exciton resonances and their field-induced tunnelling life-times on equal footing. This method is a generalization of a self-consistent approach developed recently by the authors[19] for the exciton in QW without the electric field. Second, we introduce the model of QCSE in shallow quantum wells (SQW), which allows us to obtain analytical results for the resonance positions and tunnelling widths as well as for the modified exciton "ground state" wave function. In this model we approximate SQW by a delta-functional potential. Calculations are significantly simplified in this model due to the fact that the single-particle one-dimensional problem for a particle in a delta-potential and in an applied uniform electric field can be solved exactly.

The paper is organized as follows. In Sec. II we generalize the self-consistent approach of Ref.19 for the presence of the electric field, and derive main self-consistent field equations for complex resonance energy positions for QCSE, using the method of complex scaling. In Sec. III we apply our approach to the model of SQW for calculations of the effective exciton potential. One of the results of these calculations is the phase diagram representing regions of exciton's stability in strong electric fields for different well's widths and/or barrier potential. Concluding remarks are given in Sec. IV.

II. COMPLEX SCALING SELF-CONSISTENT APPROACH FOR QCSE

One of the goals of this paper is to develop a new method for calculating excitonic characteristics in QW in the presence of the electric field due to QCSE. In order to present the method clearly we consider the simplest model of QW excitons. In particular, we assume that both conduction and valence bands are non-degenerate, and that they both have an isotropic parabolic dispersion characterized by the masses m_e and m_h, respectively. Thus, we neglect valence-band mixing[20], anisotropy of the system, and dielectric[21] and effective mass mismatch between the well and barrier materials. All these effects, which are very important for realistic computations can be, however, easily incorporated into our approach. Throughout the paper we use effective atomic units (a.u.), which means that all distances are measured in the units of the effective Bohr radius $a_B = \hbar^2 \epsilon / \mu^* e^2$, energies in the units of $\mu^* e^4 / \hbar^2 \epsilon^2 \equiv 2$ Ry, and masses in the units of reduced electron-hole mass μ^*, where $1/\mu^* = 1/m_e^* + 1/m_h^*$, and ϵ is an average background dielectric constant of the well and barrier materials. In these notations $m_{e,h} = m_{e,h}^* / \mu^*$, where $m_{e,h}^*$ are effective masses of an electron and a heavy hole.

Within the approximations explained above, and after the standard procedure of excluding the center-of-mass of the perpendicular motion in the plane of the layers[2], the excitonic Hamiltonian is given by

$$
\begin{aligned}
\hat{H} &= E_g + H_e + H_h + K_r + V_{reh}, \qquad (1) \\
H_e(z_e) &= -\frac{1}{2m_e}\frac{\partial^2}{\partial z_e^2} + U_1(z_e) - Fz_e, \\
H_h(z_h) &= -\frac{1}{2m_h}\frac{\partial^2}{\partial z_h^2} + U_2(z_h) + Fz_h, \\
K_r(r) &= -\frac{1}{2}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right], \\
V_{reh}(R) &= -\frac{1}{\sqrt{r^2 + (z_e - z_h)^2}} \equiv -\frac{1}{R},
\end{aligned}
$$

where E_g is a gap energy, z is the growth direction, r measures a relative electron-hole distance in the transverse direction $r = \sqrt{(x_e - x_h)^2 + (y_e - y_h)^2}$, $U_{1,2}$ are the quantum well confining potential in z direction for the electron and the hole, respectively, and $F = |e|E$ measures the strength of the electric field. We also assume that the quasi-bound exciton state is independent of the angle in the xy plane, and exclude the corresponding term from the kinetic energy of the relative motion K_r.

Strictly speaking, because of the possibility of tunnelling, there are no bound states in a system with uniform electric field, and the energy spectrum of Hamiltonian (1) is continuous: $E \in (-\infty, \infty)$. This means that the respective wave functions do not vanish at infinity and, therefore, are not normalizable in L^2 sense. Then a proper approach to the problem is to consider a scattering problem. The scattering matrix S contains all the physical information about the system. For example, resonances correspond to the poles of the S-matrix in the lower half of the complex energy plane. It is well known that these complex energies can also be found by solving an eigenvalue problem for the time-independent Schrödinger equation, when the wave functions are chosen to have only outgoing components, but do not have an incident wave (so called Siegert or Gamow wave functions). Formally, after matching the usual "bound-state" boundary conditions one can obtain the correct complex eigenvalues. However, the eigenfunctions

corresponding to these complex eigenvalues exponentially diverge. This circumstance prohibits an application of a standard variational principle to calculations of approximate values of the quasi-bound states for QCSE.

The complex coordinate (complex scaling) approach (see for review Refs. 22,23) is devised to circumvent this problem. The idea consists in applying the coordinate transformation $\mathbf{R} \to \mathbf{R}\exp(i\gamma)$ to all coordinates in the Hamiltonian (1). Such a transformation makes the new Hamiltonian non-Hermitian $[\hat{H} \to \hat{H}(\gamma)]$ and changes its spectrum respectively. The continuous spectrum moves[24] to $-i\infty$. In addition, a discrete set of complex points lying below the real energy appears. These complex quasi-energies correspond to the tunnelling resonances under consideration. It is important that the eigenfunctions $\Psi_\gamma(\mathbf{R})$ corresponding to these complex eigenvalues $W = E - i\Gamma/2$ are square-integrable, and, therefore, can be calculated by means of the variational principle, which requires the stationarity of the functional

$$W\left[\Psi\right] = \int \Psi_\gamma \hat{H}(\gamma)\Psi_\gamma \, dV \left/ \int \Psi_\gamma \Psi_\gamma \, dV \right. \tag{2}$$

It should be noted, however, that the biorthogonality normalization (without complex conjugation of the left eigenvector) is used in the definition of the energy functional instead of the standard scalar product. The complex quasi-energies should also be stationary with respect to changes in rotation angle γ. The method of complex scaling and methods similar to it are widely and successfully used in studies of atomic and molecular auto-decaying states[22,23].

The new variational principle, Eq. (2), for the rotated non-Hermitian Hamiltonian can be used for extension of the self-consistent method, recently developed by the authors[19], to the problem of QCSE. According to this method, we construct an approximate exciton wave function $\Psi_\gamma(z_e, z_h, r)$ with the help of the unknown functions $\psi_1, \psi_2, \ldots$, where each function ψ_k depends on a fewer number of variables than the total wave function. Considering variations of these functions independently, from the variational principle, Eq. (2), we obtain coupled integro-differential equations for ψ_k. The resulting coupled equations can be solved by successive approximations. The convergence of this procedure allows for estimating to what degree a given functional dependence of the trial function is close to the exact wave function. In the case of zero electric field and sufficiently strong localization (the exciton "z-size" is smaller than its three-dimensional Bohr radius), we found[19] that representation of the trial function in the form of a product of functions of different coordinates gives an excellent approximation for exciton energies even after only one iteration. We expect, therefore, that a similar form will give accurate results for quasi-bound states in the presence of the electric field, at least, when it is not very large. Thus, we choose the trial function for the Hamiltonian (1) in the form of the product:

$$\Psi_{\text{trial}}(r, z_e, z_h) = \psi(r)\chi_e(z_e)\chi_h(z_h). \tag{3}$$

Assuming normalization of every function in this product, we substitute function Eq. (3) in Eq. (2), vary each function in a product separately, and obtain the system of coupled integro-differential equations

$$\left[e^{-2i\gamma}K_r(r) + e^{-i\gamma}\overline{V}_r(r)\right]\psi(r) = W_X\psi(r), \tag{4}$$

$$\left[H_e(e^{i\gamma}z_e) + e^{-i\gamma}\overline{V}_e(z_e)\right]\chi_e(z_e) = W_e\chi_e(z_e), \tag{5}$$

$$\left[H_h(e^{i\gamma}z_h) + e^{-i\gamma}\overline{V}_h(z_h)\right]\chi_h(z_h) = W_h\chi_h(z_h), \tag{6}$$

where the following notations for effective potentials are introduced:

$$\overline{V}_r(r) = \langle\chi_e\chi_h| - 1/R|\chi_e\chi_h\rangle, \tag{7}$$

$$\overline{V}_{e,h}(z_{e,h}) = \langle\psi\chi_{h,e}| - 1/R|\psi\chi_{h,e}\rangle. \tag{8}$$

The angle brackets of biorthogonal inner product imply that the integration of the Coulomb potential with corresponding wave functions is carried out over two of three independent variables.

Solving the system of equations (4)–(6) we obtain the best approximation for the entire wave function in the form of a product (3). The corresponding value of the total quasi-bound energy $W = E - i\Gamma/2$ is given by Eq. (2), which can be rewritten in the form

$$W = \langle\Psi|\hat{H}|\Psi\rangle = W_e + W_h + W_X - \langle\chi_e|e^{-i\gamma}\overline{V}_e|\chi_e\rangle - \langle\chi_h|e^{-i\gamma}\overline{V}_h|\chi_h\rangle. \tag{9}$$

Eigenfunctions and corresponding complex eigenvalues of Eqs. (4)–(6) can be found with the help of successive iterations. As in the case of zero electric field, the zero order solution is obtained after neglecting the effective Coulomb terms $[\overline{V}_{e,h}^{(0)}=0]$ in single-particle Eqs. (5) and (6):

$$H_{e,h}(e^{i\gamma}z_{e,h})\chi_{e,h}^{(0)}(z) = W_{e,h}^{(0)}\chi_{e,h}^{(0)}(z). \tag{10}$$

With the help of functions $\chi_{e,h}^{(0)}$ a zero order approximation for the effective potential $\overline{V}_r^{(0)}(r)$ is calculated and substituted into Eq. (4). This effective potential has the meaning of a two-dimensional effective electron-hole interaction induced by collective effects of an attractive Coulomb interaction, quantum well potentials in the z direction, and an applied uniform electric field. The first quasi-bound state for this effective two-dimensional exciton is found from the following equation

$$\left[e^{-2i\gamma}K_r + e^{-i\gamma}\overline{V}_r^{(0)}(r)\right]\psi^{(0)}(r) = W_X^{(0)}\psi^{(0)}(r). \tag{11}$$

The eigenfunction $\psi^{(0)}(r)$ is then substituted into Eqs. (8) to calculate a new approximation $\overline{V}_{e,h}^{(1)}(z_{e,h})$ for the effective potentials. This process can be continued until the potentials are self-consistent to a high order of accuracy, i.e. until the condition

$$\langle\psi|\overline{V}_r|\psi\rangle \approx \langle\chi_e|\overline{V}_e|\chi_e\rangle \approx \langle\chi_h|\overline{V}_h|\chi_h\rangle \tag{12}$$

is fulfilled.

The main advantage of the approach described above is that it allows one to calculate, in principle, not only field-induced single-particle widths $\Gamma_{e,h}$ but the *exciton width* Γ_X as well, which describes a renormalization of the electron-hole pair life-time by the effective interaction. For moderate fields this width is a non-analytical function of F, and is small compared to $\Gamma_{e,h}$. The exact calculation of this contribution is possible only numerically. The details of such calculations for particular semiconductor structures will be presented elsewhere. Below we consider the properties of the solution of Eqs. (4)–(6) obtained after the first iteration of the self-consistent method for the case of a shallow quantum well, where some analytical results can be derived.

It should be stressed that the most important feature of the complex scaling method is the biorthogonality normalization. The other feature, the coordinate rotation itself $\mathbf{R} \to \mathbf{R}\exp(i\gamma)$, is necessary to guarantee the convergence of the integrals (7,8). Although, this rotation is important to negate the asymptotic divergence of the *exact* eigenfunctions of the quasi-bound state, it was found[23] that in the case of sharp resonances (when the width Γ is small in comparison with the real part of the energy) the optimal angle of rotation γ is close to zero. Moreover, the final answer for quasi-energy is not very sensitive to the change of γ. Therefore, for approximate calculations we will fix $\gamma = 0$ and choose the trial functions to be square integrable from the very beginning. However, we will permit variational parameters to be *complex*. The latter assumption allows us to extract the resonance width in the problem, while still keeping the problem tractable. We will follow this procedure in the subsequent sections.

III. δ-FUNCTIONAL MODEL FOR A SHALLOW QUANTUM WELL IN AN ELECTRIC FIELD

A zero approximation of a self-consistent field approach for the electron (hole) part of the wave function in the z direction, Eqs. (10), is equivalent to the standard problem of a single-particle quasi-bound state in QW. Therefore, its solution can be obtained with the help of any method described previously[8,9,10,11,12,13,14,15,16,17]. Let us first solve the problem exactly using Airy functions with complex arguments.

We define a shallow quantum well as a well in which only one bound state exists for both electrons and holes. It is well-known that, if a well's width, L, tends to zero, a shallow quantum well can be successfully described by a δ-functional well

$$V(z) = U - \alpha\delta(z), \tag{13}$$

where $\alpha = UL$ is characterizes the δ-potential strength and U is the barrier height. For convenience, the first constant term U on the left hand side of Eq. (13) will be omitted hereafter. In terms of the total Hamiltonian, Eq. (1), it means that the energy band gap, E_g, is the barrier's energy band gap: $E_g^{\text{bar}} = E_g^{\text{well}} + U_e + U_h$. The delta-functional approximation is directly applicable only either to very narrow QW[19,25] or to wells with a small band-gap offset,[25] i.e. when the well width and/or the band offsets are very small so that the carrier wave functions are mostly in the barrier region. However, the range of its applicability can be extended[19] up to the moment of the appearance of the second bound state by introducing the effective strength of the potential

$$\alpha = UL_{\text{eff}} = \sqrt{\frac{2U}{m} - \frac{\pi^2 x_1^2}{m^2 L^2}} \tag{14}$$

where x_1 is the solution of the equation

$$x = 1 - 2/\pi\arcsin\left(\frac{\pi x}{\sqrt{2mUL^2}}\right). \tag{15}$$

L_{eff} is chosen in such a way that the energy of the bound state in the δ-potential matches the ground state energy of the finite well problem[27]. In some sense, the model of the δ-functional QW is complementary to the model of an effective infinite quantum well[2] (EIQW), which is used to approximate finite QW with large widths (or barrier heights) when the number of levels in a well is large. Indeed, the more discrete levels exist in the QW the better the EIQW model works for the ground state, but it fails when the well has only one discrete level. On the other hand, the δ-functional QW is not applicable for quantum wells with more than one level. For typical parameters in $Al_{0.3}Ga_{0.7}As/GaAs$ structures the range of applicability of δ-functional SQW extends up to a well width $L \approx 40\text{\AA}$.

The advantages of the δ-functional SQW model become especially obvious in the case when a uniform electric field is applied. The simplicity of the model allows one to derive analytically *both* the electric field induced energy shift, and the tunnelling life-time. Let us first find the complex energy and the corresponding wave function of the single one-particle quasi-stationary state for the electron (the case of a hole is obtained by substituting $-F$ for F). The respective one-dimensional Schrödinger equation is

$$\left[-\frac{1}{2m}\frac{d^2}{dz^2} - \alpha\delta(z) - Fz \right]\chi(z) = E\,\chi(z). \tag{16}$$

It is convenient to introduce the dimensionless variables for the field and the wave vector,

$$f = 2mF/\kappa_0^3, \qquad \kappa = \sqrt{-2mE}/\kappa_0, \tag{17}$$

where $\kappa_0 = m\alpha$ is the ground state wave vector for an unperturbed δ-potential problem. After performing the standard coordinate transformation

$$y = \kappa_0 f^{1/3}\left(z - \frac{\kappa^2}{\kappa_0 f} \right) \tag{18}$$

we obtain

$$\frac{d^2\chi(y)}{dz^2} + y\chi(y) = -2f^{-1/3}\delta(y+y_0)\chi(y), \tag{19}$$

where $y_0 = \kappa^2 f^{-2/3}$. Everywhere except the point $z = 0$ (or equivalently, $y = -y_0$), Eq. (19) coincides with the Airy equation.[26] In order to find the quasi-bound state we have to use boundary conditions at infinity, which require that the solution does not contain incoming waves. It means that we construct our solution in the form of an evanescent wave to the left, and propagating outgoing wave to the right:

$$\chi = \begin{cases} C_1(\kappa)\left[\text{Ai}(-y) - i\text{Bi}(-y) \right], & y \to +\infty & \dfrac{C_1}{\sqrt{\pi}y^{1/4}}\exp\left(i2/3y^{3/2} \right) & z > 0 \\[3mm] C_2(\kappa)\text{Ai}(-y), & y \to -\infty & \dfrac{C_2}{\sqrt{\pi}|y|^{1/4}}\exp\left(-2/3|y|^{3/2} \right) & z < 0 \end{cases} \tag{20}$$

Note that propagating asymptotic for the right part of the wave function is valid for $z \gg \kappa^2/\kappa_0 f$, i.e. far away from the origin $z = 0$. Near the origin, the wave function decreases exponentially for both $z < 0$ and $z > 0$. For small fields the evanescent asymptotic can be used to describe the behavior of the wave function at both sides of the point $z = 0$. The unknown constants $C_{1,2}$ and complex energy are found after matching the boundary conditions at $y = -y_0$. For the normalized energy κ^2 we obtain the following equation:

$$\text{Ai}\left(\frac{\kappa^2}{f^{2/3}} \right)\text{Bi}\left(\frac{\kappa^2}{f^{2/3}} \right) + i\text{Ai}^2\left(\frac{\kappa^2}{f^{2/3}} \right) = \frac{f^{1/3}}{2\pi}. \tag{21}$$

It has one complex solution

$$\varepsilon_c \equiv \kappa^2 = \varepsilon_R(f) + i\varepsilon_I(f). \tag{22}$$

The real and the imaginary parts numerically calculated from Eq. (21) are shown in Figs. 1, 2. The notion of the quasi-bound state has sense, when the width ε_I is small in comparison with the real part of the energy. This happens at small fields, i.e. when the condition $f^{1/3} < 1$ is fulfilled. In this case the right hand side of the Eq. (21) is small, and the real part of the argument of the Airy functions is large: $\text{Re}(\kappa^2 f^{-2/3}) \gg 1$. With the help of asymptotic expansions of the Airy functions,[26] Eq. (21) can be reduced to

$$\kappa = 1 + \frac{5}{32}\frac{f^2}{\kappa^6} + \frac{1155}{2048}\frac{f^4}{\kappa^{12}} + \cdots + \frac{i}{2}\exp\left(-\frac{4\kappa}{3f} \right)\left(1 - \frac{5f}{24\kappa} + \cdots \right). \tag{23}$$
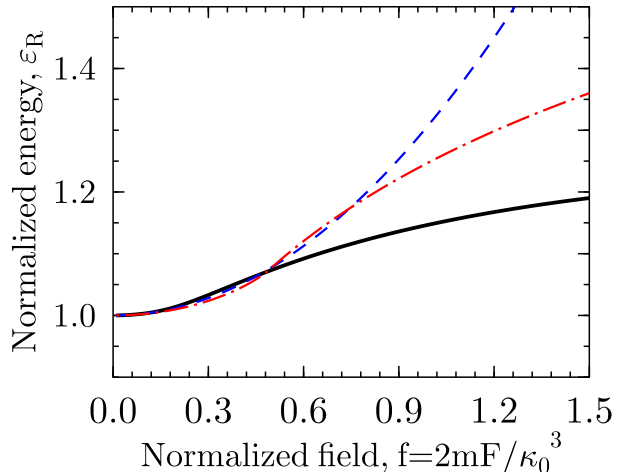
FIG. 1: The real part ε_R of the normalized energy κ^2 as a function of normalized electric field $f = 2mF/\kappa_0^3$. The solid line represents the exact solution of Eq. (21). The dashed line shows the quadratic behavior of an approximate solution, Eq. (24) for small f. The dot-dashed line is the real part for the energy, Eq. (29), obtained with the help of a variational method with a trial function (27). See below in text.

Solving this equation by iterations, we obtain after the first successive approximation

$$\varepsilon_R \approx 1 + \frac{5}{16}f^2, \quad \varepsilon_I \approx \exp\left(-\frac{4}{3f}\right). \tag{24}$$

For comparison we present these results in Figs. 1, 2 along with the results of the exact numerical solution of Eq.(21). The first two terms in the expansion of the wave function (20) near the origin with respect to the field parameter f are

$$\chi(z) \approx \sqrt{\kappa_0}e^{-\kappa_0|z|}\left[1 + \frac{f}{4}\text{sign}(z)|\kappa_0 z|(1 + |\kappa_0 z|)\right]. \tag{25}$$

The result for the real part of the energy presented in Eq. (24) can also be obtained from the second order of the standard quantum mechanical perturbation theory:

$$E_0^{(2)} = -2m\int_0^\infty \frac{|\langle\chi_{k,odd}^{(0)}(z)| - Fz|\chi_0^{(0)}(z)\rangle|^2}{\kappa_0^2 + k^2}dk, \tag{26}$$

where $\chi_{k,odd}^{(0)}(z) = \sin(kz)/\sqrt{\pi}$ are the odd wave functions of the unperturbed Hamiltonian. The non-analytical exponential dependence of the field induced broadening in Eq.(24) is typical for the Stark effect in a hydrogen-like atom $\Gamma \propto \exp\left[-(4/3)(E_0/F\ell)\right]$, where E_0 and ℓ are the absolute value of energy and the average radius of localization for the ground state without the field. In the case of QW excitons, the main contribution to E_0 comes from the single particle confinement energy, which is much larger than the exciton ground state energy $E_0/E_X \sim U^2L^2/\text{Ry}^2a_B^2 \gg 1$. Because of this circumstance, QCSE in QW is observable for very large fields.

In a strong enough electric field, the broadening quickly grows and becomes comparable to the real part of energy. In this case the resonance associated with the quasi-bound state disappears, becoming invisible on the background of the continuous spectrum. The condition of the existence of the resonance can be approximately formulated as $f \leq 1$. Since $f = 2mF/(mUL_{eff})^3$, it is easy to determine the region of parameters where quasi-bound states (and QCSE respectively) are observable. In Fig. 3 we present the phase diagram for the region of the existence of the quasi-bound states as a function of well width, L, and electric field for a GaAs-Ga$_{0.7}$Al$_{0.3}$As SQW. As expected, the larger fields and smaller widths destroy the localization of the exciton in the quantum well.

A knowledge of the complex energy and the corresponding wave function, Eq. (20), allows us, in principle, to find the corrections to the quasi-bound energy due to the effective electron-hole interaction. To this end, one would have to perform a coordinate rotation $z_{e,h} \to z_{e,h}\exp(i\gamma)$ to provide the convergence at infinity for the electron and the
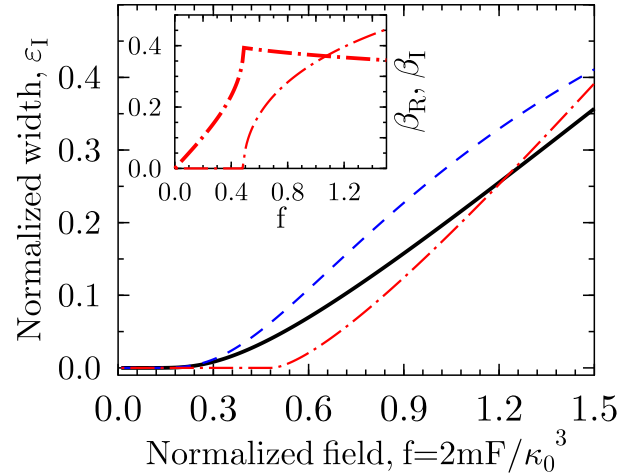
FIG. 2: The imaginary part ε_I of the normalized energy κ^2 as a function of normalized electric field $f = 2mF/\kappa_0^3$. The solid line represents the exact solution of Eq. (21). The dashed line shows the exponential non-analytical growth of an approximate solution, Eq. (24). The dot-dashed line is the imaginary part for the energy, Eq. (29), obtained with the help of a variational method with a trial function (27). The insert shows the behavior of the real and the imaginary parts of the variational parameter β
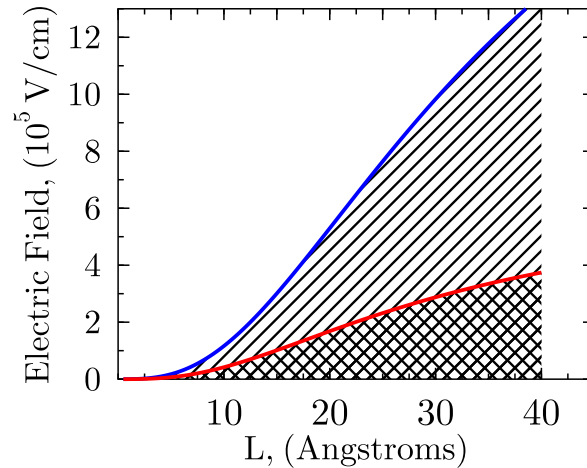
for the trial function (27).

FIG. 3: The phase diagram (L, F) for the region, where the quasi-bound states for an electron (upper curve) and a hole (lower curve) exist. The data are presented for GaAs-Ga$_{0.7}$Al$_{0.3}$As SQW. The calculations are based on the following physical constants: $m_e^* = 0.067m_0$, $m_h^* = 0.45m_0$, $U_e = 340$ meV, $U_h = 70$ meV, $\epsilon = 13.8$. The upper border for widths, $L = 40\AA$, is a limit of applicability of δ-functional model.

hole eigenfunctions (20), to substitute these wave functions into the integral in Eq. (7), and calculate the effective complex potential for the electron-hole interaction.

Unfortunately, the exact forms for the wave functions (20) lead to fairly cumbersome numerical calculations of the integral (7). However, the simple and rather accurate analytical estimates can be obtained with the help of the variational wave function of the following form

$$\chi_{trial}(z; \beta) = \sqrt{\kappa_0(1 - \beta^2)} \exp\left[\kappa_0\left(-|z| + \beta z\right)\right]. \tag{27}$$

A function of similar form has been successfully used in the past to model the real part correction to the single particle energy in quantum wells with finite width and in the presence of the electric field[7]. In our approach, however, we do not restrict the variational parameter β to be a real number, extending the range of its values on the whole complex plane. The only restriction is $\text{Re}(\beta) < 1$, which is dictated by the square integrability of the biorthogonal scalar product. Applying the variational principle to the Eq. (16) we obtain the following equations for the energy

$$\kappa^2(\beta) = 1 - \beta^2 + \frac{f\beta}{1 - \beta^2}. \tag{28}$$

The corresponding equation for the variational parameter β is

$$-f/2 + \beta - f/2\beta^2 - 2\beta^3 + \beta^5 = 0. \tag{29}$$

For small fields, the last three terms on the left hand side of Eq. (29) can be omitted, and we obtain $\beta \approx f/2$. The corresponding value for energy shift $\varepsilon_R - 1 \approx f^2/4$, which differs from Eq. (24) only by a factor of 1.25. For moderate values of the electric field this variational energy is even closer to the exact value than the perturbative result, Eq. (24). It is more important, however, that Eq. (29) also allows one to analyze the field induced decay of the electron. In order to understand how the electron acquires a finite life-time, one needs to include the third quadratic term in Eq. (29). The solution of the modified equation takes the form

$$\beta = f^{-1}\left[1 - \sqrt{1 - f^2}\right], \tag{30}$$

from which it is seen that when the electric field exceeds a critical value $f = f_{cr} = 1$, a square-root singularity appears, and the corresponding energy acquires an imaginary part. The exact solution of Eq. (29) changes the type of singular behavior of function $\beta(f)$ in the vicinity of f_{cr}, and lowers the critical field value

$$f_{cr} = 0.487. \tag{31}$$

The dependences of the real and imaginary parts of variational energy, Eq (28), on the normalized electric field, obtained from the solution of Eq. (29) are shown in Figs. 1 and 2. We can see that the variational results for the real part of the energy are in very good agreement (especially in the case of small and moderate fields) with the results of the exact solution of Eq. (21). The variational method with a simple trial function (27) also captures the effect of the field-induced decay of excitons characterized by a non-analytical dependence of the decay rate upon the electric field. Thus, the inclusion of the complex solutions of Eq. (29) for the variational parameter gives substantial physical insight into the problem of calculation of the effective exciton potential. We have to stress here that in the above procedure we performed only partial optimization of the functional (2), since we fixed $\gamma = 0$. The variational optimization of Eq. (10) with respect to the rotation angle would give a non-zero optimal angle γ_{opt} and even better agreement with the exact solution of Eq. (21). As we already mentioned, in the case of sharp resonances[23] the optimal angle of rotation γ is small. Moreover, the final answer for quasi-energy is not very sensitive to the change of γ. Therefore, the full optimization gives minimal corrections to the obtained result for the complex energy and variational parameter β, making, however, the further calculations of the exciton effective potential very cumbersome.

IV. EFFECTIVE POTENTIAL AND BINDING ENERGY CORRECTIONS FOR EXCITON

The effective potential for a quasi 2D exciton is given by the integral

$$V_{\text{eff}}(r; \kappa_0^{(e)}, \kappa_0^{(h)}, F) = -\int_{-\infty}^{\infty} dz_e \int_{-\infty}^{\infty} dz_h \frac{|\chi_e(z_e)|^2 |\chi_h(z_h)|^2}{\sqrt{r^2 + (z_e - z_h)^2}}. \tag{32}$$

For electron and hole wave functions we will use functions in a form Eq. (27) with corresponding values of the complex variational parameter β. For further calculations it is useful to introduce the following notations: we will denote wave numbers, variational parameters, and wave functions, related to the electron (hole) by index 1(2), for instance wave numbers $\kappa_i \equiv \kappa_0^{(e,h)}$, where $i = 1$ or 2. We also introduce renormalized parameters $\kappa_{iL,R}$ according to

$$\kappa_{1L,R} = \kappa_1 (1 \pm \beta_1) \tag{33}$$
$$\kappa_{2L,R} = \kappa_2 (1 \mp \beta_2) \tag{34}$$
$$\beta_i = \beta_i (2m_i F/\kappa_i^3) = \beta_{iR} + i\beta_{iI}, \quad \beta_R, \beta_I \geq 0. \tag{35}$$
$$\tag{36}$$

With these notations the wave functions (27) and effective potential, Eq. (7), can be rewritten as

$$\chi_i(z_i) = \sqrt{\frac{\kappa_{iR}\kappa_{iL}}{\kappa_i}} \begin{cases} \exp(\kappa_{i\,L} z), & z < 0 \\ \exp(-\kappa_{i\,R} z), & z > 0 \end{cases} \tag{37}$$

$$\begin{aligned} \overline{V}_r^{(0)}(r; \kappa_1, \kappa_2, F) &= -\int_0^\infty dz_1 \int_0^\infty dz_2 \left[\frac{\chi_{1L}^2 \chi_{2L}^2 + \chi_{1R}^2 \chi_{2R}^2}{\sqrt{r^2 + (z_1 - z_2)^2}} + \frac{\chi_{1L}^2 \chi_{2R}^2 + \chi_{1R}^2 \chi_{2L}^2}{\sqrt{r^2 + (z_1 + z_2)^2}} \right] \\ &\equiv V_I(\kappa_{1L}, \kappa_{2L}, r) + V_I(\kappa_{1R}, \kappa_{2R}, r) + V_{II}(\kappa_{1L}, \kappa_{2R}, r) + V_{II}(\kappa_{1R}, \kappa_{2L}, r), \end{aligned} \tag{38}$$

where the last line introduces notations for each of four terms comprising the integral representation for $\overline{V}_r^{(0)}$. As we had shown before[19] the potentials $V_{I,II}$ can be represented with the help of the function

$$T_\alpha \equiv T(\kappa_\alpha r) = \int_0^\infty \frac{\exp(-2\kappa_\alpha t) dt}{\sqrt{r^2 + t^2}} = \frac{\pi}{2} \left[\mathbf{H}_0(2\kappa_\alpha r) - Y_0(2\kappa_\alpha r) \right], \tag{39}$$

where $\mathbf{H}_0$ is the zero-order Struve function and Y_0 is the zero-order Neumann or Bessel function of the second kind.[26] Then

$$V_{I,II}(\kappa_\alpha, \kappa_\beta) = -\frac{\kappa_{1L}\kappa_{1R}\kappa_{2L}\kappa_{2R}}{2\kappa_1\kappa_2} \left[\frac{T(\kappa_\beta r) \pm T(\kappa_\alpha r)}{\kappa_\alpha \pm \kappa_\beta} \right], \tag{40}$$

and the final result for the effective exciton potential induced by QW confinement and the presence of the electric field takes the form

$$\overline{V}_r^{(0)}(r; \kappa_1, \kappa_2, F) = \frac{\kappa_1\kappa_2(1-\beta_1^2)(1-\beta_2^2)}{2} \left[\frac{T_{1L}+T_{2L}}{\kappa_{1L}+\kappa_{2L}} + \frac{T_{1R}+T_{2R}}{\kappa_{1R}+\kappa_{2R}} + \frac{T_{1L}-T_{2R}}{\kappa_{2R}-\kappa_{1L}} + \frac{T_{1R}-T_{2L}}{\kappa_{2L}-\kappa_{1R}} \right]. \tag{41}$$

Without the electric field Eq.(41) is reduced to the result obtained in Ref.[19]

$$\overline{V}_r^{(0)}(r; \kappa_1, \kappa_2, 0) = -\frac{2\kappa_1\kappa_2}{\kappa_2^2 - \kappa_1^2} \left[\kappa_2 T(\kappa_1 r) - \kappa_1 T(\kappa_2 r) \right]. \tag{42}$$

where it was shown that the properties of this potential are governed by a single parameter

$$d^2 = \frac{1}{2} \left(\frac{1}{\kappa_1^2} + \frac{1}{\kappa_2^2} \right) = \langle \chi_1(z_1)\chi_2(z_2) | (z_1 - z_2)^2 | \chi_1(z_1)\chi_1(z_2) \rangle. \tag{43}$$

This parameter has a simple physical meaning of the average square of the distance between the electron and the hole in the z direction. It controls the transition between small r and large r asymptotics of the zero-field potential (42):

$$\overline{V}_r^{(0)}(r; \kappa_1, \kappa_2, 0) \approx \begin{cases} \frac{1}{d} \ln(r/d), & r \lesssim d, \\ -\frac{1}{\sqrt{r^2+d^2}}, & r \gtrsim d. \end{cases} \tag{44}$$

The effective zero-field electron-hole interaction for the exciton in the SQW starts from the true logarithmic Coulomb potential of a point charge in two dimensions that smoothly transforms at distances $r \sim d$ to the screening potential (44) with three-dimensional Coulomb tails.

The understanding of the role played by the parameter d helps to substantially simplify calculations of the ground state energy. For example, we found that the variational energy obtained with a single parameter trial function

$$\varphi_{trial} = \frac{2\exp(d/\lambda)}{\sqrt{\lambda(\lambda + 2d)}} \exp(-\sqrt{r^2 + d^2}/\lambda) \tag{45}$$

coincides with more sophisticated numerical approaches with excellent accuracy. The respective expression for the ground state energy can be written as a sum of two terms: $E_X = E_X^{(0)}(\lambda) + E_X^{(1)}$, where

$$E_X^{(0)}(\lambda) = -\frac{2}{\lambda} \frac{1}{1 + 2d/\lambda} + \frac{1}{\lambda^2} \left[1 - \frac{(2d/\lambda)^2 E_1(1, 2d/\lambda) \exp(2d/\lambda)}{1 + 2d/\lambda} \right], \tag{46}$$
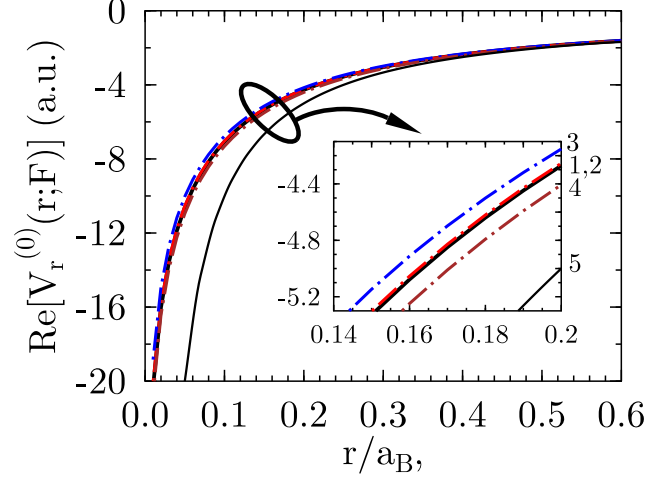
FIG. 4: The profile of the real part of the effective self-consistent exciton potential $\overline{V}_r^{(0)}(r; \kappa_1, \kappa_2, F)$ for different values of the electric field (dot-dashed lines). The thick solid line (curve 5) below the other curves represents $-1/r$ behavior, and is given for comparison. The insert is a magnified view of the circled area. The labels for the curves correspond to, curve 1, $F = 0$ V/cm, curve 2, $F = 0.4 \times 10^5$ V/cm, curve 3, $F = 0.8 \times 10^5$ V/cm, curve 4, $F = 4 \times 10^5$ V/cm. All data are for $d/a_B = 0.16$ that corresponds $L = 20\mathring{A}$ finite quantum well in AlGaAs/GaAs materials.

with $E_1(x)$ being the exponential integral.[26], and

$$E_X^{(1)} \approx -\frac{2d}{\lambda^2}\left[\frac{1}{2} - 0.557\frac{2d}{\lambda} + 0.563\left(\frac{2d}{\lambda}\right)^2 + \cdots\right]. \tag{47}$$

The first term $E_X^{(0)}$ should be taken for the optimal value of λ that brings Eq. (46) to the minimum. The second term, Eq. (47), is a small correction, which is calculated for a given optimal λ.

In order to understand how these results are modified by the electric field we study the properties of the effective potential Eq.(41). Figures 4 and 5 show the profiles of the real and the imaginary parts of this potential calculated for several different electric fields. For concreteness we chose for calculations parameters typical for GaAs-Ga$_{0.7}$Al$_{0.3}$As SQW with width $L = 20\mathring{A}$. In our calculations we used the following physical constants: $m_e^* = 0.067m_0$, $m_h^* = 0.45m_0$, $U_e = 340$ meV, $U_h = 70$ meV, $\epsilon = 13.8$. For these constants we have $\kappa_1 = 5.68$, $\kappa_2 = 7.31$, and $d = 0.16$. The latter value tells us that in a zero field the exciton is strongly localized in the QW. The critical fields $F_{1,2}^{cr}$ derived from Eqs. (31,17) are $F_h^{cr} = 0.82 \times 10^5$V/cm and $F_e^{cr} = 2.57 \times 10^5$V/cm. According to our phase diagram, Fig. 3, a field that larger than 1.7×10^5V/cm should be considered as strong, since in this case the hole has already a substantial probability to tunnel through the barrier, escaping an interaction with the electron. Results presented in Figure 4 show that effects of the electric field on the real part of the effective exciton potential are relatively small. It indicates that the corrections to the real part of quasi-bound exciton energy due to the field must also be small. The result is consistant with the previous calculations[18] for larger QW, where a trend to a substantial decrease of the Stark shift was observed with narrowing of quantum well widths up to $L = 50\mathring{A}$.

With increasing applied field the potential changes in the following way: at small fields (see curves 2,3 on the insert) both βs are real and there is no imaginary part at all. As the field is applied, the electron and the hole are pulled apart by the field. It weakens the effective attractions and the curve moves upwards, manifesting a Stark shift for the binding energy corrections. Curve 3 represents the maximal deflection from the zero-field potential. It corresponds to the moment of the first critical field, when the single particle energy for the hole in QW acquires the width and its tunnelling becomes possible. At this moment the optical (imaginary) part of the effective potential also appears. After this the real part of the potential begins swinging back. The latter can be understood if we have a look at the real part of β in the insert of Fig. 2. After the "critical field" is passed, β_R also changes its behavior and even slightly decreases with field growth. The latter explains the "effective" increasing of the attraction again. However, since now the connection with the continuum is established, the physical interpretation is not so obvious. The imaginary part of the effective potential continues to grow, which is clearly seen in Fig. 5. In order to understand the character of this growth, we fixed the radius of the potential and investigated the field dependence of the potential strength at this
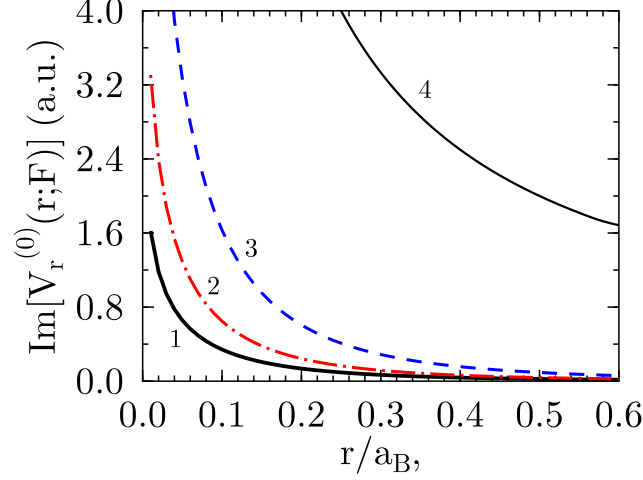
FIG. 5: The profile of the imaginary part of the effective self-consistent exciton potential $\overline{V}_r^{(0)}(r;F)$ for different values of electric field (dot-dashed lines). The upper solid line (curve 4) represents $1/r$ behavior, and is given for comparison. The labels for the curves correspond to, curve 1, $F = 10^5$ V/cm, curve 2, $F = 2. \times 10^5$ V/cm, curve 3, $F = 4 \times 10^5$ V/cm. All data are for $d/a_B = 0.16$ that corresponds to $L = 20\mathring{A}$ finite quantum well in AlGaAs/GaAs materials.
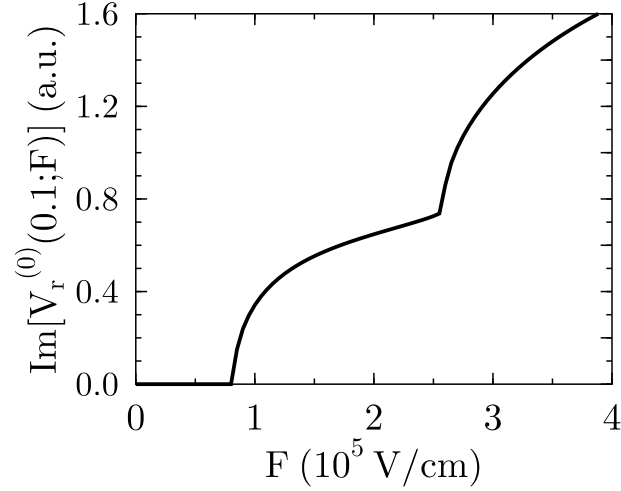

FIG. 6: The dependence on electric field of an imaginary part of the effective potential $\overline{V}_r^{(0)}(r;F)$ at fixed value of radius $r/a_B = 0.1$ Data are for $L = 20\mathring{A}$ AlGaAs/GaAs SQW.

fixed r. Fig. 6 gives corresponding results for this dependence. As we can see, it follows the behavior of the imaginary parts of $\beta_{1,2}$ (compare with Fig. 2). The second leap corresponds to the second critical field, when a new scattering channel, namely, a possibility of electron tunnelling, is open.

The smallness of the correction to the real part of the effective potential suggests that we can try to express this effective complex potential at finite field through the zero-field potential, renormalizing some of its parameters. To do so, let us look at the asymptotic behavior of the potential Eq. (41). One can show that the first two terms in the asymptotic expansion are

$$\overline{V}_r^{(0)}(r; \kappa_1, \kappa_2, F) \approx -1/r + \tilde{d}^2/(2r^3). \tag{48}$$

They are the same forms as for zero-field potential [see Eq. (44)], but with

$$\tilde{d}^2 = \frac{1}{2}\left[\frac{1}{\kappa_1^2}\frac{1+3\beta_1^2}{(1-\beta_1^2)^2} + \frac{1}{\kappa_2^2}\frac{1+3\beta_2^2}{(1-\beta_2^2)^2} + \frac{4\beta_1\beta_2}{\kappa_1\kappa_2(1-\beta_1^2)(1-\beta_2^2)}\right] \tag{49}$$

It is also easy to see that this new parameter is the average square of the distance between the electron and the hole in the z direction, when the electric field applied:

$$\tilde{d}^2 = \langle\chi_1(z_1)\chi_2(z_2)|(z_1-z_2)^2|\chi_1(z_1)\chi_1(z_2)\rangle. \tag{50}$$

This parameter is complex now, and its imaginary part provides the coefficient for the asymptotic of the imaginary part of the effective exciton potential. With this finding, it is easy to understand how we should renormalize the wave numbers $\kappa_{1,2}$ to adjust corrections in binding energy, induced by electric field. The easiest way is the following:

$$\frac{1}{\tilde{\kappa}_1}^2 = \frac{1}{\kappa_1^2}\frac{1+3\beta_1^2}{(1-\beta_1^2)^2} + \frac{2\beta_1\beta_2}{\kappa_1\kappa_2(1-\beta_1^2)(1-\beta_2^2)}, \tag{51}$$

$$\frac{1}{\tilde{\kappa}_2}^2 = \frac{1}{\kappa_2^2}\frac{1+3\beta_2^2}{(1-\beta_2^2)^2} + \frac{2\beta_1\beta_2}{\kappa_1\kappa_2(1-\beta_1^2)(1-\beta_2^2)}. \tag{52}$$

Then, for small applied fields the potential, Eq. (41) coincides with the modified potential for zero field Eq. (42) up to the third degree in the electric field expansion,

$$\overline{V}_r^{(0)}(r;\kappa_1,\kappa_2,F) \approx \overline{V}_r^{(0)}(r;\tilde{\kappa}_1,\tilde{\kappa}_2,0). \tag{53}$$

Therefore, the expressions (46,47) for exciton binding energy in zero field with renormalized parameter $\tilde{d}^2$ are valid for non-zero electric fields.

V. CONCLUSIONS

We developed a self-consistent complex scaling approach for calculations of field-induced complex energies of single particle states as well as of the exciton quasi-energy in QWs. This technique is a generalization of the self-consistent approach recently developed by the authors[19] for the exciton in a QW without the presence of the electric field. For the case of strong confinement, we represented the trial function in factorized form and obtained the corresponding coupled self-consistent equations (4–6), which include the effective potentials (7,8). These effective potentials are results of averaging over z coordinates of the Coulomb interaction and the quantum well potential. We would like to note, that, although the resulting equations are obtained for a separable wave function, the approach itself has a broader range of applicability, and can be employed for different forms of trial functions.

We further applied our approach to the case of a shallow quantum well. To this goal we developed the model of QCSE in a δ-functional quantum well, which allows us to obtain analytical results for the resonance positions and widths and the behavior of the modified exciton "ground state" wave function. This occurs because the single-particle one-dimensional problem in delta-potential and applied uniform electric field can be solved exactly. We also compared the exact results for single-particle complex energies with the complex scaling variational method results for a trial function in a simple form of two decaying exponents with different coefficients of decay. The obtained energy has both the real and the imaginary parts, and their values are in a very good agreement with the exact solution for quasi-energy within a wide range of the parameters. The non-zero imaginary part gives additional physical insight into the problem. The simple variational functions for the electron and the hole allow us to calculate the effective exciton potential. This potential has real and imaginary (optical) parts. We found that the real part of the potential is insensitive to changes of external electric field up to the QCSE ionization threshold. This allows us to express exciton quasi-bound state at some field through the renormalized expression for the binding energy in zero field.

Acknowledgments

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