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One-dimensional δ-potential in external fields

O Olendski†

Atomic and Molecular Engineering Laboratory, Belarussian State University, Skarina Avenue 4, Minsk 220050, Belarus

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Abstract. The 1D δ-potential with strength Ω in an external in-plane magnetic field $\boldsymbol{B}$ is considered theoretically. Energy dependences on Ω and d (with d being normalized to the magnetic radial $r_B = (\hbar/eB)^{1/2}$ distance between the δ-potential and the vertex of the magnetic parabola) are calculated and analysed in detail in the whole ranges of d and Ω. It is shown that at $d = d_{jk}$ the jth Landau level is not affected by the presence of the potential, where d_{jk} are the zeros of the jth-degree Hermite polynomial. For $d = 0$, every excited even level with number j changes its energy normalized to $\hbar\omega_B$ (ω_B is the cyclotron frequency) from $j - \frac{1}{2}$ at $\Omega = -\infty$ through $j + \frac{1}{2}$ at $\Omega = 0$ to $j + \frac{3}{2} (\Omega = +\infty)$. However, the ground-state energy asymptotically tends to $-\infty$ while Ω varies from $+\infty$ to $-\infty$. A simple physical explanation of the results obtained is given. Anticrossings of the levels in the dispersion relations are investigated for all values of Ω. For fixed positive (negative) Ω, every jth level ($j = 0, 1, \ldots$) has, on the d axis, j minima (maxima) with absolute value $j + \frac{1}{2}$, which are achieved at d_{jk}. It is derived that, in the anticrossing picture, gaps between levels at the points d_{jk} decrease on increase in $|\Omega|$, and levels cross at $\Omega = \pm\infty$. For large negative Ω a picture of the interaction of the ground state with excited levels is given. The proposed model with the simplest modification is used to investigate the combined influence of the crossed electric and magnetic fields. This problem enables comparison with earlier results for a δ-like quantum object in a uniform electric field.

A problem of increasing interest is the influence of an external magnetic field $\boldsymbol{B}$ on the electronic, transport and optical properties of semiconductors [1]. In previous investigations (see, e.g., [1–12], and references therein), nanostructures were modelled by means of a quantum well (or sequence of wells) with a finite width and a finite or infinite height of the barrier or barriers. To the great surprise of the present author, no complete solution of the similar problem for a one-dimensional (1D) δ-potential has been found in the literature. The main goal of the present paper is to achieve this. This extremely simplified model allows one to obtain physically clear conclusions for both a δ barrier and a δ well and, in a sense, is a generalization of previous studies. Another advantage lies in the fact that with the simplest modification it can be applied to the combined influence of the crossed electric and magnetic fields which in the case of the vanishing magnetic field enables comparison with earlier results for a quantum well or barrier in a uniform electric field.

In the absence of external fields, the behaviour of a particle in a 1D potential of the form $V(y) = (\hbar^2/m)\Omega\delta(y - y_P)$ (m is the mass of the particle and y_P is the location of the potential on the y axis) is well known [13, 14]. For $\Omega > 0$ there are no bound states, and the reflection and transmission coefficients are easily calculated [13, 14]. For $\Omega < 0$ there is one bound state with energy $-\hbar^2\Omega^2/2m$ [13, 14]. Now let us apply a magnetic field $\boldsymbol{B} = (0, 0, B)$, which lies in the plane of the potential. The opposite configuration

† Present address: Department of Physics, Chonnam National University, Kwangju, 500-757, Republic of Korea.

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with the field perpendicular to the plane is trivial and will not be discussed here. As usual in the Landau gauge, we use a vector potential of the form $A = (-By, 0, 0)$. In that case the variables x and z with the help of plane waves are factorized out, and the y-dependent part of the Schrödinger equation describes particle behaviour on the superposition of two potentials: the δ-like profile and the usual magnetic parabola. The corresponding solutions for the wavefunction are

$$\chi(y) = A_{-}U(\nu, -\xi(y)) \qquad y < y_P \tag{1a}$$

$$\chi(y) = A_{+}U(\nu, \xi(y)) \qquad y > y_P \tag{1b}$$

with

$$\nu = -c \tag{2a}$$

$$\xi(y) = 2^{1/2}(y - y_0)/r_B \tag{2b}$$

$$c = (E - p_z^2/2m)/\hbar\omega_B. \tag{3}$$

Here $\omega_B = eB/m$, $r_B = (\hbar/eB)^{1/2}$, $y_0 = -p_x/eB$, p_x and p_z are the x and z components of the kinetic momentum $\boldsymbol{p}$ and $U(\nu, \xi)$ is the Weber parabolic cylinder function [15, 16]. In deriving (1), use has been made of the properties of the Weber functions, i.e. solutions which increase with $y \to \pm\infty$ and which contain the functions $V(\nu, \xi)$ have been omitted. The usual procedure of matching the wavefunctions in the presence of the δ-potential [13, 14] gives a universal equation for the determination of the energy spectrum (the prime on $U(\nu, \xi)$ denotes the derivative of the Weber function with respect to the second argument):

$$U(\nu, 2^{1/2}d)U'(\nu, -2^{1/2}d) + U'(\nu, 2^{1/2}d)U(\nu, -2^{1/2}d) - \Omega_B U(\nu, 2^{1/2}d)U(\nu, -2^{1/2}d) = 0 \tag{4}$$

$$\Omega_B = 2^{1/2} r_B \Omega \tag{5}$$

$$d = \Delta \tag{6}$$

with Δ being normalized to the magnetic radial distance between the potential and the centre of the magnetic oscillations:

$$\Delta = (y_P - y_0)/r_B. \tag{7}$$

We wish to note that, contrary to the uniform magnetic field, unperturbed by potentials, when Hamiltonian eigenvalues are independent of p_x, in our case the energy strongly depends on the x component of kinetic momentum which, in turn, determines the vertex of the parabola. This is clearly seen from equation (4) which links together the energy E, the field B, the opacity Ω and the kinetic momentum p_x. It is worthwhile to point out also that (4) is invariant with respect to the change in sign of d. Therefore, below (figures 2 and 3), only the case $d > 0$ is considered.

For $d = 0$, (4) can be simplified to

$$U(\nu, 0)[2U'(\nu, 0) - \Omega_B U(\nu, 0)] = 0$$

or, using the properties of the parabolic cylinder functions [16], one immediately finds that odd Landau levels are not affected by the presence of the δ-potential at the vertex of the parabola, i.e.

$$c_{\mathrm{odd}}(d=0) = 2i + \tfrac{3}{2} \qquad i = 0, 1, 2, \ldots \tag{8a}$$

and even states satisfy the equation (see also [17, 18] where a similar expression has been derived using other methods)

$$\Omega_B = -\frac{2^{3/2}\Gamma(-c/2+\frac{3}{4})}{\Gamma(-c/2+\frac{1}{4})}. \tag{8b}$$

Equation (8*a*) is a particular case of the well known result that a quantum system does not 'feel' the external δ-potential if the δ-potential is located at one of the nodes of the wavefunction [13, 17, 18]. Some preliminary results may be derived for the limiting cases $\Omega_B = 0$ and $\Omega_B \to \pm\infty$ without numerical solutions of (4) and (8*b*). For instance, for $\Omega_B = 0$, one gets, as expected, the spectrum of the usual Landau levels. The case $\Omega_B \to +\infty$ corresponds physically to magnetic fields small compared with the opacity of the quantum barrier. In this case we have a system of two non-interacting constrained quantum-mechanical harmonic oscillators [19] with a common impenetrable boundary. At $\Omega_B \to +\infty$ and $d = 0$ we can conclude, using the properties of the Γ-function (figure 6.1 in [16]), that the energy of every even Landau state tends to the nearest odd level above. For $\Omega_B \to -\infty$, every even state (except the ground state) approaches the energy of the corresponding odd level from the direction of the higher energies. However, in this case the ground-state solution of (8*b*) on increase in $|\Omega_B|$ tends asymptotically to the value

$$c_0(d=0; \Omega_B \to -\infty) = -\tfrac{1}{4}\Omega_B^2$$

which appears to be the ground-state energy (in units of $\hbar\omega_B$) in the absence of an external field. This last result may be easily explained from the physical point of view also, namely that small magnetic fields produce little effect on the quantum well.

In figure 1 the c dependence on Ω_B is shown for $d = 0$, i.e. for the case when the singular potential coincides with the vertex of the magnetic parabola. As we discussed earlier, every even state with number j (except $j = 0$) changes its energy from $j - \frac{1}{2}$ at $\Omega_B = -\infty$ through $j + \frac{1}{2}$ at $\Omega_B = 0$ to $j + \frac{3}{2}$ at $\Omega_B = +\infty$. Similar to the previous configurations [4, 9], for higher-lying even states, transformations to odd-state energies occur at higher $|\Omega_B|$.

In figures 2 and 3 the energy dependences on d for a few positive and negative Ω_B-values, respectively, are shown. For positive (negative) Ω_B, every jth level ($j = 0, 1, 2, \ldots$) has, on the d axis ($-\infty < d < +\infty$), j minima (maxima) with absolute value $j + \frac{1}{2}$, which are achieved at d_{jk}, with d_{jk} being the kth zero of the jth-degree Hermite polynomial:

$$c_{\min}^{(j)}(\Omega_B > 0) = c^{(j)}(d_{jk}, \Omega_B > 0) = j + \tfrac{1}{2} \tag{9a}$$

$$c_{\max}^{(j)}(\Omega_B < 0) = c^{(j)}(d_{jk}, \Omega_B < 0) = j + \tfrac{1}{2}. \tag{9b}$$

The d_{jk} values may be found, for example, in table 25.10 in [16]. Equations (9) are due to the above-mentioned fact that the δ-potential cannot affect properties of the quantum states if it is located in one of the nodes of the corresponding wavefunction [2, 13, 19].

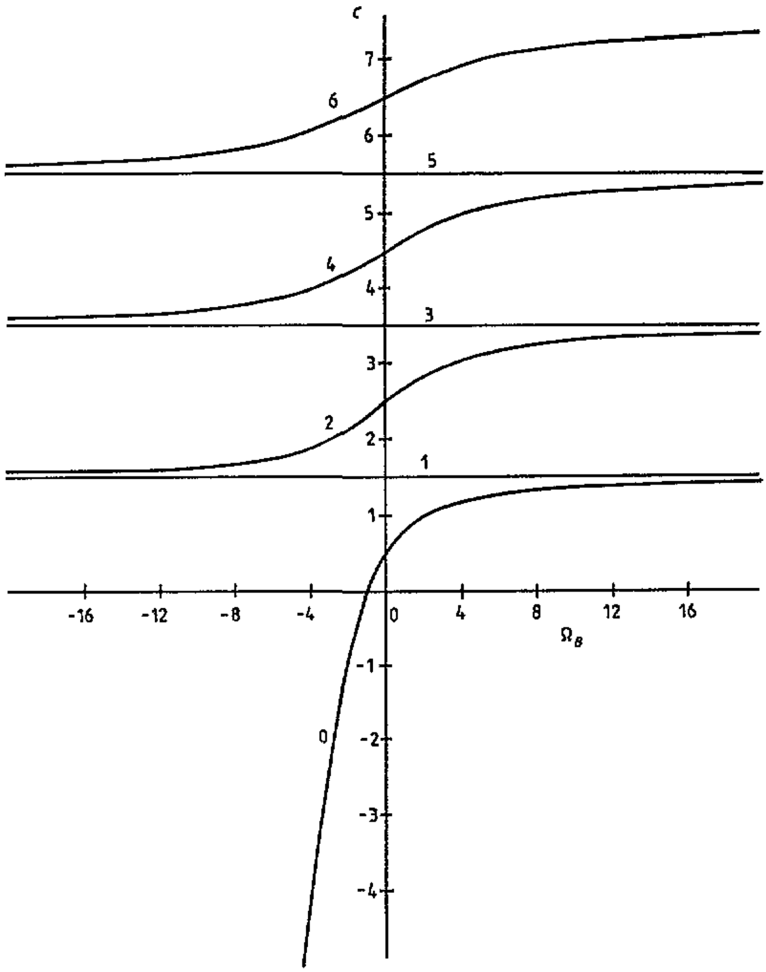

Figure 1. Dependence of the normalized energy c on Ω_B at $d = 0$ (compare with figure 8 of [18]). The numbers near the curves denotes the levels: 0, ground state; 1–6, excited levels.

The characteristic features of similar systems which have been widely discussed earlier [1, 2, 5, 6, 8, 10–12] are anticrossings of the levels in dispersion relations. The model of the δ-potential in an external field proposed here allows one to elucidate this property for the barrier ($\Omega_B > 0$) and the well ($\Omega_B < 0$). That is, as is seen from figures 2(a) and 3(a), at small $|\Omega_B|$ there are small deviations in the energies from the Landau states on varying d which, in turn, linearly depends on the kinetic momentum p_x. It is even difficult in this case to consider any interaction between levels. However, on increase in $|\Omega_B|$ (figures 2(b), 2(c) and 3(b)–3(d)) the levels become closer and closer to each other at the points d_{jk}. With increasing $|\Omega_B|$ the gaps between states decrease but remain finite and not equal to zero. The gaps are wider for higher states, and only at $|\Omega_B| = \pm\infty$ do levels cross at the points d_{jk} (figure 2(d)). It should be mentioned also that, as expected, at large d the levels are the usual Landau states. At fixed Ω_B for higher states, this occurs at larger d. The same is also true for fixed j and varying $|\Omega_B|$. The explanation for this is similar to that in previous studies [2, 4, 9, 19].

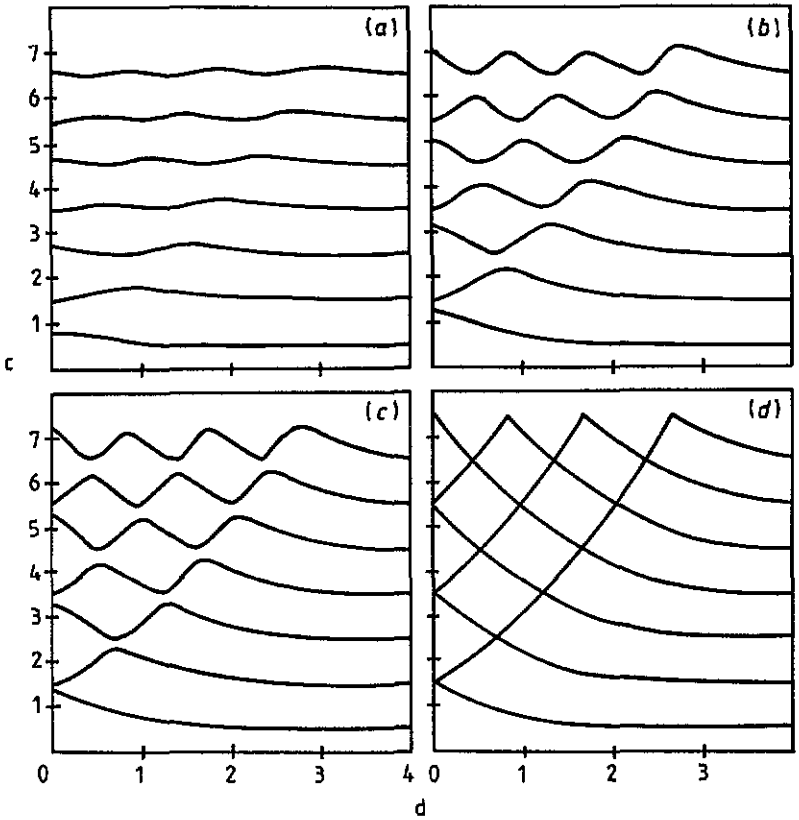

Figure 2. Dispersion relations for (*a*) $\Omega_B = 1$, (*b*) $\Omega_B = 5$, (*c*) $\Omega_B = 10$ and (*d*) $\Omega_B = \infty$. The case $\Omega_B = \infty$ may be obtained as a replica of a plot for a constrained quantum mechanical harmonic oscillator folded along the energy axis (figure 2 in [19]).

Another interesting phenomenon consists of the repulsions of the levels at $\Omega_B < 0$. Similar to the above-discussed anticrossings, this phenomenon is clearly manifested at large $|\Omega_B|$ when, as mentioned above, the ground state has a large negative energy. In this case on increase in d the first excited state approaches and attains the energy $c_0 = \frac{1}{2}$, the second excited state $c_1 = \frac{3}{2}$, etc. On the other hand, increasing d causes the ground-state energy to increase also, and finally it is shifted from the negative part of the spectrum and approaches the value $c_0 = \frac{1}{2}$, causing the first excited level to move upwards because of repulsion; it maintains this energy on further increase in the distance. In turn, the level which is moved upwards attains the value $c_1 = \frac{3}{2}$, and the whole picture is repeated, etc. For larger $|\Omega_B|$ (i.e. for deeper wells) the repulsions just described occur at larger d, the slope of the curve being steeper and the transformations sharper. Using the properties of the Weber functions [15, 16], one can easily show from equation (4) that at large $|\Omega_B|$ the location of these anticrossings on the d axis linearly depends on $|\Omega_B|$. All other properties are similar to the anticrossings discussed earlier in this paper. In our model this is completely analogous to the behaviour of magnetic levels near the potential step [1, 5] or in the finite superlattice [1, 11].

Finally we should point out that, as at $\Omega_B = -\infty$ infinite energy is available while achieving the ground state, the dispersion relation for $\Omega_B = -\infty$ is the same as for

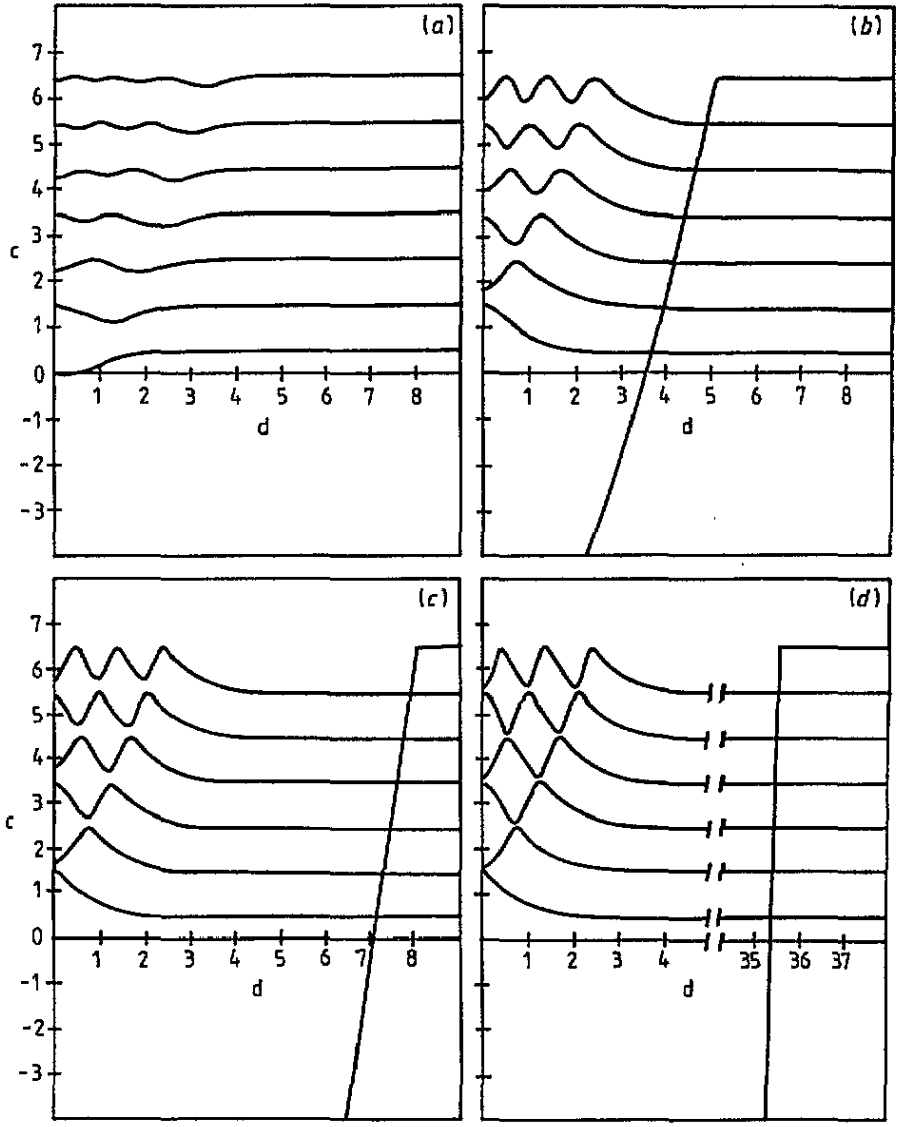

Figure 3. Dispersion relations for (*a*) $\Omega_B = -1$, (*b*) $\Omega_B = -5$, (*c*) $\Omega_B = -10$ and (*d*) $\Omega_B = -50$. Because of the chosen scale, the gaps between the states for the ground-state interaction with excited levels are not resolved in (*b*)–(*d*).

$\Omega_B = +\infty$. This is seen also directly from equation (4), which for the case $\Omega_B = \pm\infty$ is

$$U(\nu, 2^{1/2}d)U(\nu, -2^{1/2}d) = 0.$$

The only difference is that the odd and even states have changed places.

It is instructive to compare the results presented here with the predictions of classical electrodynamics. This states that a charged particle does not 'feel' a barrier (to be specific, in the classical limit we shall talk about a barrier) if $d > 1$. In this case one has the usual cyclotron orbit in a uniform magnetic field, without average displacement along the x or

y axes [20]. This is in a some accordance with quantum theory where also for large d the influence of the potential on magnetic states is negligible. If the orbit hits the barrier ($d < 1$), which in classical theory is impenetrable for all values $\Omega > 0$, the particle begins to move along a skipping orbit, acquiring an average velocity along the barrier, perpendicular to the magnetic field. It can be readily shown that this velocity has only an x component and its value is

$$\langle v_x \rangle = v_\perp^B \frac{\sin(\pi - \alpha)}{\pi - \alpha} \tag{10}$$

with $v_\perp^B$ being the transverse velocity of the classical particle in the unperturbed uniform magnetic field. α satisfies the equation

$$\cos\alpha = d$$

and for d the classical definition of the magnetic radius is used:

$$r_B^{\mathrm{cl}} = \frac{(2mE - p_z^2)^{1/2}}{eB}.$$

For two limiting cases of d we have the following: for case (i), $d = 0$, $\langle v_x \rangle = (2/\pi)v_\perp^B$, the largest value; for case (ii), $d = 1$, $\langle v_x \rangle = 0$, as expected. It is also seen from (10) that $\langle v_x \rangle$ is larger for higher energies. Again, this is in agreement with the results of the wave mechanics presented above.

There is no difficulty in extending the quantum model proposed here to the case of the simultaneous influence of the crossed magnetic field $\boldsymbol{B}$ and electric field $\boldsymbol{F}$, the latter being directed along the y axis. In this case the wavefunction is expressed by equation (1) also with

$$\nu = -(c + \eta y_{0B} + \eta^2) \tag{11a}$$

$$\xi(y) = 2^{1/2}[(y - y_0)/r_B - \eta] \tag{11b}$$

$$\eta = eFr_B/\hbar\omega_B \tag{12}$$

$$y_{0B} = y_0/r_B.$$

Equation (4) also holds with

$$d = \Delta - \eta. \tag{13}$$

Therefore, we see that all the conclusions derived above will be valid in the case of crossed fields with the corresponding choice of ν and d according to (11)–(13). At this point we note the quadratic dependence of normalized energies c on F in two limiting cases: case I, $\eta \to 0$ (the electric field is small compared with the magnetic field); case II, $\eta \to +\infty$ (the magnetic field is small in comparison with the electric field). Both cases may be easily explained physically. For case II we obtain superposition of the crossed fields [14] with the δ-potential as a small perturbation. The larger η, the smaller is the perturbation. Case I with the auxiliary condition $\Delta = 0$ (and $\Omega_B < 0$) corresponds to the problem of the δ well in a small uniform electric field when the energy also quadratically depends on F [14]. However, our approach has some advantages, since we do not have to use Airy functions with complex arguments, as has been done in [14] for the δ well and in [21, 22] for a finite quantum potential. This can be explained by the fact that, in our method, because of the presence of the magnetic field we have true bound states and, in [14, 21, 22], only a quasi-bound state exists.

Finally, we indicate some obvious extensions of the present work. Firstly, on increasing the number of the barriers or the wells, we come to the Kronig–Penney δ model of the solid state in external fields (a similar procedure for finite wells and barriers has been discussed in [1, 11]). Secondly, comparing the results presented here with those in [9, 21], we can calculate the electronic and optical properties of the finite quantum well in crossed electric and magnetic fields, which enables a comparison to be made with different methods of investigating the quantum well in the uniform electric field [21, 23–28]. Detailed discussions of these investigations will be reported elsewhere.

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