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Charged donor in a narrow quantum well in the presence of in-plane crossed magnetic and electric fields

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Abstract

An analytical approach to the problem of a negatively charged donor in a narrow quantum well (QW) in the presence of crossed magnetic and electric fields is developed. The width of the QW is taken to be much less than the impurity radius and the magnetic length. Both magnetic and electric fields are directed parallel to the heteroplanes. The impurity centre is positioned anywhere within the QW. The adiabatic approximation is used: the motion of the electron in the direction perpendicular to the heteroplanes is much faster than that parallel to the heteroplanes. The explicit dependences of the total energy of the charged donor upon the parameters of the well and external field strengths are obtained. The dependences of the binding energy of the charged donor on the width of the well and the position of the impurity within the well are studied. It is shown that a displacement of the impurity centre from the mid-point of the QW leads to a decrease of the binding energy. The relative position of the impurity within the narrow well affects strongly the dependence of the binding energy on the width of the well. A red shift of the energy and the detachment rate of the quasi-two-dimensional charged donor both caused by the weak electric field are calculated explicitly. The red shift can be balanced by the blue shift induced by the magnetic field. Using the parameters associated with GaAs and InGaN QWs estimates of the values expected for an experiment are made.

1. Introduction

The problem of a negatively charged donor consisting of the neutral donor and a weakly bound extra electron, which are confined within low-dimensional heterostructures, has attracted considerable attention in recent years. Semiconductor systems based on GaAs/GaAlAs structures, particularly isolated single quantum wells (QWs), were a major focus of interest

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during the last decade. Of special interest is the narrow QW with a width which is much less than the radius of the impurity. This is due to the fact that the quasi-two-dimensional charged donor in the narrow QW is considerably more stable than that in bulk material. It was shown in [1] that the binding energy E_b of the two-dimensional (2D) negatively charged hydrogenic donor (D^-) scaled to the impurity Rydberg constant Ryd is about $E_b \approx 0.48$ Ryd whereas for the bulk semiconductor we have $E_b \approx 0.055$ Ryd [2]. Although the problem of a single D^- has so far been addressed in many papers the interest in multielectron charged donors and acceptors, in particular the Mg acceptor, in dimensionally quantized structures has recently been renewed (see [3] and references therein). It was suggested [3] that the origin of the main photoluminescence band in InGaN/GaN QW structures is due to novel 2D inter-impurity recombination between 2D donors and Mg acceptors.

It is common knowledge that the external fields strongly modify the confined states of the charged donors. An increase in the binding energy of the D^- in the presence of a magnetic field $\boldsymbol{B}$ directed perpendicular to the heteroplanes was found to occur (see [4, 5] and references therein). Although the magnetic field directed perpendicular to the heteroplanes has been studied in many papers the in-plane magnetic field attracts considerable attention. This is because the in-plane magnetic field interacts with the confinement that in turn influences significantly the bound systems in the QW structures [6, 7].

There is also much current interest in the study of effects of combined electric $\boldsymbol{E}$ and magnetic $\boldsymbol{B}$ fields but little work on this has been published to date. Optical spectroscopy of the QWs subject to an electric field directed perpendicular to the heteroplanes and parallel ($\boldsymbol{B} \parallel \boldsymbol{E}$) [8] and crossed ($\boldsymbol{B} \perp \boldsymbol{E}$) [9] magnetic field has been investigated. Recently the optical properties of the QWs in the presence of in-plane electric field and crossed ($\boldsymbol{B} \perp \boldsymbol{E}$) magnetic field were studied in [10]. A configuration of crossed both in-plane electric and magnetic fields to be considered in this paper has not been studied yet. However this geometry is of interest. In particularly the effect of the balance of the donor energy shifts induced by in-plane crossed fields will be shown to occur.

The majority of papers on the problem of the charged donor are based on numerical calculations, which usually rely upon a variational method. However, the numerical approach requires a lot of computational effort. In parallel with this the detailed study of the evolution of the charged donor states as a function of the parameters of the well and magnitudes of the fields remains unavailable. Thus studies via analytical methods are of great interest because they make the basic physics of the problem transparent throughout the analysis. In addition a combination of the analytical and numerical methods improves the accuracy of the calculation of the impurity states in the QWs [11].

In this paper an analytical approach to the problem of a negatively charged donor in a QW in the presence of crossed electric and magnetic fields is developed. The case of the narrow QW considered below is most important, because the states in the wide QW closely resemble those in the bulk material. In order for the effect of the confinement to be more pronounced the width of the QW is taken to be much less than the impurity radius and the magnetic length. In case of a narrow QW an electric field directed perpendicular to the heteroplanes would produces only a minor effect [6]. Both fields are therefore assumed to lie within the heteroplanes. The impurity is positioned anywhere within the QW. We emphasize that we are not in competition with the variational calculations or numerical methods requiring cumbersome computing and pretending to the comprehensive quantitative results. The main aim of the paper is the analytical study of the effects specifically provided by the confinement i.e. the dependences on the width of the QW and the position of the impurity in the presence of the fields. The motion of the weakly bound ideal 2D extra electron in the absence of the external fields is considered to be governed by the model short range potential (SRP) associated with the neutral donor and the binding energy of the 2D extra electron is treated as the only parameter. This approach is reminiscent of the use of model potentials in atomic physics (see [12] and references therein). The dependences of the total energy of the charged donor in the ground state upon the parameters of the well and the magnitudes of the fields are obtained in an explicit form. A red shift of the energy level and the detachment rate of the (SRP) extra electron both induced by the weak electric field are calculated analytically and then compared with those for the three-dimensional weakly bound particle. Estimates of the expected effects are made for the parameters of the narrow GaAs QW.

This paper is organized as follows: in section 2 the details of the analytical approach are presented. In section 3 we test the accuracy of our technique by applying it to the quasi-2D neutral donor and comparing the results with those obtained by variational calculations. The binding energy of the charged donor as a function of the width of the QW and strength of the electric field is calculated in section 4. We discuss these results in section 5 and provide the conclusions in section 6.

2. General theory

The z-axis is chosen parallel to the uniform magnetic field vector $\boldsymbol{B}$, which is applied in plane to a single QW of width d bounded by the infinite barriers at the planes $y = \pm d/2$. The uniform electric field $\boldsymbol{E}$ is directed parallel to the heteroplanes namely to the x-axis. The other parameters relevant to the calculation are the impurity radius (a_0), in particularly the Bohr radius for the D^-, and the magnetic length (a_B). They are defined as usual by

$$a_0 = \frac{4\pi\varepsilon_0\varepsilon\hbar^2}{\mu e^2} \qquad a_B = \left(\frac{\hbar}{eB}\right)^{1/2}$$

where μ is the electron effective mass and ε is the dielectric constant. The impurity centre is positioned at the distance b from the mid-point of the QW that is taken to be the point $y = 0$. We take the conduction band to be parabolic non-degenerate and separated from the valence band by a wide energy gap.

In general the problem of the charged donor subject to confinement and external fields cannot be solved analytically. Nevertheless below we consider the specific case in which an approximate analytical solution can be obtained in an explicit form. Our approach is based on the adiabatic approximation. The width of the QW is assumed to be much less than the radius of the impurity and the magnetic length, i.e.

$$d \ll a_0, a_B. \tag{2.1}$$

We consider the charged donor formed by the neutral system and extra electron at a position $\boldsymbol{r}$. The neutral donor consists of an attractive centre of charge $+Ne$ and N 'inner' electrons having the coordinates $\boldsymbol{r}_j$ ($j = 1, \ldots, N$). In the effective mass approximation the equation for the wave function $\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N, \boldsymbol{r})$ of the charged donor subject to the external uniform magnetic $\boldsymbol{B}$ and electric $\boldsymbol{E}$ fields has the form

$$\left\{\frac{1}{2\mu}(-\mathrm{i}\hbar\nabla - eBy\boldsymbol{e}_x)^2 - eEx - \frac{Ne^2}{4\pi\varepsilon_0\varepsilon|\boldsymbol{r} - b\boldsymbol{e}_y|} + \sum_{j=1}^{N}\frac{e^2}{4\pi\varepsilon_0\varepsilon|\boldsymbol{r} - \boldsymbol{r}_j|} + H_0\right\}\Psi = E\Psi \tag{2.2}$$

where

$$H_0 = \sum_{j=1}^{N}\left[\frac{1}{2\mu}(-\mathrm{i}\hbar\nabla_j - eBy_j\boldsymbol{e}_x)^2 - eEx_j - \frac{Ne^2}{4\pi\varepsilon\varepsilon_0|\boldsymbol{r}_j - b\boldsymbol{e}_y|} + \sum_{i\neq j=1}^{N}\frac{e^2}{4\pi\varepsilon\varepsilon_0|\boldsymbol{r}_j - \boldsymbol{r}_i|}\right] \tag{2.3}$$

is the Hamiltonian describing the neutral donor in the presence of external fields and where $\boldsymbol{e}_x$ and $\boldsymbol{e}_y$ are the unit vectors. By solving this equation subject to the boundary conditions

$$\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N, \boldsymbol{r}) = 0 \qquad \text{at } y_j, y = \pm\frac{d}{2} \qquad j = 1, \ldots, N \tag{2.4}$$

the total energy E and wave function Ψ can be found in principle.

Further we assume as usual that the motion of the weakly bound extra electron is adiabatically slower than that of the 'inner' electrons. Under the condition (2.1) and leaving aside the correlation effects the solution to equation (2.2) for the ground state of a charged donor satisfying the boundary conditions (2.4), may be written in the form

$$\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N, \boldsymbol{r}) = \chi(y_1)\ldots\chi(y_N)\chi(y)f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N)\varphi(\boldsymbol{\rho}) \tag{2.5}$$

where

$$\chi(y) = \left(\frac{2}{d}\right)^{1/2} \cos\frac{\pi y}{d} \tag{2.6}$$

is the wave function of the ground state of the electron in the one-dimensional QW and where $f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N)$ and $\varphi(\boldsymbol{\rho})$ ($\boldsymbol{\rho} = x\boldsymbol{e}_x + z\boldsymbol{e}_z$) are the two-dimensional wave functions of the 'inner' and extra electrons respectively. The wave function $f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N)$ and energy E_0 of the neutral donor can be found by solving the equation

$$\langle y_1, \ldots, y_N|H_0|y_1, \ldots, y_N\rangle f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N) = E_0 f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N) \tag{2.7}$$

where $\langle y_1, \ldots, y_N|\ldots|y_1, \ldots, y_N\rangle$ is an average with respect to the function $\chi(y_1)\ldots\chi(y_N)$. Averaging the equation (2.2) with respect to the function $\chi(y_1)\ldots\chi(y_N)\chi(y)f(\rho_1, \ldots, \rho_N)$ we obtain

$$\left[-\frac{\hbar^2}{2\mu}\nabla_\rho^2 + U_0(\boldsymbol{\rho}) + U_1(\boldsymbol{\rho}) - eE_x\right]\varphi(\boldsymbol{\rho}) = W\varphi(\boldsymbol{\rho}) \tag{2.8}$$

where

$$U_0(\boldsymbol{\rho}) = -\frac{e^2}{4\pi\varepsilon\varepsilon_0}\left[\frac{N}{\rho} - \sum_{j=1}^{N}\left\langle f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N)\left|\frac{1}{\boldsymbol{\rho} - \boldsymbol{\rho}_j}\right|f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N)\right\rangle\right] \tag{2.9}$$

and where

$$U_1(\boldsymbol{\rho}) = \frac{e^2}{4\pi\varepsilon\varepsilon_0}\left[\frac{N}{\rho} - \left\langle y\left|\frac{N}{|\boldsymbol{r} - b\boldsymbol{e}_y|}\right|y\right\rangle + \sum_{j=1}^{N}\left\langle y_1, \ldots, y_N, y, f\left|\frac{1}{\boldsymbol{r} - \boldsymbol{r}_j}\right|y_1, \ldots, y_N, y, f\right\rangle\right.$$
$$\left. - \sum_{j=1}^{N}\left\langle f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N)\left|\frac{1}{|\boldsymbol{\rho} - \boldsymbol{\rho}_j|}\right|f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N)\right\rangle\right]. \tag{2.10}$$

The energy W is defined as follows

$$E = \frac{\hbar^2\pi^2}{2\mu d^2} + \frac{e^2B^2d^2}{24\mu}\left(1 - \frac{6}{\pi^2}\right) + E_0 + W \tag{2.11}$$

where the first and second terms on the right-hand side of equation (2.11) are the energy of the spatial quantization of the extra electron in the y-direction and its energy red shift induced by the magnetic field. The potentials (2.9) and (2.10) describe the ideal 2D extra electron and the effect of the finite width d of the QW respectively. Following the above mentioned ideas the energy of the ideal 2D extra electron in the absence of the electric field ($E = 0$) $W_0 = -\hbar^2q_0^2/2\mu$ is considered as a parameter determined from numerical calculations or experimental data. Furthermore we replace the potential (2.9) by the model short range potential (SRP) U_0 providing the weak binding properties of the extra electron positioned far away from the 'inner' electrons. The wave function relevant to the energy W_0 is $\varphi_0(\boldsymbol{\rho}) \sim \exp(-q_0\boldsymbol{\rho})$ whereas the exponential factor of the wave function of the neutral donor has the form $f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N) \sim \prod_{j=1}^{N} \exp(-\mathrm{i}\rho_j/a_{0j})$ where a_{0j} are the effective radii of the 'inner' electrons with $q_0^{-1} \gg a_{0j}$. Under this condition an estimation of the last two terms on the right-hand side of equation (2.10) taken for $\rho \approx q_0^{-1}$ yields

$$U_1(\boldsymbol{\rho}) = \frac{e^2 N}{4\pi\varepsilon\varepsilon_0}\left[-\left\langle y\left|\frac{N}{|\boldsymbol{r} - b\boldsymbol{e}_y|}\right|y\right\rangle + \left\langle y', y\left|\frac{1}{\sqrt{\boldsymbol{r} - y'\boldsymbol{e}_y}}\right|y', y\right\rangle\right]. \tag{2.12}$$

Note that the potential $U_1(\boldsymbol{\rho})$ does not depend on the distribution of the charge of the neutral 2D donor in contrast to the potential $U_0(\boldsymbol{\rho})$ affected by the wave function f [13]. Thus the expression (2.12) is of general character and can be used in order to describe the effect of the finite width d of the QW and the arbitrary position b of the donor.

3. Stark effect of the quasi-two-dimensional neutral donor

Obviously the qualitative comparison of the results obtained below for the charged donor with those for the neutral centre is desirable. For this purpose we impart to equation (2.7) for the function $f(\boldsymbol{\rho}_1, \ldots, \boldsymbol{\rho}_N)$ describing the neutral donor an explicit form

$$\left\{\sum_{j=1}^{N}\left[-\frac{\hbar^2}{2\mu}\nabla^2_{\rho_j} - \frac{e^2}{4\pi\varepsilon\varepsilon_0}\left\langle y_1, \ldots, y_N\left|\frac{N}{|\boldsymbol{r}_j - b\boldsymbol{e}_y|}\right.\right.\right.\right.$$
$$\left.\left.\left.\left. - \sum_{i\neq j=1}^{N}\frac{1}{|\boldsymbol{r}_j - \boldsymbol{r}_i|}\right|y_1, \ldots, y_N\right\rangle - eEx_j\right]\right\}f = \Lambda f \tag{3.1}$$

where

$$\Lambda_N = E_0 - N\left[\frac{\hbar^2\pi^2}{2\mu d^2} + \frac{e^2B^2d^2}{24\mu}\left(1 - \frac{6}{\pi^2}\right)\right]. \tag{3.2}$$

Let us consider for an example the simplest case of the D^0 donor ($N = 1$). Equation (3.1) becomes

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0\varepsilon\rho} + V(\boldsymbol{\rho}) - eEx\right]f(\boldsymbol{\rho}) = \Lambda_1 f(\boldsymbol{\rho}) \tag{3.3}$$

where the potential

$$V(\boldsymbol{\rho}) = \frac{e^2}{4\pi\varepsilon_0\varepsilon}\left(\frac{1}{\rho} - \left\langle y\left|\frac{1}{\sqrt{\boldsymbol{\rho}^2 + (y-b)^2}}\right|y\right\rangle\right) \tag{3.4}$$

describes the effect of the finite width d of the QW on the ideal 2D neutral hydrogen-like donor.

In first order perturbation theory the correction to the ground energy level $\Lambda_1^{(0)} = -4$ Ryd (Ryd $= -\hbar^2/2\mu a_0^2$ is the impurity Rydberg constant) caused by the finite width d is determined by the matrix element of the potential $V(\boldsymbol{\rho})$ in equation (3.4) calculated with respect to the unperturbed wave functions of the 2D ground state

$$f(\rho) = \frac{4}{\sqrt{2\pi}a_0}\exp\left(-\frac{2\rho}{a_0}\right). \tag{3.5}$$

The effect of the electric field on the 2D Coulomb states was considered in [14] and the corresponding complex energies have been obtained. The real part of the energy includes a red shift of the energy level and the imaginary part determines the ionization rate. Both effects are caused by the electric field. Using the results obtained in [14] and the analytical expression for the matrix element of the potential $V(\boldsymbol{\rho})$ (3.4) we obtain for the ground state of the quasi-2D D^0 subjected to a weak electric field

$$\Lambda_1 = -4\mathrm{Ryd}\left\{1 - \frac{2d}{\pi^2 a_0}\left(\pi^2 + \varphi_0^2 - 4 + 4\sin^2\frac{\varphi_0}{2}\right)\right.$$
$$-\left(\frac{2d}{\pi a_0}\right)^2 \frac{1}{\pi}\left[\left(\frac{\pi^3}{3} - 2\pi + \pi\varphi_0^2\right)\left(\ln\frac{d}{\pi a_0} + C - \frac{1}{2}\right) + \Phi(\varphi_0) + \Phi(-\varphi_0)\right]$$
$$\left. + \frac{21}{2^9}\left(\frac{E}{E_0}\right)^2 + \mathrm{i}8\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{E}{E_0}\right)^{1/2}\exp\left(-\frac{16E_0}{E}\right)\right\} \tag{3.6}$$

where

$$\Phi(\varphi_0) = (\pi + \varphi_0)\left(\frac{1}{6}(\pi + \varphi_0)^2 - 1\right)\ln(\pi + \varphi_0) - \frac{1}{18}(\pi + \varphi_0)^3$$
$$+ \cos\varphi_0\,\mathrm{si}(\pi + \varphi_0) - \sin\varphi_0\,\mathrm{ci}(\pi + \varphi_0) - \pi\sin^2\frac{\varphi_0}{2} \qquad \varphi_0 = \frac{2\pi b}{d}$$

and where $\mathrm{ci}(x)$ and $\mathrm{si}(x)$ are the integral cosine and sine, respectively. In the above expression $C(\approx 0.577)$ is the Euler constant and $E_0 = e(4\pi\varepsilon_0\varepsilon a_0^2)^{-1}$ is the effective electric field of the impurity. The expression for the energy Λ_1 in equation (3.6) is valid under the condition (2.1) and for a weak electric field $E \ll E_0$.

For the narrow QW the energy $(-\Lambda_1)$ can be treated as the binding energy of the neutral donor. It is clear from equation (3.6) that an increase in the width of the QW d leads to a decrease in the binding energy $(-\Lambda_1)$. The dependence of the binding energy of D^0 i.e. of $(-\Lambda_1)$ on the width d of the QW is shown in figure 1. A similar effect holds when the impurity shifts away from the mid-point of the well ($\varphi_0 \neq 0$), i.e. the binding energy decreases and reaches a minimum in the case that the impurity centre is at the edge of the QW ($\varphi_0 = \pi$). Figure 2 shows the binding energy $(-\Lambda_1)$ as a function of the displacement $\varphi_0 = 2\pi|b|/d$ of the impurity from the mid-point of the QW for different widths d. These results are in line with those obtained numerically in papers published during the last two decades (see [15] and [11] and references therein). Keeping the leading term in equation (3.6) $\sim d/a_0$ we obtain that for small displacements of the impurity from the mid-point of the QW ($\varphi_0 \ll 1$) the correction to the 2D ground level $\Delta\Lambda_1(d, b)$ caused by the finite width d is given by

$$\Delta\Lambda_1(d, b) \approx 8\ \mathrm{Ryd}\left(\frac{d}{\pi^2 a_0}\right)\left(\pi^2 - 4 + \frac{8\pi^2 b^2}{d^2}\right). \tag{3.7}$$

This expression coincides completely with that derived from the variational equations given in [15]. Thus our perturbation approach to the description of the effects of the finite width d of the QW is justified.

Also it follows from (3.6) that for an increase of the electric field strength the energy Λ_1 decreases and $\Delta\Lambda_1(E) \approx -(21/2^7)(E/E_0)^2$ Ryd. The ionization rate P of D^0 is defined as usual by $P = -(2/\hbar)\mathrm{Im}\,\Lambda_1$. A comparison of the effect of the electric field on 2D Coulomb states with that on three-dimensional states is given in [14].

4. Stark effect of the weakly bound quasi-two-dimensional extra electron

The wave function $\varphi(\boldsymbol{\rho})$ and the energy W of the extra electron satisfy the equation (2.8). The motion of the extra electron is determined by the potential $U_0(\boldsymbol{\rho})$ (2.9) perturbed by the potential $U_1(\boldsymbol{\rho})$ (2.10) and the potential $-Eex$ induced by the electric field E. Since the effective radius

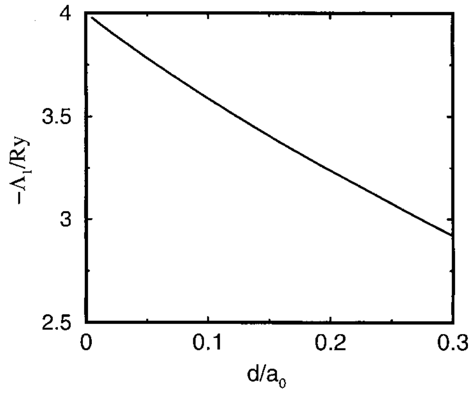

Figure 1. The dimensionless binding energy ($-\Lambda_1$) of the D^0 centre defined by equation (3.6) for $E = 0$ scaled to the impurity Rydberg constant Ryd as a function of the dimensionless width d/a_0 of the QW, where a_0 is the impurity Bohr radius. The impurity is taken to be at the mid-point of the QW ($\varphi_0 = 0$).

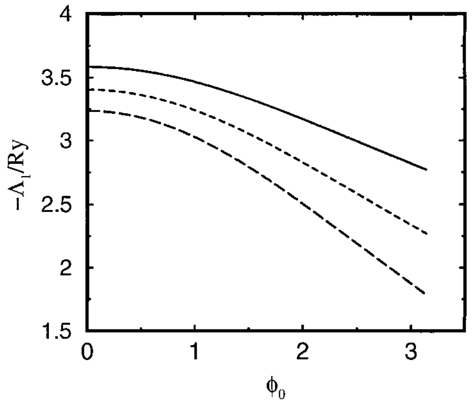

Figure 2. The dependence of the binding energy $-\Lambda_1/\text{Ryd}$ (Ryd is the Rydberg constant) calculated from equation (3.6) for $E = 0$ of the D^0 centre in the QW of width $d = 0.1a_0$—solid curve; $d = 0.15a_0$—dashed curve; $d = 0.20a_0$—long dashed curve (a_0 is the Bohr radius) on the displacement of the impurity $|b| = (\varphi_0 d)/2\pi$ from the centre of the QW with width d.

of the wave function $\varphi_0(\boldsymbol{\rho})$ of the weakly bound extra electron exceeds considerably the effective radius of the potential $U_0(\boldsymbol{\rho})$ the approximation of a zero-range potential will be used in the following. This approximation is based on the replacement of the potential $U_0(\boldsymbol{\rho})$ by the δ-function potential $\sim\delta(\boldsymbol{\rho})$. The details of this approach can be found in [16].

Following the main idea of the approximation of a zero-range potential [16] we assume that the unperturbed ground energy level $W_0 = -\hbar^2 q_0^2/2\mu$ relevant to the potential U_0 and considered below as the parameter of the theory is determined from numerical calculations or experimental data. The wave function of the ground state $\varphi_0(\boldsymbol{\rho})$ associated with the energy level W_0 has the form

$$\varphi_0(\boldsymbol{\rho}) = DK_0(q_0\rho) \tag{4.1}$$

where D is a constant and where $K_0(x)$ is the McDonald function (i.e. modified Bessel function) [17].

The effect of the electric field E on the energy level W_0 is described by the equation (see [18])

$$(\nabla^2 + Fx - q^2)\varphi(\boldsymbol{\rho}) = -\delta(\boldsymbol{\rho}) \tag{4.2}$$

where

$$F = \frac{2\mu e E}{\hbar^2} \qquad \text{and} \qquad q^2 = -\frac{2\mu W_E}{\hbar^2}.$$

By solving this equation subject to the boundary condition

$$\varphi(\boldsymbol{\rho}) = \varphi_0(\boldsymbol{\rho}) \qquad \text{for } \boldsymbol{\rho} \to 0 \tag{4.3}$$

the energy of the extra electron W_E in the presence of an electric field can be found. To avoid cumbersome mathematics only an outline of the calculation will be given below.

The solution to equation (4.2) can be written in the form

$$\varphi(x, z) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}kz} g(x, k)\,\mathrm{d}k \tag{4.4}$$

where $g(x, k)$ is the Green function satisfying the equation

$$\left(\frac{\mathrm{d}}{\mathrm{d}x^2} + Fx - p^2\right) g(x, k) = -\delta(x) \tag{4.5}$$

and where $p^2 = k^2 + q^2$.

The Green function $g(x, k)$ for the region $x \geqslant 0$ is given by

$$g(x, k) = \pi F^{-1/3}\mathrm{Ai}(-\eta_0)[\mathrm{Bi}(-\eta) + \mathrm{Ai}(-\eta)] \tag{4.6}$$

where $\eta(x) = F^{1/3}(x - x_0)$; $\eta_0 = \eta(0)$; $x_0 = F^{-1}p^2$ and where $\mathrm{Ai}(u)$ and $\mathrm{Bi}(u)$ are the Airy functions [17]. The expression for the Green function $g(x, k)$ for the region $x \leqslant 0$ can be obtained from equation (4.6) by replacing the parameter η_0 by η and *vice versa*.

On using the asymptotic expansion of the Airy functions for $\eta < 0$, $|\eta| \gg 1$ [17] we obtain from (4.6) for the region $x \ll x_0$ the result

$$g(x, k) = \frac{1}{2p}\left[\left(1 + \frac{5F^2}{32p^6}\right)\exp(-px) + \frac{\mathrm{i}}{2}\exp\left(-\frac{4p^3}{3F}\right)\right]. \tag{4.7}$$

Substituting the expression (4.7) in equation (4.4) we have for $y = 0$

$$\varphi(x, 0) = \frac{1}{2\pi}\left[K_0(qx) + \frac{F^2}{12q^6} + \frac{\mathrm{i}}{2}\left(\frac{\pi}{6}\right)^{1/2}\left(\frac{4q^3}{3F}\right)^{-1/2}\exp\left(-\frac{4q^3}{3F}\right)\right]. \tag{4.8}$$

Substituting the expressions (4.1) with $D = (2\pi)^{-1}$ and (4.8) into the boundary conditions (4.3) taken for $z = 0$ we use for the McDonald functions $K_0(u) = -\ln(u/2) - C$ for $u \ll 1$. The equation for the parameter q that in turn determines the energy W_E becomes

$$\ln q = \ln q_0 + \frac{F^2}{12q^6} + \frac{\mathrm{i}}{2}\left(\frac{\pi}{6}\right)^{1/2}\left(\frac{4q^3}{3F}\right)^{-1/2}\exp\left(-\frac{4q^3}{3F}\right). \tag{4.9}$$

In first order perturbation theory a correction to the ground level W_0 caused by the finite width of the QW d is governed by the matrix element of the potential $U_1(\boldsymbol{\rho})$ (2.10) calculated with respect to the normalized wave functions $\varphi_0(\boldsymbol{\rho})$ in equation (4.1) ($D = q_0\pi^{-1/2}$). Taking into account the effect of the electric field E and the confinement effects caused by the QW we arrive at the expression for the energy of the extra electron W

$$W = W_0 + W_E + \langle\varphi_0(\boldsymbol{\rho})|U_1(\boldsymbol{\rho})|\varphi_0(\boldsymbol{\rho})\rangle. \tag{4.10}$$

Taking for an example the expression (2.10) for $N = 1$ (D^-) we have from (4.10)

$$W = -|W_0|\left\{1 + \frac{1}{6}\left(\frac{E}{E_1}\right)^2 - \frac{4d}{a_0}\left[\left(\ln\frac{q_0 d}{4\pi} + C\right)^2\left(\frac{1 - \pi^2/3 + \varphi_0^2 + 4\sin 2(\varphi_0/2)}{4\pi^2}\right)\right.\right.$$
$$\left.\left. +2\left(\ln\frac{q_0 d}{4\pi} + C\right)(S(\varphi_0) - \langle S\rangle) + R(\varphi_0) - \langle R\rangle\right]\right\} - \mathrm{i}\frac{\hbar}{2}K \tag{4.11}$$

where

$$S(\varphi_0) = \frac{1}{(2\pi)^2}\int_{-\pi}^{+\pi} \mathrm{d}\varphi|\varphi - \varphi_0|(1 + \cos\varphi)\ln|\varphi - \varphi_0| \tag{4.12}$$

$$R(\varphi_0) = \frac{1}{(2\pi)^2}\int_{-\pi}^{+\pi} \mathrm{d}\varphi|\varphi - \varphi_0|(1 + \cos\varphi)\ln^2|\varphi - \varphi_0| \tag{4.13}$$

and correspondingly

$$\langle S\rangle = \frac{1}{2\pi}\int_{-\pi}^{+\pi} \mathrm{d}\varphi_0(1 + \cos\varphi_0)S(\varphi_0)$$

$$\langle R\rangle = \frac{1}{2\pi}\int_{-\pi}^{+\pi} \mathrm{d}\varphi_0(1 + \cos\varphi_0)R(\varphi_0).$$

In equation (4.12) $E_1 = [(2\mu)^{1/2}/e\hbar]|W_0|^{3/2}$ is the effective electric field associated with the SRP $U_0(\boldsymbol{\rho})$. The last term on the right-hand side of the equation (4.12) determines the detachment rate K of the 2D charged donor

$$K = \frac{|W_0|}{\hbar}\left(\frac{\pi E}{2E_1}\right)^{1/2}\exp\left(-\frac{4E_1}{3E}\right). \tag{4.14}$$

The expressions (4.11)–(4.14) for the energy W are valid for the narrow QW ($q_0^{-1} \gg a_0 \gg d$) and for a weak electric field $E \ll E_1$. The total energy of the charged donor in the narrow QW subject to crossed electric and magnetic fields can be obtained from equation (2.11).

5. Results and discussion

It follows from (4.11) that the electric field E leads to a red shift of the energy $\Delta W(E)$ such that

$$\Delta W(E) = -\frac{1}{6}\left(\frac{E}{E_1}\right)^2|W_0|. \tag{5.1}$$

A comparison of the 2D shift $\Delta W(E) = \Delta W_{2D}(E)$ (5.1) with that calculated in [18] for a three-dimensional (3D) weakly bound electron

$$\Delta W_{3D}(E) = -\frac{1}{16}\left(\frac{E}{E_{13D}}\right)^2|W_{03D}| \tag{5.2}$$

is desirable at this point. From the equations (5.1) for which $W_0 \equiv W_{02D}$ and $E_1 = E_{12D}$ are implied, and equation (5.2), we have

$$\frac{\Delta W_{3D}(E)}{\Delta W_{2D}(E)} = \frac{3}{8}\left(\frac{W_{02D}}{W_{03D}}\right)^2. \tag{5.3}$$

Estimates of the suitable values for the parameters for D^- are made further. Using the values $|W_{02D}| = 0.48$ Ryd and $|W_{03D}| = 0.055$ Ryd calculated in [1] and [2] respectively, we obtain $\Delta W_{3D}(E)/\Delta W_{2D}(E) = 28.6$. Thus in the presence of the electric fields of equal strength the shift of the energy of the 3D charged donor considerably exceeds that of the 2D structure.

An effect specific to the narrow QW subject to in-plane fields occurs. It follows from equations (2.11) and (4.11) that under the condition

$$\frac{e^2B^2d^2}{24\mu}\left(1-\frac{6}{\pi^2}\right)-|W_0|\frac{1}{6}\left(\frac{E}{E_1}\right)^2=0 \tag{5.4}$$

the blue and red shifts of the energy of the extra electron induced by the magnetic B and electric E fields respectively are balanced.

Taking the expression (4.14) for the detachment rate K_{2D} of the 2D system and relating it to the detachment rate K_{3D} result (see equation (13) in ref. [18]) we obtain

$$\frac{K_{3D}}{K_{2D}}=\frac{1}{\sqrt{2\pi}}\left|\frac{W_{03D}}{W_{02D}}\right|^{1/4}\left(\frac{E}{E_{13D}}\right)^{1/2}\exp\left\{-\frac{4E_{13D}}{3E}\left[1-\left(\frac{W_{02D}}{W_{03D}}\right)^{3/2}\right]\right\}. \tag{5.5}$$

Because of the ratio $W_{02D}/W_{03D}=8.7$ the detachment rate of the 3D D^- is much greater than that of the 2D charged donor. As expected it turns out that generally the quasi-2D charged donor in the narrow QW is far more stable with respect to field ionization than the similar system in the bulk semiconductor.

The dependences of the energy W on the width d of the QW and the position $b=d(\varphi_0/2\pi)$ of the impurity centre are described by the factor $4d/a_0$ multiplied by the term in the square brackets in equation (4.11). In order for the qualitative analysis to be simplified the logarithmic approximation ($q_0d/4\pi\ll 1$, $|\ln(q_0d/4\pi)|\gg 1$) is used. For this case we avoid the cumbersome expressions associated with the functions $S(\varphi_0)$ (4.12) and $R(\varphi_0)$ (4.13). Note that in principle these functions can be calculated analytically. In the above mentioned approximation a correction to the 2D binding energy $\Delta E_b(d,\varphi_0)=-\Delta W(d,\varphi_0)$ caused by the finite width of the QW and the position of the impurity can be written in the form

$$\Delta E_b\approx|W_0|\frac{d}{\pi^2a_0}\left(\ln\frac{q_0d}{4\pi}+C\right)^2G(\varphi_0) \tag{5.6}$$

where

$$G(\varphi_0)=\frac{\pi^2}{3}-1-\varphi_0^2-4\sin^2\frac{\varphi_0}{2}. \tag{5.7}$$

It follows from (5.6) that as the impurity centre shifts away from the mid-point of the QW ($\varphi_0=0$) the energy increases and the binding energy decreases and reaches a minimum in the case where the impurity is at the edge of the QW ($\varphi_0=\pi$). This result coincides with those obtained numerically by a variational approach [5, 19, 20]. The dependence of the shift of the binding energy $\Delta E_b(d,\varphi_0)$ in equations (5.6) and (5.7) on the displacement b of the impurity from the mid-point of the QW of different widths d is depicted in figure 3. The reason for the decrease of the binding energy is that the electrons in the ground size-quantization state (2.6) are localized close to the centre of the QW ($y=0$) regardless of the position of the impurity. When the impurity is displaced from the point $y=0$ towards the edge of the QW the electron–impurity centre attraction decreases which as a consequence leads to a decrease in the binding energy. We emphasize that in the narrow QW the effect of the displacement of the impurity centre increases with increasing width of the well d. For the wide QW this dependence is completely the contrary. With an increase of the width of the well the effect caused by the position of the impurity becomes less pronounced. The wide QW of width $d=2a_0$ and $d=8a_0$ considered in [5, 19] and [20] respectively makes a quantitative comparison of our results and those obtained in the given papers difficult.

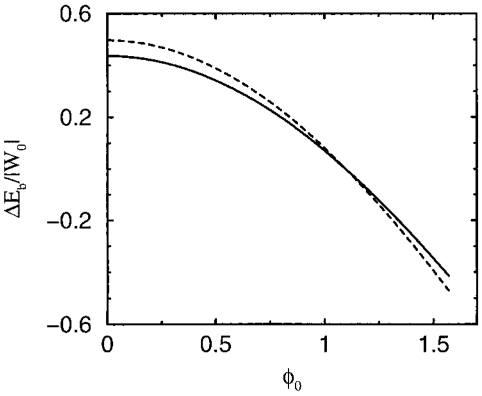

Figure 3. The dimensionless shift of the binding energy ΔE_b in equations (5.6), (5.7) of the D^- centre scaled to the binding energy of the ideal 2D charged donor $|W_0| = 0.48$ Ryd ($q_0 a_0 = 0.69$) as a function of the position of the donor $|b| = (\varphi_0 d)/2\pi$ within the QW of width $d = 0.1a_0$—dashed curve; $d = 0.08a_0$—solid curve.

A change of the sign of the shift ΔE_b as a function of the width d with the position b of the impurity can be seen to occur according to equation (5.7). For the impurity centre positioned at the mid-point of the QW ($\varphi_0 = 0$) the function $G(0) = \frac{1}{3}\pi^2 - 1 > 0$ and the binding energy increases with increasing width of the QW. If the impurity is localized close to the edge of the QW ($\varphi_0 = \pi$) the function $G(\pi) = -(\frac{2}{3}\pi^2 + 5) < 0$ and the wider the QW the smaller the binding energy. Figure 4 shows the energy shift ΔE_b given by the equations (5.6) and (5.7) as a function of the width d for the impurity positioned at the centre of the QW and at $|b| = d/4$. The differences between the dependences of the energy shift $\Delta E_b(d, \varphi_0)$ can be explained by the screening of the impurity centre produced by the electronic cloud associated with the neutral donor. For the case $b/d \approx 0$ the neutral donor is localized close to the point $y = 0$ and the screening effect is pronounced. With the increase of the width of the QW the wave function $\chi(y)$ (2.6) becomes widely distributed, screening decreases and the binding energy of the extra electron increases. The electronic cloud has a smaller effect on the distant impurity, positioned close to the edge of the QW. The wider the QW the less is the electron–impurity centre attraction and the less the binding energy.

It should be particularly emphasized that the strong logarithmic approximation providing a simplified and interpretable form of the equations (5.6) and (5.7) preserves the qualitative, though not the rigorous quantitative, character of these equations and figures 3 and 4. Also this approximation constrains considerably the width of the QW. Taking into account in equation (4.14) the terms (4.12), (4.13), $\langle S\rangle$ and $\langle R\rangle$ the obtained result can be extended comfortably to the more accurate description of the narrow QWs of typical width $d \approx (0.2\text{–}0.3)a_0$. Particularly the crossing of the energy shifts ΔE_b at $\varphi_0 \approx 1.1$ (see figure 3) can be turned into an anticrossing. It follows from (3.5) that the effective radius of the quasi-'inner' electron $a_{0j} = 0.5a_0$. The parameter $q_0 a_0$ chosen in figures 3 and 4 means that the parameter $q_0 a_{0j} \approx 0.35 < 1$ and applicability of the equations (4.11), (5.6) and (5.7) is justified qualitatively.

In view of possible experiments, concrete values for the parameters of a GaAs QW are $\mu = 0.067m_0$ and a narrow well of width $d = 20$ Å is assumed. Following [1] we take for the binding energy of the ideal 2D charged donor $|W_0| = 0.48$ Ryd to give in turn for the effective electric field $E_1 = 2.02 \times 10^5$ V m^{-1}. For the electric field $E = 0.31E_1$ the red shift of the energy $\Delta W(E)$ can be found from equation (5.1) such that $\Delta W(E) \approx 0.050$ meV. This red shift

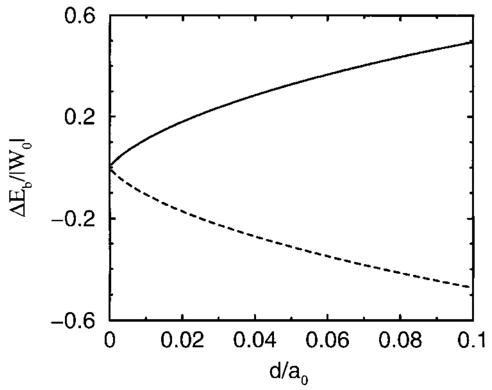

Figure 4. The dependence of the shift of the binding energy ΔE_b in equations (5.6), (5.7) of the D^- centre on the width d of the QW for the impurity positioned: at the centre of the QW ($\varphi_0 = 0$)—solid curve; at the intermediate point ($\varphi_0 = \pi/2$)—dashed curve. The binding energy of the ideal 2D charged donor $|W_0|$ is taken to be $|W_0| = 0.48$ Ryd ($q_0 a_0 = 0.69$).

would be cancelled by a blue shift of the energy of the extra electron induced by the magnetic field $B \approx 18.3$ T. The above electric field produces a detachment rate $K \approx 4.35 \times 10^{10}$ s^{-1} according to equation (4.14). Though the GaAs structures remain in the focus of study the InGaN/GaN material system has attached great interest because of use for the fabrication of blue–green light-emitting diodes and laser diodes [21]. Particularly the investigations of the InGaN extremely narrow QWs up to 12 Å are under way [22]. In order to estimate the expected values we take $\mu = 0.2m_0$ and $\varepsilon = 8.2$ (see [21] and references therein) for the InGaN QW of width $d = 18$ Å. For $E = 0.16E_1$ where the effective electric field E_1 is found to be $E_1 = 6.0 \times 10^6$ V m^{-1}, the red shift of the energy $\Delta W(E)$ defined by equation (5.1) gives the result $\Delta W(E) \approx 0.1$ meV. To cancel this red shift the magnetic field $B \approx 40$ T used widely in strong magnetic field physics [23] would be applied. The detachment rate induced by the electric field $E = 0.16E_0$ is $K \approx 3.5 \times 10^9$ s^{-1}. When the electric field is approaching the effective value E_1 the red shift $\Delta W(E)$ becomes more detectable in an experiment. The wider the QW the less the magnetic field $B \sim d^{-1}$ counterbalancing the red shift $\Delta W(E)$. Thus the effects of crossed electric and magnetic fields on the charged donor in the practically implied and intensively studied narrow QW are experimentally accessible. For the intermediate values of the width of the QW ($d \leqslant a_0$) and electric field ($E \leqslant E_1$) the results obtained above remain qualitatively valid. The correct quantitative description requires numerical methods.

6. Conclusion

An analytical approach to the problem of a charged donor in a narrow QW in the presence of crossed electric and magnetic fields both directed parallel to the heteroplanes is developed originally. Within our theoretical model the extra electron is governed by a δ-function type 2D potential. The explicit dependences of the total energy of the charged donor on the parameters of the well and the magnitudes of the external fields are obtained. The dependences of the binding energy of the charged donor on the width of the well and the position of the impurity within the well are studied. As the impurity centre shifts from the mid-point of the QW, the binding energy decreases. With the increase of the width of the narrow QW the effect of the displacement of the impurity becomes more pronounced. The impact of the relative position of the impurity within the QW on the dependence of the binding energy on the width of the well is studied. The red shift of the energy and the detachment rate of the extra electron both induced by the weak electric field are calculated using a well established procedure. The red and blue shifts of the energy caused by the electric and magnetic fields respectively can be balanced by specifically chosen fields. The quasi-two-dimensional charged donor is found to be far more stable with respect to the effect of the electric field than the charged donor in the bulk material. Estimates of the expected values associated with a GaAs and InGaN QWs show that the effects of the confinement and external fields on the charged donor states can be observed experimentally.

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