Impurity center in a single quantum well in the presence of a strong magnetic field

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The states and energies of an impurity electron confined within a single quantum well (QW) in the presence of a strong magnetic field directed perpendicular to the layers are derived. An analytical model in which the impurity may be positioned anywhere between the midpoint and edge of the QW is developed. The dependencies of the electron energies upon the magnitude of the magnetic field, the width of the QW, and the position of the impurity within the well are derived explicitly. Expressions for the levels of lowest energy are obtained, and have a quasi-Coulomb character, while the expressions for levels of higher energy are of the form of the size quantization levels, which form the excited subbands. Both types of levels are derived from the same original equations. The results obtained are compared with those of existing numerical calculations and specifically for the quantum numbers $N=m=0$. The relation between the states and the labels derived here and those obtained by others is also given. [S0163-1829(96)04320-2]

I. INTRODUCTION

During the last decade, the subject of shallow-donor impurities in quasi-two-dimensional systems has been studied extensively both experimentally and theoretically. The wealth of data obtained experimentally has been possible on account of the advances made in growth techniques and control by the development of molecular-beam epitaxy and metal-organic chemical vapor deposition methods of manufacturing specific structures. Also, improvements in the techniques frequently used in the experiments, such as far-infrared and intersubband spectroscopy, have resulted in the availability of more accurate and reliable data. Much of this work has concentrated on the $GaAs/Ga_xAl_{1-x}As$ system. The study of impurities in such systems is very important because the optical and transport properties of devices made from these materials are greatly affected by the presence of shallow impurities. References to a selection of the results that have been obtained experimentally may be found in the recent paper by Shi, Peeters, and Devresse.[1]

In parallel with the experiments, a considerable literature of theoretical work has developed in order to provide accurate explanations of these data. This is summarized also by Shi, Peeters, and Devresse.[1] Much of this theoretical work has involved variational-type calculations of the energies and wave functions of the isolated impurity particularly in an isolated single quantum well (SQW) and also in multiple-quantum-well (MQW) systems. Various additional contributions to the energies of the impurity states have also been included in many of these analyses, particularly the effects due to band nonparabolicity and resonant and nonresonant polaron corrections arising from the vibronic coupling of the impurity electron to the longitudinal optical phonons.

In addition to the many variational-type calculations that have been cited in Shi, Peeters, and Devresse,[1] other alternative theoretical approaches have been used. Dunn and Bates have been involved in a matrix diagonalization procedure (MDP) developed originally by Dunn and Pearl[2] and extended in Barmby *et al.*,[3–5] in the case of magnetic fields pointing at different angles relative to the layers in a MQW system. They have also been involved in calculations of impurity transition energies involving the metastable states;[6] one nonvariational approach to such calculations is to integrate directly the Schrödinger equation using an iterative technique for the whole range of magnetic field values.[7]

Monozon has been involved in analytical calculations of shallow-donor impurity states and energy levels in cases of a large magnetic field[8,9] acting perpendicular to the layers by extending the approach used originally by Hasegawa and Howard[10] for confined systems. This theory[8] does not contain any free parameters but was limited because it did not allow for the possibility that the impurity may be positioned very close to the boundary of the QW.

In this paper, we extend and improve the analytical model[8] to the case when the impurity can be positioned anywhere between the midpoint and edge of the QW. This analytical approach introduces a free parameter, which may be defined from a comparison with either the previous results[8] or with experiment. Both the low-energy quasi-Coulomb impurity states and the high-energy size quantization states in the QW are found as different solutions to the same equation.

II. BACKGROUND

Let us consider a single QW of width d bounded by infinite barriers at the planes $z=\mp\frac{1}{2}d$ containing an impurity at a position b such that $-\frac{1}{2}d\leqslant b\leqslant\frac{1}{2}d$. In the effective mass approximation and using cylindrical coordinates, the equation describing the electron of mass μ at position $\mathbf{r}(\boldsymbol{\rho},z)$ in a magnetic field $\mathbf{B}$ parallel to the z axis in a medium with

relative permittivity κ has the form

$$\left\{\frac{1}{2\mu}(-i\hbar\nabla+\tfrac{1}{2}e[\mathbf{B}\times\mathbf{r}])^2 - \frac{e^2}{4\pi\epsilon_0\kappa\sqrt{\rho^2+(z-b)^2}}\right\}\Psi(\boldsymbol{\rho},z)=E\Psi(\boldsymbol{\rho},z). \quad (2.1)$$

By solving this equation, the energy E of this electron and its wave function $\Psi(\boldsymbol{\rho},z)$ can be found in principle, which satisfy the boundary conditions

$$\Psi(\boldsymbol{\rho},\pm\tfrac{1}{2}d)=0. \quad (2.2)$$

The characteristic dimensional parameters of the problem are the impurity radius $a_0=(4\pi\hbar^2\epsilon_0\kappa/\mu e^2)$, the magnetic length $a_H[=(\hbar/eB)^{1/2}]$, and the width of the QW d.

In the strong magnetic field limit for which $a_H/a_0\ll 1$, the effect of the magnetic field is much greater than that of the Coulomb field of the impurity. Under these conditions, the solution to (2.1) may be written in the form

$$\Psi_{N,m}(\mathbf{r})=X_{\perp N,m}(\boldsymbol{\rho})f^{(N,m)}(z), \quad (2.3)$$

where the function $X_{\perp N,m}(\boldsymbol{\rho})$ describes the motion of the electron in the magnetic field in the x-y plane. Its corresponding Landau energy $E_{\perp N,m}$, including the spin term, is given by

$$E_{\perp N,m}=\mathscr{E}_g+\frac{\hbar eB}{2\mu}(2N+|m|+m+1)\pm\mu_B B. \quad (2.4)$$

$\mathscr{E}_g$ is the QW energy gap, μ_B is the effective Bohr magneton for the electron, and the quantum numbers are N,m, where $N=0,1,2,\ldots$ and $m=0,\pm1,\pm2,\ldots$.

The function $f^{(N,m)}(z)$ describes the motion in the z direction and satisfies the equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2f^{(N,m)}(z)}{dz^2}+V_{N,m}(z)f^{(N,m)}(z)=\mathscr{E}^{(N,m)}f^{(N,m)}(z), \quad (2.5)$$

with the boundary conditions

$$f^{(N,m)}(\pm\tfrac{1}{2}d)=0, \quad (2.6)$$

with

$$V_{N,m}(z)=-\frac{e^2}{4\pi\epsilon_0\kappa}\int\frac{|X_{\perp N,m}(\boldsymbol{\rho})|^2}{[\rho^2+(z-b)^2]^{1/2}}\,d\boldsymbol{\rho},$$

$$\mathscr{E}^{(N,m)}=E-E_{\tau N,m}. \quad (2.7)$$

The potential $V_{N,m}(z)$ has the following characteristic properties:

(i) Its depth is given by

$$V_{N,m}(b)\sim-\frac{e^2}{4\pi\epsilon_0\kappa a_H}. \quad (2.8)$$

(ii) If $|z-b|\gg a_H$, it reduces to the Coulomb form

$$V_{N,m}(z)=-\frac{e^2}{4\pi\epsilon_0\kappa|z-b|}. \quad (2.9)$$

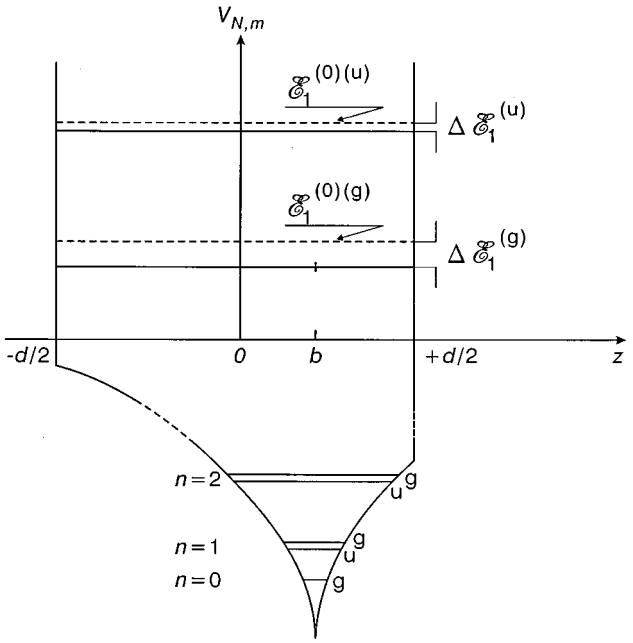

FIG. 1. The schematic form of the potential function $V_{N,m}$ given by (2.7) and (2.11). The solid lines refer to the ground ($n=0$) and first two excited Coulomb levels ($n=1,2$) of energy $\mathscr{E}_\lambda$ given by (3.1) and also the two lowest size quantization levels $\mathscr{E}_s$ given by (5.10) for even- [Eqs. (5.11) and (5.12)] and odd-parity [Eqs. (5.19) and (5.20)] states. The dashed lines are the unperturbed levels $\mathscr{E}_1^{(0)}$ of the even- (5.11) and odd-parity (5.19) states.

Unfortunately,[8] it is impossible to use the above form for the potential function (2.7) when the impurity is positioned close to the boundaries of the QW at positions for which

$$|b\pm\tfrac{1}{2}d|\leqslant a_H. \quad (2.10)$$

Consequently, our approach here is based on the replacement of the exact potential (2.7) by the model potential

$$V_{N,m}(z)=-\frac{e^2}{4\pi\epsilon_0\kappa(\alpha_{N,m}a_H+|z-b|)}, \quad (2.11)$$

where $\alpha_{N,m}$ is the free parameter of the theory. It can be determined by comparison of either the solutions to Eq. (2.5) with the potentials (2.7) and (2.11) or from the comparison with the experimental data. The form of the potential function given in (2.11) has been used previously[11] for an analysis of excitons in bulk semiconductors. It is important to note that the latter expression for the potential has properties similar to those contained in the earlier expressions (2.8) and (2.9) but it avoids the limitation given by Eq. (2.10). This is because the solution to (2.5) with the potential (2.11) can be obtained in analytical form for any values of b. The schematic form of the potentials (2.7) and (2.11) is shown in Fig. 1.

III. THE SPECTRUM IN THE REGION OF NEGATIVE ENERGIES: THE QUASI-COULOMB SPECTRUM

The mathematical problem is to obtain solutions to Eq. (2.5) with the potential function (2.11), which satisfy the boundary conditions given by (2.6). At $z=b$, the solutions

and their first derivatives are continuous. It is convenient to attach a parameter λ to the function $f^{(N,m)}$, which then becomes $f_\lambda^{(N,m)}$ such that λ is defined by the expression

$$\mathscr{E}^{(N,m)} \rightrightarrows \mathscr{E}_\lambda = -\frac{\hbar^2}{2\mu a_0^2 \lambda^2} \tag{3.1}$$

for the energy. Writing f_λ for $f_\lambda^{(N,m)}$ the differential equation (2.5) becomes

$$f''_\lambda(u) + \left(\frac{\lambda}{|u|+g}\right) f_\lambda(u) - \tfrac{1}{4} f_\lambda(u) = 0 \tag{3.2}$$

in which the new variables are defined by

$$u = \frac{2(z-b)}{a_0\lambda}, \quad g = \alpha_{N,m}\frac{2a_H}{a_0\lambda}, \quad \text{where } g \ll 1 \tag{3.3}$$

and where the primes denote the appropriate differentiation. The boundary condition (2.6) becomes

$$f_\lambda(u_{1,2}) = 0, \quad \text{where } u_{1,2} = \frac{d}{a_0\lambda}\left(\pm 1 - \frac{2b}{d}\right). \tag{3.4}$$

For $u>0$ and writing u for $|u|$, the general solution to Eq. (3.2) can be written in the form

$$f_{1\lambda}(x) = A_1 W_{\lambda,1/2}(x) + B_1 M_{\lambda,1/2}(x), \tag{3.5}$$

where $x = u+g > 0$ and where $W_{\lambda,1/2}(x)$ and $M_{\lambda,1/2}(x)$ are Whittaker functions.[12,13]

In the region $u<0$ (i.e., $|u| = -u$), the general solution to (3.2) is

$$f_{2\lambda}(y) = A_2 W_{\lambda,1/2}(y) + B_2 M_{\lambda,1/2}(y), \tag{3.6}$$

where $y(=-u+g)>0$. The two boundary conditions (3.4), the continuity condition for the two functions

$$f_{1\lambda}(u) = f_{2\lambda}(u) \quad \text{for } u=0 \quad (\text{that is, } z=b), \tag{3.7}$$

and for their first derivatives

$$\frac{df_{1\lambda}(u)}{du} = \frac{df_{2\lambda}(u)}{du} \quad \text{for } u=0 \tag{3.8}$$

lead to the following set of four homogeneous algebraic equations for the coefficients A_1, A_2, B_1, and B_2:

$$\begin{aligned} A_1 W_1 + B_1 M_1 &= 0, \\ A_2 W_2 + B_2 M_2 &= 0, \\ A_1 W + B_1 M &= A_2 W + B_2 M, \\ A_1 W' + B_1 M' &= -A_2 W' - B_2 M', \end{aligned} \tag{3.9}$$

where

$$\begin{aligned} W_{1,2} &\equiv W_{\lambda,1/2}(x_{1,2}), \quad M_{1,2} \equiv M_{\lambda,1/2}(x_{1,2}), \\ W(g) &\equiv W_{\lambda,1/2}(g), \quad M(g) \equiv M_{\lambda,1/2}(g) \end{aligned} \tag{3.10}$$

and where

$$x_{1,2} = \frac{d}{a_0\lambda}\left(1 + \frac{a_0\lambda g}{d} \mp \frac{2b}{d}\right) \tag{3.11}$$

with the labels 1 and 2 corresponding to the signs $-$ and $+$, respectively.

The coefficients $A_{1,2}$ and $B_{1,2}$ may be determined by solving Eqs. (3.9). After a considerable amount of algebraic manipulation, the condition that these equations are solvable may be expressed by the equation

$$\left[\frac{W_2}{M_2} + \frac{W_1}{M_1} - 2\frac{W'}{M'} + \Phi\right]\left[\frac{W_2}{M_2} + \frac{W_1}{M_1} - 2\frac{W}{M} - \Phi\right] = 0, \tag{3.12}$$

where

$$\Phi = \frac{-1}{\Gamma(-\lambda+1)MM'} - \left[\left(-\frac{1}{\Gamma(-\lambda+1)MM'}\right)^2 + \left(\frac{W_2}{M_2} - \frac{W_1}{M_1}\right)^2\right]^{1/2}. \tag{3.13}$$

In deriving the above, use has been made of the Wronskian of the functions $W(g)$ and $M(g)$ from which we have

$$\frac{W'(g)}{M'(g)} - \frac{W(g)}{M(g)} = -\frac{1}{\Gamma(-\lambda+1)M(g)M'(g)}, \tag{3.14}$$

where Γ is the Γ function.[12]

The roots λ_n, with $n=0,1,2,...$, of Eq. (3.12) give the required energies $\mathscr{E}_n$ of the problem and the coefficients $A_{1,2}(n)$ and $B_{1,2}(n)$ give the required wave functions $f_{1\lambda}^n(u)$ and $f_{2\lambda}^n(u)$. Equation (3.12) is an exact equation that is valid for any values of the variables x_1 and x_2 for the case when $g \ll 1$. However, special considerations are needed in their evaluation for the two particular cases when the impurity is close to the center of the well ($x>1$) and when the impurity is close to the barrier ($x \ll 1$). It is thus necessary to look at these special cases in more detail and this is discussed in the next section. In this connection, the Appendix contains approximate expressions for the Whittaker functions appropriate to these two limits.

IV. ANALYSIS OF SPECIAL CASES

A. Impurity close to the midpoint of the QW ($b=0$)

In this case, the approximation for small x given in the Appendix may be used so that we rewrite the expressions for $x_{1,2}$ given in (3.10) in the form

$$x_{1,2} = x_0(1 \mp S),$$

where

$$x_0 = \frac{d}{a_0\lambda}\left(1 + \frac{a_0\lambda g}{d}\right), \quad S = \frac{2b}{d + a_0\lambda g}, \tag{4.1}$$

with

$$x_0 > 1, \quad S \ll 1$$

so that

$$\frac{W_2}{M_2} - \frac{W_1}{M_1} \ll 1. \tag{4.2}$$

Then, Eq. (3.12) simplifies to

$$\left[\left(\frac{W_2}{M_2}+\frac{W_1}{M_1}\right)-2\frac{W'(g)}{M'(g)}\right]\left[\left(\frac{W_2}{M_2}+\frac{W_1}{M_1}\right)-2\frac{W(g)}{M(g)}\right]=0. \tag{4.3}$$

If the impurity is at the exact center of the QW (i.e., $b=0$) we have

$$x_1=x_2=x_0, \quad \frac{W_2}{M_2}=\frac{W_1}{M_1}=\frac{W_{\lambda,1/2}(x_0)}{M_{\lambda,1/2}(x_0)}. \tag{4.4}$$

On equating the left-hand square bracket of Eq. (4.3) to zero, the solutions are found to satisfy the relationships $A_1=A_2$ and $B_1=B_2$. The functions $f_\lambda(z)$ are then *even* such that $f_\lambda(z)=f_\lambda(-z)$. Thus the energy levels described by the left-hand brackets of Eqs. (4.3) and (3.12) can be classified as *quasi-even* (g) levels. Similarly, under the same conditions, on equating the right hand of (4.3) to zero, the solutions satisfy the relationships $A_1=-A_2$ and $B_1=-B_2$. The functions $f_\lambda(z)$ then become *odd* such that $f_\lambda(z)=-f_\lambda(-z)$ and thus the energy levels described by the right-hand brackets of Eqs. (4.3) and (3.12) can be classified as *quasi-odd* (u) levels. We discuss now these two solutions in turn.

1. Quasi-even levels

The condition for the quasi-even energy levels is obtained by using Eqs. (4.1) and (4.2) to obtain $W'(g)$ and $M'(g)$ for $g\ll 1$. Thus we find

$$\ln g+\Psi(1-\lambda)+2C+\frac{1}{2\lambda}-\frac{1}{2}\Gamma(-\lambda)\left[\frac{W_2}{M_2}+\frac{W_1}{M_1}\right]=0. \tag{4.5}$$

This equation can be used to obtain a definition for the parameter α. It will be shown that the effect of the parameter g on the energies of the quasi-even levels is of order $(-\ln g)^{-1}$ and on the quasi-odd levels it has a magnitude of (ng) as found previously.[8,10] However, as $g\ll 1$, then $[(ng)\ln g]\ll 1$. Therefore, it is advantageous to use Eq. (4.5) for the quasi-even levels rather than the corresponding equation for the quasi-odd solutions. In particular, from the theory of Monozon and Zhilich,[8] the potential $V_{0,0}(z)$ given in (2.7) leads to the equation

$$\ln\frac{\sqrt{2}a_H}{a_0\lambda}+\Psi(1-\lambda)+2C+\frac{1}{2\lambda}-\frac{1}{2}C-\frac{1}{2}\Gamma(-\lambda)\left[\frac{W_2}{M_2}+\frac{W_1}{M_1}\right]=0, \tag{4.6}$$

which describes the quasi-even levels. Thus from Eqs. (4.5) and (4.6) we obtain the expression

$$g=\sqrt{2}e^{-(1/2)C}\frac{a_H}{a_0\lambda}. \tag{4.7}$$

Using Eq. (3.3) for g, we can define the unknown parameter $\alpha_{0,0}$ of the theory by

$$\alpha_{0,0}=\frac{e^{-(1/2)C}}{\sqrt{2}}\simeq 0.5. \tag{4.8}$$

In the case of a general potential $V_{N,m}(z)$, the corresponding unknown parameter $\alpha_{N,m}$ is given by

$$\alpha_{N,m}=\sqrt{1/2}e^{(1/2)\psi(N+|m|+1)}.$$

In order to further simplify the analysis, we use the asymptotic expansions (A.3) and (A.4) given in the Appendix for $W_{\lambda,1/2}$ and $M_{\lambda,1/2}$ for $x_0\gg 1$ and the logarithmic approximation $g\ll 1$. This implies that $|\ln g|\gg 1$. On substituting $\lambda=n+\delta_n^{(g)}$ into (4.5) and using Eq. (A.5) for Ψ and Γ, we obtain for the $n=0$ ground state, the result

$$\frac{1}{\delta_0^{(g)}(S)}=\frac{1}{g_0^{(g)}(0)}(1-\beta_0 S^2), \tag{4.9}$$

where

$$\frac{1}{\delta_0^{(g)}(0)}=-2(\ln\overline{g})(1-2e^{-x_0}),$$

where

$$\overline{g}=g(\lambda=1), \quad \beta_0=x_0^2e^{-x_0}. \tag{4.10}$$

For the $n=1,2,3,...$ excited states we obtain similarly

$$\frac{1}{\delta_n^{(g)}(S)}=\frac{1}{\delta_n^{(g)}(0)}(1-\beta_n S^2), \tag{4.11}$$

where

$$\frac{1}{\delta_n^{(g)}(0)}=-\ln g-\frac{n}{(n!)^2}(\ln g)^2x_0^{2n}e^{-x_0} \tag{4.12}$$

and

$$\beta_n=\frac{n}{2(n!)^2}|\ln g|x_0^{2n}e^{-x_0}(x_0-2n)^2. \tag{4.13}$$

2. Quasi-odd levels

On equating the right-hand brackets in Eq. (4.3) to zero, and using Eq. (A.1) for $W(g)$ and (A.2) for $M(g)$ with $g\ll 1$ from the Appendix, we obtain

$$-\frac{1}{\lambda g}+\ln g+\Psi(1-\lambda)+2C-1+\frac{1}{2\lambda}-\frac{1}{2}\Gamma(-\lambda)\left[\frac{W_2}{M_2}+\frac{W_1}{M_1}\right]=0. \tag{4.14}$$

Following the same procedure as above, by substituting $\lambda=n+\delta_n^{(u)}$ $(n=1,2,3,...)$ into (4.14), we obtain the expression

$$\frac{1}{\delta_n^{(u)}(S)}=\frac{1}{\delta_n^{(u)}(0)}[1-\gamma_n S^2], \tag{4.15}$$

where

$$\frac{1}{\delta_n^{(u)}(0)}=\frac{1}{ng}-\frac{n}{(n!)^2(ng)^2}x_0^{2\lambda}e^{-x_0} \tag{4.16}$$

and

$$\gamma_n=\frac{1}{2(n!)^2g}x_0^{2n}e^{-x_0}(x_0-2n)^2. \tag{4.17}$$

The formal solution to Eq. (4.14) is given by

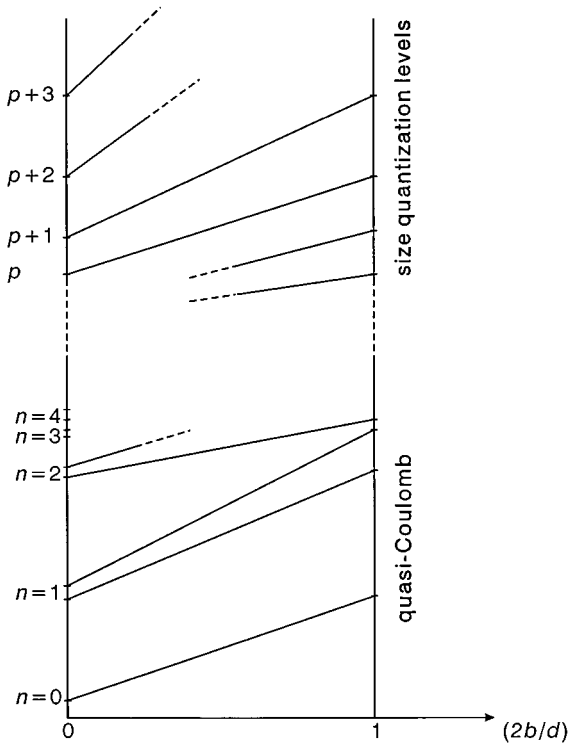

FIG. 2. The correlation diagram of the quasi-Coulomb levels (3.1) $\mathscr{E}_\lambda$, $\lambda = n + \delta_n^{(u,g)}$ and the size quantization levels (5.1) $\mathscr{E}_s$ for $s[=d/(\pi a_0 p)] \ll 1$ vs the displacement of the center b relative to the QW boundary $\frac{1}{2}d$ for $N=m=0$.

$$\lambda = \delta_0 \simeq \left(\frac{2}{\lambda g}\right)^{-1} \approx \frac{a_H}{a_0}$$

for $n=0$ but, as it does not satisfy the condition (3.3), it should be dropped.

3. The energy-level pattern

If the center is close to the midpoint of the QW, the above calculations have shown that the energy spectrum consists of a singlet ground level ($n=0$, $\delta_0 \ll 1$). In contrast, all excited levels form pairs of states that are very close in energy. They consist of quasi-even ($\lambda^{(g)} = n + \delta_n^{(g)}$) and quasi-odd ($\lambda^{(u)} = n + \delta_n^{(u)}$) components with $n=1,2,3,\ldots$. It is also easy to see from Eqs. (4.9), (4.11), and (4.15) that the final result for the energies $\mathscr{E}_\lambda(S)$, as defined originally in Eq. (3.1), are given by the approximate relation:

$$\mathscr{E}_\lambda(S) \sim -[n + \delta_n(S)]^{-2} \tag{4.18}$$

and that they increase with S. This result is indicated schematically in the lower part of Fig. 2.

We have also found that the binding energies $|\mathscr{E}_\lambda|$ decrease with the displacement of the impurity from the center of the QW. For $x>2$, the shift of the ground state exceeds that of the excited states. As a consequence, the transition energy from the ground state decreases with the displacement of the impurity from the midpoint of the QW. It follows from Eqs. (4.9), (4.11), and (4.15) that the reciprocal of the derivative of the transition energy with respect to the central position b is proportional b^{-1}. With the narrowing of the QW, the positive shifts of the extended excited states exceed that of the localized ground state. As a result, the transition energy from the ground state increases as the width of the QW decreases. All these conclusions are confirmed by numerical calculations.[2,14]

B. Impurity at the edge of the QW

In this case, we have $b=\frac{1}{2}d$, $x_1 = g \ll 1$, and

$$x_s \to \overline{x_2} = \frac{2d}{a_0\lambda}\left(1 + \frac{a_0\lambda g}{2d}\right) \simeq 2x_0 . \tag{4.19}$$

The right-hand brackets in (3.12), which gave the quasi-odd solutions previously, are equal to zero under the condition

$$\frac{W_{\lambda,1/2}(g)}{M_{\lambda,1/2}(g)} - \frac{W_{\lambda,1/2}(\overline{x_2})}{M_{\lambda,1/2}(\overline{x_2})} = 0. \tag{4.20}$$

In contrast, the left-hand bracket in (3.12), which corresponded previously to the quasi-even solutions, cannot be equated to zero for any values of λ so that this equation has no roots and should be dropped.

Equation (4.20) can be formally obtained from (4.14) by the substitution

$$\frac{1}{2}\left(\frac{W_2}{M_2} + \frac{W_1}{M_1}\right) \to \frac{W_{\lambda,1/2}(\overline{x_2})}{M_{\lambda,1/2}(\overline{x_2})}. \tag{4.21}$$

The roots of (4.20) have the form $\lambda = n + \delta_n$ where $n=1,2,3,\ldots$. The expression for δ_n can be obtained from (4.16) by the substitution of $\overline{x_2}$ for x_0. Therefore, if the impurity is at the edge of the QW, all energy levels are very clearly nondegenerate as shown in the lower part of Fig. 2 for those states for which $N=m=0$. (This was pointed out originally by Green and Lane.[15]) These ground and the first excited states are defined by the quantum numbers $\lambda = 1 + \delta_1$ and $\lambda = 2 + \delta_2$, respectively.

The transition energy $\Delta\mathscr{E}_{\lambda,\lambda'}(b)$ is readily deduced and is given by

$$\Delta\mathscr{E}_{\lambda,\lambda'}(b) = |\mathscr{E}_\lambda(b) - \mathscr{E}_{\lambda'}(b)| \tag{4.22}$$

so that, if $\delta_{1,2} \ll 1$, then

$$\Delta\mathscr{E}_{12}(\tfrac{1}{2}d) \cong \Delta\mathscr{E}_{02}(0) - \Delta\mathscr{E}_{01}(0). \tag{4.23}$$

These calculations are in good qualitative agreement with the results obtained using other numerical methods.[16]

V. THE SPECTRUM IN THE REGION OF POSITIVE ENERGY: THE SIZE QUANTIZATION SPECTRUM

In the above, we have considered the solutions to (2.5) in which the energy $\mathscr{E}_\lambda$ given by (3.1) is negative. We consider now the region for which this energy is positive (see Fig. 1). In bulk semiconductors, for which d is effectively infinite, a continuous spectrum results but in a quantum well of finite width, the spectrum is quantised.

A. Definitions

In order to consider this region, we introduce a new set of parameters X, γ, and s, which replace u, g, and λ, respectively used previously in Sec. III. They are defined by

$$\mathscr{E}^{(N,m)} \rightrightarrows \mathscr{E}_s = \frac{\hbar^2}{2\mu a_0 s^2}, \quad X = \frac{2|z-b|}{ia_0 s} + \gamma,$$

$$\text{where } \gamma = \frac{2\alpha a_H}{ia_0 s}, \quad \alpha_{N,m} \rightrightarrows \alpha \text{ with } |\gamma| \ll 1. \quad (5.1)$$

Thus Eq. (2.5) may be written in the form

$$\frac{d^2 f_s(X)}{dX^2} + \frac{is}{X} f_s(X) - \tfrac{1}{4} f_s(X) = 0 \quad (5.2)$$

for the function $f_s(X)$. On choosing the two linear independent solutions to (5.2) in the form

$$W_{is,1/2}(X), \quad W_{-is,1/2}(-X)$$

the general solution to (5.2) for $z \geqslant b$ is given by

$$f_s(X) = e^{i\theta} W_{is,1/2}(X) + e^{-i\theta} W_{-is,1/2}(-X) \quad (5.3)$$

and for $z \leqslant b$, we have

$$f_s(X) = D[e^{i\phi} W_{is,1/2}(X) + e^{-i\phi} W_{-is,1/2}(-X)]. \quad (5.4)$$

Much of what follows is similar to Sec. III as the boundary conditions (2.6) on the function $f_s(X)$ are as before. These conditions and the requirements of the continuity of the function $f_s(X)$ and its first derivative for $z = \pm \frac{1}{2} d$ lead again to a set of four homogeneous algebraic equations for the coefficients involving $De^{\pm i\phi}$ and $e^{\pm i\theta}$ similar to those given by (3.9). Thus by requiring that the equations are solvable we obtain the equation

$$\left[\frac{W_{+,2}}{W_{-,2}} + \frac{W_{+,1}}{W_{-,1}} + 2\frac{W'_+}{W'_-} + F\right]\left[\frac{W_{+,2}}{W_{-,2}} + \frac{W_{+,1}}{W_{-,1}} - 2\frac{W_+}{W_-} - F\right] = 0, \quad (5.5)$$

where

$$W_{\pm 1,2} = W_{\pm is,1/2}(y_{1,2}),$$

$$\text{where } y_{1,2} = \frac{d}{ia_0 s}\left[1 + \frac{ia_0 s\gamma}{d} \mp \frac{2b}{d}\right]$$

and where

$$W_\pm = W_{\pm is,1/2}(\pm\gamma), \quad W'_\pm = W'_{\pm is,1/2}(\pm\gamma)$$

and

$$F = \frac{e^{s\pi}}{W_- W'_-} - \left[\frac{e^{2s\pi}}{(W_- W'_-)^2} + \left(\frac{W_{+,2}}{W_{-,2}} - \frac{W_{+,1}}{W_{-,1}}\right)^2\right]^{1/2}.$$

In obtaining Eq. (5.5), we have taken into account that the Wronskian of the functions $W_{is,1/2}(X)$ and $W_{-is,1/2}(-X)$ is equal to $-\exp(s\pi)$. As $|\gamma| \ll 1$, the expression (A1) for W and for its derivative are used. The roots s_n with $n = 1,2,3,...$ of (5.5) define the energy levels $\mathscr{E}_s$. This equation is exact and it is valid for any values of $y_{1,2}$. Analogous to our previous treatment of Eq. (3.12), the left- and right-hand brackets separately give rise to quasi-even and quasi-odd states, respectively. The expressions simplify if we assume that the impurity is situated near the midpoint of the QW for which

$$b \simeq 0, \quad y_1 \simeq y_2 \simeq y_0 = \frac{d}{ia_0 s}\left(1 + \frac{i\gamma a_0 s}{d}\right), \quad F = 0.$$

B. The quasi-even states

On setting the left-hand bracket of (5.5) to zero, the equation describing the quasi-even states becomes

$$\frac{W_{is,1/2}(y_0)}{W_{-is,1/2}(-y_0)} + \frac{W'_{is,1/2}(\gamma)}{W'_{-is,1/2}(-\gamma)} = 0. \quad (5.6)$$

Let us consider the excited energy levels with $s \ll 1$, $|y_0| \gg 1$. On substituting the asymptotic expansion from (A3) for the functions $W_{\pm is,1/2}(\pm y_0)$ and from (A1) for $W_{\pm is,1/2}(\pm\gamma)$, we obtain, for the real part, the result

$$\mathrm{Re}\left\{\exp[\tfrac{1}{2} y_0 - is\,\ln(-y_0)]\,\frac{1}{\Gamma(-is)}\,[\ln\gamma + \psi(1-is) + 2C - \tfrac{1}{2} i s^{-1}]\right\} = 0. \quad (5.7)$$

Using the limiting values

$$\Gamma(-is) \simeq is^{-1} \quad \text{and} \quad \Psi(1-is) \simeq \Psi(1) = -C \quad \text{for } s \ll 1$$

Eq. (5.7) becomes

$$-\cot\left[\frac{d}{2a_0 s}\left(1 + \frac{ia_0 s\gamma}{d}\right) + s\,\ln\left(\frac{d}{a_0 s}\right)\left(1 + \frac{ia_0 s\gamma}{d}\right)\right] = s\left[\ln\left(\frac{2\alpha a_H}{a_0 s}\right)^2 + 2C\right]. \quad (5.8)$$

This equation can be solved by the method of iteration. In the zeroth approximation setting $s = 0$, we find that $s_0^{-1} = (\pi a_0/d)(2p-1)]$ with $p = 1,2,3,...$ so that

$$\frac{1}{s} = \frac{1}{s_0}\left[1 + \frac{2a_0 s_0^2}{d}\left[\ln\left\{\left(\frac{2\alpha a_H}{a_0 s}\right)^2 \frac{a_0 s_0}{d}\right\} + 2C\right]\right]. \quad (5.9)$$

From the latter equation (5.9), the energies $\mathscr{E}_s$ of the quasi-even states can be written in the form

$$\mathscr{E}_s = \mathscr{E}_p(0) + \Delta\mathscr{E}_p, \quad (5.10)$$

where

$$\mathscr{E}_p(0) = \frac{\hbar^2 \pi^2}{2\mu d^2}(2p-1)^2 \quad (5.11)$$

and

$$\Delta\mathscr{E}_p = \Delta\mathscr{E}_p^{(g)} = \frac{\hbar^2}{2\mu d^2}\,4\,\frac{d}{a_0}\left[\ln\left\{\pi(2p-1)\left(\frac{2\alpha a_H}{d}\right)^2\right\} + 2C\right]. \quad (5.12)$$

The expressions (5.10)–(5.12) are valid under the conditions

$$\frac{d}{a_0 \pi^2 (2p-1)} \ll 1, \quad \frac{(2p-1)\pi a_H}{d} \ll 1.$$

The energies $\mathscr{E}_p(0)$ given by (5.11) are the unperturbed size quantized energy levels of the even-parity states. The energies $\Delta\mathscr{E}_p^{(g)}<0$ from (5.12) are caused by the one-dimensional Coulomb impurity potential $V(z)$ given in (2.11).

The condition $(d/a_0)/[(2p-1)\pi^2]\ll 1$ means that impurity potential $V(z)$ can be regarded as a perturbation to the size quantized states. In first-order perturbation theory, the additional energy $\Delta\mathscr{E}_p^{(g)}$ has been defined by the diagonal matrix element of the potential $V(z)$, namely,

$$\Delta\mathscr{E}_p^{(g)}=\int_{-(1/2)d}^{+(1/2)d}\psi_p^*(z)V(z)\ \psi_p(z)\ dz, \tag{5.13}$$

where

$$\psi_p(z)=\left(\frac{2}{d}\right)^{1/2}\cos\left(\frac{(2p-1)\pi z}{d}\right) \tag{5.14}$$

are the unperturbed even-parity wave functions.

Under the other condition $(a_H/d)\pi(2p-1)\ll 1$, the integral in (5.13) can be calculated explicitly. The energy $\Delta\mathscr{E}_p^{(g)}$ obtained differs from the energy given by (5.12) by the Euler constant C, which is considerably less than the logarithmic term. This difference is likely to be a consequence of the different approximations used (namely, that of iteration versus perturbation theory).

C. The quasi-odd states

The quasi-odd states can be considered in much the same way as the quasi-even states. Equating the right-hand bracket of (5.5) to zero, the equation describing the quasi-odd levels can be written in the form

$$\frac{W_{is,1/2}(y_0)}{W_{-is,1/2}(-y_0)}-\frac{W_{is,1/2}(\gamma)}{W_{-is,1/2}(-\gamma)}=0. \tag{5.15}$$

On substituting for the asymptotic expansions from (A3) for the functions $W_{\pm is,1/2}(\pm y_0)$ and from (A1) for $W_{\pm is,1/2}(\pm\gamma)$ into (5.15) under the conditions $s\ll 1$, $|y_0|\gg 1$, and $|\gamma|\ll 1$, we obtain from the imaginary part the result

$$\mathrm{Im}\Bigg(\exp[\tfrac{1}{2}y_0-is\ \ln(-y_0)]\ \frac{1}{\Gamma(-is)}\times[is^{-1}+\gamma\{\ln\gamma+\Psi(1-is)+2C-1-\tfrac{1}{2}is^{-1}\}]\Bigg)=0 \tag{5.16}$$

and then

$$\tan\left[\frac{d}{2a_0s}\left(1+\frac{ia_0s\gamma}{d}\right)+s\ \ln\left(\frac{d}{a_0s}\right)\left(1+\frac{ia_0s\gamma}{d}\right)\right]=\frac{\alpha a_H}{a_0sG}, \tag{5.17}$$

where

$$G=1-\left(\frac{2\alpha a_H}{a_0}\right)\left[\ln\left(\frac{2\alpha a_H}{a_0s}\right)+C-1\right].$$

As $(\alpha a_H)/(a_0s)\sim\gamma\ll 1$, the right-hand part of (5.17) is much smaller than unity. In the zeroth approximation, obtained by equating this right hand part to zero, and also by putting $s=0$, we find that, by taking $s_0^{-1}=2pa_0\pi/d$ with $p=1,2,3,...$, we have

$$\frac{1}{s}=\frac{1}{s_0}\left[1-\frac{2a_0s_0^2}{d}\ln\left(\frac{d}{a_0s_0}\right)\right]. \tag{5.18}$$

The energies $\mathscr{E}_s$ of the quasi-odd states are given by (5.10) where

$$\mathscr{E}_p^{(0)}=\frac{\hbar^2\pi^2}{2\mu d^2}\ (2p)^2 \tag{5.19}$$

and

$$\Delta\mathscr{E}_p=\Delta\mathscr{E}_p^{(u)}=-\frac{\hbar^2}{2\mu d^2}\,4\,\frac{d}{a_0}\ln(2\pi p). \tag{5.20}$$

The conditions of validity of Eq. (5.19) and (5.20) are the same as those of Eqs. (5.10) to (5.12).

The energies $\mathscr{E}_p(0)$ are the unperturbed energies due to the size quantization of the odd-parity states. The energy changes $\Delta\mathscr{E}_p^{(u)}$ are caused by the impurity potential $V(z)$ as given in (2.11). On treating the potential as a perturbation, this change in energy is given by the right-hand part of (5.13) where

$$\psi_p(z)=\left(\frac{2}{d}\right)^{1/2}\sin(2p\pi z/d) \tag{5.21}$$

are the unperturbed odd-parity wave functions. Under the condition $2p\pi a_H/d\ll 1$, $\Delta\mathscr{E}_p^{(u)}$ can be obtained from (5.20) by replacing $[\ln(2\pi p)]$ by $[\ln(2\pi p)+C)]$. We note that, for the excited states considered above for which $p>1$, $C\ll\ln(2\pi p)$.

The above results are equivalent to those obtained in Sec. IV and reflect their complementary characteristics. Thus it is possible to describe any impurity states in the QW with both a Coulomb form ($\mathscr{E}_\lambda<0$) and also the form of the size quantized states for which $\mathscr{E}_s>0$. The correlation diagram of the energy levels versus the impurity center displacement b is given in the upper part of Fig. 2, which is also simplified to show states belonging to the lowest Landau level only ($N=m=0$). It is based on the general properties of the eigenvalues of the differential equation (2.5) and (2.11). It is clear that, as the impurity moves from a position with $b=0$ to the position where $b=\frac{1}{2}d$, the energy increases.

VI. FINAL RESULTS AND CONCLUSIONS

The previous sections have concentrated on the Coulomb and size quantization parts of the energy-level spectra of the impurity electron in a QW in the presence of a strong magnetic field associated with a given Landau level. The results are shown schematically in Fig. 2 for $N=m=0$ to illustrate the basic physics involved. It has been found that the levels of lowest energy have a quasi-Coulomb character while the levels of high energy are size quantization levels. It should be noted that all energies have been derived analytically using a common approach.

The results derived above have been used to obtain the explicit dependence of the lowest-energy levels as a function of the displacement of the impurity. The results are displayed

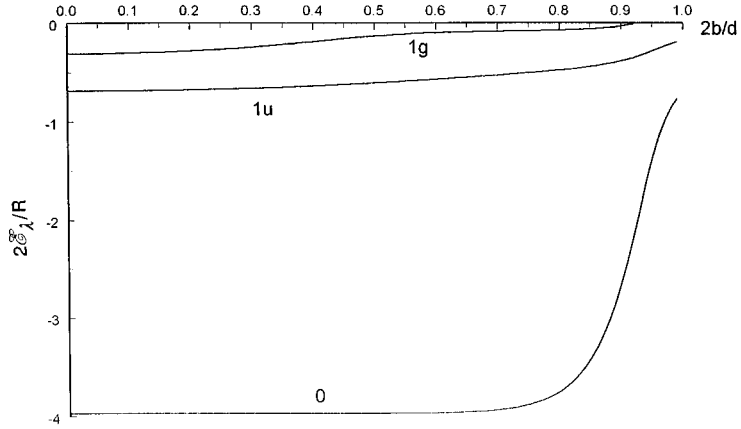

FIG. 3. The calculated energies $\mathscr{E}$ [given by Eqs. (3.2) and (3.12)] where $\mathscr{E}=-R/(2\lambda^2)$ and where $R(=\hbar^2/\mu a_0^2)$ is the impurity Rydberg constant, of the ground state ($\lambda=\lambda_0$), the first excited quasi-even state ($\lambda=\lambda_{1g}$), and of the quasi-odd ($\lambda=\lambda_{1u}$) states as a function of the displacement b of the impurity from the center of the well for $N=m=0$. [The other parameters are given by $d/a_0=11.0$, $a_H/a_0=0.30$].

in Fig. 3; as expected, this dependence is in agreement with the schematic diagram (Fig. 2). The curves are similar to each other in that their slopes are initially shallow for $b\leqslant b_\lambda$ but then they have relatively steep slopes in the region $b>b_\lambda$ where b_λ is a critical center position defined by the boundary. As can be seen from Fig. 3, $b_{1g}<b_{1u}<b_0$. This means that the QW boundary has a relatively large effect on the first excited quasi-even state, a medium effect on the first excited quasi-odd state and little effect on the ground state.

These results can be explained by the dependencies of the quantum number λ upon the width of the well d, which are shown in Fig. 4 for $N=0$. These in turn are defined by the forms of the wave functions of the relevant states (Fig. 5). It follows from Fig. 5 that the ground state is localized at the center of the well ($z=0$), the first excited quasi-odd state has its maximum probability at $z=1.5a_0=0.15d$ and at $z=2.5a_0=0.25d$ for the quasi-even state. The greater the distance by which the maxima of the wave packets are removed from the center of the well, the larger is the effect of the boundary. This is consistent with the dependencies of the quantum numbers λ upon the width of the well d. The first excited quasi-even state is affected by the boundary of a sufficiently wide well, the first excited quasi-odd state by the medium wide well, and the ground state by the boundary of a relatively narrow well. From the values of the quantum number λ given in Fig. 4, the binding energy $\mathscr{E}$ of the ground state, measured in terms of the impurity Rydberg constant R, is given by $-2\mathscr{E}/R=1/\lambda^2=3.2$ with $d/a_0=2$ and $a_H/a_0=0.3$. This value is in reasonable agreement with that obtained for $a_H/a_0=0.7$ by a variational-type numerical method,[16] which gives $-2\mathscr{E}/R=3.0$. The small difference between the two values can be attributed to the differences between the magnetic fields used in the two calculations and the replacement of barriers of finite size as used in Ref. 16 with the infinite barriers used here.

Further direct comparisons are difficult to make as our calculations are applicable for wider quantum wells and larger magnetic fields than those commonly used by other authors (see, e.g., Refs. 15, 16). However, Fig. 6 shows the variation of the energy of the ground state with the scaled magnetic field, which has been calculated from our model above for a very wide well (of thickness $\sim 20a_0$) and the data from Makado and McGill[23] appropriate to bulk GaAs. It is seen that there is very good agreement between the two sets of data, which goes a long way towards justifying the accuracy of the analytical model proposed.

It follows from Eqs. (4.10), (4.12), and (4.16) that the effect of the QW boundary on the impurity states is considerable under the condition

$$\frac{d}{a_0}<\nu_n,$$

where ν_n are the critical values defined by the inequalities

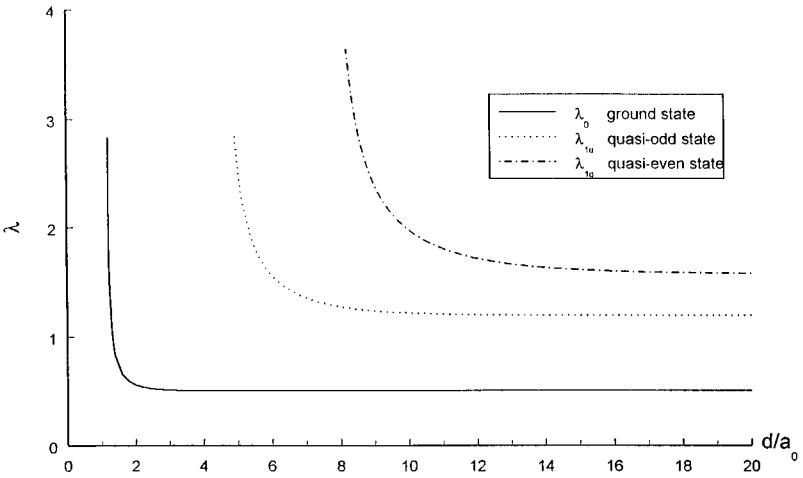

FIG. 4. The dependencies of the quantum numbers of the ground state (λ_0) and of the first excited even (λ_{1g}) and odd (λ_{1u}) states upon the width of the well d for the case when the impurity is positioned at the center of the well [Eqs. (3.2) and (3.12)] for $N=m=0$ and with $a_H/a_0=0.30$.

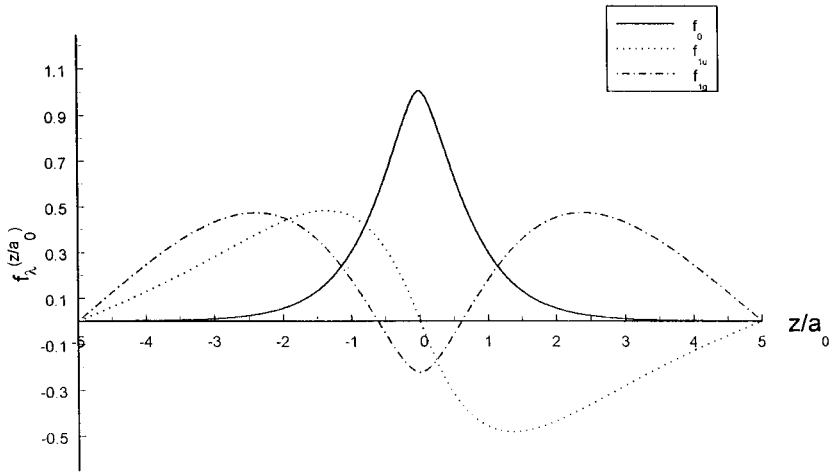

FIG. 5. The wave functions of the ground (f_0) and the first excited even (f_{1g}) and odd (f_{1u}) states for the case when impurity center is positioned at the center of the well obtained from solving Eq. (3.2) numerically for the case when $N=m=0$, $a_H/a_0=0.30$ and $d/a_0=10.0$.

$$\frac{\nu_0}{\bar{\lambda}_0}>1, \quad \frac{1}{\bar{\delta}_{1u,g}}\left(\frac{\nu_{1u,g}}{\bar{\lambda}_{1u,g}}\right)^{2\bar{\lambda}_{1u,g}} \exp^{-\nu_{1u,g}/\bar{\lambda}_1 u,g}\simeq 1, \quad (6.1)$$

where $\bar{\lambda}_n=n+\bar{\delta}_n$ and where δ_n is the quantum defect of the relevant state in the bulk semiconductor. As is seen from Fig. 4, $\bar{\lambda}_0\simeq 0.5$, $\bar{\delta}_{1u}\simeq 0.2$, and $\bar{\delta}_{1g}\simeq 0.6$ such that the calculated values are $\nu_0>0.5$, $\nu_{1u}\simeq 7.0$, and $\nu_{1g}\simeq 10.4$. These results are consistent with the graphs drawn in Fig. 4 ($\nu_0\simeq 1$, $\nu_{1u}\simeq 7.5$, $\nu_{1g}\simeq 11.0$).

In order to obtain the complete energy-level pattern, the results derived above for each Landau level, labeled by the quantum number N, with each magnetic component, labeled by the quantum number m are superposed. Together, they reconvert the problem to one in three dimensions. Resonance effects can arise therefore if the energy of one of the size quantization levels associated with the Landau state for which $N=N'$ has exactly the same energy as a state of the Coulomb spectrum associated with $N=(N'+1)$ Landau state particularly when their m values are the same. However, this is unlikely to be important for QW's of the usual size (for which d is typically 150 Å) where the magnetic and Landau splittings are much smaller than the size quantization (or subband) splittings. As the magnetic field used in an experiment increases, the probability of the resonance effect described above increases.

The final set of results includes both hydrogenlike[1] and the so-called metastable[6,7] states. However, it is usual to label the metastable states by an additional quantum number ν as well as N and m where ν gives the number of nodes in the wave function in the z direction (apart from at $\pm\infty$ for bulk systems and at the edges of the well in MQW systems). Obviously, ν is related to λ but it also includes m. Both types of states (hydrogenlike and metastable) can thus be expressed explicitly in terms of the set of quantum numbers (N,m,ν) even though the notation[17] has been developed specifically for high fields.

It is clear from the definitions and Fig. 5 that the ground state shown in Fig. 2 is the hydrogenlike state $1s_0$ and the metastable state (000). The first excited ''quasi-even'' state is $2s_0$ and (002) and the first excited ''quasi-odd'' state is $2p_0$ and (001) in the two notations. Work is currently in progress to correlate all the remaining states derived from our analysis with others existing in the literature and full details of these results will be published later. However, this is not straightforward because of the need to obtain the cor-

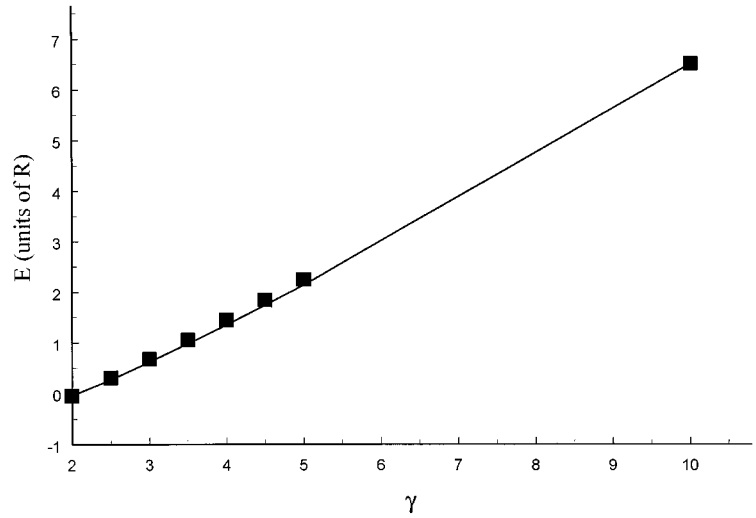

FIG. 6. The calculated values for the energy of the ground state (in units of R) as a function of the scaled magnetic field $\gamma(=0.147B$, where B is given in Tesla). The corresponding values calculated by Makado and McGill (Ref. 23) are denoted by ■.

rect relationships between the label λ introduced here and the quantum numbers N, m, and ν used in these other publications.

There have been a few attempts[17–20] to calculate analytically the energy spectrum for bulk systems but even less work has been done on QW systems before that described here. It is interesting to note that the empirical relation for energy-level splittings quoted by von Klarenbosch *et al.*,[21] from an earlier paper[19] on shallow-donor impurities in bulk GaAs, has a very similar form to that derived here. Thus the effects of the confining barriers in cases of large magnetic fields are not thought to be large though they do play a very important role in determining the fine structure in the spectrum in such cases. It is also clear from previous work[7] that the approximation of modeling a MQW system by a single QW is valid in most cases and thus the theory described above can be applied with only minor modifications to MQW systems. In conclusion, it should be stated that the approach developed above for a large magnetic field is not particularly sensitive to the actual magnitude of the magnetic field. As shown previously,[22] the maximum error incurred by reducing the magnitude of the magnetic field, such that the parameter g remains ~ 1, does not exceed approximately 20%.

Finally, it is worth noting that the results obtained above for the Coulomb states of an impurity electron ($\mathscr{E}_\lambda < 0$) can be readily extended to an exciton formed by an electron (e) and a hole (h) with very different effective masses ($m_e \ll m_h$). In this case, the adiabatic approximation can be used.

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APPENDIX: SOME LIMITING VALUES OF THE SPECIAL FUNCTIONS

The special functions used above have relatively simple forms in the limiting cases that are applicable here. For example, for small values of $x(\ll 1)$, we have[13]

$$W_{\lambda,1/2}(x) = \frac{1}{\Gamma(-\lambda)}\left[-\frac{1}{\lambda} + x\,\ln x + x\left\{\Psi(1-\lambda) + 2C - 1 + \frac{1}{2\lambda}\right\}\right], \quad \text{(A1)}$$

$$M_{\lambda,1/2}(x) = x(1 - 1/2\lambda x) \quad \text{(A2)}$$

and for large values of $x(\gg 1)$, we find

$$W_{\lambda,1/2}(x) = x^{\lambda} e^{-x/2}, \quad \text{(A3)}$$

$$M_{\lambda,1/2}(x) = \frac{1}{\Gamma(1-\lambda)}\, x^{-\lambda} e^{x/2}. \quad \text{(A4)}$$

In the above, $\Psi(x) = d[\ln \Gamma(x)]/dx$ is the logarithmic derivative of the Γ function $\Gamma(x)$. In particular, $\Psi(1) = -C$, where $C(=0.577)$ is the Euler constant. We note also that, if the argument of $\Gamma(x)$ or $\Psi(x)$ has a value close to a negative integer, the following approximations may be used:

$$\Gamma(-n-1-\delta) = \frac{(-1)^n}{(n+1)!\,\delta}, \quad \Psi(-n-\delta) = \frac{1}{\delta},$$

$$\Gamma(-\delta) = -\frac{1}{\delta} \quad \text{for } \delta \ll 1 \quad \text{and } n = 0,1,2,\ldots . \quad \text{(A5)}$$

Between the two limits, no simplification is possible.

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