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The shifted-$1/N$-expansion method for two-dimensional hydrogenic donor states in an arbitrary magnetic field

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Abstract. The shifted-$1/N$-expansion method has been used to study the energy levels for a 2D donor impurity in the presence of an arbitrary magnetic field. Exact analytical expressions for the energy levels at zero- and high-field limits are obtained. The calculations are carried out to the third-order correction of the shifted-$1/N$-expansion energy series. The results appear to be in excellent agreement with those of Martin *et al*.

1. Introduction

In recent years the problem of two-dimensional (2D) hydrogenic energy levels in an arbitrary magnetic field has received much attention (MacDonald and Ritchie 1986, Whittaker and Elliot 1988, Zhu *et al* 1990, Martin and Baker 1991, Larsen and McCann 1992, Martin *et al* 1992). Work on this problem is motivated by interest in quantum well (QW) and multiple-quantum-well (superlattice) systems. The most commonly studied semiconductor superlattice consists of regions of GaAs which act as wells for the conduction electrons separated by regions of $Ga_{1-x}Al_xAs$ which act as barriers. The magnetic field dependence of the donor levels has been studied by Greene and Bajaj (1985). Experimentally, shallow donor levels have been studied by photoluminescence Raman spectroscopy (Shanabrook *et al* 1984), and by far-infrared magnetoabsorption spectroscopy (Jarosik *et al* 1985), where the magnetic field dependence plays a useful role in identifying absorption features.

Perturbation treatments of this problem can handle the weak- and strong-field limits. In the weak-field limit the energy levels are given in an expansion in powers of the coupling constant γ, while in the strong-field limit the Coulombic potential is considered as a perturbative term and the expansion is given in powers of $x = (\pi/2\gamma)^{1/2}$. The parameter γ is defined as

$$\gamma = \epsilon^2\hbar^2 B/ce^3m^{*2} \tag{1}$$

where m^* is the effective mass and ϵ the dielectric constant of the host (GaAs) material. However, such treatments cannot provide information about how the energy shifts with the magnetic field in the intermediate range, which is in fact of experimental interest in QW systems. Therefore, one has to go through interpolation approximations between the weak- and strong-field limits. For example, MacDonald

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and Ritchie (1986) have used two-point Padé approximations, but no regular pattern appears and the results become unreliable. Martin *et al* (1992) have used appropriate forms of the two-quasi-fractional approximation and found better interpolation between the two field limits.

In the absence of highly accurate analytical solutions, even for the simplest case of the 2D hydrogenic state in a uniform magnetic field, numerical solution of the Schrödinger equation could, in principle, resolve this issue (Duggan 1988, Whittaker and Elliot 1988).

In this paper the shifted-$1/N$-expansion method (Imbo *et al* 1984, Imbo and Sukhatme 1985) is introduced to study the 2D hydrogenic donor states in the presence of a magnetic field. The method has a non-perturbative character as it is not an expansion in powers of a coupling constant. The remarkable success of this method has been shown through a large number of potential models of physical interest (Imbo *et al* 1984, Imbo and Sukhatme 1985, Varshni 1988, Christiansen *et al* 1989, Mustafa and Sever 1991a, b).

In section 2 we consider a 2D electron gas in the x–y plane in the presence of a hydrogenic potential, representing the interaction between the conduction electron and the donor impurity centre and an external magnetic field of intensity B along the growth axis of the heterostructure, i.e. the z axis. This problem is discussed within the shifted-$1/N$-expansion method. In section 3 we give the analytical results for the energy at the zero- and high-field limits. We also compare our results with those of Martin *et al* (1992). We draw our conclusions in section 4.

2. The method

We shall consider the Hamiltonian which describes the Coulomb interaction between a conduction electron and a donor impurity centre when a magnetic field is applied perpendicular to the x–y plane. If we adopt the symmetric gauge $A = (B/2)(-y, x, 0)$, the Hamiltonian is expressed as

$$H = -\nabla^2 - 2w'/\rho + \gamma L_z + \gamma^2\rho^2/4 \tag{2}$$

where w' is introduced for convenience ($w' = 0.1$). ∇^2 is the two-dimensional Laplacian. L_z is the angular momentum operator $-i\partial/\partial\phi$ with the eigenvalue m, the magnetic quantum number. The units of energy and length are the effective Rydberg $R^* = m^*e^4/2\hbar^2\epsilon^2$, and the effective Bohr radius $a^* = \hbar^2\epsilon/m^*e^2$, respectively. Let the two-dimensional Laplacian be transformed to N dimensions (Nieto 1979) and be substituted in the Schrödinger equation to obtain

$$[\![-\{d^2/d\rho^2 + [(N-1)/\rho]d/d\rho - l(l+N-2)/\rho^2\} + V(\rho)]\!]\, R(\rho) = ER(\rho) \tag{3}$$

where

$$V(\rho) = -2w'/\rho + m\gamma + \gamma^2\rho^2/4 \tag{4}$$

with m being the magnetic quantum number and

$$\rho^2 = \sum_{i=1}^{N} x_i^2 \qquad N = 1, 2, 3, \ldots. \tag{5}$$

For $N = 2, x_1 = \rho\cos\phi, x_2 = \rho\sin\phi$ and $l = |m|$. The first derivative in equation (3) is removed by defining

$$R(\rho) = \rho^{-(N-1)/2}\Phi(\rho). \tag{6}$$

Equation (3), together with equation (6), gives

$$[-\mathrm{d}^2/\mathrm{d}\rho^2 + (\bar{k} + a - 1)(\bar{k} + a - 3)/4\rho^2 + V(\rho)]\Phi(\rho) = E\Phi(\rho) \tag{7}$$

where $\bar{k} = N + 2l - a$ and a is a suitable shift which has the meaning of an additional degree of freedom. Invoking now the formal procedure of the shifted-$1/N$-expansion method (see Imbo *et al* (1984) and Mustafa and Sever (1991a,b) and references therein), we obtain, from (7), the following results:

$$E = E_0 + (1/\rho_0^2)[(1-a)(3-a)/4 + \alpha_1] + \alpha_2/\bar{k}\rho_0^2 \tag{8}$$

$$E_0 = V(\rho_0) + \bar{k}^2/4\rho_0^2 \tag{9}$$

$$a = 2 - (2n_\rho + 1)w \tag{10}$$

$$w = \sqrt{3 + \rho_0 V''(\rho_0)/V'(\rho_0)}. \tag{11}$$

ρ_0 can be determined through the relation

$$\sqrt{2\rho_0^3 V'(\rho_0)} = 2 + 2l - a = Q^{1/2}. \tag{12}$$

n_ρ is the radial quantum number, and α_1 and α_2 are given in the appendix.

3. Results and discussion

Considering equations (8)–(12), we have obtained the limiting values of the energy at the zero- and high-field limits as

$$E_{\text{donor}} = -(n_\rho + |m| + \tfrac{1}{2})^{-2} \tag{13}$$

and

$$E_{\text{Landau}} = \gamma(2n_\rho + |m| + m + 1). \tag{14}$$

It is worthwhile to point out that E_{donor} and E_{Landau} are obtained (for comparison see Whittaker and Elliot (1988)) by the leading energy term E_0 where higher-order terms vanish identically.

For donor states in an arbitrary magnetic field, we have numerically solved equation (12) through equations (10) and (11) to find the energy eigenvalues presented by equation (8).

Figures 1–3 show the results of the shifted $1/N$ expansion for the ground state 1S and the excited states $2P^-$ and $3D^-$. The results show excellent agreement with those of Martin *et al* (1992). However, the only disagreement is noted at the point $\gamma = \gamma' = 0$ for $2P^-$ and $3D^-$ excited states. This disagreement should have arisen from using the principal quantum number n (Martin *et al* 1992). Thereupon, when the magnetic field is applied to a donor impurity, the principal quantum number n is no longer a good quantum number. However, the magnetic quantum number m, and the radial quantum number n_ρ, retain their meanings and so can be used to follow the states from the donor impurity to Landau levels (Whittaker and Elliot 1988).

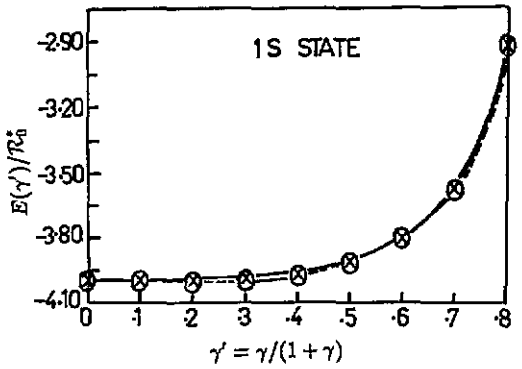

Figure 1. The 2D donor energy versus γ' for the 1S state: —×—, results of Martin *et al* (1992); – – –, best-fit line of our predictions (○).

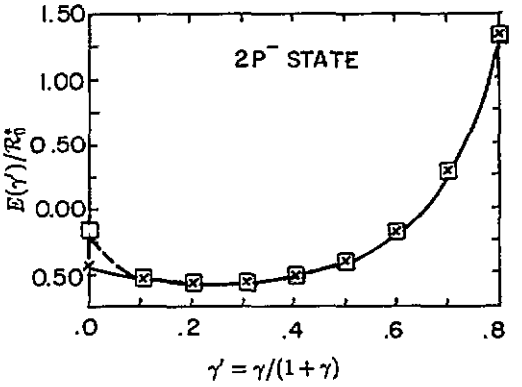

Figure 2. The 2D donor energy versus γ' for the $2P^-$ state: —×—, results of Martin *et al* (1992); – – –, best-fit line of our predictions (□).

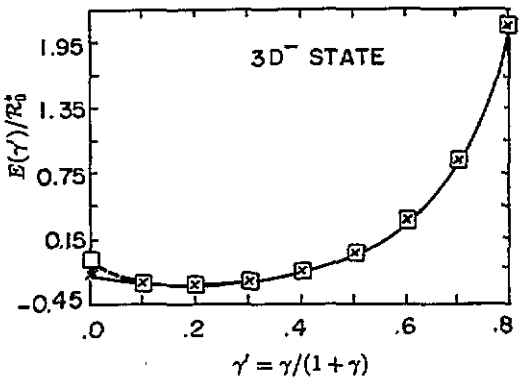

Figure 3. The 2D donor energy versus γ' for the $3D^-$ state: —×—, results of Martin *et al* (1992); – – –, best-fit line of our predictions (□).

4. Conclusions

We have used the shifted-$1/N$-expansion method to obtain the 2D donor impurity states in the presence of an arbitrary magnetic field. The convergence of this method is noted to be very fast in the sense that the dominating contribution to the energy is the leading term E_0 of equation (8). We have obtained exact analytical results for the zero- and high-field limits. The method leads to very accurate analytical results and its domain of applicability can be extended to include problems of magneto-exciton binding energy and others of solid state interest.

Appendix

Although the following definitions can be found in many references we would like to repeat them so as to make this paper self-contained:

$$\alpha_1 = [(1+2n_\rho)e_2 + 3(1+2n_\rho+2n_\rho^2)e_4] - w^{-1}[e_1^2 + 6(1+2n_\rho)e_1e_3 + (11+30n_\rho+30n_\rho^2)e_3^2] \tag{A1}$$

$$\begin{aligned}\alpha_2 = {} & (1+2n_\rho)d_2 + 3(1+2n_\rho+2n_\rho^2)d_4 + 5(3+8n_\rho+6n_\rho^2+4n_\rho^3)d_6 \\ & - w^{-1}[(1+2n_\rho)e_2^2 + 12(1+2n_\rho+2n_\rho^2)e_2e_4 + 2e_1d_1 \\ & + 2(21+59n_\rho+51n_\rho^2+34n_\rho^3)e_4^2 + 6(1+2n_\rho)e_1d_3 \\ & + 30(1+2n_\rho+2n_\rho^2)e_1d_5 + 6(1+2n_\rho)e_3d_1 + 2(11+30n_\rho+30n_\rho^2)e_3d_3 \\ & + 10(13+40n_\rho+42n_\rho^2+28n_\rho^3)e_3d_5] + w^{-2}[4e_1^2e_2 + 36(1+2n_\rho)e_1e_2e_3 \\ & + 8(11+30n_\rho+30n_\rho^2)e_2e_3^2 + 24(1+n_\rho)e_1^2e_4 + 8(31+78n_\rho+78n_\rho^2)e_1e_3e_4 \\ & + 12(57+189n_\rho+225n_\rho^2+150n_\rho^3)e_3^2e_4] - w^{-3}[8e_1^3e_3 + 108(1+2n_\rho)e_1^2e_3^2 \\ & + 48(11+30n_\rho+30n_\rho^2)e_1e_3^3 + 30(31+109n_\rho+141n_\rho^2+94n_\rho^3)e_3^4]\end{aligned} \tag{A2}$$

with

$$e_j = \epsilon_j / w^{j/2} \qquad d_i = \delta_i / w^{i/2} \tag{A3}$$

where $j = 1,2,3,4$, and $i = 1,2,3,4,5,6$.

The definitions of ϵ_j- and δ_i-values are

$$\epsilon_1 = (2-a) \qquad \epsilon_2 = -3(2-a)/2 \tag{A4}$$

$$\epsilon_3 = -1 + \rho_0^5 V'''(\rho_0)/6Q \qquad \epsilon_4 = \tfrac{5}{4} + \rho_0^6 V''''(\rho_0)/24Q \tag{A5}$$

$$\delta_1 = -(1-a)(3-a)/2 \qquad \delta_2 = 3(1-a)(3-a)/4 \tag{A6}$$

$$\delta_3 = 2(2-a) \qquad \delta_4 = -5(2-a)/2 \tag{A7}$$

$$\delta_5 = -\tfrac{3}{2} + \rho_0^7 V'''''(\rho_0)/120Q \qquad \delta_6 = \tfrac{7}{4} + \rho_0^8 V''''''(\rho_0)/720Q. \tag{A8}$$

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