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Theoretical calculations of shallow donor impurity states in GaAs/GaAlAs multi-quantum wells with magnetic fields applied parallel to the layers

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Abstract. A method is presented for the calculation of the energy eigenvalues and eigenstates of the electron associated with a shallow donor impurity in a GaAs/GaAlAs multi-quantum well structure in the presence of a magnetic field parallel to the layers. Compared to the case of an impurity in a magnetic field directed perpendicular to the layers, the problem is complicated by the lack of cylindrical symmetry. This lack of symmetry is reflected in the form chosen here for the basis states that describe the donor electron. By formulating the Hamiltonian and operating on these states, the energies and orthonormal ground and excited state wavefunctions of the donor electron are determined by matrix diagonalization procedures. Calculations of the transition probability between the ground and excited states yield the theoretically most probable transition energy for a given magnetic field. These calculated values are compared to available experimental data and deviations between the theory and experiments at large fields are discussed.

1. Introduction

Sakai *et al* (1993) showed that donor impurities can affect the observed current–voltage curves in magnetotunnelling experiments on laterally gated, n-type δ-doped multi-quantum well (MQW) devices. Resonances are seen, which are detected far below the threshold voltage expected for tunnelling through the lowest 2D sub-band of the well. Further very recent experiments (e.g. Sakai *et al* 1994, Fromhold *et al* 1995, Langerak *et al* 1994, Geim *et al* 1994a, b) have confirmed the earlier results that these resonances arise from a donor impurity whose energy matches that of the incoming electron. Preliminary calculations of the voltage and magnetic field dependence of the normalized magnetocurrent for such devices using the Bardeen–Transfer Hamiltonian approach were presented earlier (Barmby *et al* 1994c). However, the donor wavefunctions used in the latter calculations were not known accurately as, in these experiments, the magnetic field is directed parallel to the layers. Most existing theories concern fields applied perpendicular to the layers. The object of this paper is to develop a more accurate theory for the calculation of the energy levels of a donor impurity in a parallel magnetic field, which in turn will enable us to improve the accuracy of the calculation of the magnetotunnelling current.

The model chosen for the calculations is based on a matrix diagonalization procedure (MDP) developed originally by Dunn and Pearl (1991) for magnetic fields directed perpendicular to the layers. Subsequently Barmby *et al* (1993, 1994a) extended the model to magnetic fields tilted by an angle θ to the perpendicular by modifying the choice of basis states. However, the form of the wavefunctions was still principally that for a perpendicular

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field, so the results for large tilt angles are poor. Although results were obtained for a tilt angle of 90°, which corresponds to the case of a parallel field, they were not found to reproduce known experimental results very accurately. In this paper, new results will be obtained using basis functions specifically designed for the case of a magnetic field in the plane of the heterolayers. The model will be tested against the experimental data of Brozak *et al* (1989) for a particular MQW system.

2. Theory

2.1. The Hamiltonian

We assume that the donor impurity is positioned at the centre of one of the wells. The coordinate of its electron is defined to be r, where $r^2 = x^2 + y^2 + z^2$. The direction of growth of the MQW is defined to be the z direction and the direction of the magnetic field $\boldsymbol{B}$, which is parallel to the plane of the layers, to be the x direction, with the origin at the donor nucleus. A symmetric form for the gauge of the magnetic field is chosen so that the field is presented by the vector potential

$$\boldsymbol{A} = (0, -\tfrac{1}{2}zB, \tfrac{1}{2}yB). \tag{2.1}$$

The form of the Hamiltonian for the donor electron in the MQW is then given by

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_\parallel \tag{2.2}$$

where

$$\begin{aligned} \mathcal{H}_0 &= -\nabla^2 - 2/r + V_b(z) \\ \mathcal{H}_\parallel &= (\gamma/\mathrm{i})(y\partial/\partial z - z\partial/\partial y) + (\gamma^2/4)(y^2 + z^2). \end{aligned} \tag{2.3}$$

$\mathcal{H}_0$ is the field-independent part of the Hamiltonian and $\mathcal{H}_\parallel$ is the component of the Hamiltonian due to the presence of the parallel magnetic field. The Hamiltonian is expressed in dimensionless form with all lengths and energies expressed in units of effective Bohr radii a_0^* and effective Rydberg R^* respectively, where $a_0^* = 100.06$ Å and $R^* = 46.11$ cm^{-1} for GaAs. γ is the dimensionless form of the magnetic field, defined by

$$\gamma = (a_0^{*2}e/\hbar)B = 0.152B \tag{2.4}$$

where B is in tesla and the constant ϵ is the permittivity of GaAs. The effective mass m^* of the donor electron in GaAs, given by $0.0665m_e$, includes the non-resonant polaron correction (Devresse 1972, Barmby *et al* 1994b). To simplify the calculations, we assume that these values are the same in the GaAlAs barriers as they are in the GaAs wells. $V_b(z)$ is the potential energy due to the varying conduction band profile of the heterostructure with

$$V_b(z) = \begin{cases} 0 & \text{in the wells} \\ V_0 & \text{in the barriers.} \end{cases} \tag{2.5}$$

The height of the potential barrier V_0 with the GaAlAs layer having an aluminium fraction x is given by (Lee *et al* 1980)

$$V_0 = 0.6(1.155x + 0.37x^2)\ \text{eV}. \tag{2.6}$$

2.2. The form of the wavefunctions

The wavefunctions used to describe the behaviour of the donor electron are based on those derived originally by Lane and Greene (1986) for donor impurities located in an MQW in perpendicular magnetic fields. The form of their wavefunctions must be modified to take into account the change in the direction of the magnetic field. As the periodic potential of the MQW breaks the cylindrical symmetry of the system in the y–z plane, basis states of different m_i will be mixed together. Thus for the parallel-field case the wavefunctions are of the form

$$\Psi = \sum_{m_i} \sum_{i} c_{i,m_i} \psi_{i,m_i} \tag{2.7}$$

with the sum covering basis states with different values of m_i. The basis states are given by

$$\psi_{i,m_i} = f(z) x^q (z \mp \mathrm{i}y)^{|m_i|} \, \mathrm{e}^{-(\alpha_i+\delta)(y^2+z^2)} \, \mathrm{e}^{-\beta_i x^2} \tag{2.8}$$

where q is the parity of the wavefunction in the direction of the magnetic field and m_i is the orbital angular momentum quantum number associated with a given basis state. The $(z \mp \mathrm{i}y)^{|m|}$ term is analogous to the $\rho^{|m|} \, \mathrm{e}^{\mathrm{i}m\phi}$ term given by Lane and Greene (1986). Also the Slater-like functions applicable to a hydrogen atom are replaced by a summation over a series of Gaussian functions for ease of manipulation. The coefficients of the Gaussians are taken from the set of values $A_k = 13.4$, 2.01, 0.454, 0.123, 0.0324 and 0.007 17 (Dunn and Pearl 1991) while the coefficients α_i and β_i are chosen from the set with the restriction that $\alpha_i = A_k \Rightarrow \beta_i = A_k$ or $A_{k\pm1}$. The parameter $\delta = 0.1\gamma$ is added to the coefficients of the Gaussians to account for the constraining effect on the y and z components of the wavefunction with increasing magnetic field. Finally, $f(z)$ represents the free-particle behaviour of the electron in the MQW. It is given by the standard square-well solutions

$$f(z) = \begin{cases} \cos(kz) & \text{in the wells} \\ A \, \mathrm{e}^{\kappa z} + B \, \mathrm{e}^{-\kappa z} & \text{in the barriers.} \end{cases} \tag{2.9}$$

The function is defined to repeat periodically over the heterostructure while the parameters k, κ, A and B are deduced by matching the function and its derivative at the well/barrier boundaries.

The eigenvalues and eigenstates of the donor electron in the case of parallel magnetic fields are found from solving the Schrödinger equation

$$\mathcal{H}\Psi = E\mathbf{U}\Psi \tag{2.10}$$

where $\mathcal{H}$ represents the matrix formulation of the Hamiltonian, $\mathbf{U}$ is the overlap matrix and E represents the set of energy eigenvalues that are to be deduced. The matrix elements within the Hamiltonian and overlap have been calculated from the Hamiltonian and the donor electron wavefunction given in (2.2) and (2.8) respectively. These matrices were diagonalized by computational means, giving the energies E and wavefunctions Ψ for the ground and excited states. As the states result from a diagonalization procedure, they are automatically orthogonal to each other.

2.3. Transition probabilities

The energies of transition for the donor electron have been calculated from the ground and excited state energy eigenvalues. However, due to the mixing of basis states of different values of m_i, it is no longer possible to attribute a given eigenstate to a particular value of m_i. It is therefore difficult to pick out the dominant transition in the case of parallel magnetic fields, in contrast to the perpendicular-field case, where the spectra are dominated by transitions to the $2p_{\pm 1}$ hydrogenic states. Therefore, the transition probability to each excited state from the ground state has been calculated in order to deduce which transition is most likely to dominate the spectrum in the parallel-field case.

We assume that the main mechanism of transition is that of the interaction of the electric dipole moment of the impurity electron with the electric field component of the applied radiation. To a first approximation, this interaction Hamiltonian is given by

$$\mathcal{H}_{ed} = e\boldsymbol{r} \cdot \boldsymbol{E} \tag{2.11}$$

where $\boldsymbol{E}$ is the electric field vector associated with the radiation, given by

$$\boldsymbol{E} = \sum_{E_x, E_y} (E_x \boldsymbol{i} + E_y \boldsymbol{j}). \tag{2.12}$$

The applied radiation is initially assumed to be unpolarized and thus a summation over the individual electric field components has been carried out. By substituting this expression for the electric field into the interaction Hamiltonian $\mathcal{H}_{ed}$, the transition probabilities between the ground and excited states of the impurity are found to be given by

$$|\langle \Psi_e | \mathcal{H}_{ed} | \Psi_g \rangle|^2 = e^2 \sum_{E_x} E_x^2 |\langle \Psi_e | x | \Psi_g \rangle|^2 + e^2 \sum_{E_y} E_y^2 |\langle \Psi_e | y | \Psi_g \rangle|^2 \tag{2.13}$$

where Ψ_g and Ψ_e are the ground and excited state wavefunctions respectively. Because the ground state wavefunction has even parity, the x component of the electric field picks out transitions to odd-parity excited states. Conversely, the y component of the electric field will pick out transitions to even-parity excited states. Thus by calculating the magnitude of the transition probability for each excited donor state, the most likely transition can be deduced and the corresponding transition energy calculated.

3. Results

In order to test the accuracy of our calculations, the results have been compared with the experimental results of Brozak *et al* (1989) obtained from a GaAs/GaAlAs MQW sample having well widths of 450 Å, barrier widths of 125 Å and with the aluminium fraction x in the barrier layers equal to 0.25. In their experiments, Brozak *et al* (1989) used electromagnetic radiation polarized in the y direction and magnetic fields up to 10 T. Our calculations were thus carried out for even-parity excited states only. To simplify the calculation, only those basis states having orbital angular momentum quantum numbers $m_i = 0, \pm 1, \pm 2$ and ± 3 were considered. In addition, both the ground and excited state energies were corrected for the effects of non-parabolicity of the conduction band to give a corrected energy E given by (Peeters *et al* 1992)

$$E = E^0(1 - \delta' E^0 / E_g) \tag{3.1}$$

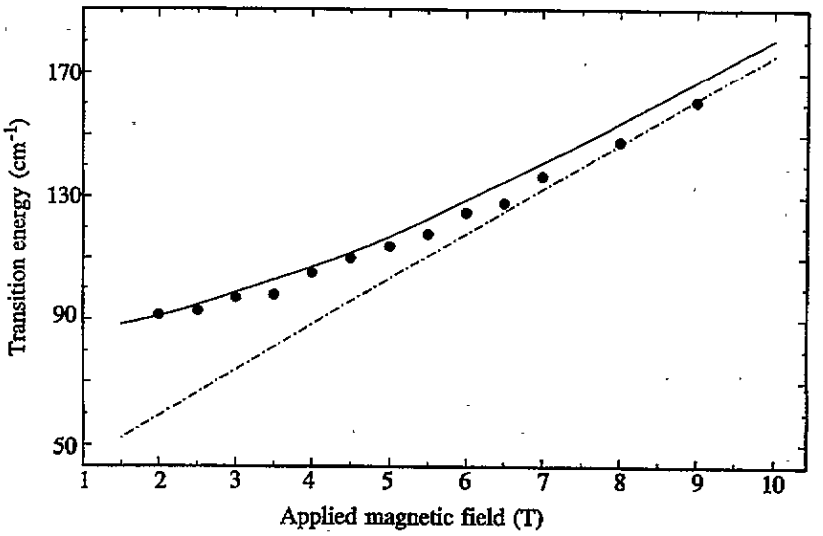

Figure 1. A plot of the calculated transition energies for the 1s–2p$_+$ transition for bulk GaAs, indicated by the broken curve, and for the main transition in an MQW system, indicated by the continuous curve. Results are shown for a GaAs/GaAlAs system in which the well width is 450 Å, the barrier width is 125 Å and $x = 0.25$. Experimental data obtained by Brozak *et al* (1989) are also given.

where E^0 is the energy calculated for a parabolic conduction band and E_g (= 1520 meV) is the GaAs band gap. The parameter δ' was chosen to be 0.73 (Vrehen 1968). The calculated transition energies for the dominant transition covering a range of magnetic field values is compared to the experimental data in figure 1. For comparison, the calculated transition energies for the 1s to 2p$_{+1}$ transition in bulk GaAs are also plotted.

As a further check on the accuracy of our results, further calculations have been undertaken by reducing the number of Gaussian coefficients used in the basis sets from the six used here down to three (which correspond to 13 and six basis states respectively). We find that the difference between the calculated transition energies using six rather than five coefficients is of the order of 0.02 cm^{-1} and further that the convergence is rapid.

4. Discussion

The effect of increasing the magnetic field is to further confine the electron in the well containing the impurity. As a result, the effect of the heterostructure barriers on the donor electron wavefunction decreases with increasing field. This is illustrated in figure 1, with the calculated heterostructure transition energies tending towards that of the bulk case as the field increases. It is also clear that the effect of the mixing of states with different values of m_i is more pronounced at lower fields where the barriers have greater influence. Comparing our calculations with the experimental data, it can be deduced that a sufficient number of values of m_i were included in the calculations for the lower values of field to obtain an accurate description of the donor electron wavefunctions, as the fit to the experimental data points is good.

At larger values of magnetic field, it can be seen that the calculated transition energies become increasingly larger than the experimental values. The probable cause of this

deviation is the so-called polaron interaction between the donor electron and the longitudinal optical (LO) phonons in the GaAs lattice. Resonant polaron corrections result in the lowering of the electron transition energy (Barmby *et al* 1994b), so the transition energies predicted by the above theory, where this vibronic coupling has not been taken into account, can be expected to be larger than the corresponding experimental data values. Whilst it is possible to include polaron corrections in our results (Barmby *et al* 1994b), the corrections take much computing time to evaluate, so this has not been attempted in this paper.

5. Summary

A method for the calculation of the energy eigenvalues and eigenstates of an electron associated with a shallow donor impurity in a GaAs/GaAlAs MQW structure with a magnetic field acting parallel to the layers has been presented. On testing the model with experimental data, it has been found that accurate estimations of the transition energies have been obtained especially at lower values of applied field. At higher fields, deviations occur probably due to the neglect of the effects of vibronic coupling involving the LO phonons. This will enable us to undertake a more accurate calculation of the effects of donor impurities in magnetotunnelling. Details of these calculations will be presented later.

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