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Theoretical calculations of the transition energies of a hydrogenic impurity in GaAs/GaAlAs multi-quantum wells in magnetic fields applied at any angle

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Abstract. Calculations are made of the energies of the dominant transition (1s to $2p_{+1}$-like) of a hydrogenic donor impurity in a multi-quantum-well (MQW) system subject to a magnetic field applied at an angle θ to the direction of growth of the MQW layers. The model used involves constructing suitable basis states, and then performing a matrix diagonalization procedure. The results are compared to the available experimental data, including the extreme cases of fields perpendicular ($\theta = 0°$) and parallel ($\theta = 90°$) to the layers. The results are also found to compare well with the results of existing variational calculations.

1. Introduction

Many studies have been made of the problem of the neutral hydrogenic donor (D^0) in multi-quantum wells (MQWs) subject to magnetic fields applied along the growth direction. More recently, a few studies have also been made when the magnetic field is applied at an angle θ to the growth direction. Far-infrared photoconductivity (FIR PC) results on GaAs/GaAlAs MQWs in tilted fields have been reported (Mueller *et al* 1991, Barmby *et al* 1993a). This is an interesting situation to consider as it allows confinement effects to be investigated. The idea of tilted fields is also useful in other situations, such as the tunnelling through bound impurity states of resonant tunnelling electrons (Barmby *et al* 1993b). In addition, some measurements have been made on impurities in magnetic fields applied parallel to the layers (Brozak *et al* 1989).

Variational calculations have been carried out to describe the states of the D^0 impurity in an MQW and under a tilted magnetic field (Mueller *et al* 1991) and a parallel field (Brozak *et al* 1989). In an earlier paper by the present authors (Barmby *et al* 1993a) a theoretical model was presented to describe the states of impurities in fields tilted by an angle of up to around 30°. The method involved employing a matrix diagonalization procedure (MDP) using basis states with a form appropriate to hydrogen with the exponentials expanded in terms of a sum of Gaussians. This was based on a procedure developed originally for the more common case of magnetic fields perpendicular to the layers (Dunn and Pearl 1991). The results compared favourably with the variational calculations of Mueller *et al* (1991). However, the model became unreliable for tilt angles above 30°, where the form of wavefunction used was inappropriate. In this paper, the model will be modified to apply to larger tilt angles by the use of improved basis wavefunctions.

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2. The theoretical model

Coordinates are chosen to describe the problem in which the z axis lies in the growth direction of the heterostructure, i.e. perpendicular to the semiconductor layers, and such that the applied magnetic field is in the x–z plane, tilted at an angle θ to the z axis. The origin is taken to be at the centre of a quantum well. The system, according to convention in this topic, is described by a Hamiltonian in dimensionless form, where the units of energy and length are the effective Rydberg energy and Bohr radius in GaAs (5.83 meV and 98.7 Å respectively). γ is used as a dimensionless magnetic field parameter, which equates to $0.148B$ for the magnetic field B in Teslas. The expression for the magnetic field is therefore given by $\gamma = \gamma_x i + \gamma_z k$, where $\gamma_z = \gamma\cos\theta$ and $\gamma_x = \gamma\sin\theta$. A symmetric gauge is chosen for the vector potential A, so that $A = (-\frac{1}{2}y\gamma_z, \frac{1}{2}(x\gamma_z - z\gamma_x), \frac{1}{2}y\gamma_x)$. The choice of a symmetric gauge (which is different to that used in our previous calculations) allows the Hamiltonian to be broken down into four component parts:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_\perp + \mathcal{H}_\parallel + \mathcal{H}_\angle \tag{2.1}$$

where $\mathcal{H}_0$ describes the behaviour of the donor atom in the MQW before the application of a magnetic field, $\mathcal{H}_\perp$ and $\mathcal{H}_\parallel$ describe the action of the perpendicular ($\theta = 0°$) and parallel ($\theta = 90°$) components of the magnetic field respectively, and $\mathcal{H}_\angle$ is the remaining part, which contributes only when the field is applied at an angle between the perpendicular and the parallel directions. (Note that, as in Barmby *et al* (1993a), we have found no advantage in using a gauge with a variable constant as used in the variational calculations of Mueller *et al* (1991).)

More explicitly,

$$\begin{aligned} \mathcal{H}_0 &= -\nabla^2 - 2/r + V_B(z) \qquad & \mathcal{H}_\perp &= \gamma_z l_z + (\gamma_z^2/4)(x^2 + y^2) \\ \mathcal{H}_\parallel &= \gamma_x l_x + (\gamma_x^2/4)(y^2 + z^2) \qquad & \mathcal{H}_\angle &= -(\gamma_x\gamma_z/2)xz. \end{aligned} \tag{2.2}$$

$V_B(z)$ is the barrier potential in the heterostructure given by zero in the GaAs wells and by V_0, the dimensionless form of the barrier height potential, in the barriers. V_0 is taken to be 60% of the band gap difference ΔE_g between GaAs and GaAlAs, where ΔE_g, for a fractional Al concentration x in the barriers, is estimated to be $(1.155x + 0.37x^2)$ eV (Lee *et al* 1980).

The wavefunction Ψ of the donor electron, as in our previous work, is taken to be a product of the free-particle-like behaviour of the donor electron in the MQW and its hydrogen-like behaviour about the positively charged donor ion (Greene and Bajaj 1985). In the case of an applied magnetic field perpendicular to the semiconductor layers, the wavefunction is written in the form

$$\Psi = \sum_i C_i f(z) g_i(\rho, z, \phi) \tag{2.3}$$

where the C_i are constants. $f(z)$ is a periodic function representing the free-particle-like behaviour, given by

$$f(z) = \begin{cases} \cos(kz) & \text{in the wells} \\ A_1 e^{\kappa z} + A_2 e^{-\kappa z} & \text{in the barriers} \end{cases} \tag{2.4}$$

where $k^2 = E_0$ and $\kappa^2 = V_0 - E_0$, with E_0 being the lowest eigenvalue of the square well solution. A_1 and A_2 are constants determined by matching the continuity and periodicity conditions in the MQW (Lane and Greene 1986). $g_i(\rho, z, \phi)$ is a basis state given by

$$g_i(\rho, z, \phi) = \rho^{|m_i|} e^{im_i\phi} (z - z_1)^{q_i} e^{-\alpha_i (z-z_1)^2} e^{-(\beta_i + \delta)\rho^2} \tag{2.5}$$

where m_i is the orbital angular momentum quantum number for the given basis state. q_i is a parameter that takes the value zero when the parity of the state in the z direction is even and unity when it is odd. z_1 is the position of the donor atom with respect to the centre of the GaAs well. The Slater-type part of the hydrogenic state is approximated by a summation over a series of Gaussians (Huzinaga 1965), and therefore α_i and β_i are numbers chosen to give the best fit to this approximation (Dunn and Pearl 1991). These are taken from a set of six parameters A_k, with the choices $\alpha_i = A_k$ and $\beta_i = A_k$, A_{k+1} or A_{k-1} (with the A_k listed monotonically). δ is a field-dependent parameter that allows for the constriction of the wavefunction about the magnetic field axis.

This form of the wavefunction, whilst written in cylindrical coordinates, is however suitable only for the magnetic field along the z axis. The cylindrical symmetry of the system is broken when the field is tilted away from the axis. To generalize the method for any angle θ, the waveform is rewritten in terms of Cartesian coordinates, allowing different constriction factors δ_1, δ_2 and δ_3 for the z-, y- and x-dependent Gaussians respectively. In addition, a set of numbers ϵ_i is introduced to allow the coefficients of the Gaussians in y to differ from those of x if required. The ϵ_i are chosen from the same set of numbers A_k as α_i and β_i. A general form for Ψ is therefore

$$\Psi = \sum_i C_i f(z)(z - z_1)^{q_i} (x \pm \mathrm{i}y)^{|m_i|} e^{-(\alpha_i + \delta_1)(z-z_1)^2} e^{-(\beta_i + \delta_2)x^2} e^{-(\epsilon_i + \delta_3)y^2} \tag{2.6}$$

where $\delta_1 = \delta\gamma_x$, $\delta_2 = \delta\gamma_z$ and $\delta_3 = \delta_1 + \delta_2$, with δ taken to be a suitably chosen coefficient. It was found that the transition energies subsequently calculated were not very sensitive to the precise value of this parameter, and so a value of 0.1 was chosen. This coincides with that used for perpendicular fields in our earlier work (Barmby *et al* 1993a).

By operating on each of the individual basis states of the wavefunction, the Hamiltonian and the overlap matrices are determined. Due to the asymmetry of the system, mixing between states of different orbital angular momentum occurs, and therefore, strictly speaking, all values of m_i should be taken into account in the calculations. However, for the sake of simplicity, only the states where $|m_i| \leqslant 2$ are considered here. By solving the generalized Hamiltonian equation

$$\mathcal{H}\Psi = EU\Psi \tag{2.7}$$

where U is the overlap matrix, the possible eigenvalues E and eigenvectors Ψ of the system can be determined.

As we diagonalize a matrix with a large number of basis states, we obtain a large number of eigenvalues. In magnetic fields perpendicular to the layers ($\theta = 0°$), only the lowest-energy states with given values of m_i and q_i have any physical significance. However, it is not so straightforward to select those states that have any physical significance under tilted fields as m is not a good quantum number. We therefore select the ground state and those excited states for which a large probability of transition from the ground state is predicted, assuming that the dominant mechanism is that of electric dipole transitions under the Faraday geometry, and evaluating integrals in the same manner as those used to determine $\mathcal{H}$. The details of this procedure are given in our previous article (Barmby *et al* 1993a). We find that this procedure does select the correct states for 1s and $2p_{+1}$ for the $\theta = 0°$ case, giving us confidence in the validity of this method.

3. Results and discussion

Firstly, calculations were carried out for the parameters $L = 178$ Å, $b = 167$ Å, $x = 0.33$ and $z_1 = 0$, at $\theta = 0°$, $\theta = 31°$ and $\theta = 42°$. These theoretical results can be compared to the results of the FIR PC experiments performed at Nottingham (Barmby *et al* 1993a), with the results shown in figure 1. It can be seen that the agreement is good at 0°, and acceptable at 31°. However, the agreement at 42° is poor. Indeed, no improvement in the agreement has been achieved compared to the less sophisticated methods of Barmby *et al* (1993a), despite separating the x and y coordinates of the wavefunctions by allowing the different coefficients β_i and ϵ_i in the Gaussian terms. In fact, the theoretical transition energies are altered very little when taking different values for β_i and ϵ_i. Logically, the x and y Gaussian terms should still be split up due to the asymmetry of the physical system, but subsequently in the calculations carried out ϵ_i was put equal to β_i, thereby reducing the number of basis states making up the wavefunction. This reduced the number of integrals to be evaluated, and so less time was required to calculate the eigenvalues and eigenvectors of the problem.

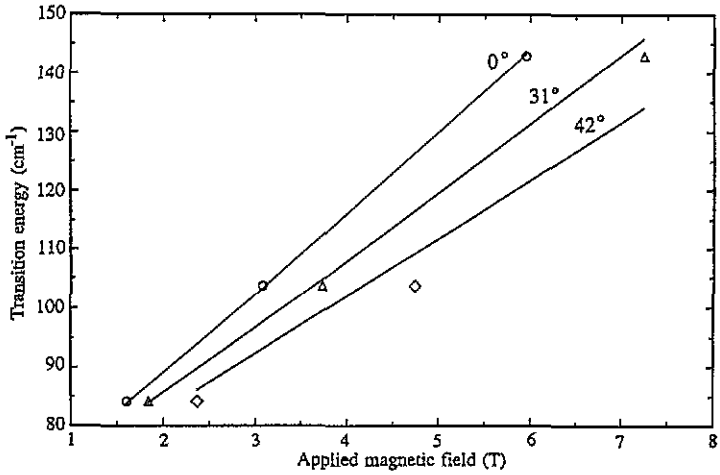

Figure 1. The experimental data of Barmby *et al* (1993a) for tilt angle of 0° (○), 31° (△) and 42° (◇), together with the corresponding calculated energies for the dominant transition (1s to $2p_{+1}$ like).

An explanation for the poor theoretical fit at $\theta = 42°$ might be that in our calculations, only a few values of m_i were considered, rather than the whole range of orbital angular momentum quantum numbers. For $\theta = 42°$ and at a magnetic field of 4.73 T, when basis states of orbital angular momentum $|m_i| \leqslant 1$ only were considered, the transition energy was calculated to be 110.7 cm^{-1}, whereas when considering $m_i = -2$ and 2 as well, the theoretical transition energy was 109.4 cm^{-1}. As θ is increased, the degree of mixing between states of different angular momentum increases, and therefore the approximation becomes less valid for the higher values of θ. Subsequently, the theoretical fit is less satisfactory for these higher values of θ.

Although there has been no improvement in this model at the tilt angle of 42°, an advantage of using this general field approach is that calculations should also be valid for the extreme case of $\theta = 90°$. We therefore carried out calculations for $\theta = 90°$ using the

data parameters of Mueller *et al* (1991) ($L = 500$ Å, $b = 350$ Å, $x = 0.2$ and $z_I = 0$), and Brozak *et al* (1989) ($L = 450$ Å, $b = 125$ Å, $x = 0.25$ and $z_I = 0$). The results are shown in figures 2 and 3 respectively. As can be seen, good agreement is obtained for both sets of data.

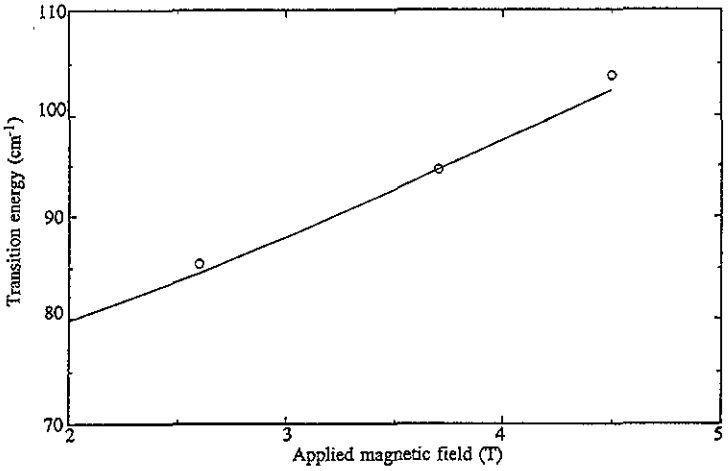

Figure 2. The experimental data of Mueller *et al* (1991) (○), together with the corresponding energy for the dominant transition (1s to $2p_{+1}$ like), calculated for magnetic fields applied parallel to the MQW layers ($\theta = 90°$) (solid line).

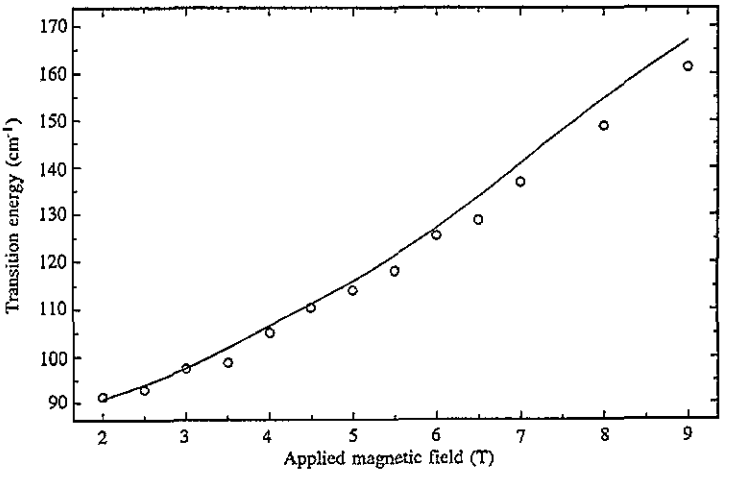

Figure 3. The experimental data of Brozak *et al* (1989) (○), together with the corresponding energy for the dominant transition (1s to $2p_{+1}$ like), calculated for magnetic fields applied parallel to the MQW layers ($\theta = 90°$) (solid line).

The fact that good agreement is obtained at $\theta = 90°$ can be explained by looking at the expression (2.1) for the Hamiltonian. It can be seen that the $\mathcal{H}_{\mathcal{L}}$ component of the Hamiltonian disappears at $\theta = 90°$, and therefore does not contribute to the mixing of the

different orbital angular momentum states. Therefore, the degree of mixing of the different states will be less at $\theta = 90°$ than at $\theta = 42°$.

4. Conclusions

We have attempted to produce a theoretical model to describe the transition energies observed from impurities in magnetic fields applied at any angle to the sample. The agreement between the theory and the available experimental results is found to be good for tilt angles from zero (i.e. a field perpendicular to the layers) up to around 30°, and also for $\theta = 90°$ (i.e. a field parallel to the layers). However, the agreement is not so good for intermediate tilt angles, where the mixing between basis states with different orbital quantum numbers m_i is largest. In principle, it should be possible to improve the model by including basis states with $|m_i| > 2$. However, this has not been attempted as it would involve a very large amount of computing time to evaluate the integrals required to determine the necessary matrix elements.

The only other theoretical calculations known to us are the variational calculations of *Mueller et al (1991) for angles up to 31° and those of Brozak et al (1989) for* $\theta = 90°$. The agreement between our results and those of the variational calculations is found to be good. Overall, our model is remarkably good considering that it essentially has no adjustable parameters and that it describes very well the two physically very different cases of magnetic fields parallel and perpendicular to the layers.

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