SPIN-FLIP ASSISTED RESONANT TUNNELING

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We present a theory of resonant tunneling via Zeeman split Landau levels in diluted magnetic semiconductor triple barrier heterostructures. In such a system, the tunneling current through two quasistationary discrete levels with high degeneracy exhibits sharp peaks as a function of bias. The spin fluctuations in the localized spin system produce, via the exchange interaction, additional peaks in the tunnel current. These peaks change with temperature in position and height. The results may provide an experimental tool to study the magnetic behaviour of thin layers by tunnel currents.

Resonant tunneling through quasistationary states in a single quantum well has been the subject of numerous experimental [1] and theoretical [2-7] work, since it became possible to grow semiconductor heterostructures by molecular beam epitaxy. Application of strong magnetic fields result in quantization, with a large degeneracy, in the x and y direction, in addition to the size quantization, in quantum wells, in the z direction. Resonant tunneling through one well in a magnetic field has been investigated [8-10]. Up to now, less attention has been paid to the fact that the energetical alignment of two discrete quasistationary states with large degeneracy is a general tool to produce a sharp current peak. The sharp current peaks provide the possibility to investigate such fundamental problems as Landau level broadening [11,12] and, as we will show here, the exchange interaction between band electrons and magnetic impurities in the barriers.

Recent progress in growing of quantum wells based on II-VI compounds, such as Cd$_{1-x}$Mn$_x$Te-CdTe has introduced a new set of physical problems, following from a strong interaction between the conduction electrons and the localized spins of the Mn$^{2+}$ ions. Wharamok et al [13] have shown, measuring the photo-luminescence in a high magnetic field, that significant penetration of the carrier wave function in the CdTe quantum well into the barriers with Mn$^{2+}$ results in a strong influence of the exchange interaction on the electronic properties. Awschalom et al [14] investigated carrier confinement in diluted magnetic semiconductor [15,16] quantum wells by optically induced magnetization.

The importance of the spin interactions in heterostructures and superlattices for studying the electronic properties under the quantum Hall effect conditions was suggested by Vagner and Maniv [17], and impressively demonstrated by Dobers et al [18]. The magnetic behaviour of microscopic layers (2D-spin system) is a field of growing interest [19,20] but the problem of detecting the magnetization of a small number of spins is still a limiting point in experiment [21].

In tunneling through one barrier with magnetic impurities the exchange interaction causes a conduction peak at zero bias [22]. Based on the transfer Hamiltonian method [23] Appelbaum [24,25] calculated the conductance across a metallic junction in analogy to the Kondo scattering [26]. In this paper we present a model to include the exchange interaction into tunneling using a transfer matrix technique for spinors. Since in a semiconductor the electrons have much longer wavelength than in metals, they interact simultaneously with a large number of magnetic impurities. In this case the classical approximation to the Heisenberg Hamiltonian can be applied and the formalism can be written in a simple way. This allows the application to more complicated structures than the one barrier case. As a result of the exchange interaction we predict additional resonances in the tunnel current through a triple barrier heterostructure including magnetic impurities and with a magnetic field applied per-
randomly distributed impurities has the following form

\[ H = \frac{1}{2m} (\vec{p} - e\vec{A})^2 + V_0 + \frac{g}{2} \mu_B \sigma \vec{B} + \sum_i V(\vec{r} - \vec{R}_i) \]

\[ - \sum_i J(\vec{r} - \vec{R}_i) \vec{S}_i \sigma \]

The exchange interaction is described in the last term by a Heisenberg Hamiltonian [27]. Here \( m \) is the effective mass, \( V_0 \) any potential energy, \( g \) the electron g-factor, \( \sigma \) the electron spin operator, \( V(\vec{r} - \vec{R}_i) \) the spin independent part of the interaction, \( \sum_i J(\vec{r} - \vec{R}_i) \) the exchange integral and \( \vec{S}_i \) the localized electron spin operator. Inelastic processes are not included in this description.

Since electrons in semiconductors have a large wavelength they interact simultaneously with a large number of impurities and thus we can approximate (virtual crystal approximation) the sum over the randomly distributed impurities by a sum over all lattice sites, \( \vec{R} \), times the concentration, \( \gamma \), of impurities

\[ M_{op} = -\gamma \sum_{\vec{R}} J(\vec{r} - \vec{R}) \vec{S}_R \]

Furthermore the simultaneous interaction of the band electron with many localized electrons leaves the exchange integral \( J(\vec{r} - \vec{R}) \) non-vanishing even for large distance, \( |\vec{r} - \vec{R}| \). Thus the sum in (2) collects many localized spins and the spin vector operator \( M_{op} \) becomes sufficiently large to be treated as a classical vector \( \vec{M}_e \).

Within this approximation the exchange interaction is described by the simple term \( M_{op} \sigma \) in the Hamiltonian (1). For the calculation of band-structures it is common practice in the theory of diluted magnetic semiconductors [15,16] to use the thermal average \( \langle \vec{M}_e \rangle_T \) as a representative numerical value for \( \vec{M}_e \) in the Hamiltonian. For an applied magnetic field in the \( z \)-direction, only \( \langle M_{e,z} \rangle_T \) is non-zero. Although this approximation might be valid for the calculation of band-structures, it is certainly not for the calculations of transport processes including spin-flip transitions, since it loses information about fluctuations of the localized spin system and it is these fluctuations which cause spin-flips of the band electrons.

However the transmission coefficient, \( D \), through the barriers can be calculated, keeping \( \vec{M}_e \) as a parameter. Since in the classical approximation the system has rotational symmetry around the direction of the applied magnetic field (\( z \)-direction), the transmission coefficient is a function of \( M_{e,x}^2 + M_{e,y}^2 \) and \( M_{e,z} \), i.e., it contains no terms of odd power in \( M_{e,x} \) or \( M_{e,y} \). This has also been checked numerically. Similar to the approximation described in the previous paragraph, as representative values for \( M_{e,x}^2 \), \( M_{e,y}^2 \) and \( M_{e,z} \) we use the thermal averages \( \langle M_{e,i} \rangle_T \) and

Fig. 1: HgCdSe heterostructures with two wells of different thickness and Mn ions in the central barrier.

The width of the barriers and wells from the left to the right are 30, 100, 50, 75, 30 Å. The barrier heights are \( V = 0.8eV \). The barrier material is \( \text{Hg}_{1-x}\text{Cd}_x\text{Se} \) with \( x = 0.62 \). The electrode and well material is \( \text{Hg}_{1-y}\text{Cd}_y\text{Se} \) with \( y = 0.16 \). The central barrier material is \( \text{Hg}_{1-z}\text{Cd}_z\text{Mn}_x\text{Se} \) with \( z = 0.12 \) and \( z' = 0.25 \). For the effective mass \( m \) in the well and barrier we took 0.04 and 0.06. The g-factor is \( g = 2 \). The Fermi energy \( E_F \) was chosen to be 90 meV. The exchange integral is -400 meV [15,16]. All material parameters are from Ref. [30,31]. The first resonances in the transmission coefficient are inserted as the energy levels (for Landau level index \( n=0 \)) of the quasibound states in the left and right wells.

The effective mass Hamiltonian for a band electron in an external magnetic field \( \vec{B} \) and experiencing the exchange interaction with localized electrons bound at the interfaces (see Fig. 1). This result may stimulate further investigation on the connection between electronic and magnetic properties of diluted magnetic semiconductor heterostructures. Most interestingly it provides the opportunity to probe the magnetic behaviour of a several Ångstrom wide layer by a tunnel current and it is of importance in the research on 2D-spin systems [19-21].
\[ (M_{x}, T) = x^2 \sum_{\mathbf{R}} J(\mathbf{r} - \mathbf{R}) (S_{x}^2)_{T} \]
\[ + z^2 \sum_{\mathbf{R} \neq \mathbf{R}'} J(\mathbf{r} - \mathbf{R}) J(\mathbf{r} - \mathbf{R}') (S_{x}^{2})_{T} (S_{z})_{T} \]  

For a diluted spin system the spins are assumed uncorrelated and the last term vanishes. For a homogeneous system the thermal average is the same on all lattice sites, thus \( \langle S_{x}^{2} \rangle_{T} = \langle S_{x}^{2} \rangle_{T} \). Due to the rotational symmetry around \( z \), it is \( \langle M_{x}^{2} \rangle_{T} = \langle M_{y}^{2} \rangle_{T} \). The key point in this approximation is that the fluctuations of the localized spin system are retained.

Since an analytic expression for the transmission coefficient through a triple-barrier structure is a bit cumbersome to obtain, it is desired to perform the calculation numerically. For this purpose we replace \( \tilde{M} \) in the Hamiltonian by

\[ \tilde{M} = \frac{\sqrt{(M_{x}^{2})_{T}}}{\sqrt{(M_{x}^{2})_{T}}} = -x \sum_{\mathbf{R}} J(\mathbf{r} - \mathbf{R}) \left( \frac{\sqrt{(S_{x}^{2})_{T}}}{\langle S_{x}^{2} \rangle_{T}} \right) \]

which is equivalent to the replacement of \( M_{x}, M_{y} \) and \( M_{z} \) by their thermal averages in the transmission coefficient. The replacement of \( \tilde{M} \) by \( \tilde{M} \) in the Hamiltonian is a technical trick which is only possible since the transmission coefficient is a function of \( M_{x}, M_{y} \) and \( M_{z} \) only. In other words due to the quadratic functional dependence \( D(M_{x}^{2}) \), caused by the rotational symmetry around \( z \), the replacement of \( M_{x}, M_{y} \) by its representative value \( (M_{x}^{2})_{T} \) in the transmission coefficient is equivalent to the replacement of \( \tilde{M} \) by \( \tilde{M} \) in the Hamiltonian.

Finally we add \( V_{0} \) and \( \sum_{r} V(\mathbf{r} - \mathbf{R}) \) into a total potential \( V(z) \) and end up with a Pauli equation:

\[ \left[ \frac{1}{2m} \left( \frac{\hbar^{2} \phi_{x}}{c} \right)^{2} + V(z) + \frac{\hbar}{2} \mu_{B} B \mathbf{\hat{B}} + \mathbf{\tilde{M}} \right] \left( \begin{array}{c} \psi_{1} \\ \psi_{2} \end{array} \right) = E \left( \begin{array}{c} \psi_{1} \\ \psi_{2} \end{array} \right) \]

The bulk solutions for each layer are found by separating into a space- and spin-part. The solutions of the space part are well known [28]. The spin-part has the eigenvalues

\[ \epsilon_{\pm} = \pm \left[ \frac{\hbar}{2} \mu_{B} B + M_{z} \right]^{1/2} \]

and eigenvectors

\[ \left( \begin{array}{c} \alpha_{+} \\ \beta_{+} \end{array} \right) = N_{+} \left( \begin{array}{c} \frac{\hbar}{2} \mu_{B} + M_{z} + \epsilon_{-} \\ M_{z} + iM_{y} \end{array} \right), \left( \begin{array}{c} \alpha_{-} \\ \beta_{-} \end{array} \right) = N_{-} \left( \begin{array}{c} -M_{z} + iM_{y} \\ \frac{\hbar}{2} \mu_{B} B + M_{z} + \epsilon_{-} \end{array} \right) \]

where \( N_{+} \) and \( N_{-} \) are normalization factors. In each region of constant potential \( V(z) = \text{const} \) (see Fig. 1) the wavefunction \( \psi(r) \) is a linear combination of bulk solutions for a given \( E \) and Landau level \( n \) with corresponding \( k_{z} = \pm k_{z}^{b} \), where the index \( \pm \) refers to the spin state in Eq. (7). For example in region (b) (see Fig. 1):

\[ \psi^{b}(r) = |b_{1}\left( \begin{array}{c} \alpha_{+} \\ \beta_{+} \end{array} \right) e^{i k_{z}^{b} z} + b_{2}\left( \begin{array}{c} \alpha_{-} \\ \beta_{-} \end{array} \right) e^{i k_{z}^{b} z} + b_{3}\left( \begin{array}{c} \alpha_{+} \\ \beta_{+} \end{array} \right) e^{-i k_{z}^{b} z} + b_{4}\left( \begin{array}{c} \alpha_{-} \\ \beta_{-} \end{array} \right) e^{-i k_{z}^{b} z} \right| \phi(x,y) \equiv \Phi^{b}(z) \phi(x,y) \]

\[ k_{z} \text{ is derived from} \]

\[ E = \frac{\hbar^{2} \kappa^{2}}{2m(b)} + \frac{\hbar|\mathbf{B}|}{m(b)c(n + \frac{1}{2})} + V^{(n)} + \epsilon^{(n)} \]

Since \( \phi(x,y) \) is equal in all layers the boundary conditions are \( \Phi(z) \) and

\[ \left( \begin{array}{cc} \frac{1}{m(z)} \frac{\partial}{\partial z} & 0 \\ 0 & \frac{1}{m(z)} \frac{\partial}{\partial z} \end{array} \right) \Phi(z) \]

continues at interfaces. The matching procedure at each interface is then carried out with a transfer matrix technique [7]. The transmission amplitudes \( t_{1}, t_{2} \) as a function of the incoming amplitudes \( a_{1}, a_{2} \) are

\[ \left( \begin{array}{c} t_{1} \\ t_{2} \end{array} \right) = M_{12}^{-1} \cdot M_{11} \cdot M_{21}^{-1} \cdot M_{1} \left( \begin{array}{c} a_{1} \\ a_{2} \end{array} \right) \]

The transmission coefficient is for example for an incoming spin-up state

\[ D_{1} = \frac{j_{\text{out}}}{j_{\text{in}}} = N_{1}|t_{1}|^{2} \]

\[ D_{2} = \frac{j_{\text{out}}}{j_{\text{in}}} = N_{2}|t_{2}|^{2} \]

where \( N_{1}, N_{2} \) are normalization factors and \( j_{\text{in}} = \frac{\hbar k_{z}^{b}}{m(z)} |a_{1}|^{2} \).

For a fixed \( k_{z}^{b} \) (parallel to the interfaces) the transmission coefficient \( D \) for two wells of different width shows resonances at the energy \( E_{1}^{b}, E_{2}^{b} \) of the quasi-bound states of the wells. The wells are decoupled if a sufficiently large central barrier is assumed (see
In a magnetic field $\mathbf{B}$ (z-direction) perpendicular to the interfaces the electronic motion parallel to the interfaces is quantized and the first resonances through the Landau level $n = 0$ occur at higher energy $E_L, E_R$ shifted by $\frac{1}{2} \hbar \omega_0$ [8-10], where $\omega_0 = \frac{eB}{m^*}$. For well materials with large g-factors each Landau level splits into two, separated by several meV (for example InAs $g = -15, B = 10T, \Delta E \simeq 9meV$). Landau level splitting is caused as well by the exchange interaction with localized spins (Eq. (6)). If the localized spins sit in the barrier the splitting depends on the penetration of the band electron wave function. The splitting is therefore smaller for larger energy difference $(V-E)$ (see Fig. 1). The transmission coefficient for a HgCdSe heterostructure with Mn ions in the central barrier has been calculated (with parameters as in Fig. 1). The energies $E_{R,L}$ of the first resonances are inserted in Fig. 1.

The electrical current density from occupied states on the left to empty states on the right in a magnetic field for zero temperature is [29]

$$ j = \left( \frac{e}{2} \right)^2 \frac{B}{c} \sum_{s=1}^{2} \int_{\max(E_R-E,U)}^{E_F} \sum_{n=0}^{n_{\max}(E)} D_s(E, n, V, U) $$

(13)

where the sum over $s$ runs over the two spin states.

The result for a HgCdSe heterostructure with Mn ions in the central barrier is shown by the full line in Fig. 2. The four peaks correspond to the alignment of the energies of the quasi-bound states in the two wells with different spin splitting.

In particular, from the leftmost to the rightmost peak, we find the following alignments:

$$ E_L^+ = E_R^-, E_L^- = E_R^+, E_L^+ = E_R^-, E_L^- = E_R^+. $$

The first and the last peaks are possible only since the band electrons in the left well is in a mixed state, Eq. (7), in the barrier due to the exchange interaction with the localized electrons. The spin-fluctuations of the localized spin system generate the off-diagonal elements in Eq. (5), which produce the mixing.

In terms of spin-flip (time-dependent description) this means that the band electron flips from a spin-up to a spin-down state (first peak for example), while tunneling through the central barrier. The spin projection on the z-direction is conserved by a simultaneous flip of a localized spin.

The second peak is larger and broader than the third, since $\kappa < \kappa_4$ in the barrier, where $\kappa_4 = \left( \frac{2}{\hbar^2} \right) (V + \hbar \omega_0 (n + \frac{1}{2}) + \epsilon_\pm - E) \frac{1}{2}$, and $\epsilon_\pm$ is defined in Eq. (6).

Additional Mn ions in equal concentration in both wells would increase the spin splitting in both wells by the same amount and therefore only the first and the last peaks are shifted to smaller and higher bias by several mV.

Changing the temperature from 4.2 to 30 K changes the values of the thermal averaging in Eq. (4) (fluctuations increase). As a result the first and the last peaks shift to smaller and higher bias by several mV and increase by a factor of about 3.

It is also of interest to replace the thermal average terms in Eq. (4) by non-equilibrium values by exciting the localized spin system with an electromagnetic pulse similar to the experiment described in Ref. [17,18]. The spin relaxation time can be investigated in this way.

We show in Fig. 2 (dashed line) the tunnel current for the case without Mn ions. Due to the small g-factor ($g \approx 2$) there is no spin splitting visible in a magnetic field of 10T. Nevertheless such a sharp current peak ($\Delta V_{FWHM} \simeq 2mV$) may be of interest by itself for applications [1]. The reason for the sharp peak is the alignment of two (highly degenerated) quasistationary states quantized in the $x$ and $y$ direction by a magnetic field and in the $z$ direction by size quantization in each well. Up to now less attention has been paid to this physical situation. We found similar sharp peaks for a GaAs-AlAs heterostructure. The width of the peak can be decreased with thicker barriers and is only limited by the Landau level broadening.

In summary we pointed out that the energetic alignment of two quantum levels with a large degener-
acy is a general tool to produce a sharp current peak. Such systems provide the possibility to study, for example, Landau level broadening [12] or exchange interaction [27] with a tunnel current.

We have presented a simple formalism to include the exchange interaction between band electrons and magnetic impurities into tunneling. The formalism is based on a classical approximation and uses a transfer matrix technique. The formalism is applied to HgCdSe triple barrier heterostructure with Mn ions in the central barrier and different well widths.

The exchange interaction causes a spin splitting of the Landau levels. An applied bias aligns the levels of the two wells at certain bias values and the current shows 4 distinct peaks. Two of the peaks (first and last) are only possible if the band electrons in the barriers are in mixed spin states (spin flip). The mixing is produced by the fluctuations of the localized spin system (Eqs. (4) and (5)). The existence of such current peaks, and their change in position and height with temperature, could be observed and provide an experimental test of our calculations.

On the other hand the peaks in the tunnel current might serve as a probe for the magnetic behaviour of a barrier with a few Angstrom only. This result may stimulate further research of 2D-spin systems.

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REFERENCES

15. N.B. Brandt and V.V. Moshchalkov, Advances in Physics 33, 193, 1984