Spin-flip Scattering Contribution to Resonant-Tunneling Current in Semimagnetic Semiconductor Heterostructures

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We calculate the characteristic current-voltage curve of a tunneling device based on semimagnetic semiconductor materials. The device is a heterostructure with layers of $Cd_{1-x}Mn_xTe$ in which the magnetic ions Mn^{2+} interact strongly with the conducting electrons via the *s-d* exchange interaction. Thermal fluctuations of Mn^{2+} magnetic moments cause spin-dependent electron scattering that modifies the characteristic current-voltage curve. Our calculation shows how this electron-ion scattering is expected to affect the spin dynamics in transport measurements.

I Introduction

Recent advances in the growth of semimagnetic semiconductor (SMS) quantum structures have renewed the interest in the long-standing study of carriers interacting with magnetic ions.[1] SMS quantum structures are versatile systems in which to conduct such study because they make possible the adjust of the spatial overlap between the carrier wave functions and the magnetic ions.[2]

Optical spectroscopy with polarized light have contributed greatly to the understanding of the carrier spin dynamics in undoped SMS quantum structures.[3] That is because angular momentum conservation at the absorption of a polarized photon allows creation of carriers in definite spin states. Furthermore, detection of the polarization of the luminescence reveals the spin states of the carriers at the moment they recombine; from this it is possible to study the role of different spin relaxation mechanisms on the spin population initially photoexcited. On the other hand, most of the transport measurements do not give access to the spin state of the conducting carriers, which complicates the study of the spin dynamics. Also, such measurements usually require doped SMS samples that only recently have been grown with reliable quality. Despite these difficulties, preliminary investigations have shown interesting behaviors that are attributed to the spin polarization of the conducting carriers.[4]

In this work we investigate a tunneling device made out of layers of $Cd_{1-x}Mn_xTe$ materials, where the magnetic moments arise from the half-filled *d* shell of the ions Mn^{2+}. An external magnetic field **B** is applied along the growth axis (z-axis) to align the localized moments and to create a magnetization proportional the average ion spin $\langle S_z \rangle$, which acts on the electrons via the *s-d* exchange interaction. This effect can be seen, in the mean-field approximation, as a change in the potential profiles; electrons with spins up see a different potential than electrons with spins down.[2] Several devices have been proposed[5] based on this difference in potential profiles to create tunneling current with some degree of spin polarization.

II Spin-dependent potential profiles

The coupling between electrons and the magnetic ions is given by the *s-d* exchange interaction term $\sum_i J_{s-d}\widehat{\sigma}\cdot\mathbf{S}_i$ in the electron Hamiltonian, where $\widehat{\sigma}$ is the electron-spin operator, $\mathbf{S}_i$'s are the ion spins, and J_{s-d} the exchange coupling constant. As discussed above, in the mean-field approximation, the Hamiltonian can be written as

$$H_0^{\pm} = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V(z) \pm \frac{g\mu_B}{2}B \mp \alpha N_0 \frac{x\langle S_z\rangle}{2} + E_l, \quad (1)$$

with the $\pm$ signs corresponding to the electron spin components $|\sigma_p = \pm 1/2\rangle$. m is the electron effective mass and $V(z)$ is the band-edge potential of the SMS heterostructure. The quantized motion in the xy-plane yields the Landau level ladder with $E_l = \hbar e B(l + \frac{1}{2})/m$. The Zeeman spin splitting is $g\mu_B B$ and the average spin $\langle S_z\rangle$ gives the so-called giant-Zeeman splitting that cause the aforementioned change in the potential profile. Also, in Eq. (1), $N_0 = 1/\Omega_0$, with Ω_0 as the volume of the primitive cell, $\alpha = \langle u_c| J_{s-d} |u_c\rangle$, where u_c is the periodic part of the conducton band Bloch function, and x is the Mn^{2+} molar fraction.[6]

The eigenstates of $H_0^{\pm}$ that we are concerned with are those involved in the tunneling current. We use a short-handed notation for these eigenstates $|p\rangle = |p_z, p_\parallel, \sigma_p\rangle$,

$$\langle \mathbf{r}|p\rangle = \psi_{p_z}^{\sigma_p}(z)\varphi_{p_\parallel}(\mathbf{r}_\parallel)u_c(\mathbf{r})\,|\sigma_p\rangle\,, \quad (2)$$

where $\psi_{p_z}(z)$, with $p_z = (E_p, k_{zp})$, gives the solution of the z-direction problem for an electron with longitudinal energy E_p, propagating to the right ($k_{zp} > 0$) or left ($k_{zp} < 0$). To obtain $\psi_{p_z}(z)$, we have used open boundary conditions when solving numerically the Schrödinger equation with the Hamiltonian $H_0^{\pm}$. The solution of the xy-plane motion gives $\varphi_{p_\parallel}(\mathbf{r}_\parallel)$, with $p_\parallel = (l_p, k_{y_p})$, as the l_p-th Landau level state.

An electron in a state $|p\rangle$, when tunneling potential barriers of SMS material, has a transmission coefficient $T^0_{E_p,\sigma_p}$, which can be easily calculated from the eigestates $\psi_{p_z}(z)$ and depends on the longitudinal energy $E_p = \frac{\hbar^2 {k_{z_p}}^2}{2m^*}$ and spin σ_p. By considering the thermal fluctuations of the Mn^{2+} moments (see next section), we allow for transitions from the initial state $|p\rangle$ to other states $|q\rangle$ with a probability rate per second that we call W_{pq}. The resulting transmission T_{E_p,σ_p} is then obtained using a semi-classical Boltzmann equation[7] in the first Born approximation

$$T_{E_p,\sigma_p} = T^0_{E_p,\sigma_p} + \frac{Lm}{\hbar k_{zp}} \sum_q W_{pq}(T^0_{E_q,\sigma_q} - T^0_{E_p,\sigma_p}), \quad (3)$$

where L is the system size, which includes the well and barrier regions, and

$$k_{zp} = \sqrt{2m[E_p - V(z)]/\hbar^2} \quad (4)$$

is the electron wave vector at the emitter, where $z = -L/2$.

The tunneling current emitter-to-collector is calculated as the product of the electron change ($e < 0$) and the probability current, summed over the occupied states $|p\rangle$ at the emitter that are moving toward the collector, yielding

$$J_{e\to c} = \frac{e^2 B}{(2\pi\hbar)^2} \sum_{l_p,\sigma_p} \int_0^\infty dE_p f^e_{l_p}(E_p)\widetilde{T}_{E_p,\sigma_p}, \quad (5)$$

where f^e is the emitter Fermi distribution function, and $\widetilde{T}_{E_p,\sigma_p}$ is given in Eq. (3) with the substitution $T^0_{E_q,\sigma_q} \to T^0_{E_q,\sigma_q}(1 - f^c(E_q))$ to account for the restriction due to the exclusion principle on the occupation of the collector states. A similar result is found for the collector-to-emitter current $J_{c\to e}$, and the net current is then obtained as $J = J_{e\to c} - J_{c\to e}$.

III Scattering by thermal fluctuations

An additional contribution of the s-d exchange interaction to the electron motion comes from the thermal fluctuations of the magnetic moments. Although the average magnetization components normal to $\mathbf{B}$ vanish, since $\langle S_x\rangle = \langle S_y\rangle = 0$, thermal fluctuations allow a finite normal magnetization component proportional to $\sqrt{\langle S^2_{x,y}\rangle}$ that is varying in time. Fluctuations of the longitudinal component $\langle S_z\rangle$ is also expected. The time-dependent Hamiltonian accounting for these contributions is written as

$$H_1(t) = -\sum_i J(|\mathbf{r} - \mathbf{R}_i|)\,[(S_{z,i}(t) - \langle S_{z,i}\rangle)\,\widehat{\sigma}_z + \frac{1}{2}\,(S_{+,i}(t)\widehat{\sigma}_- + S_{-,i}(t)\widehat{\sigma}_+)], \quad (6)$$

where the electron-spin raising and lowering operators $\widehat{\sigma}_\pm = \widehat{\sigma}_x \pm i\widehat{\sigma}_y$ have been used. Similarly, for the ion spins, $S_{\pm,i}(t) = S_{x,i}(t) \pm iS_{y,i}(t)$, which are not operators. $H_1(t)$ is treated as a perturbation in second order. The rate W_{pq}

for the transition $|p\rangle \rightarrow |q\rangle$ between eigenstates of $H_0^{\pm}$ is proportional[8] to the Fourier transform of the correlation function

$$G_{pq}(\tau) \equiv \langle \langle q| H_1(t-\tau) |p\rangle \langle p| H_1(t) |q\rangle \rangle_{\rm av} \, , \tag{7}$$

where $\langle \quad \rangle_{\rm av}$ means an average over ensembles accounting for the random dependence of $H_1(t)$ on time, as well as the average on the ion positions in the lattice sites. We assume an exponential decay $G_{pq}(\tau) \propto \exp(-|\tau|/\tau_c)$, with τ_c setting the time scale of the ion-spin auto-correlations $G_{pq}(\tau) \propto \sum_{i,j} \langle S_{\alpha,i}(\tau) S_{\alpha',j}(0)\rangle$ that Eqs. (6) and (7) imply. The transition rate is then

$$W_{pq} = \frac{1}{\hbar^2}\int_{-\infty}^{+\infty} G_{pq}(\tau) e^{-i(E_q-E_p)\tau/\hbar} d\tau = |\langle p\,|H_1|\,q\rangle|^2 \frac{2\tau_c}{\hbar^2 + (E_q - E_p)^2\tau_c^2}, \tag{8}$$

which is a Lorentzian function of the transferred energy $E_q - E_p$ between the initial and final scattering states of the transition.

The matrix element $\langle p| H_1 |q\rangle$ in Eq. (8) is then calculated as follows. The integral of the spatial parts can be performed using the short-range nature of $J(r)$ and the periodicity of the Bloch functions. Using the states Eq. (2),

$$\begin{aligned} & -\int_V \left[\psi_{q_z}^{\sigma_q}(z)\varphi_{q_\parallel}(\mathbf{r}_\parallel)u_c(\mathbf{r})\right]^* J\left(|\mathbf{r}-\mathbf{R}_i|\right)\psi_{p_z}^{\sigma_p}(z)\varphi_{p_\parallel}(\mathbf{r}_\parallel)u_c(\mathbf{r})d\mathbf{r} \\ = & \; -\alpha\left[\psi_{q_z}^{\sigma_q}(Z_i)\varphi_{q_\parallel}(\mathbf{R}_{i\parallel})\right]^* \psi_{p_z}^{\sigma_p}(Z_i)\varphi_{p_\parallel}(\mathbf{R}_{i\parallel}), \end{aligned} \tag{9}$$

where the magnetic ion positions are $\mathbf{R}_i$=$(\mathbf{R}_{i\parallel}, Z_i)$. Calculating the spin-dependent part we obtain

$$\begin{aligned} \langle p| H_1 |q\rangle \;\; = \;\; & -\alpha \sum_i \left[\psi_{q_z}^{\sigma_q}(Z_i)\varphi_{q_\parallel}(\mathbf{R}_{i\parallel})\right]^* \psi_{p_z}^{\sigma_p}(Z_i)\varphi_{p_\parallel}(\mathbf{R}_{i\parallel}) \\ & \times[\delta_{\sigma_q,\sigma_p}\sigma_p \Delta S_{z,i}(t) + \frac{1}{2}\delta_{\sigma_q,\mp\frac{1}{2}}\delta_{\sigma_p,\pm\frac{1}{2}} S_{\pm,i}(t)], \end{aligned} \tag{10}$$

where $\Delta S_{z,i}(t)$=$S_{z,i}(t) - \langle S_{z,i}\rangle$ and the upper (lower) signs holding for the spin-up to spin-down transitions (vice-versa)

To proceed with the calculation of $G_{pq}(\tau) \propto \sum_{i,j} \langle S_{\alpha,i}(\tau)S_{\alpha',j}(0)\rangle$, we assume in this work no correlation between spins of different ions, i.e.

$$\langle S_{\alpha,i}(\tau)S_{\alpha',j}(0)\rangle = \delta_{\alpha',\alpha}\delta_{i,j}\,\langle S_\alpha(\tau)S_\alpha(0)\rangle\,, \tag{11}$$

with α=x, y, z. This neglects the fact that pairing of spins in antiferromagnetic states is actually expected in the systems investigated; which is however accounted for in an approximated manner in the effective concentration x.[6] The transition probability Eq. (8) then becomes

$$W_{pq} = \frac{\alpha^2}{4\hbar^2}\sum_i \left|\psi_{q_z}^{\sigma_q}(Z_i)\right|^2 \left|\psi_{p_z}^{\sigma_p}(Z_i)\right|^2 \left|\varphi_{q_\parallel}(\mathbf{R}_{i\parallel})\right|^2 \left|\varphi_{p_\parallel}(\mathbf{R}_{i\parallel})\right|^2 F(\omega_{pq}), \tag{12}$$

with ω_{pq}=$(E_q - E_p)/\hbar$ and

$$F^{sf}(\omega) = \int_{-\infty}^{+\infty} \langle S_\pm(\tau)S_\mp(0)\rangle\, e^{-i\omega\tau} d\tau, \tag{13}$$

for the spin-flip (sf) scattering $(\sigma_q$=$-\sigma_p)$ and

$$F^{sc}(\omega) = \int_{-\infty}^{+\infty} \langle \Delta S_z(\tau)\Delta S_z(0)\rangle\, e^{-i\omega\tau} d\tau \tag{14}$$

for the spin-conserving (sc) scattering $(\sigma_q$=$\sigma_p)$.

The summation over the final states, given in Eq. (3), allows us to perform the integration over the planar spin distribution

$$\widetilde{W}_{pq_z} \equiv \sum_{q_\parallel=(l_q,k_{y_q})} W_{pq} = \frac{(\alpha/\Omega_0)^2}{4\hbar^2} A\,(eB/h)\left(\frac{\Omega_0}{A}\right)^2 \sum_{l_q,n} N_n \left|\psi_{q_z}^{\sigma_q}(Z_n)\right|^2 \left|\psi_{p_z}^{\sigma_p}(Z_n)\right|^2 F(\omega_{pq}), \tag{15}$$

where A is the system area and N_n is the number of ions in the n^{th} layer.

Finally, using the exponential decay of the spin correlations $G_{pq}(\tau) \propto \exp(-|\tau|/\tau_c)$, Eq. (13) gives

$$F^{sf}(\omega_{pq}) = [S(S+1) - \langle S_z^2 \rangle \pm \langle S_z \rangle] \frac{2\tau_c}{1+\omega_{pq}^2 \tau_c^2}. \tag{16}$$

For the spin-conserving scattering, a similar expression is obtained by changing $[S(S{+}1) - \langle S_z^2 \rangle \pm \langle S_z \rangle] \leftrightarrow [\langle S_z^2 \rangle - \langle S_z \rangle^2]$. Note that $\widetilde{W}_{pq_z}$ is proportional to the product of probabilities of finding the electron in a primitive unit cell of the n^{th} layer, i.e. $\frac{\Omega_0}{A}|\psi_p(Z_n)|^2$, for the initial and final states, times the number N_n of such cells containing a magnetic ion in that layer. The sum over the Landau orbits gives the number of states $A(eB/h)$ in the degenerate levels l_q. The thermal equilibrium averages used above are $\langle S_z \rangle = -SB_S(y)$ and $\langle S_z^2 \rangle = \langle S_z \rangle^2 + S^2 \frac{d}{dy} B_S(y)$, where $B_S(y)$ is the spin-S Brillouin function, with $y = (g_{Mn}\mu_B SB)/(k_B T)$ and S=5/2 for Mn^{2+}.

IV Results

The tunneling device we investigate has the potential profile depicted in Fig. 1, where the material compositions are indicated and the percentages shown are the Mn^{2+} molar fraction x. The levels drawn in the wells A and B of the potential profile are the energies of the peaks of the transmission coefficients corresponding to the quasi-bound spin-up (+) and spin-down (−) states in these wells. For zero magnetic field B these levels are degenerate (solid line in Fig. 1). They split for $B \neq 0$ due to the s-d exchange term in the Hamiltonian. We have chosen the system parameters in such a way that the resonant conditions for the tunneling through the levels of similar spins, A_--B_- and A_+-B_+, occur at the same gate voltage. In this way, *when scattering is neglected*, only one peak is expected in the characteristic current-voltage (I-V) curve of this device, exactly at the voltage that align those levels. By including scattering by the thermal fluctuations, alignments of the levels of opposite spins, A_+-B_- and A_+-B_-, are also allowed to contribute to the tunneling current. This is seen in Figs.2(a) and 2(b) for different values of magnetic field, where the main peaks are due to spin-conserving tunneling and the smaller peaks at lower and higher voltages appear because of the spin-flip scattering.[9]

Experimental data [3] indicate long correlation times τ_c (~250 ps). Since the width of the transmission coefficient in Eq. (3) is much larger than the Lorentzian width $\hbar/\tau_c$ in the expression Eq. (8) for W_{pq}, in this work the Lorentzian was used as a δ-function.

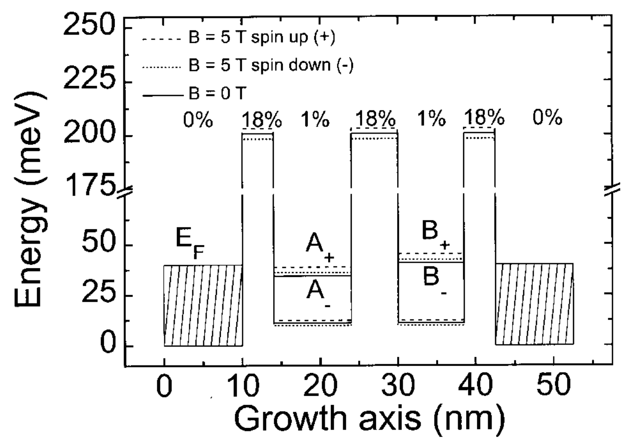

Figure 1. Effective potential profile. Solid line is the potential for electrons in zero magnetic field. In nonzero field the spin degeneracy is lifted, such that there are different potential profiles for spin-up (dashed line) and spin-down (dotted line) electrons. Levels in the wells A and B indicate the energies of the quasi-bound states of spins up (+) and down (−). The materials in the layers of the heterostructure are $Cd_{1-x}Mn_xTe$, with x being given by the percentages shown. For this figure the bias voltage is zero and Fermi energy is set to E_F=30 meV in both emitter and collector, corresponding to an In doping concentration 1×10^{18} cm^{-3}.

It may be worthwhile mentioning that we had better resolved the spin-flip scattering contributions, as in Fig. 2, when the spin splitting was large (large values of B), otherwise the overlap with the main resonant tunneling peak obscures the spin-flip peaks. The effect of temperature is twofold on the results of Fig. 2. First, temperature enters the Fermi distribution functions $f(E)$ in Eq. (5) for the emitter and collector.[10] Second, the alignment of the magnetic moments and their thermal fluctuations depend on T, which affects the observation of the spin-flip peaks in the I-V curve. For small temperatures the spin splittings are large, but the thermal fluctuations are reduced, and consequently the spin-flip scattering is weakened. For high temperatures the thermal fluctuations are enhanced, but the spin splittings are smaller and the I-V peaks are broadened. Some important contributions to the tunneling current, which are however beyond the scope of this paper, have not been treated in our model calculation, such as phonon-assisted and sequential tunneling, as well as charge accumulation effects and higher-order electron–magnetic-ion interactions.[1]

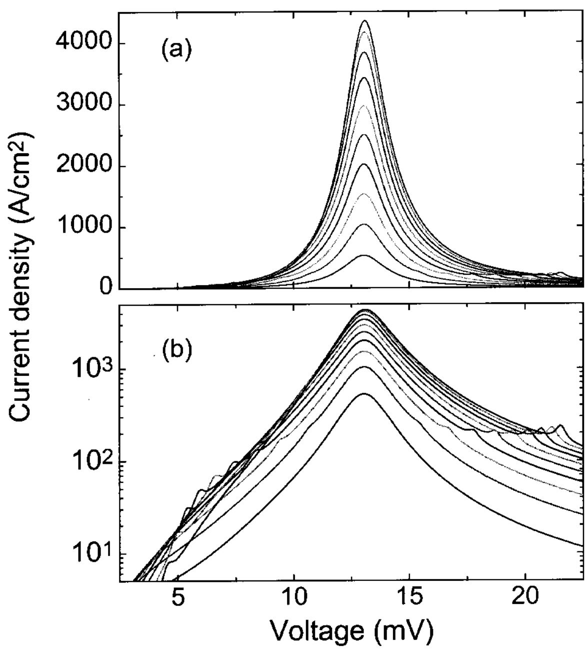

Figure 2. (a) Tunneling current density versus bias voltage for different values of magnetic field (B=1 T up to 10 T, for increasing values of current). (b) Same as above but in logarithmic scale. Scattering by Mn^{2+} thermal fluctuations gives the small peaks at lower and higher voltages. For these results the Lorentzian in Eq. (8) is taken in the δ-limit, i.e. $\tau_c \rightarrow \infty$. The increase of current with the magnitude of the magnetic field is due to the number of states in the Landau levels [factor $A(eB/h)$ in Eq. (15)].

Acknowledgments

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[6] Actually, an effective Mn^{2+} molar fraction $x_{\rm eff}=x(1-x)^{12}$ is used to account for the antiferromagnetic pair formation.

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[9] As a conservative approximation that underestimates the spin-flip scattering we have taken $x_{\rm eff}=x(1-x)^{12}$ as the molar fraction, assuming the antiferromagnetic pair states not taking part on the scatterings. See, e.g., G. Bastard and L. L. Chang, Phys. Rev. B **41**, 7899 (1990).

[10] This is a minor effect for the triple-barrier SMS system because, at relatively low temperatures, the condition for resonant tunneling is satisfied only for states that are deep into the emitter Fermi sea and away form the collector Fermi level (see Fig. 1).