Transport Properties of a $Ga_{1-x}Mn_xAs/Ga_{1-y}Al_yAs$ Double-Barrier

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We study the transport properties of a spin filter consisting of a double-barrier resonant tunneling device in which the well is made of a semimagnetic material. Even if the device could be made of several materials, we discuss here the case of a $Ga_{1-x}Mn_xAs/Ga_{1-y}Al_yAs$ system because it can be integrated into the well known $AlAs/GaAs$ technology. We solve the Hamiltonian $\mathcal{H} = \mathcal{H}_K + \mathcal{H}_P + \mathcal{H}_E + \mathcal{H}_M + \mathcal{H}_{h-i} + \mathcal{H}_{h-h}$. Its terms represent the kinetic energy, the double-barrier profile, the applied bias, the magnetic interaction, the hole-impurity attraction and the hole-hole repulsion, respectively. A very simple one-dimensional Green function is introduced to solve self-consistently the Poisson equation for the profile due to the charge distribution. A real space renormalization formalism is used to calculate exactly the currents. In a previous work we have shown that the Rashba effect is weak. Therefore the results show very well defined spin-polarized currents. Our results confirm that this system is a good device for spintronics.

Keywords: Double barrier spin polarizer; Diluted magnetic semiconductors; Spintronic devices

I. INTRODUCTION

The system studied here consists of a double-barrier in which the well is made of a diluted magnetic semiconductor (DMS). The magnetization of the well produces resonant peaks that have well defined spin polarization. Therefore the current tunneling through the structure is also spin polarized. The device could be made of several materials. We discuss here the case of a $Ga_{1-x}Mn_xAs/Ga_{1-y}Al_yAs$ system because it can be integrated into the well known $AlAs/GaAs$ technology.

The Mn^{2+} cations have a magnetic moment due to their spin $S = \frac{5}{2}\hbar$. In addition, The Mn ion binds a hole to satisfy charge neutrality. Homogeneous samples of $Ga_{1-x}Mn_xAs$ alloys with x up to 10% have been produced by molecular beam epitaxy at low temperatures, avoiding the formation of $MnAs$ clusters that could turn the material to be non-magnetic [1–3]. This kind of DMS introduces an interesting problem from the physical point of view: Mn in the alloy is a strong p dopant, the free hole concentration reaching even $p = 10^{20-21} cm^{-3}$. At small Mn concentrations, the alloy is a paramagnetic insulator. As x increases, it becomes ferromagnetic, going through a non-metal/metal transition for higher concentrations ($x \approx 0.03$) and keeping its ferromagnetic phase. For x above 5%, the alloy becomes a ferromagnetic insulator. In the metallic phase, the ferromagnetic transition is observed in the range of $30-110$K, depending on the value of x. In samples of $Ga_{1-x}Mn_xAs$ with selective $p-$doping [12] it was reported a Curie temperature $T_c \sim 172K$. Today it is possible to make semiconductors that are ferromagnetic at room temperature [4–7]. Several spintronic devices like spin valves, spin filters, polarizers and analyzers have been made using heterostructures including DMS [8–11].

II. SELF-CONSISTENT PROFILE AND LEVELS

Our tight-binding Hamiltonian is

$$\mathcal{H} = \mathcal{H}_K + \mathcal{H}_P + \mathcal{H}_E + \mathcal{H}_M + \mathcal{H}_{h-i} + \mathcal{H}_{h-h}. \tag{1}$$

where $\mathcal{H}_K$ is the kinetic energy, $\mathcal{H}_P$ describes the double-barrier profile and $\mathcal{H}_E$ represents the electric field due to the applied bias. The magnetic $\mathcal{H}_M$, the hole-impurity $\mathcal{H}_{h-i}$ and the hole-hole $\mathcal{H}_{h-h}$ terms are included in the mean field approximation. The profile and the charge distribution are calculated self-consistently by solving the Poisson equation $\nabla^2\phi = -\rho/\varepsilon$, where $\rho = \rho_i + \rho_h$ includes both the impurity and hole contributions. This potential gives a contribution

$$\mathcal{H}_{h-i} + \mathcal{H}_{h-h} = e\phi. \tag{2}$$

As the Hamiltonian is modified by this term so are modified its wave functions, from which the hole charge density ρ_h is calculated.

Usually the Poisson equation is solved in the momentum space because it becomes an algebraic equation. On the other side, to solve the Hamiltonian (1) in the reciprocal space requires a big computational effort. In the context of a tight-binding calculation it is natural to express the Poisson equation in a finite difference formalism, in which it turns out to be a simple $N \times N$ matricial equation,

$$\phi_{j-1} - 2\phi_j + \phi_{j+1} = -\frac{a^2}{\varepsilon}\rho_j, \tag{3}$$

where a is the distance between layers. The inverse operator of the discretized one-dimensional Laplacian (its Green function) is obtained easily as

$$G_{ij} = -\frac{1}{(N+1)} i(N+1-j) \qquad for\ \ i \leq j \tag{4}$$

and it is symmetric. Using this Green function it is easy to obtain the potential as

$$\phi_j = -\frac{\varepsilon}{a^2}\sum_k^N G_{jk}\rho_k \ .$$

Let us discuss now the mean field approximation used for the magnetic term. The hole interaction with the magnetic impurities is described through the contact potential,

$$\mathcal{H}_M(\mathbf{r}) = -I\sum_{\mathbf{i=1}}^{\mathbf{N_i}} \mathbf{s}(\mathbf{r}).\mathbf{S}(\mathbf{R_i})\delta(\mathbf{r}-\mathbf{R_i}),$$

where I is the $p-d$ exchange coupling constant, $\mathbf{R_i}$ denotes the positions of the N_i impurities of Mn, $\mathbf{S}(\mathbf{R_i})$ is the (classical) spin of the impurity, and $\mathbf{s}(\mathbf{r})$ is the spin of the hole. We assume the layer in its metallic and ferromagnetic phase. Thus, the spin of the hole is well defined in that direction, being polarized either up (parallel) or down (anti-parallel). In order to write the magnetic term in the new basis we have to integrate over $\mathbf{r}$. To do that, the magnetic impurities are assumed to be uniformly distributed in the $Ga_{1-x}Mn_xAs$ DMS layer, having the same magnetization $< M >$. Therefore, a net Mn magnetization $< M >$ polarizes the hole gas by introducing an additional effective confining potential given by

$$\mathcal{H}_M(z) = -N_0\beta x(\sigma/2) < M >,$$

for z inside the well. Here $\sigma = \pm 1$ for the hole spin and $N_0\beta = I/v_0$.

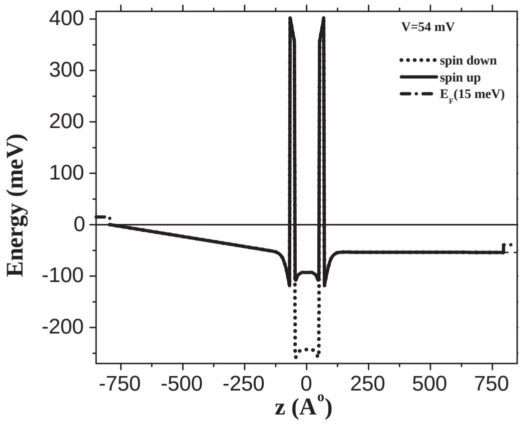

FIG. 1: The self-consistent potential for an applied bias $V = 54mV$

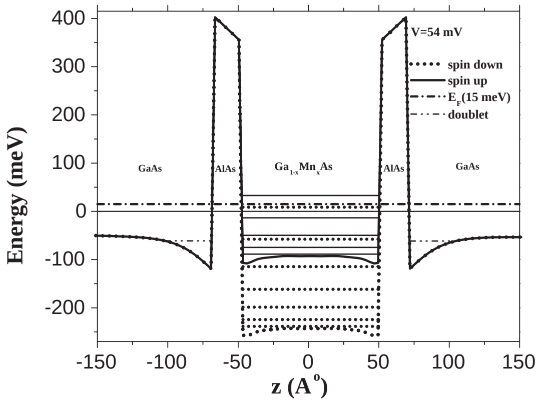

FIG. 2: The resonant levels.

III. THE SPIN POLARIZED CURRENTS

We are dealing here with an open system, but the Hamiltonian given by equation (1) is first solved in a finite region including the double barrier and a small part of the contacts where the band bending, due to charge accumulation, occurs. This region can be seen in Fig. 1.

Outside this region the profile is flat. Therefore the solutions are plane waves for energies above the Fermi level and evanescent modes below it. The total Hamiltonian can be written as $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where $\mathcal{H}_0 = \mathcal{H}_L + \mathcal{H}_S + \mathcal{H}_R$ describes three uncoupled regions: the left contact, the scattering region and the right contact. Thus each part of $\mathcal{H}_0$ can be diagonalized exactly.

The diagonalization of $\mathcal{H}_S$ yields the spin polarized resonant levels shown in Fig. 2. Besides, other non-resonant states are obtained that are necessary to get the exact solution.

We shall connect the three regions depicted in Fig.3 to get the exact solution for the open system. This method is the extension of the standard procedure described in elementary quantum text books, to the tight binding formalism.

For this device the scattering region for each spin is depicted in Fig. 4. To relate the plane wave amplitudes at right and left of the double barrier we reconnect the three regions using the Hamiltonian

$$\mathcal{H}_1 = v(c_{-1}^{+}c_0 + c_0^{+}c_{-1}) + v(c_{N-1}^{+}c_N + c_N^{+}c_{N-1})$$

where v is the hopping that gives the effective mass m^*. Here the left region goes from $-\infty$ to -1, the N sites from 0 to $N-1$ belong to the scattering region and labels from N to ∞ correspond to the right region. By labeling $m = 0,\ldots,N-1$ the scattering region eigenstates, that come out from the numerical diagonalization of $\mathcal{H}_S$, we can represent the reconnected regions by the diagram of Fig.5.

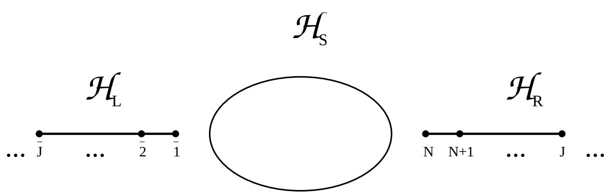

FIG. 3: The scheme for solving a tight-binding Hamiltonian for an open system.

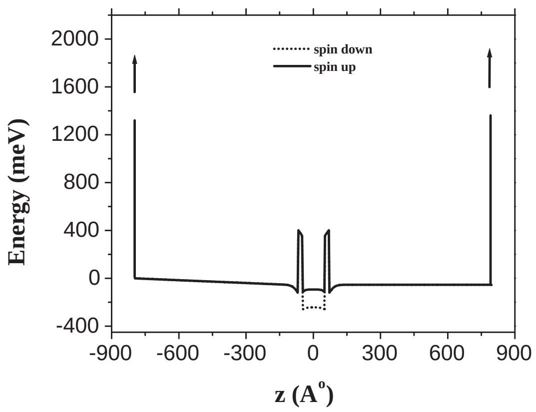

FIG. 4: The scattering region profile.

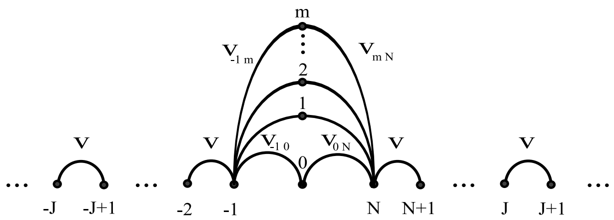

FIG. 5: The scheme for reconnection.

Here, $v_{\bar{1}m} = \langle \bar{1}|\mathcal{H}_1|m\rangle = v\langle \bar{1}|m\rangle$ are the hoppings from the left contact to the levels of the scattering region. In similar way we get $v_{m1} = v\langle m|1\rangle$. It is easy to see that $\langle m|1\rangle = u_{Nm}$, i. e., the last component of the m-th eigenvector.

Now it is easy to decimate all the states in the well. The result is a renormalization of the energies at sites -1 and N and the effective hopping between them. We get

$$
\begin{aligned}
\tilde{\varepsilon}_{\bar{1}} &= \varepsilon_{\bar{1}} + \sum_m v_{\bar{1}m}^2/(\hbar\omega - E_m) \\
\tilde{\varepsilon}_N &= \varepsilon_N + \sum_m v_{mN}^2/(\hbar\omega - E_m) \\
\tilde{v}_{\bar{1}N} &= \sum_m v_{\bar{1}m} v_{mN}/(\hbar\omega - E_m)
\end{aligned}
$$

where we denote the site -1 as $\bar{1}$ to simplify the notation.

After that, we obtain directly the transmittance and therefore the current.

We emphasize that this procedure is non-perturbative. Thus the results are exact. The diagram representing the renormalized equations is shown in Fig. 6, where we have renamed the layers from N to ∞ as $1, 2, \ldots, \infty$.

Now the solutions at the emitter (layers $\bar{1}$ and $\bar{2}$) can be easily connected with the solutions at the collector (Layers 1 and 2) to obtain the transmittance. Finally we get the current using the Landauer-Bütiker formalism.

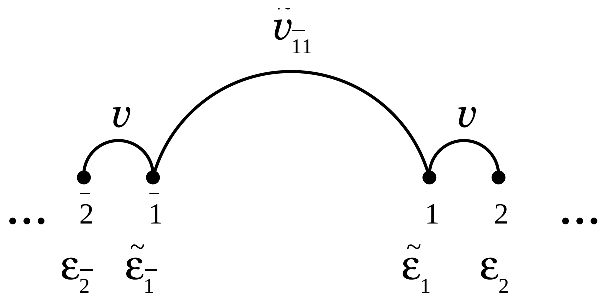

FIG. 6: The renormalized diagram.

IV. RESULTS

Due to the very high hole density inside the well, a simple iterative procedure to get selfconsistency does not converge. Instead, a quasi-Newton procedure for solving non-linear systems is used. It requires to diagonalize $\mathcal{H}_S$ many times for each applied potential. However the diagonalization of $\mathcal{H}_S$ is very fast because it is a finite tridiagonal matrix.
After this process, the selfconsistent profile and the spin polarized levels shown in Fig.2 are obtained. Through the procedure described in the previous section we get the electronic current as a function of the applied bias shown in Fig.7.
It is easy to see that the three polarized levels above the Fermi in Fig.2 begin to descend. When one of these levels is in between the Fermi level and the bottom of the band a current peak appears.

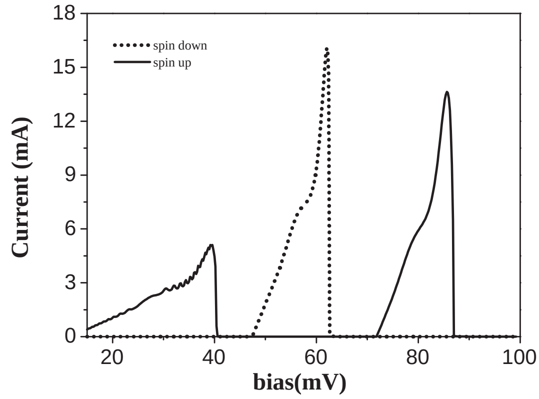

FIG. 7: The spin polarized currents.

V. CONCLUSIONS

Using a decimation technique in a tight binding model we obtained the transmission probability and the current as a function of the bias. The strong spin-polarization inside the quantum well gives rise to a separation of the resonant peaks for each spin polarization of the order of $0.15eV$, providing an excellent diode for applications in spin filtering [16–20].

As discussed in previous works [13–15] the device described here produces a current strongly polarized. Without taken into account the Rashba effect, the polarization is almost total. The only spin mixture is due to the very small tail of a $-\sigma$ transmittance peak at the central region of a σ peak.

In a previous work [21] the peaks were not completely polarized because we considered the Rashba effect at the well walls that flip the spin of the carriers. Nevertheless this effect is quadratic in the small Rashba parameter α. Therefore the depolarization is small.

We conclude that a double-barrier heterostructure with a diluted ferromagnetic semiconductor at the well can be a very effective spin polarizer. Other effects, such as the disordered distribution of magnetic impurities have to be studied to confirm this prediction.

Acknowledgments

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[1] H. Ohno, Science **281**, 951 (1998).

[2] R. Fiederling, M. Keim, G. Reuscher, W. Ossau, G. Schmidt, A. Waag, and L. W. Molenkamp, Nature **402**, 787 (1999).

[3] Y. Ohno, D. K. Young, B. Beschoten, F. Matsukura, H. Ohno, and D. D. Awschalom, Nature **402**, 790 (1999).

[4] Y. Matsumoto, M. Murakami, T. Shono, T. Hasegawa, T. Fukumura, M. Kawasaki, P. Ahmet, T. Chikyow, S. Koshihara, and H. Koinuma, Science **291**, 854 (2001).

[5] Y. Matsumoto, Science **294**, 1003 (2001).

[6] K. Ueda, H. Tabata, and T. Kawai, Appl. Phys. Lett. **79**, 988 (2001).

[7] G. T. Thaler, M. E. Overberg, B. Gila, R. Frazier, C. R. Abernathy, S. J. Pearton, J. L. Lee, S. Y. Lee, Y. D. Park, Z. G. Khim, J. Kim, and F. Ren, Appl. Phys. Lett. **80**, (21): 3964 (2002).

[8] G. A. Prinz, Phys. Today (Apr 1995) 58.

[9] J. Gregg et al, J. Magn. Magn. Mater. **175**, 1 (1997).

[10] S. Das Sarma, J. Fabian, X. Hu, and I. Žutic, Solid State Commun. **119**, 207 (2001).

[11] M. Oestreich, Nature **402**, 735 (1999).

[12] A. M. Nazmul, S. Kobayashi, S. Sugahara, and M. Tanaka Physica E **21**, 937 (2004).

[13] S. S. Makler, M. A. Boselli, J. Weberszpil, X. F. Wang, and I. C. da Cunha Lima, Physica B **320**, 396 (2002).

[14] L. L. da Silva, M. A. Boselli, X.-F. Wang, J. Weberszpil, S. S. Makler, and I. C. da Cunha Lima, Braz. J. Phys. **32**, 433 (2002).

[15] S. S. Makler, M. A. Boselli, and I. C. da Cunha Lima, *proceedings of the 26th International Conference on the Physics of Semiconductors* (ICPS-26) Edimburgh - UK, P152 (2002).

[16] J. C. Egues, Phys. Rev. Lett. **80**, 4578 (1998).

[17] J. C. Egues and J. W. Wilkins, Phys. Rev. B **58**, R16 012 (1998).

[18] P. Bruno and J. Wunderlich, J. Appl. Phys. **84,** 978 (1998).

[19] V. A. Chitta, M. Z. Maiale, S. A. Leão, and M. A. Degani, Appl. Phys. Lett. **74**, 2845 (1999).

[20] E. A. de Andrada e Silva and G. C. La Rocca, Braz. J. Phys. **29**, 719 (1999).

[21] S. S. Makler, J. G. Zelcovit, M. A. Boselli, and I. C. da Cunha Lima, Physica B **354**, 348 (2004).