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Solvable model of spin-dependent transport through a finite array of quantum dots

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Abstract

The problem of spin-dependent transport of electrons through a finite array of quantum dots attached to a 1D quantum wire (spin gun) for various semiconductor materials is studied. The Breit–Fermi term for spin–spin interaction in the effective Hamiltonian of the device is shown to result in a dependence of transmission coefficient on the spin orientation. The difference of transmission probabilities for singlet and triplet channels can reach a few per cent for a single quantum dot. For several quantum dots in the array due to interference effects it can reach approximately 100% for some energy intervals. For the same energy intervals the conductance of the device reaches the value ≈ 1 in $[e^2/\pi\hbar]$ units. As a result a model of the spin gun which transforms the spin-unpolarized electron beam into a completely polarized one is suggested.

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1. Introduction

Spintronics is a novel branch of nanoscience which exploits spin properties of electrons or nuclei instead of charge degrees of freedom [1]. Perhaps the most current efforts in designing and manufacturing the spintronics devices are focused on finding novel ways of both generation and utilization of spin-polarized currents. This, in particular, includes the study of spin-dependent transport in semiconductor nanostructures, which can operate as spin polarizers or spin filters. Although spintronics can have a lot of practical applications [2–8], one of them is most interesting and ambitious: the application of electron or nuclear spins to quantum information processing and quantum computation [9–13].

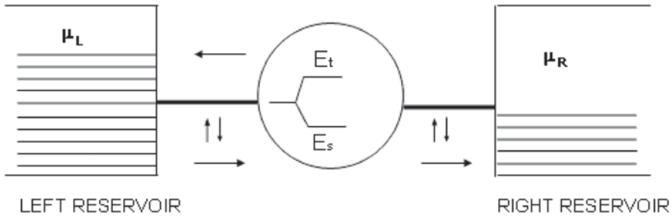

Figure 1. Schematic representation of one quantum dot attached to quantum wires. The left and right reservoirs are at different chemical potentials μ_L and μ_R. The horizontal arrows represent the incident, transmitted and reflected electronic wave. The quantum dot carries spin $s = \frac{1}{2}$. The singlet and triplet states are denoted by E_s and E_t. The electron spin projection $s_3 = \pm\frac{1}{2}$ before and after the scattering by the quantum dot is denoted by $\uparrow\downarrow$. If the small voltage $eV = \mu_L - \mu_R$ is applied a non-equilibrium situation is induced and spin-dependent current will flow through the device.

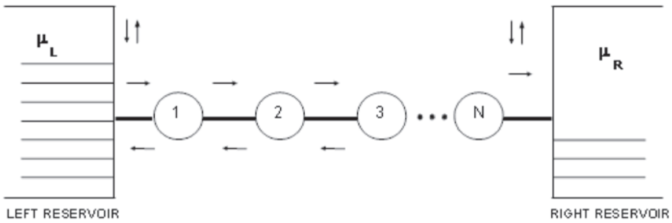

Figure 2. Schematic representation of spin filter device (spin gun) fabricated from *N* quantum dots and quantum wires. For details see the caption for figure 1.

In this paper we suggest a new type of spin polarizer constructed from a finite array of semiconducting quantum dots (QD) attached to a quantum wire (QW).

All dots of the array are identical and each of them carries the spin 1/2. The schematic construction of the proposed device is shown for a single dot in figure 1 and for a finite array of dots in figure 2.

Using the mathematical modelling based on zero-range potentials [14, 15], we reduce the problem of spin-dependent transport in the device to an exactly solvable scattering problem. In terms of the scattering data, in particular of spin-dependent transmission coefficients through the device, we calculate the most important measurable characteristics: the polarization efficiency $P(k)$ and the conductance $G(k)$ of the device.

2. Assumptions, constraints and choice of model parameters

In this section we formulate the physical conditions under which our mathematical modelling is relevant. We assume that, in the quantum wire connected with a quantum dot, one-mode propagation of electrons in a ballistic regime can be realized. For the ballistic propagation of electrons through the QW, the de Broglie wavelength [17] $\lambda_B = 2\pi\hbar/\sqrt{2m^* k_B T}$ has to be much greater than both the mean free path l_{mfp} in the material of QW and the length d of QW between the neighbouring quantum dots, i.e. $\lambda_B \gg l_{\mathrm{mfp}}$ and $\lambda_B \gg d$.

On the other hand, in order to use zero-range potentials for mathematical modelling of scattering by quantum dots, the de Broglie wavelength has to be greater than the mean size r_0 of the dot: $\lambda_B \gg r_0$ [14]. There are different ways of manufacturing quantum dots (see, e.g., [18–20]). Depending on technology the mean size of quantum dots varies from 20 nm for small dots up to more than 100 nm for the large dots. In order to satisfy all the constraints

Table 1. Physical characteristics of narrow-gap semiconductors [21].

Semiconductor	E_g (eV) (285 K)	$\frac{m^*}{m_e}$	λ_B (nm) (285 K)	λ_B (nm) (77 K)
GaAs	1.430	0.068	29.9	57.7
InAs	0.360	0.022	52.8	101.5
$Cd_xHg_{1-x}Te$				
$x = 0.20$	0.150	0.013	68.6	131.9
$x = 0.30$	0.290	0.021	54.0	103.9
HgTe	−0.117	0.012	71.4	137.4
$Zn_{0.15}Hg_{0.85}Te$	0.190	0.015	63.9	122.9
InSb		0.014	66.1	127.2

mentioned above, we have to assume that spin gun can be realized on relatively small QD using narrow-gap semiconductors (i.e. semiconductors with small E_g—see table 1). For such materials (see table 1) λ_B is about 50 nm at room temperature and more than 100 nm at the liquid nitrogen temperature.

It means that we have either to use in our modelling the parameters $d, r_0 \ll 100$ nm or to assume the working temperature of the device less than $T = 77$ K. In section 5 we shall take into account these limitations in our numerical simulations of the device operation.

3. A mathematical model of spin transport through a single quantum dot

In this section we consider a model for scattering of a 1D electron on a quantum dot attached to the quantum wire. Both 1D electron and quantum dot are assigned to have spin 1/2 ($s_e = 1/2, s_d = 1/2$) and the possible spin projections on a fixed axis are $(s_3)_{e,d} = \pm 1/2$. We emphasize that in the model in question the quantum dot is treated as unstructured uncharged scatterer carrying spin 1/2 as a whole.

Due to the Breit–Fermi theory [22], the spin–spin interaction in frames of this simplest model leads to a singular interaction V^s in the model Hamiltonian: $V^s = \hat{\gamma}_s \delta(x) \otimes \langle \hat{s}(1), \hat{s}(2)\rangle$, where x is the distance between the electron and the quantum dot, $\delta(x)$ is the 1D delta function, $\hat{\gamma}_s$ is the coupling constant, $\hat{s}(1)$ and $\hat{s}(2)$ are the electron and the quantum dot spin operators respectively: $\hat{s}(j) = (s_1(j), s_2(j), s_3(j)), j = 1, 2, s_i = \frac{\hbar}{2}\sigma_i$ where $\sigma_i, i = 1, 2, 3$, are the Pauli matrices and $\langle \hat{s}(1), \hat{s}(2)\rangle = s_1(1) \otimes s_1(2) + s_2(1) \otimes s_2(2) + s_3(1) \otimes s_3(2)$.

Thus, the Schrödinger equation relevant to the proposed model has the form

$$\left[-\frac{d^2}{dx^2} \otimes I_4 + \gamma_s \delta(x) \otimes \langle s(1), s(2)\rangle\right] \Psi(x, s_3(1), s_3(2)) = k^2 \Psi(x, s_3(1), s_3(2)). \tag{1}$$

Here I_4 is the unit operator in the total spin space $\mathbf{C}^2 \otimes \mathbf{C}^2$ and m^* is the effective mass of electron in semiconductor material of the quantum wire and $\otimes$ means the tensor product, $k^2 = E\frac{2m^*}{\hbar^2}$, $s(j) = \hbar^{-1}\hat{s}(j)$, $\gamma_s = 2m^*\hat{\gamma}_s$. The wavefunction Ψ depends on the coordinate variable x, and $s_3(1), s_3(2)$ can take the values $\pm 1/2$.

In accordance with the extension theory approach [15], equation (1) is equivalent to the following boundary problem:

$$\left(-\frac{d^2}{dx^2} \otimes I_4\right)\Psi = k^2\Psi \tag{2}$$

$$\begin{aligned} &\Psi|_{x=+0} = \Psi|_{x=-0} \\ &\Psi'|_{x=+0} - \Psi'|_{x=-0} = \gamma_s \langle s(1), s(2)\rangle \Psi|_{x=0}. \end{aligned} \tag{3}$$

In order to solve the problem (2), (3), one has to separate the spin variables, i.e. to calculate the matrix elements of the Hamiltonian from equation (1) in the spin basis constructed below. Let us denote by $\chi_\pm(1)$ and $\chi_\pm(2)$ the spin part of the electron and the dot wavefunctions respectively with the value of spin projection $s_3(j) = \pm 1/2$, $j = 1, 2$. One can take these spinors in the form $\chi_+(j) = \binom{1}{0}$, $\chi_-(j) = \binom{0}{1}$. It is well known [23] that the two-spin space $\mathcal{H}_{s_1} \otimes \mathcal{H}_{s_2} \simeq \mathbf{C}^2 \otimes \mathbf{C}^2$ can be decomposed into the direct sum of two invariant (with respect to operators of representation of the group of rotation) subspaces: $\mathcal{H}_{s_1} \otimes \mathcal{H}_{s_2} = D_0 \oplus D_1$, where D_0 is the singlet space (subspace of the total spin $S = 0$) which is spanned on the spinor $\chi_{0,0}$, $\dim D_0 = 1$ and D_1 is the triplet space (subspace of the total spin $S = 1$) which is spanned on three spinors $\{\chi_{1,1}, \chi_{1,0}, \chi_{1,-1}\}$, $\dim D_1 = 3$.

The orthonormal basis of spinors in the triplet subspace has the form [23] $\chi_{1,1} = \chi_+(1) \otimes \chi_+(2)$, $\chi_{1,-1} = \chi_-(1) \otimes \chi_-(2)$, $\chi_{1,0} = \frac{1}{\sqrt{2}}(\chi_+(1) \otimes \chi_-(2) + \chi_-(1) \otimes \chi_+(2))$. The second index in χ_{1,S_3} means the values of the total spin projection $S_3 = 1, 0, -1$. The basis vector in the singlet subspace reads $\chi_{0,0} = \frac{1}{\sqrt{2}}(\chi_+(1) \otimes \chi_-(2) - \chi_-(1) \otimes \chi_+(2))$. The above-described spinors form the orthonormal basis in the total spin space $\mathcal{H}_{s_1} \otimes \mathcal{H}_{s_2} \simeq \mathbf{C}^2 \otimes \mathbf{C}^2$. Hence the total wavefunction $\Psi(x, s_3(1), s_3(2))$ can be decomposed as follows:

$$\Psi(x, s_3(1), s_3(2)) = \psi_{1,1}(x)\chi_{1,1} + \psi_{1,0}(x)\chi_{1,0} + \psi_{1,-1}(x)\chi_{1,-1} + \psi_{0,0}(x)\chi_{0,0}. \tag{4}$$

In order to separate the spin variables in the problem (2), (3), it is sufficient to calculate the action of the operator $\langle s(1), s(2)\rangle$ on these spinors. One can easily verify that $\langle s(1), s(2)\rangle\chi_{1,S_3} = \frac{1}{4}\chi_{1,S_3}$, where $S_3 = 1, 0, -1$ and $\langle s(1), s(2)\rangle\chi_{0,0} = -\frac{3}{4}\chi_{0,0}$.

Since the chosen basis of spinors is an orthonormal system, the separation of spin variables in the channel $S = 0$ and $S = 1$ gives the following boundary value problem for the coordinate parts of the wavefunction (4):

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} \otimes I_2 - k^2\right)\psi = 0 \tag{5}$$

$$\begin{aligned} &\psi(+0) = \psi(-0) \\ &\psi'|_{x=+0} - \psi'|_{x=-0} = \begin{pmatrix} \gamma_{11} & 0 \\ 0 & \gamma_{00} \end{pmatrix}\psi(0). \end{aligned} \tag{6}$$

Here ψ is a two-component vector $\psi = \binom{\psi_{1,S_3}}{\psi_{0,0}}(x)$, where $S_3 = 1, 0, -1$, $\gamma_{00} = -\frac{3}{4}\gamma_s$ is the coupling constant in the singlet channel and $\gamma_{11} = \frac{1}{4}\gamma_s$ is the coupling constant in the triplet channel. In the proposed model in the absence of relativistic effects, the total spin S conserves and the triplet–singlet and singlet–triplet transitions are forbidden. As a consequence, the antidiagonal elements of the coupling matrix in boundary condition (6) are equal to zero. Since the projection of the total spin S_3 also conserves, one can choose in the boundary problem above any value of this projection. In what follows we set $S_3 = 1$.

4. Scattering on a periodic array of *N* quantum dots

The single-dot Hamiltonian (7) for the case of a periodic array of N quantum dots is modified as follows:

$$H^{(N)} = -\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \otimes I_4 + \sum_{l=1}^{l=N} \hat{\gamma}_s \delta(x - y_l) \otimes \langle \hat{s}(1), \hat{s}(2)\rangle, \tag{7}$$

where points y_l are separated by distance d.

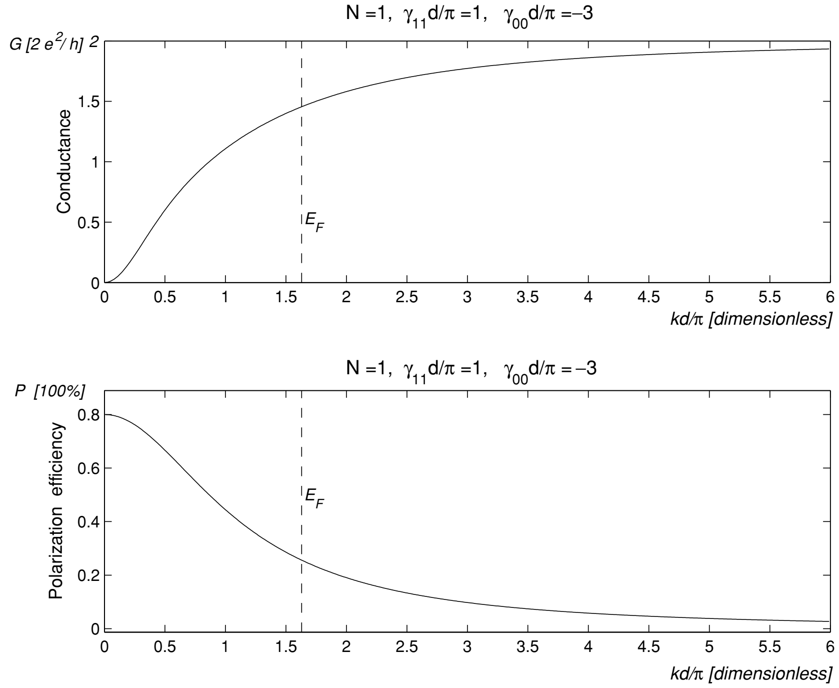

Figure 3. The conductance G and polarization efficiency P versus dimensionless momentum $\hat{k} = k\frac{d}{\pi}$ of incident electrons in the case of one quantum dot. The Fermi level $E_F = 35$ meV in InSb is indicated by the dashed line. The interdot distance $d = 45$ nm.

All the constructions of the previous section are easily generalized for this case. Hence after separation of spin variables in the equation $H^{(N)}\Psi^{(N)} = E\Psi^{(N)}$, one obtains for the coordinate part $\psi^{(N)}(x) = \binom{\psi^{(N)}_{1,1}}{\psi^{(N)}_{0,0}}(x)$ of the total wavefunction $\Psi^{(N)}$ the following boundary value problem:

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} \otimes I_2 - k^2\right)\psi^{(N)} = 0 \tag{8}$$

$$\begin{aligned} &\psi^{(N)}(y_l + 0) = \psi^{(N)}(y_l - 0) \\ &\psi^{(N)\prime}|_{x=y_l+0} - \psi^{(N)\prime}|_{x=y_l-0} = \begin{pmatrix} \gamma_{11} & 0 \\ 0 & \gamma_{00} \end{pmatrix} \psi^{(N)}(y_l), \qquad l = 1, 2, \ldots, N. \end{aligned} \tag{9}$$

The transmission coefficients in the triplet channel $T^{(N)}_{11}(k)$ and singlet channel $T^{(N)}_{00}(k)$ are calculated in terms of elements of the 4×4 matrix $\hat{\mathbf{T}} = t_{ij}, i, j = 1, 2, 3, 4$ (i is the line number, j is the column number), which is the product of transition matrices through dots and wire-connected dots. It reads $\hat{\mathbf{T}} = Q^{N-1}Q_1$, where

$$Q = \frac{1}{2\mathrm{i}k}\begin{pmatrix} \gamma_{11} + 2\mathrm{i}k & 0 & \mathrm{e}^{-2\mathrm{i}dk}\gamma_{11} & 0 \\ 0 & \gamma_{00} + 2\mathrm{i}k & 0 & \mathrm{e}^{-2\mathrm{i}dk}\gamma_{00} \\ -\gamma_{11} & 0 & \mathrm{e}^{-2\mathrm{i}dk}(2\mathrm{i}k - \gamma_{11}) & 0 \\ 0 & -\gamma_{00} & 0 & \mathrm{e}^{-2\mathrm{i}dk}(2\mathrm{i}k - \gamma_{00}) \end{pmatrix}. \tag{10}$$

The matrix Q_1 differs from Q by the absence of multiplier $\mathrm{e}^{-2\mathrm{i}dk}$ in its matrix elements. Here d is the distance between the centres y_l, where δ-functions are localized. As applied

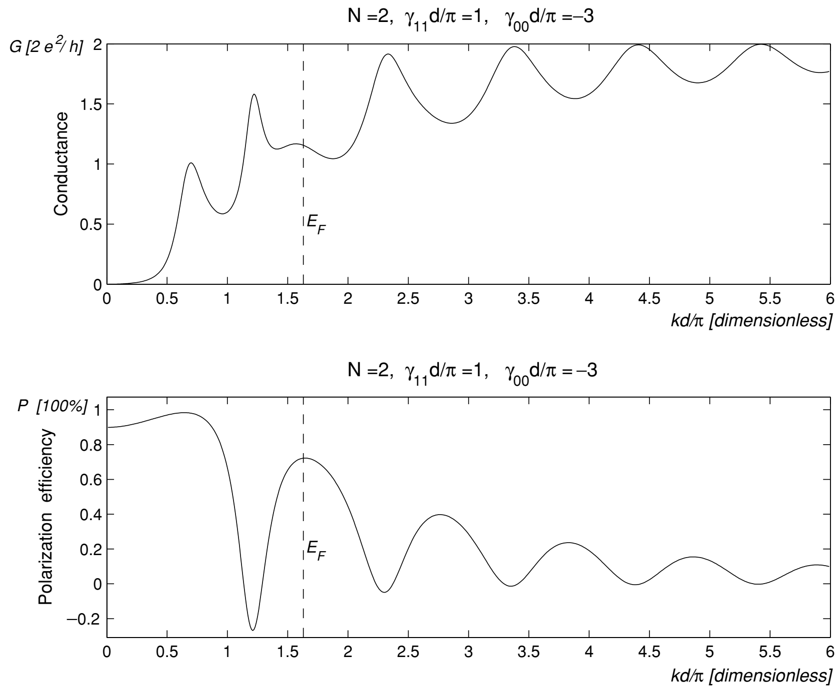

Figure 4. The conductance G and polarization efficiency P versus dimensionless momentum $\hat{k} = k\frac{d}{\pi}$ of incident electrons in the case of two quantum dots. The Fermi level $E_F = 35$ meV in InSb is indicated by the dashed line. The interdot distance $d = 45$ nm.

to the physical situation we are modelling d is the length of a quantum wire connecting two neighbour dots. The transmission coefficients have the form $T_{11}^{(N)} = t_{11} + t_{13}\,\mathrm{e}^{-2\mathrm{i}ky_1} R_{11}^{(N)}$, $T_{00}^{(N)} = t_{22} + t_{24}\,\mathrm{e}^{-2\mathrm{i}ky_1} R_{00}^{(N)}$. The reflection coefficients $R_{11}^{(N)}$, $R_{00}^{(N)}$ in the triplet and singlet channels respectively are given by the equations $R_{11}^{(N)} = \mathrm{e}^{2\mathrm{i}ky_1} D^{-1}(t_{41}t_{34} - t_{31}t_{44})$, $R_{00}^{(N)} = \mathrm{e}^{2\mathrm{i}ky_1} D^{-1}(t_{43}t_{32} - t_{33}t_{42})$, where $D = t_{33}t_{44} - t_{34}t_{43}$. The relations $\left|T_{jj}^{(N)}\right|^2 + \left|R_{jj}^{(N)}\right|^2 = 1$ $(j = 0, 1)$ which imply the unitarity of scattering has been checked by means of an analytical calculation package.

In the case $N = 1$ one has $T_{jj}^{(1)} = 2\mathrm{i}k(2\mathrm{i}k - \gamma_{jj})^{-1}$, $R_{jj}^{(1)} = \mathrm{e}^{2\mathrm{i}ky_1}\gamma_{jj}(2\mathrm{i}k - \gamma_{jj})^{-1}$ $(j = 0, 1)$.

5. Results and discussions

In this section we present the results of the numerical calculations of the operation regime characteristics for the spin gun and discuss the proper choice of the model parameters as well as the choice of semiconductor materials for QW and QD. We use the applied bias $V : eV = \mu_L - \mu_R$ for tuning the spin polarization effects in the device.

In order to calculate the conductance G of the device we exploit the two-channel Landauer formula at zero-temperature limit:

$$G = \frac{e^2}{\pi\hbar}\left[\left|T_{00}^{(N)}(E_F + eV)\right|^2 + \left|T_{11}^{(N)}(E_F + eV)\right|^2\right],$$

where E_F is the Fermi level of QW.

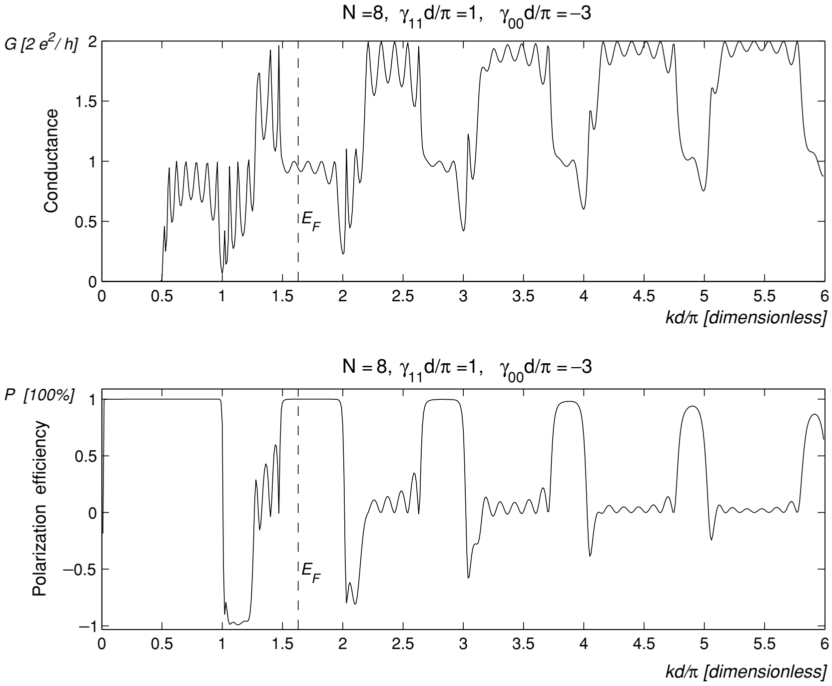

Figure 5. The conductance G and polarization efficiency P versus dimensionless momentum $\hat{k} = k\frac{d}{\pi}$ of incident electrons in the case of 8 quantum dots. The Fermi level $E_F = 35$ meV in InSb is indicated by the dashed line. The interdot distance $d = 45$ nm.

For an unpolarized incident beam of electrons, the scattering by the QD array in the triplet and singlet channels leads to different transmission coefficients $T_{11}^{(N)}$ and $T_{00}^{(N)}$. Following [26] we shall use the polarization efficiency

$$P = \frac{\left|T_{11}^{(N)}\right|^2 - \left|T_{00}^{(N)}\right|^2}{\left|T_{11}^{(N)}\right|^2 + \left|T_{00}^{(N)}\right|^2}$$

which determines the difference of transmission probabilities through the spin gun for the triplet and singlet spin states.

At a given wave number k the conductance G and polarization efficiency P of the device both depend on the model parameters: the distance d, the coupling constants γ_{11}, γ_{00} and the number N of QD. They also both depend on the choice of semiconductor materials from which the QD and QW are fabricated, i.e. effective mass m^*, Fermi energy E_F and mean size r_0 of quantum dots. Varying the bias applied one can calculate the dependence of G and P on $k = \sqrt{2m^*(E_F + eV)/\hbar^2}$ at fixed model parameters and chosen m^*, E_F and r_0. Let us mention that from the spin analysis in section 3 one has $\gamma_{00} = -3\gamma_{11}$. Since d and N are free parameters of the model, the only parameter that has to be fixed is γ_{11}. The reasonable way to fix this parameter is to take it proportional to the inverse mean size of the quantum dot. For relatively small QD $r_0 \approx$ 20–30 nm. Hence $\gamma_{11} \approx$ 0.03–0.05 nm^{-1}. Taking $d \approx 50$ nm, we obtain the value of order $\approx$1 for the dimensionless parameter $\hat{\gamma}_{11} = \gamma_{11}\frac{d}{\pi}$.

In figures 3–5 we show the dependence of G and P on the dimensionless parameter $\hat{k} = k\frac{d}{\pi}$ for $\gamma_{11}\frac{d}{\pi} = 1$ in the cases $N = 1, 2, 8$. We also indicate the position of the Fermi level $E_F = 35$ meV in InSb ($m^* = 0.014m_e$) and fix the inter-dot distance $d = 45$ nm.

The general behaviour of the conductance G and polarization efficiency P for a wide range of parameter variation is the following. On the $\hat{k}$-axis with the growth of the number N of quantum dots there arise the so-called working windows (see figure 5), i.e. intervals $[\hat{k}_1, \hat{k}_2]$, $[\hat{k}_3, \hat{k}_4], \ldots$ in which P and G are sufficiently high simultaneously. Due to the interference processes in a QD array at $N \sim 8$–10 the values of P and G on the working windows approach $P \approx 100\%$ and $G \approx \frac{e^2}{\pi\hbar}$ which is equal to one half of its upper limit. It means that at $\hat{k}$ lying in the working windows the spin gun really produces the fully polarized spin beam and conducts at fairly high level. In figures 3–5 the working windows lie on the right of E_F up to the value of $\hat{k} = (d/\pi)\sqrt{2m^*(E_F + eV)/\hbar^2}$ which corresponds to the bias applied.

6. Plans and prospect

There are a lot of interesting modifications of the model we constructed. For example, we are going to take into account the internal structure of quantum dots. We plan to supply the quantum dot by prescribed internal structure keeping the model exactly solvable. Another interesting modification is to take into account the Coulomb interaction between the electron and quantum dot if the dot is charged. We shall prove that if we switch on the Coulomb interaction the modified model remains exactly solvable. Finally we are going to incorporate in our model the magnetic field in order to manipulate spins in QW and QD.

Acknowledgments

The idea to use interference effect in finite periodic structures in order to amplify the polarization of an electronic beam and the name of a such types of spintronic devices (spin gun) were proposed by N T Bagraev and B S Pavlov[4]. The authors are very grateful to B S Pavlov for supplying the manuscript and for numerous fruitful discussions.

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