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Spin-dependent tunnelling through an indirect double-barrier structure*

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We use the transfer matrix method to study the quantum tunnelling through an indirect-band-gap double-barrier like the GaAs/AlAs/GaAs/AlAs/GaAs heterostructures along the [001] axis, which is described by the tight-binding model. The X-valley quasi-bound state gives rise to the Fano resonance different from the direct double-barrier transition in a resonance-tunnelling diode. The quantitative calculations demonstrate that a relatively high spin-polarization of the transmission probability can be achieved as compared with the single-barrier tunnelling case. Moreover the extension to the multi-barrier device is provided and leads to an important observation that the spin polarization increases with the number of barriers.

Keywords: spin-polarized, spin–orbit interaction, indirect-barrier
PACC: 7210, 7225, 2570E

1. Introduction

Traditional electronics is based on the charge transport while the spin degree of electron does not play a role. The idea of electronic devices that exploit both charge and spin degrees of electron has led to a new branch of physics and technology, known as spintronics. Spin-polarized transports in semiconductor heterostructures have attracted considerable attention recently, which not only exhibit the new fundamental physics but also have promising applications in the emerging technologies of spintronics and quantum information.[1−3] Recent experimental advances in spintronics have given an impetus to the study of spin-polarized transport through such quantum devices in which the spin–orbit (SO) interaction couples the spin states and the spatial motion of electrons. The spin-polarized transmission probability is controllable by using external electric fields or gate voltages.[4−17] The SO interaction originating from the relativistic effect is believed to have a substantial increase in some semiconductors and has attracted great attention recently. Two mechanisms are shown to be responsible for the spin-dependent transport: one is the Rashba SO coupling in asymmetric non-magnetic heterostructures (for example, the spin precessions in a spin-transistor) and the other is the spin-dependent k^3 coupling that is called the Dresselhaus SO coupling in symmetric materials (for example: spin precessions in the Zinc-blende-Lattice semiconductors). Recent theoretical studies show that when an electron tunnels through a Zinc-blende semiconductor single[18] or double-barrier[19] structure, it can be highly spin polarized and the generation of spin-polarized transport can be analysed in terms of the electron Hamiltonian[20] in the effective-mass approximation with an additional Dresselhaus-interaction-term.[21,22] It was subsequently demonstrated that in the study of spin-polarization tunnelling we must consider both the $\Gamma - \Gamma - \Gamma$ direct tunnelling in a higher Γ valley and the $\Gamma - X - \Gamma$ indirect transition through a quasi-bound state in the X valley[23] (see Fig.1(a)). The transmission is therefore characterized by the $\Gamma-$ and the $X-$ point Hamiltonians and the Fano resonances.[23] However the spin-polarization is rather small, evaluated theoretically with the parameters of effective masses, band offsets, and the Dresselhaus coefficients.[23] It is of interest and importance to see whether the spin-polarization can be enhanced by the multi-barrier tunnelling.

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To this end we consider the double-indirect-barrier (GaAs/AlAs/GaAs/AlAs/GaAs) tunnelling as shown in Fig.1(a), where $\Gamma-$ band and the $X-$ band edges are indicated by solid and dashed lines respectively, and E_1 and E_2 are the X-valley quasi-bound states in the AlAs barrier. The direct tunnelling ($\Gamma-\Gamma-\Gamma$) and indirect transition ($\Gamma-X-\Gamma$) are depicted by the solid wavy arrow and dotted wavy arrows respectively. By using the tight-binding (TB) approximation, the above system can be reduced to a simpler model that is shown in Fig.1(b), then we can evaluate the transmission probability of electron by using the transfer-matrix method. The indirect barrier tunnelling leads to the Fano-type resonances different from that caused by the direct double-barrier tunnelling, known as the resonant tunnelling diode (RTD). The Fano-type resonances and the spin polarization are compared quantitatively with the result of single-barrier tunnelling.

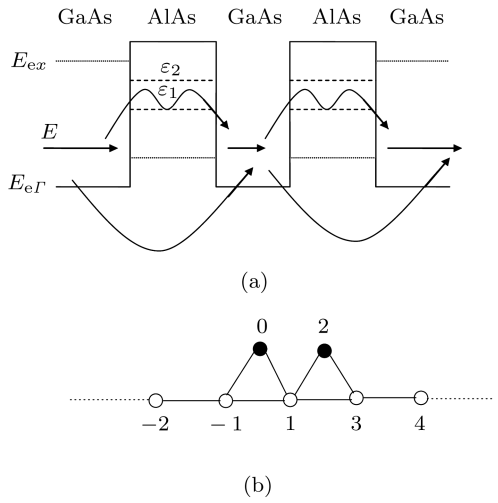


Fig.1. Indirect double-barrier tunnelling and the effective TB model.

The paper is organized as follows: in Section 2, we present the tight-binding Hamiltonian and the formulation of transmission matrix. Its generalization to the multi-barrier tunnelling is provided in Section 3, while the numerical results and the corresponding discussion are given in Section 4.

2. Tight-binding model and formulation

The double-barrier tunnelling together with X-valley quasi-bound-state transition can be formulated by a simple TB model where spin states are assumed to be degenerate in the left lead and the right lead (bulk-like states) and the degeneracy is removed in the barrier due to the SO coupling. The Hamiltonian of the second quantization can be written as (see Fig.1(b))

$$\begin{aligned} H = & \sum_{n=-\infty,\sigma=\uparrow,\downarrow}^{-2} [\epsilon a_{n,\sigma}^{+} a_{n,\sigma} + (t a_{n-1,\sigma}^{+} a_{n,\sigma} + \text{h.c.})] \\ & + \sum_{n=4,\sigma=\uparrow,\downarrow}^{\infty} [\epsilon a_{n,\sigma}^{+} a_{n,\sigma} + (t a_{n,\sigma}^{+} a_{n-1,\sigma} + \text{h.c.})] \\ & + \sum_{j=-1,1,3;\sigma=\uparrow,\downarrow} \epsilon a_{j,\sigma}^{+} a_{j,\sigma} + \sum_{j=0,2;\sigma=\uparrow,\downarrow} \epsilon_\sigma a_{j,\sigma}^{+} a_{j,\sigma} \\ & + \sum_{\sigma=\uparrow,\downarrow} [(V_\sigma a_{0,\sigma}^{+} a_{-1,\sigma} + V_\sigma a_{1,\sigma}^{+} a_{0,\sigma} + \text{h.c.})] \\ & + \sum_{\sigma=\uparrow,\downarrow} (t_\sigma a_{1,\sigma}^{+} a_{-1,\sigma} + \text{h.c.}) \\ & + \sum_{\sigma=\uparrow,\downarrow} [(V_\sigma a_{2,\sigma}^{+} a_{1,\sigma} + V_\sigma a_{3,\sigma}^{+} a_{2,\sigma} + \text{h.c.})] \\ & + \sum_{\sigma=\uparrow,\downarrow} (t_\sigma a_{3,\sigma}^{+} a_{1,\sigma} + \text{h.c.}), \end{aligned} \tag{1}$$

here $\uparrow$ and $\downarrow$ denote spin up and spin down, respectively. In Eq.(1), the first two terms on the right-hand side describe the electrodes (i.e. the left lead and the right lead), ϵ is the on-site energy, t is the transfer integral, and $a_{n,\sigma}^{+}$ ($a_{n,\sigma}$) is the creation (annihilation) operator of the electron with spin-σ on the site-n. The two electrodes are connected with the tunnelling device at sites $n=-2$ and $n=4$ respectively (Fig.1(b)). The potential well and two contacts connected with the left electrode and the right electrode are regarded as three quantum-dots numbered as 1, -1 and 3 respectively, which are described by the third term of the Hamiltonian. The X-valley quasi-bound states are also considered as two quantum dots ($j=0,2$) with an energy ϵ_σ (see the fourth term). The last four terms represent the couplings among the X-valley QDs $(0,2)$ and the QDs $(-1,1,3)$, where $-1\rightarrow 1$ and $1\rightarrow 3$ correspond to the two-barrier ($\Gamma-\Gamma-\Gamma$) direct tunnelling with t_σ being the hopping integral constant and $-1\rightarrow 0\rightarrow 1$ and $1\rightarrow 2\rightarrow 3$ denote the ($\Gamma-X-\Gamma$) indirect transitions with V_σ being the coupling parameter. It is worth pointing out that both V_σ and t_σ are spin-dependent due to the SO interaction.

Since there is no spin-flipping mechanism, the eigenvalue problem can be solved for each spin-component separately. Thus we begin with the stationary Schrödinger equation for the spin-up component

$$H\,|\,\Psi_\uparrow\rangle = E\,|\,\Psi_\uparrow\rangle\,,$$

which possesses a general solution in the following form:

$$|\Psi_{\uparrow}\rangle = \sum_{n=-\infty,}^{\infty} C_{n,\uparrow} a_{n,\uparrow}^{+} |0\rangle , \tag{2}$$

where $a_{n,\uparrow}^{+}$ is the creation operator of electron on site n with spin-component ($\uparrow$), and $|0\rangle$ denotes the vacuum state. The Dresselhaus Hamiltonians for both the direct tunnelling and the indirect transition can be diagonalized by

$$\chi_{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mp \mathrm{e}^{-\mathrm{i}\phi} \end{pmatrix},$$

where the spinors $\chi_{\pm}$ with the polar angle ϕ of the electron wave-vector in the plane perpendicular to the [001] axis correspond to our spin-up ($\uparrow$) and spin-down ($\downarrow$) states respectively. Inserting expression (2) into the above stationary Schrödinger equation, we find the following recurring equation for the electron-occupation-amplitude $\{C_{n,\uparrow}\}$ on the site-n

$$\begin{aligned} &(E-\varepsilon)C_{n,\uparrow} - tC_{n-1,\uparrow} - tC_{n+1,\uparrow} = 0, \\ &n \leq -2 \quad \text{and} \quad n \geq 4, \end{aligned} \tag{3}$$

$$\begin{aligned} &(E-\varepsilon)C_{-1,\uparrow} - tC_{-2,\uparrow} - V_{\uparrow}C_{0,\uparrow} - t_{\uparrow}C_{1,\uparrow} = 0, \\ &\quad n = -1, \\ &(E-\varepsilon_{\uparrow})C_{0,\uparrow} - V_{\uparrow}C_{-1,\uparrow} - V_{\uparrow}C_{1,\uparrow} = 0, \quad n = 0, \end{aligned}$$

$$\begin{aligned} &(E-\varepsilon)C_{1,\uparrow} - V_{\uparrow}C_{2,\uparrow} - V_{\uparrow}C_{0,\uparrow} - t_{\uparrow}C_{-1,\uparrow} \\ &\qquad -t_{\uparrow}C_{3,\uparrow} = 0, \qquad n = 1, \\ &(E-\varepsilon_{\uparrow})C_{2,\uparrow} - V_{\uparrow}C_{1,\uparrow} - V_{\uparrow}C_{3,\uparrow} = 0, \quad n = 2, \end{aligned}$$

and

$$\begin{aligned} &(E-\varepsilon)C_{3,\uparrow} - tC_{4,\uparrow} - V_{\uparrow}C_{2,\uparrow} - t_{\uparrow}C_{1,\uparrow} = 0, \\ &\quad n = 3, \end{aligned} \tag{4}$$

which can be written as a matrix equation,

$$\begin{pmatrix} C_{n+1,\uparrow} \\ C_{n,\uparrow} \end{pmatrix} = M(n,E) \begin{pmatrix} C_{n,\uparrow} \\ C_{n-1,\uparrow} \end{pmatrix}, \tag{5}$$

where the transfer matrix $M(n,E)$, which links the expansion coefficients $(C_{n+1,\uparrow}, C_{n,\uparrow})^{\mathrm{T}}$ with $(C_{n,\uparrow}, C_{n-1,\uparrow})^{\mathrm{T}}$, is defined as

$$M(n,E) = \begin{bmatrix} \dfrac{E-\varepsilon}{t} & -1 \\ 1 & 0 \end{bmatrix}, \quad (n \leqslant -2, \quad \text{and} \quad n \geqslant 4,).$$

$$\begin{aligned} &M(-1,E) \\ &= \begin{bmatrix} \dfrac{E-\varepsilon+t_{\uparrow}}{V_{\uparrow}+\dfrac{t_{\uparrow}}{V_{\uparrow}}(E-\varepsilon_{\uparrow})} & -\dfrac{t}{V_{\uparrow}+\dfrac{t_{\uparrow}}{V_{\uparrow}}(E-\varepsilon_{\uparrow})} \\ 1 & 0 \end{bmatrix}, \end{aligned}$$

$$M(2,E) = M(0,E) = \begin{bmatrix} \dfrac{E-\varepsilon_{\uparrow}}{V_{\uparrow}} & -1 \\ 1 & 0 \end{bmatrix},$$

$$M(1,E) = \begin{bmatrix} \dfrac{E-\varepsilon+2t_{\uparrow}}{V_{\uparrow}+\dfrac{t_{\uparrow}}{V_{\uparrow}}(E-\varepsilon_{\uparrow})} & -1 \\ 1 & 0 \end{bmatrix},$$

and

$$\begin{aligned} &M(3,E) \\ &= \begin{bmatrix} \dfrac{E-\varepsilon+t_{\uparrow}}{t} & -\dfrac{V_{\uparrow}+\dfrac{t_{\uparrow}}{V_{\uparrow}}(E-\varepsilon_{\uparrow})}{t} \\ 1 & 0 \end{bmatrix}. \end{aligned} \tag{6}$$

In the left-hand-side electrode the eigenfunctions are in the form of $\{\exp(\pm k_{\uparrow} na)\}$ with the positive (negative) sign representing the right- (left-) going waves while only the transmitting wave of amplitude t exists in the right-hand-side electrode, taking which into account the occupation coefficients on the site-n in the two electrode-regions can be written as

$$C_{n,\uparrow} = \mathrm{e}^{\mathrm{i}K_{\uparrow}^{L} na} + r\mathrm{e}^{-\mathrm{i}K_{\uparrow}^{L} na}, \qquad n \leq -2,$$

and

$$C_{n,\uparrow} = t\mathrm{e}^{\mathrm{i}K_{\uparrow}^{R} na}, \quad n \geq 4. \tag{7}$$

It can be shown that the transmitting amplitude $t_{\uparrow}$ is related to the reflection coefficient $r_{\uparrow}$ via the equation

$$\begin{pmatrix} t_{\uparrow} \\ 0 \end{pmatrix} = S(E) \begin{pmatrix} 1 \\ r_{\uparrow} \end{pmatrix}, \tag{8}$$

where the transfer matrix $S(E)$ is given by

$$\begin{aligned} S(E) = &\begin{bmatrix} \mathrm{e}^{-\mathrm{i}5K_{\uparrow}^{R}a} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}5K_{\uparrow}^{R}a} \end{bmatrix} \\ &\times \begin{bmatrix} \mathrm{e}^{\mathrm{i}k_{\uparrow}^{R}a} & \mathrm{e}^{-\mathrm{i}k_{\uparrow}^{R}a} \\ 1 & 1 \end{bmatrix} \prod_{n=4}^{-2} M(n,E) \\ &\times \begin{bmatrix} \mathrm{e}^{\mathrm{i}k_{\uparrow}^{L}a} & \mathrm{e}^{-\mathrm{i}k_{\uparrow}^{L}a} \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \mathrm{e}^{\mathrm{i}K_{\uparrow}^{L}a} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}K_{\uparrow}^{L}a} \end{bmatrix}. \end{aligned} \tag{9}$$

Thus we can obtain from Eq.(8) the reflection amplitude $r_{\uparrow}$ and transmission amplitude $t_{\uparrow}$ as

$$r_{\uparrow} = -\frac{S_{21}}{S_{22}},$$

and

$$t_{\uparrow} = \frac{S_{11}S_{22} - S_{12}S_{21}}{S_{22}} = \frac{\mathrm{Det}[S]}{S_{22}}. \tag{10}$$

While the spin-up (↑) reflection and transmission probabilities are

$$R_{\uparrow}(E) = |r_{\uparrow}|^2,$$

and

$$T_{\uparrow}(E) = |t_{\uparrow}|^2. \tag{11}$$

In the same way we can obtain the spin-down (↓) reflection and transmission probabilities $R_{\downarrow}(E)$ and $T_{\downarrow}(E)$. Then the spin-polarized transmission probability can be evaluated as

$$P = \frac{T_{\uparrow} - T_{\downarrow}}{T_{\uparrow} + T_{\downarrow}}. \tag{12}$$

When the size of structure is small with respect to the coherent length, the transmission probability plays an essential role in the quantum transport. For example, we can obtain the conductivity of the devices from the transmission probability with the help of the Laudauer–Büticker formula. Various methods[24−30] have been developed for the numerical calculation of the transmission probability.[31−34]

2.1. Generalization to multi-barrier tunnelling

The generalization to the N-barrier tunnelling is straight forward, with Eqs.(3) and (4) replaced by

$$\begin{aligned}
&(E-\varepsilon)C_{n,\uparrow} - tC_{n-1,\uparrow} - tC_{n+1,\uparrow} = 0,\\
&\quad n \le -2 \ \text{ and } \ n \ge 4(N+1),
\end{aligned}$$

$$\begin{aligned}
&(E-\varepsilon)C_{-1,\uparrow} - tC_{-2,\uparrow} - V_{\uparrow}C_{0,\uparrow} - t_{\uparrow}C_{1,\uparrow} = 0,\\
&\quad n = -1 + 4\mathrm{i},\\
&(E-\varepsilon_{\uparrow})C_{0,\uparrow} - V_{\uparrow}C_{-1,\uparrow} - V_{\uparrow}C_{1,\uparrow} = 0, \ n = 0 + 4\mathrm{i},\\
&(E-\varepsilon)C_{1,\uparrow} - V_{\uparrow}C_{2,\uparrow} - V_{\uparrow}C_{0,\uparrow} - t_{\uparrow}C_{-1,\uparrow}\\
&\qquad -t_{\uparrow}C_{3,\uparrow} = 0, \qquad n = 1 + 4\mathrm{i},\\
&(E-\varepsilon_{\uparrow})C_{2,\uparrow} - V_{\uparrow}C_{1,\uparrow} - V_{\uparrow}C_{3,\uparrow} = 0, \quad n = 2 + 4\mathrm{i},
\end{aligned}$$

and

$$\begin{aligned}
&(E-\varepsilon)C_{3,\uparrow} - tC_{4,\uparrow} - V_{\uparrow}C_{2,\uparrow} - t_{\uparrow}C_{1,\uparrow} = 0,\\
&n = 3 + 4\mathrm{i},
\end{aligned}$$

where $i = 0, 1, \ldots, N$ with N denoting the number of the barriers. The corresponding transfer matrix $M(n, E)$ in Eq.(5) and expression (6) should be replaced by $M(n+4\mathrm{i}, E)$ for $n = -1, 0, 1, 2$, and $M(3, E)$ by $M(3 + 4N, E)$. Thus the transmission probability can be obtained in terms of the transfer matrix $S(E)$ defined as expression (9).

3. Qualitative results and discussion

The transmission spectrum $T(E)$ of double-barrier tunnelling defined by expression (11) can be evaluated with expressions (9) and (10) for the given matrix elements of $M(n, E)$. Theoretical and experimental methods have been developed to determine the Dresselhaus SO interaction coefficients γ and β which depend on the bulk properties of the material.[35−38] So the parameters such as V_{σ} and t_{σ} can be evaluated according to the values of γ and β. We shall take t as the unit of energy and set $V_{\uparrow} = t_{\uparrow} = 0.05$, $V_{\downarrow} = t_{\downarrow} = 0.052$, and the on-site energies $\epsilon_{\uparrow} = 0.17$ and $\epsilon_{\downarrow} = 0.175$. Figure 2 displays the numerical results of the transmission probability, where the dotted line shows the direct double-barrier tunnelling i.e. the RTD that has two resonance-peaks without antiresonance. The X-valley quasi-bound states result in the Fano-type resonances with two resonance peaks for both spin-up and spin-down components (solid line).

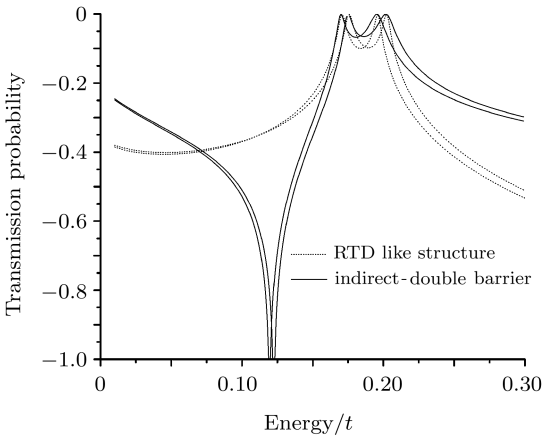


Fig.2. Transmission probability versus the incident energy as the unit of t through an indirect double-barrier (solid line) and direct double-barrier tunnelling (dotted line).

The existence of the antiresonance can be understood from expression (6): when the energy satisfies the condition $E = \epsilon_i - \dfrac{(V_i)^2}{t_i}$, $(i = 1, 2)$, the matrix element approaches the infinity, thus the transmission probability (Eq.(10)) vanishes. Since the hopping integral t is basically the conduction bandwidth and $t_1(t_2)$ and

$V_1(V_2)$ are the tunnelling rates, the first resonance (i.e. the first pole) occurs approximately at an energy value (E) of $\epsilon_1 - 2\frac{V_1^2}{t}\mathrm{e}^{\mathrm{i}ka}\left(\epsilon_2 - 2\frac{V_2^2}{t}\mathrm{e}^{\mathrm{i}ka}\right)$ with $V_1, t_1(V_2, t_2) \ll t$. The difference in energy between two resonance peaks, ΔE, is $(\epsilon_2 - \epsilon_1) - \frac{2}{t}(V_2^2 - V_1^2)\mathrm{e}^{\mathrm{i}ka}$, which is a much small value. While the difference in energy between the peaks of resonance and antiresonance, ΔE, is about $\frac{(V_i)^2}{t_i}$, we then can obtain a more wide energy window, ΔE, by decreasing t_i or increasing V_i. Figure 3 shows the spin polarization of transmission probability defined as expression (12) for indirect double-barrier tunnelling (solid line) and the RTD case (dotted line).

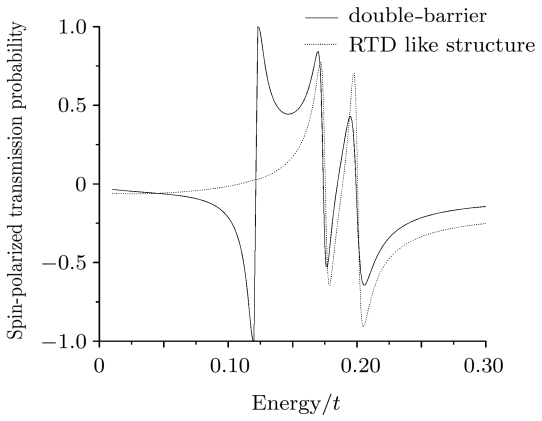


Fig.3. Spin-polarized transmission probabilities for indirect barrier tunnelling (solid line) and direct double-barrier tunnelling (dotted line) versus the incident energy as the unit of t.

The main goal of our study for the multi-barrier tunnelling is to seek a possibility to obtain a higher spin-polarization and therefore we compare the spin-polarized transmission probability of the indirect double-barrier tunnelling (solid line in Fig.4) with that in the single-barrier case (dotted line) studied before. An additional resonance peak occurs due to the resonant tunnelling in the double-barrier case, and the quantitative results show that a large polarization indeed can be obtained. For example, the spin-polarization for the double-barrier is 60% higher than that for the single barrier case in an energy range from $0.124t$ to $0.172t$. Especially, the polarization-value at an energy point $0.172t$ is 0.63 that is more than twice that for the single-barrier case, 0.30.

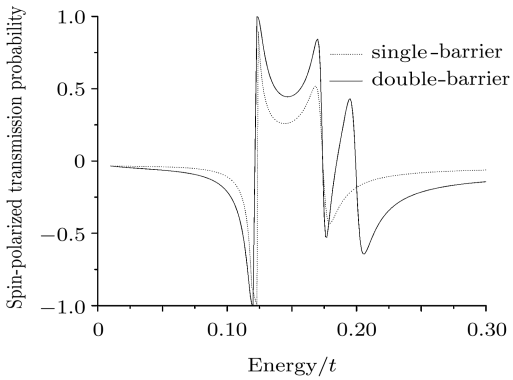


Fig.4. Spin-polarized transmission probabilities versus the incident energy as the unit of t for indirect double-barrier (solid line) and single-barrier (dotted line).

In Fig.5, we show the transmission probabilities of ten barriers. We find ten resonance peaks for both spin-up and the spin-down components and a large relative shifts of peak-positions between spin-up and the spin-down components, resulting in a much higher polarization value as shown in Fig.6. The polarization value in an energy region from $0.15t$ to $0.173t$ is about 164% higher than that for the single-barrier case. So the spin polarization of transmission probability increases with the number of barriers.

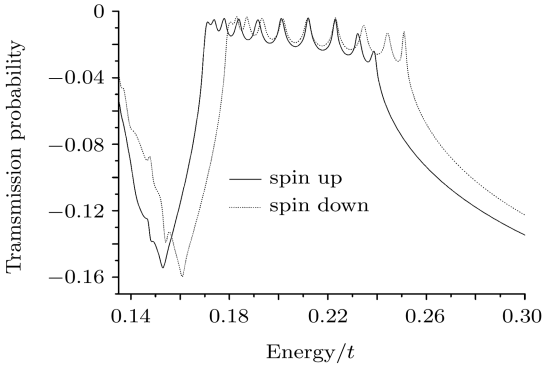


Fig.5. Transmission probability of ten barriers versus the incident energy as the unit of t.

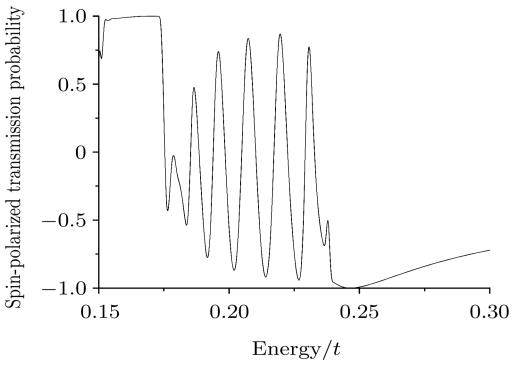


Fig.6. Spin-polarized transmission probabilities for ten barriers versus the incident energy as the unit of t.

4. Conclusion

The quantum transport through an indirect-band-gap double-barrier like the GaAs/AlAs/GaAs/AlAs/GaAs heterostructures along the [001] axis described by the tight-binding model is studied by using the transfer matrix method, where the Dresselhaus SO coupling will lead to the spin-polarization dependent transmission probability. Fano-type resonances occur, which are different from the case of direct double-barrier tunnelling i.e. the RTD case. Compared with the single indirect barrier tunnelling, a higher spin polarization is obtained when electrons tunnel through the indirect double-barrier. The transmission probability through a multi-barrier device is also obtained and the spin polarization increases with the number of barriers. This observation is useful for seeking the device of high spin-polarization in future experiment.

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