Resonant Tunneling and the Pauli Principle

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Abstract

A new method based on modified optical Bloch equations is proposed for studying resonant tunneling in semiconductor heterostructures. The method manifestly takes account of electrons’ statistics, which enables to investigate the influence of the Pauli principle on resonant tunneling in presence of inelastic scattering. Being applied to evaluation of the resonant current in semiconductor heterostructures, our approach predicts considerable deviations from the one-electron picture.

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The impressive progress in microfabrication technology has considerably enhanced the interest to quantum transport through multilayered semiconductor heterostructures [1]. A good number of theoretical approaches have been developed to describe resonant tunneling in these devices. However, the problem has been mostly treated within the one-electron picture. The existing many-electron approaches (see, e.g., [2–5]) are very complicated, owing to which the influence of many-body effects in resonant tunneling problems remains insufficiently elucidated yet. One of them is the effect of the Pauli exclusion principle, which is expected to be especially important in presence of inelastic scattering [5,6].

We propose here a novel method of handling resonant-tunneling problems. This method is based on modified master equations suited for problems, where “classical” (incoherent) and “quantum” (coherent) phenomena are in interplay. Being technically simpler than the other approaches, it has nevertheless a many-body nature and takes account of the Pauli principle from the very beginning.

Let us consider a mesoscopic “device” consisting of coupled quantum wells. The device is connected with two separate electron reservoirs. We assume that the density of states in the reservoirs is very high (continuum). However, each of the quantum wells in the device contains only a small number of discrete energy levels. For the sake of simplicity we consider the reservoirs at zero temperature, where the carriers (electrons) occupy all the states in the left reservoir up to the Fermi level \( E_F^{(l)} \) and in the right reservoir up to the level \( E_F^{(r)} < E_F^{(l)} \). As a result, a current is flowing through the device from the left reservoir to the right one. The device is also coupled to an additional phonon reservoir (also at zero temperature), which enables inelastic transitions between the discrete levels in the quantum wells. We assume that the system is described by a tunneling Hamiltonian, i.e. only the couplings between the adjacent wells are taken into account.

The general idea of our approach follows from the observation that the electron transport in the system can be fully determined in terms of the density submatrix of the device solely, without resorting to the complicated density matrix of the entire system including the reservoirs. This density submatrix contains full information about currents and particle
accumulation, and the only problem is to determine its time evolution. This problem can be solved by using, with some modifications, the technique of NMR theory [7] or the Bloch-Maxwell equations [8].

Let us assume that the reservoirs’ states remain unchanged during the process. We designate the density submatrix of the device as $\sigma_{ab}(t)$ in terms of all possible electrons’ states ($|a\rangle$, $|b\rangle$, $|c\rangle$, . . .) inside the device. For instance, $|a\rangle$ denotes the state where there are no carriers inside the device; $|b\rangle$ – one electron occupies the upper level in the first well, and so on. In the spirit of Bloch-Maxwell equations [8], we write the equations for diagonal and off-diagonal matrix elements of the density submatrix as

$$\dot{\sigma}_{aa} = -i[H, \sigma]_{aa} - \sigma_{aa} \sum_{n(\neq a)} \Gamma_{a\rightarrow n} + \sum_{c(\neq a)} \sigma_{cc} \Gamma_{c\rightarrow a} ,$$  \hspace{1cm} (1a)$$

$$\dot{\sigma}_{ab} = -i[H, \sigma]_{ab} - \frac{1}{2} \sigma_{ab} \left( \sum_{n(\neq a)} \Gamma_{a\rightarrow n} + \sum_{n(\neq b)} \Gamma_{b\rightarrow n} \right) ,$$  \hspace{1cm} (1b)$$

where $H$ is the matrix of the “internal” (without reservoirs) Hamiltonian, and $\Gamma_{a\rightarrow n}$ is the probability per unit time for the system to make a transition from the state $|a\rangle$ to the state $|n\rangle$ of the device due to the tunneling to (or from) the reservoirs, or due to interaction with the phonon bath. The commutator in these equations describes the coherent (“quantum”) motion of carriers inside the device, and the remaining terms describe the incoherent (“classical”) motion of the carriers. By neglecting the commutator one obtains the “classical” kinetic master equations.

Now we can use our basic assumption that the system is described by a tunneling Hamiltonian, which takes into account only the couplings between the nearest neighbors. Then we can rewrite Eqs. (1) explicitly as

$$\dot{\sigma}_{aa} = i \sum_{b(\neq a)} \Omega_{ab}(\sigma_{ab} - \sigma_{ba}) - \sigma_{aa} \sum_{n(\neq a)} \Gamma_{a\rightarrow n} + \sum_{c(\neq a)} \sigma_{cc} \Gamma_{c\rightarrow a} ,$$  \hspace{1cm} (2a)$$

$$\dot{\sigma}_{ab} = i(E_b - E_a)\sigma_{ab} + i \left( \sum_{b'(\neq b)} \sigma_{ab'} \Omega_{b'b} - \sum_{a'(\neq a)} \Omega_{aa'} \sigma_{a'b} \right) - \frac{1}{2} \left( \sum_{n(\neq a)} \Gamma_{a\rightarrow n} + \sum_{n(\neq b)} \Gamma_{b\rightarrow n} \right) \sigma_{ab} ,$$  \hspace{1cm} (2b)$$
where $\Omega_{ij}$ denote the couplings between the levels in adjacent wells, and $a_{ba} = a^*_{ab}$.

By solving Eqs. (2), one can find the diagonal elements of the density submatrix, which determine the charge density of the corresponding quantum states of the device. Then the current flowing into the right reservoir is

$$J(t) = \sum_i \sigma_{ii} \Gamma_{R}^{(i)} ,$$

where the sum is taken over only those states $|i\rangle$ that contain electrons in the well adjacent to the right reservoir; $\Gamma_{R}^{(i)}$ is the partial width of the state $|i\rangle$ due to tunneling to the right reservoir [9]. The stationary current $I$ is obtained from Eq. (3) as $I = J(t \to \infty)$ and does not depend on the initial state of the device [9,10].

Now we give some examples of application of our method to resonant tunneling problems. Although the method can be applied to many different problems, we concentrate in this letter on the Pauli exclusion effects in resonant tunneling. In all the examples we neglect transitions to motion parallel to the layers, by assuming that the scattering on impurities and layers irregularities is small. This makes the problem essentially one-dimensional. For the sake of simplicity we also neglect the electron spin effects, assuming only that two electrons cannot occupy the same quantum state.

Let us start with the well-known case of penetration through a double-barrier heterostructure with one discrete level $E_1$ inside the well, Fig. 1(a). In this case the device has only two possible states, namely: $|a\rangle$ – the level $E_1$ is empty, and $|b\rangle$ – the level $E_1$ is occupied. There are two possible interstate transitions: $|a\rangle \to |b\rangle$ via $\Gamma_L$ (an electron tunnels from the left reservoir), and $|b\rangle \to |a\rangle$ via $\Gamma_R$ (an electron tunnels to the right reservoir). Hence Eqs. (2a) give

$$\dot{\sigma}_{aa} = -\Gamma_L \sigma_{aa} + \Gamma_R \sigma_{bb} ,$$

$$\dot{\sigma}_{bb} = \Gamma_L \sigma_{aa} - \Gamma_R \sigma_{bb} ,$$

where $\Gamma_{L,R}$ are the partial widths of the level $E_1$ due to tunneling to the left and the right reservoirs. Solving Eqs. (3) with the initial condition either $\sigma_{aa}(0) = 1$, $\sigma_{bb} = 0$, or
\( \sigma_{aa}(0) = 0, \sigma_{bb} = 1 \), and using Eq. (3), we obtain for the resonant current \( I \) the standard result

\[
I = \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}.
\]  

(5)

Notice that the coherent (quantum) effects in the resonant current are absent here. As it follows from Eqs. (2), such effects can appear only due to coupling between discrete levels in adjacent quantum wells, whereas in the considered example there is only one quantum well. Hence, the transport through this system is described by classical master equations. It thus might be not surprising that “coherent” and “sequential” approaches to the resonant tunneling produce the same answer in this case, [11].

Next we consider the resonant tunneling through double-well potential structure shown in Fig. 1b. As in the previous case, there are no inelastic transitions due to interaction with the phonon reservoir, since each of the wells contains only one level. However, the coherent tunneling between the wells can take place in this structure. Let us enumerate all possible electron states in the device. There are just four of them: \( |a \rangle \) – the levels \( E_{1,2} \) are empty; \( |b \rangle \) – the level \( E_1 \) is occupied; \( |c \rangle \) – the level \( E_2 \) is occupied; \( |d \rangle \) – both the levels \( E_1 \) and \( E_2 \) are occupied. Taking account of all possible transition between these states, one obtains from Eqs. (2)

\[
\begin{align*}
\dot{\sigma}_{aa} &= -\Gamma_L \sigma_{aa} + \Gamma_R \sigma_{cc}, \\
\dot{\sigma}_{bb} &= \Gamma_L \sigma_{aa} + \Gamma_R \sigma_{dd} + i\Omega(\sigma_{bc} - \sigma_{cb}), \\
\dot{\sigma}_{cc} &= -\Gamma_R \sigma_{cc} - \Gamma_L \sigma_{cc} + i\Omega(\sigma_{cb} - \sigma_{bc}), \\
\dot{\sigma}_{dd} &= -\Gamma_R \sigma_{dd} + \Gamma_L \sigma_{cc} , \\
\dot{\sigma}_{bc} &= i(E_2 - E_1)\sigma_{bc} + i\Omega(\sigma_{bb} - \sigma_{cc}) - \frac{1}{2}(\Gamma_L + \Gamma_R)\sigma_{bc}.
\end{align*}
\]  

(6a)

(6b)

(6c)

(6d)

(6e)

The total current \( I \), according to Eq. (3), is \( I = (\sigma_{cc} + \sigma_{dd})\Gamma_R \), where \( \sigma_{ii} \equiv \sigma_{ii}(t \to \infty) \). Eqs. (6) can be easily solved, so that we finally get for the resonant current

\[
I = \left( \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \right) \frac{\Omega^2}{\Omega^2 + \Gamma_L \Gamma_R/4 + \epsilon^2 \Gamma_L \Gamma_R/((\Gamma_L + \Gamma_R)^2)} ,
\]  

(7)
where \( \epsilon = E_2 - E_1 \). This result coincides with the one found in the framework of one-electron approach \([10,12]\). At first sight, such a coincidence looks surprising. Indeed, our treatment explicitly excludes the states when two or more electrons occupy the same level. On the other hand, these states are implicitly present within the one-particle picture. Nevertheless, a more detailed analysis shows that this coincidence is not accidental. One can demonstrate that in the absence of inelastic scattering the Pauli forbidden configurations in the one-electron picture do not contribute to the resonant current \([13]\). However, in the presence of inelastic scattering, the influence of Pauli forbidden terms is very essential.

Let us consider two other examples of the resonant tunneling, now in presence of inelastic scattering. The first case is shown in Fig. 2a. It corresponds to the double-barrier structure discussed above, but now the quantum well contains two levels, the upper one \( E_0 \) and the lower one \( E_1 \). An electron which tunnels from the left reservoir into the upper level \( E_0 \) can either relax inelastically into the lower state with the transition rate \( \Gamma_{\text{in}} \), and then tunnel out into the right reservoir, or tunnel out directly into the right reservoir. There are four possible electron states of the device: \(|a\rangle\) – the levels \( E_{0,1} \) are empty; \(|b\rangle\) – the upper level, \( E_0 \), is occupied; \(|c\rangle\) – the lower level, \( E_1 \), is occupied; \(|d\rangle\) – both levels \( E_0 \) and \( E_1 \) are occupied. The possible interstate transitions are: \(|a\rangle \to |b\rangle\) via \( \Gamma_L \), which is the tunneling rate from the left reservoir; \(|b\rangle \to |a\rangle\) via \( \Gamma_{\text{R0}} \), which is the tunneling rate to the right reservoir from the upper level; \(|b\rangle \to |c\rangle\) via \( \Gamma_{\text{in}} \); \(|c\rangle \to |a\rangle\) via \( \Gamma_{\text{R1}} \) which is the tunneling rate to the right reservoir from the lower level; \(|c\rangle \to |d\rangle\) via \( \Gamma_L \); \(|d\rangle \to |b\rangle\) via \( \Gamma_{\text{R1}} \); \(|d\rangle \to |c\rangle\) via \( \Gamma_{\text{R0}} \).

Accordingly, using Eqs. (2) we get

\[
\dot{\sigma}_{aa} = -\Gamma_L \sigma_{aa} + \Gamma_{\text{R0}} \sigma_{bb} + \Gamma_{\text{R1}} \sigma_{cc},
\]

\[
\dot{\sigma}_{bb} = \Gamma_L \sigma_{aa} - (\Gamma_{\text{R0}} + \Gamma_{\text{in}}) \sigma_{bb} + \Gamma_{\text{R1}} \sigma_{dd},
\]

\[
\dot{\sigma}_{cc} = \Gamma_{\text{in}} \sigma_{bb} - (\Gamma_L + \Gamma_{\text{R1}}) \sigma_{cc} + \Gamma_{\text{R0}} \sigma_{dd},
\]

\[
\dot{\sigma}_{dd} = \Gamma_L \sigma_{cc} - (\Gamma_{\text{R0}} + \Gamma_{\text{R1}}) \sigma_{dd}.
\]

The total current \( I = I_{\text{R0}} + I_{\text{R1}} \) is given by Eq. (3), where \( I_{\text{R0}} = f_0 \Gamma_{\text{R0}} \) is the current flowing to the right reservoir from the upper level, and \( I_{\text{R1}} = f_1 \Gamma_{\text{R1}} \) is the current flowing from the
lower level (the “inelastic current”). Here \( f_0 = \bar{\sigma}_{bb} + \bar{\sigma}_{dd} \) and \( f_1 = \bar{\sigma}_{cc} + \bar{\sigma}_{dd} \) are the electron densities on the upper and the lower levels, correspondingly. After solution of Eqs. (8) we obtain

\[
I_{R0} = \frac{\Gamma_L \Gamma_{R0}(1 + \alpha)}{\Gamma_T + \alpha(\Gamma_L + \Gamma_{R0})}, \quad I_{R1} = \frac{\Gamma_L \Gamma_{in}}{\Gamma_T + \alpha(\Gamma_L + \Gamma_{R0})},
\]

where \( \Gamma_T = \Gamma_L + \Gamma_{R0} + \Gamma_{in} \) and \( \alpha = \Gamma_L \Gamma_{in}/[\Gamma_{R1}(\Gamma_L + \Gamma_{R0} + \Gamma_{R1})] \).

This result is quite different from the stationary resonant current \( I^{(\text{one-el})} \) having been found within the one-electron framework [9,14],

\[
I^{(\text{one-el})}_{R0} = \frac{\Gamma_L \Gamma_{R0}}{\Gamma_T}, \quad I^{(\text{one-el})}_{R1} = \frac{\Gamma_L \Gamma_{in}}{\Gamma_T}.
\]

Notice that \( \Gamma_{R1} \) does not enter Eq. (10), and therefore the stationary current in the one-electron approach does not depend on subsequent processes following the electron relaxation to the lower level. This follows from the irreversibility of the inelastic scattering, which disconnects the inelastic flux from the initial channel [9,14]. Hence, it is very remarkable that the \( \Gamma_{R1} \)–dependence of the resonant current appears in Eq. (9). It means that, when the exclusion principle is taken into account, the irreversibility does not totally disconnect the processes taking place before and after the relaxation.

One can show [9] that the inelastic current \( I^{(\text{one-el})}_{R1} \) in the one-electron approach, Eq. (10), can be represented as \( I^{(\text{one-el})}_{R1} = f_0 \Gamma_{in} \), where \( f_0 \) is the electron density on the upper level. Therefore one may tempt to account for the exclusion principle by writing the inelastic current as \( I_{R1} = f_0(1 - f_1)\Gamma_{in} \), where \( f_1 \) is the electron density on the lower level, Eq. (3). However, one can easily check, by using Eq. (9), that this assumption does not hold. This example shows explicitly that \textit{ad hoc} introduction of the additional factor \((1 - f)\) cannot be correct in general for taking account of the Pauli principle in quantum transport [5,6,15].

It is important to mention that the total current \( I = I_{R0} + I_{R1} \), Eq. (9), always increases with \( \Gamma_{in} \). It is similar to the result of the one-electron treatment, Eq. (10). However, the account for the exclusion principle leads to restriction of the total resonant current \( I \) when \( \Gamma_{in} \to \infty \) (as can be easily seen from Eq. (9)).
The most spectacular manifestation of the Pauli exclusion principle would take place in the resonant tunneling through double-well structures, in presence of inelastic transitions. As an example we consider the system shown in Fig. 2b, where a resonant current flows due to inelastic transitions from the upper to the lower levels in the left well. We investigate the case where the lower level in the left well, $E_1$, and the level $E_2$ in the right well are aligned, i.e. $E_1 = E_2$, so the electrons may oscillate between the wells. As a result, the exclusion principle generates non-trivial quantum interference effects in the course of inelastic transitions from the upper level $E_0$ to the lower one $E_1$.[8]

Enumerating all possible electron states one can straightforwardly write down the system of linear coupled equations, Eqs. (2), for all transitions in the device. We do not present these equations here, since the procedure is exactly the same as in all the previous examples. Here we give only the final expression for the resonant current, Eq. (3), when the inelastic rate $\Gamma_{in} \gg \Gamma_{L,R}, \Omega$:

$$I = \frac{M\Gamma_L \Gamma_R}{N + P\Gamma_{in}/2\Omega^2}.$$  \hspace{1cm} (11)

Here the coefficients $M$, $N$ and $P$ are functions of the tunneling widths, $\Gamma_{L,R}$, and the coupling $\Omega$ between the aligned levels, namely

$$M = \Omega^2(\Gamma_L^2 + 4\Gamma^2) + 2\Gamma_L \Gamma_1 \Gamma^2,$$  \hspace{1cm} (12a)

$$N = \Gamma_L(2\Omega^2 + \Gamma_1 \Gamma)(4\Gamma^2 - \Gamma_L \Gamma_R) + \frac{\Gamma_R^2 \Gamma_L}{4} \left( \Gamma_R^2 - \Gamma_L^2 + \frac{\Gamma_L \Gamma_R^2}{\Omega^2} \right),$$  \hspace{1cm} (12b)

$$P = \Gamma_1 \Gamma_L \Gamma_R (\Omega^2 + \Gamma^2),$$  \hspace{1cm} (12c)

where $\Gamma = (\Gamma_L + \Gamma_R)/2$ and $\Gamma_1 = (2\Gamma_L + \Gamma_R)/2$. It follows from Eq. (11) that, contrary to expectations, the resonant current decreases to zero when the inelastic rate $\Gamma_{in}$ increases. Such a strange behavior of the tunneling (inelastic) current is a result of quantum interference effects due to the Pauli principle. Indeed, since the tunneling time from the left well to the right one is much larger than the time of inelastic transition from the upper level, an electron from the upper level should have arrived the second well “simultaneously” with the previous electron. It leads to an effective localization of electrons at the upper and the lower levels.
in the left well, and therefore to the decrease of the inelastic resonant current.

One can also consider a configuration where the level $E_1$ in Fig. 2b is above the bottom of the Fermi sea in the left reservoir. Then the total resonant current has two components: the first one from the inelastic transitions from the upper level $E_0$, and the second one from the direct tunneling to the level $E_1$. In this case, too, the first component interferes destructively with the second one. As a result, the total resonant current increases when the first component is “switched off” (i.e. when $E_F < E_0$).

All the discussed deviations from the single particle picture can be verified in experiments with semiconductor quantum wells. Yet, one should take into account that inelastic transitions with subsequent rescattering on impurities, with the momentum transfer to directions parallel to the layers, may decrease the expected deviations.
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The one-electron treatment produces the same result for the inelastic resonant current, as in the previous example, namely $I^{(\text{one-el})} = \Gamma_L \Gamma_{in}/(\Gamma_L + \Gamma_{in})$. It follows from the disconnection of the inelastic flux from the initial channel, when the exclusion principle is disregarded.
FIGURES

FIG. 1. Resonant tunneling through (a) double-barrier and (b) triple-barrier heterostructures in absence of inelastic scattering.

FIG. 2. Resonant tunneling through (a) double-barrier and (b) triple-barrier heterostructures in presence of inelastic scattering.