Microscopic derivation of rate equations for quantum transport

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(Received 6 November 1995; revised manuscript received 23 February 1996)

It is shown that under certain conditions the resonant transport in mesoscopic systems can be described by modified (quantum) rate equations, which resemble the optical Bloch equations with some additional terms. Detailed microscopic derivation from the many-body Schrödinger equation is presented. Special attention is paid to the Coulomb blockade and quantum coherence effects in coupled quantum dot systems. The distinction between classical and quantum descriptions of resonant transport is clearly manifested in the modified rate equations. [S0163-1829(96)00323-2]

I. INTRODUCTION

Over the past decade great interest has been paid to artificially fabricated nanostructures containing a discrete number of quantum states. The discreteness of quantum states manifests itself in peculiar transport properties of these systems as, for instance, in the Coulomb blockade oscillations.[1] Actually, the study has been mostly concentrated on the quantum transport through single devices (quantum dots). In fact, more interesting quantum mechanical effects can be found in *coupled* nanostructures devices, where the quantum interference may strongly influence the resonance current. The impressive progress in microfabrication technology now allows us to extend the experimental investigation to these systems too. For instance, the transport properties of coupled dots are presently under intensive study.[2,3]

For description of quantum transport through a single quantum dot (quantum well), the ''classical'' rate equations are usually used.[4–6] They can be derived either by using nonequilibrium Green's functions technique,[7] or directly from the Schrödinger equation.[8] The situation is different for coupled wells with aligned levels. The quantum transport through these devices goes on via quantum superposition between the states in adjacent wells. It is thus quite obvious that nondiagonal density matrix elements would appear in the equations of motion. These terms have no classical counterparts, and therefore the classical rate equations have to be modified. A plausible modification of master equations for some particular cases of the resonance tunneling through double-dot structures has been proposed by Nazarov.[9] A more general case, though without account of Coulomb interaction, has been considered in Ref. 10, where modified rate equations have been proposed by using an analogy to the optical Bloch equations.[11] However, no microscopic derivation of the modified rate equations has been presented yet.

In this paper, we derive the rate equations for a general case of resonant transport through mesoscopic systems, starting with the many-body Schrödinger equation, with special attention being paid to the Coulomb blockade and coherent quantum mechanical effects. Our main goals are, first, to substantiate and generalize the previously suggested rate equations and second, to determine the region of validity of the rate equations for the description of quantum transport in general. Also, we believe that the microscopic derivation of the rate equations will provide a better understanding of the correspondence between quantum and classical description of carrier transport in mesoscopic systems.

The plan of the paper is the following. In Sec. II, we give a detailed derivation of the transport rate equations through a single quantum well (dot). In order to present our method most lucidly, we neglect in this section the Coulomb interaction and spin effects. These effects are considered in Sec. III. In Sec. IV, we derive the modified rate equations for coupled well structures, taking into account the Coulomb and spin effects. An example of coherent resonant transport with inelastic transitions is studied in Sec. V. The derivation of rate equations performed in this case allows us to establish their correct form valid in a general case of quantum transport. The general case and an example of coherent resonant transport with inelastic transitions in the presence of strong Coulomb blockade are presented in Sec. VI. The last section is a summary.

II. SINGLE-WELL STRUCTURE

Let us consider a mesoscopic ''device'' consisting of a quantum well (dot), coupled to two separate electron reservoirs. The density of states in the reservoirs is very high (continuum). The dot, however, contains only isolated levels. We first demonstrate how to achieve the reduction of a many-body Schrödinger equation to the rate equation in the simplest example, Fig. 1, with only one level, E_1, inside the dot. We also ignore the Coulomb electron-electron interaction inside the well and the spin degrees of freedom. Hence, only one electron may occupy the well. With the stand simplifications, the tunneling Hamiltonian of the entire system in the occupation number representation is

$$\mathcal{H}=\sum_l E_l a_l^\dagger a_l + E_1 a_1^\dagger a_1 + \sum_r E_r a_r^\dagger a_r + \sum_l \Omega_l (a_l^\dagger a_1 + a_1^\dagger a_l) + \sum_r \Omega_r (a_r^\dagger a_1 + a_1^\dagger a_r). \tag{2.1}$$

Here, the subscripts l and r enumerate correspondingly the (very dense) levels in the left (emitter) and right (collector) reservoirs. For simplicity, we restrict ourselves to the zero

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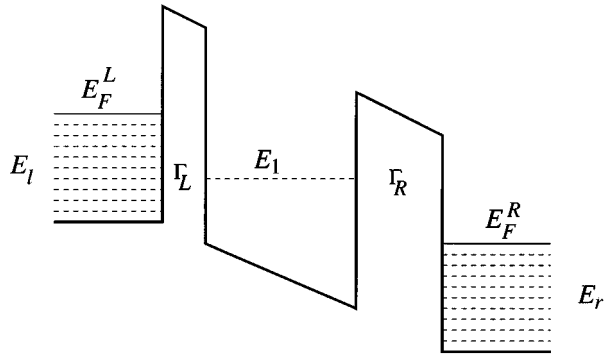

FIG. 1. Resonant transport through a single quantum well structure.

temperature case. All the levels in the emitter and the collector are initially filled with electrons up to the Fermi energy E_F^L and E_F^R, respectively. This situation will be treated as the ''vacuum'' state $|0\rangle$.

This vacuum state is unstable; the Hamiltonian Eq. (2.1) requires it to decay exponentially to a continuum state having the form $a_1^\dagger a_l|0\rangle$ with an electron in the level E_1 and a hole in the emitter continuum. These continuum states are also unstable and decay to states $a_r^\dagger a_l|0\rangle$, having a particle in the collector continuum as well as a hole in the emitter continuum, and no electron in the level E_1. The latter, in turn, are decaying into the states $a_1^\dagger a_r^\dagger a_l a_{l'}|0\rangle$ and so on. The evolution of the whole system is described by the many-particle wave function, which is represented as

$$|\Psi(t)\rangle=\Bigg[b_0(t)+\sum_l b_{1l}(t)a_1^\dagger a_l+\sum_{l,r} b_{lr}(t)a_r^\dagger a_l + \sum_{l<l',r} b_{1ll'r}(t)a_1^\dagger a_r^\dagger a_l a_{l'}+\cdots\Bigg]|0\rangle, \tag{2.2}$$

where $b(t)$ are the time-dependent probability amplitudes for finding the system in the corresponding states described above with the initial condition $b_0(0)=1$, and all the other $b(0)$'s are zeros. Substituting Eq. (2.2) into the Schrödinger equation $i|\dot\Psi(t)\rangle=\mathcal{H}|\Psi(t)\rangle$, results in an infinite set of coupled linear differential equations for the amplitudes $b(t)$. Applying the Laplace transform

$$\tilde b(E)=\int_0^\infty e^{iEt}b(t)dt \tag{2.3}$$

and taking account of the initial conditions, we transform the linear differential equations for $b(t)$ into an infinite set of algebraic equations for the amplitudes $\tilde b(E)$,

$$E\tilde b_0(E)-\sum_l \Omega_l\tilde b_{1l}(E)=i, \tag{2.4a}$$

$$(E+E_l-E_1)\tilde b_{1l}(E)-\Omega_l\tilde b_0(E)-\sum_r \Omega_r\tilde b_{lr}(E)=0, \tag{2.4b}$$

$$(E+E_l-E_r)\tilde b_{lr}(E)-\Omega_r\tilde b_{1l}(E)-\sum_{l'} \Omega_{l'}\tilde b_{1ll'r}(E)=0, \tag{2.4c}$$

$$(E+E_l+E_{l'}-E_1-E_r)\tilde b_{1ll'r}(E)-\Omega_{l'}\tilde b_{lr}(E)+\Omega_l\tilde b_{l'r}(E) -\sum_{r'} \Omega_{r'}\tilde b_{ll'rr'}(E)=0, \tag{2.4d}$$

$$\cdots\ .$$

Equations (2.4) can be substantially simplified. Let us replace the amplitude $\tilde b$ in the term $\Sigma\Omega\tilde b$ of each of the equations by its expression obtained from the subsequent equation. For example, substitute $\tilde b_{1l}(E)$ from Eq. (2.4b) into Eq. (2.4a). We obtain

$$\left[E-\sum_l \frac{\Omega_l^2}{E+E_l-E_1}\right]\tilde b_0(E)-\sum_{l,r} \frac{\Omega_l\Omega_r}{E+E_l-E_1}\tilde b_{lr}(E)=i. \tag{2.5}$$

Since the states in the reservoirs are very dense (continuum), one can replace the sums over l and r by integrals, for instance, $\Sigma_l\to\int\rho_L(E_l)dE_l$, where $\rho_L(E_l)$ is the density of states in the emitter. Then the first sum in Eq. (2.5) becomes an integral, which can be split into a sum of the singular and principal value parts. The singular part yields $-i\Theta(E_F^L+E-E_1)\Gamma_L/2$, where $\Gamma_L=2\pi\rho_L(E_1)|\Omega_L(E_1)|^2$ is the level E_1 partial width, due to coupling to the emitter. Let us assume that $E_F^L\gg E_1\gg E_F^R$, i.e., the bias is large and the energy level is deeply inside the band. In this case, the integration over $E_{l(r)}$ variables can be extended to $\pm\infty$. As a result, the θ-function can be replaced by one, and the principal part is merely included into redefinition of the energy E_1. Also, the second sum (integral) in Eq. (2.5) proves to be negligibly small. Indeed, let us replace $\tilde b_{lr}\to\tilde b(E_l,E_r,E)$, and assume weak energy dependence of Ω on $E_{l(r)}$. Then one finds from Eqs. (2.4) that the poles of the integrand in the $E_l(E_r)$ variable are on one side of the integration contour, and, therefore, this term vanishes.

Applying analogous considerations to the other equations of the system (2.4), we finally arrive to the following set of equations:

$$(E+i\Gamma_L/2)\tilde b_0(E)=i, \tag{2.6a}$$

$$(E+E_l-E_1+i\Gamma_R/2)\tilde b_{1l}(E)-\Omega_l\tilde b_0(E)=0, \tag{2.6b}$$

$$(E+E_l-E_r+i\Gamma_L/2)\tilde b_{lr}(E)-\Omega_r\tilde b_{1l}(E)=0, \tag{2.6c}$$

$$(E+E_l+E_{l'}-E_1-E_r+i\Gamma_R/2)\tilde b_{1ll'r}(E)-\Omega_{l'}\tilde b_{lr}(E) +\Omega_l\tilde b_{l'r}(E)=0, \tag{2.6d}$$

$$\ldots,$$

where $\Gamma_R=2\pi\rho_R(E_1)|\Omega_R(E_1)|^2$ is the level E_1 partial width, due to coupling to the collector.

Now we introduce the density matrix of the ''device.'' The Fock space of the quantum well consists of only two possible states, namely: $|a\rangle$ — the level E_1 is empty, and $|b\rangle$ — the level E_1 is occupied. In this basis, the diagonal

elements of the density matrix of the ''device,'' σ_{aa} and σ_{bb}, give the probabilities of the resonant level being empty or occupied, respectively. In our notation, these probabilities are represented as follows:

$$\sigma_{aa}=|b_0(t)|^2+\sum_{l,r}|b_{lr}(t)|^2+\sum_{l<l',r<r'}|b_{ll'rr'}(t)|^2+\cdots \equiv\sigma_{aa}^{(0)}+\sigma_{aa}^{(1)}+\sigma_{aa}^{(2)}+\cdots, \tag{2.7a}$$

$$\sigma_{bb}=\sum_{l}|b_{1l}(t)|^2+\sum_{l<l',r}|b_{1ll'r}(t)|^2+\sum_{l<l'<l'',r<r'}|b_{1ll'l''rr'}(t)|^2+\cdots \equiv\sigma_{bb}^{(0)}+\sigma_{bb}^{(1)}+\sigma_{bb}^{(2)}+\cdots, \tag{2.7b}$$

where the index n in $\sigma^{(n)}$ denotes the number of electrons in the collector. The current $I(t)$ flowing through the system is $I(t)=e\dot{N}_R(t)$, where $N_R(t)$ is the number of electrons accumulated in the collector, i.e.,

$$N_R(t)=\sum_{n} n[\sigma_{aa}^{(n)}(t)+\sigma_{bb}^{(n)}(t)]. \tag{2.8}$$

The density submatrix elements are directly related to the amplitudes $\tilde{b}(E)$ through the inverse Laplace transform,

$$\sigma^{(n)}(t)=\sum_{l\ldots,r\ldots}\int\frac{dE\,dE'}{4\pi^2}\tilde{b}_{l\ldots r\ldots}(E)\tilde{b}^{*}_{l\ldots r\ldots}(E')\times e^{i(E'-E)t}. \tag{2.9}$$

By means of this equation, one can transform Eqs. (2.6) for the amplitudes $b(E)$ into differential equations directly for the probabilities $\sigma^{(n)}(t)$. Consider, for instance, the term $\sigma_{bb}^{(0)}(t)=\Sigma_l|b_{1l}(t)|^2$, Eq. (2.7b). Multiplying Eq. (2.6b) by $\tilde{b}^{*}_{1l}(E')$ and then subtracting the complex conjugated equation with the interchange $E\leftrightarrow E'$, we obtain

$$\int\frac{dE\,dE'}{4\pi^2}(E'-E-i\Gamma_R)\sum_l\tilde{b}_{1l}(E)\tilde{b}^{*}_{1l}(E')e^{i(E'-E)t}-\int\frac{dE\,dE'}{4\pi^2}2\,\mathrm{Im}\sum_l\Omega_l\tilde{b}_{1l}(E)\tilde{b}^{*}_{0}(E')e^{i(E'-E)t}=0. \tag{2.10}$$

One can easily deduce from Eq. (2.9) that the first integral in Eq. (2.10) equals $-i[\dot{\sigma}_{bb}^{(0)}(t)+\Gamma_R\sigma_{bb}^{(0)}(t)]$. Next, substituting

$$\tilde{b}_{1l}(E)=\frac{\Omega_l\tilde{b}_0(E)}{E+E_l-E_1+i\Gamma_R/2} \tag{2.11}$$

from Eq. (2.6b) into the second integral of Eq. (2.10), and replacing $\Sigma_l\rightarrow\int\rho_L(E_l)dE_l$, one can perform the E_l integration in the integral, thus obtaining $i\Gamma_L\sigma_{aa}^{(0)}(t)$. Ultimately, Eq. (2.10) reads $\dot{\sigma}_{bb}^{(0)}(t)=\Gamma_L\sigma_{aa}^{(0)}(t)-\Gamma_R\sigma_{bb}^{(0)}(t)$. We can go on with this algebra for all the other amplitudes $\tilde{b}(t)$. For instance, the above procedure applied to Eq. (2.6d) converts it into a differential equation for the density-matrix element $\sigma_{bb}^{(1)}$, Eq. (2.7b). The only difference with the previous example is an appearance of the ''cross terms,'' like $\Sigma\Omega_l\tilde{b}_{l'r}(E)\Omega_{l'}\tilde{b}^{*}_{lr}(E')$. Yet, these terms vanish after the integration over $E_{l(r)}$, just as the second term in Eq. (2.5). The rest of the algebra remains the same, so one obtains $\dot{\sigma}_{bb}^{(1)}(t)=\Gamma_L\sigma_{aa}^{(1)}(t)-\Gamma_R\sigma_{bb}^{(1)}(t)$. Finally, we arrive at the following infinite system of the chain equations for the diagonal elements, $\sigma_{aa}^{(n)}$ and $\sigma_{bb}^{(n)}$, of the density matrix,

$$\dot{\sigma}_{aa}^{(0)}(t)=-\Gamma_L\sigma_{aa}^{(0)}(t), \tag{2.12a}$$

$$\dot{\sigma}_{bb}^{(0)}(t)=\Gamma_L\sigma_{aa}^{(0)}(t)-\Gamma_R\sigma_{bb}^{(0)}(t), \tag{2.12b}$$

$$\dot{\sigma}_{aa}^{(1)}(t)=-\Gamma_L\sigma_{aa}^{(1)}(t)+\Gamma_R\sigma_{bb}^{(0)}(t), \tag{2.12c}$$

$$\dot{\sigma}_{bb}^{(1)}(t)=\Gamma_L\sigma_{aa}^{(1)}(t)-\Gamma_R\sigma_{bb}^{(1)}(t), \tag{2.12d}$$

$$\cdots\ .$$

Summing up these equations, one easily obtains differential equations for the total probabilities $\sigma_{aa}=\Sigma_n\sigma_{aa}^{(n)}$ and $\sigma_{bb}=\Sigma_n\sigma_{bb}^{(n)}$:

$$\dot{\sigma}_{aa}=-\Gamma_L\sigma_{aa}+\Gamma_R\sigma_{bb}, \tag{2.13a}$$

$$\dot{\sigma}_{bb}=\Gamma_L\sigma_{aa}-\Gamma_R\sigma_{bb}, \tag{2.13b}$$

which should be supplemented with the initial conditions

$$\sigma_{aa}(0)=1,\quad \sigma_{bb}(0)=0. \tag{2.14}$$

Using Eqs. (2.8) and (2.12), we obtain the total current

$$I(t)=e\dot{N}_R(t)=e\Gamma_R[\sigma_{bb}^{(0)}(t)+\sigma_{bb}^{(1)}(t)+\sigma_{bb}^{(2)}(t)+\cdots]=e\Gamma_R\sigma_{bb}(t). \tag{2.15}$$

Thus, the current $I(t)$ is directly proportional to the charge density in the well. Solving Eqs. (2.13) and substituting $\sigma_{bb}(t)$ into Eq. (2.15), we obtain (for $t\rightarrow\infty$) the standard formula for the dc resonant current,

$$I/e=\frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}. \tag{2.16}$$

Notice that, whereas the time behavior of the current $I(t)$ depends on the initial condition, the stationary current $I=I(t\rightarrow\infty)$, Eq. (2.16), does not.

Equations (2.13), derived from the many-body Schrödinger equation, coincide with the classical rate equations in the sequential picture for the resonant tunneling, obtained using nonequilibrium quantum statistical mechanics technique.[7] In contrast, our approach starts directly from the many-body Schrödinger equation and will be straightforwardly extended to more complicated situations. Note, however, that the method can be applied only when the resonance energy is inside the band, and $\Gamma_{L,R}\ll E_F^L-E_F^R$. If the resonance is near the edge of the band, but the width of the resonance is much smaller than the bandwidth, our method still can be applied, but only to the stationary case ($t\rightarrow\infty$).

Yet, the time-dependent Scrödinger equation cannot be reduced to the rate equations (2.13), and therefore this case is not a subject of this paper.

III. COULOMB BLOCKADE

Now we extend the approach of Sec. II to include the effects of Coulomb interaction. Consider again the quantum well in Fig. 1, taking into account the spin degrees of freedom (s). In this case, the tunneling Hamiltonian (2.1) becomes

$$\mathcal{H}=\sum_{l,s} E_l a_{ls}^{\dagger}a_{ls}+\sum_{s} E_1 a_{1s}^{\dagger}a_{1s}+\sum_{r,s} E_r a_{rs}^{\dagger}a_{rs} + \sum_{l,s} \Omega_l(a_{ls}^{\dagger}a_{1s}+a_{1s}^{\dagger}a_{ls})+\sum_{r,s} \Omega_r(a_{rs}^{\dagger}a_{1s}+a_{1s}^{\dagger}a_{rs}) + U a_{1s}^{\dagger}a_{1s}a_{1,-s}^{\dagger}a_{1,-s}, \tag{3.1}$$

where $s=\pm 1/2$, and U is the Coulomb repulsion energy.

Writing down the many-body wave function, $|\Psi(t)\rangle$, in the occupation number representation, just as in Eq. (2.2), and then substituting it into the Schrödinger equation $i|\dot{\Psi}(t)\rangle=\mathcal{H}|\Psi(t)\rangle$, we find a system of coupled equations for the amplitudes $b(t)$

$$E\tilde{b}_0(E)-\sum_l \Omega_l[\tilde{b}_{\uparrow l}(E)+\tilde{b}_{\downarrow l}(E)]=i, \tag{3.2a}$$

$$(E+E_l-E_1)\tilde{b}_{\uparrow l}(E)-\Omega_l\tilde{b}_0(E)-\sum_{l'} \Omega_{l'}\tilde{b}_{\uparrow\downarrow ll'}(E) - \sum_r \Omega_r\tilde{b}_{lr}(E)=0, \tag{3.2b}$$

$$(E+E_l-E_r)\tilde{b}_{lr}(E)-\Omega_r\tilde{b}_{\uparrow l}(E)-\sum_{l'} \Omega_{l'}[\tilde{b}_{\uparrow l'}(E) + \tilde{b}_{\downarrow l'}(E)]=0, \tag{3.2c}$$

$$(E+E_l+E_{l'}-2E_1-U)\tilde{b}_{\uparrow\downarrow ll'}(E)-\Omega_{l'}\tilde{b}_{\uparrow l}(E)-\Omega_l\tilde{b}_{\downarrow l'}(E) - \sum_r \Omega_r[\tilde{b}_{\uparrow ll'r}(E)+\tilde{b}_{\downarrow ll'r}(E)]=0, \tag{3.2d}$$

. . . .

In order to shorten the notations, we eliminated the index (1) of the level E_1 in the amplitudes b, so that $\tilde{b}_{\uparrow(\downarrow)\ldots}(t)$ denotes the probability amplitude for finding one electron inside the well with spin up (down), and the amplitude $\tilde{b}_{\uparrow\downarrow\ldots}(t)$ is the probability amplitude for finding two electrons inside the well.

Equations (3.2) can be simplified by using the same procedure as described in the previous section. For instance, by substituting $\tilde{b}_{lr}$ from Eq. (3.2c) and $\tilde{b}_{\uparrow\downarrow ll'}$ from Eq. (3.2d) into Eq. (3.2b), and neglecting the ''cross terms'' on the grounds of the same arguments as in the analysis of Eq. (2.5), we obtain

$$\left[E+E_l-E-\int_{-\infty}^{E_F^L}\frac{\rho_L(E_{l'})\Omega^2(E_{l'})dE_{l'}}{E+E_l+E_{l'}-2E_1-U} - \int_{E_F^R}^{\infty}\frac{\rho_R(E_r)\Omega^2(E_r)dE_r}{E+E_l-E_r}\right]\tilde{b}_{\uparrow l}(E)=0. \tag{3.3}$$

Since $E_l\sim E_1$, the singular parts of the integrals in (3.3) are, respectively, $-i\Theta(E_F^L+E-E_1+U)\Gamma_L'/2$ and $-i\Theta(E+E_1-E_F^R)\Gamma_R/2$, where

$$\Gamma_{L(R)}=2\pi\rho_{L(R)}(E_1)|\Omega_{L(R)}(E_1)|^2, \qquad \Gamma_{L(R)}'=2\pi\rho_{L(R)}(E_1+U)|\Omega_{L(R)}(E_1+U)|^2. \tag{3.4}$$

Here, $\rho_{L(R)}$ is the spin up or spin down density of states in the emitter (collector), $\rho_{L(R)}\equiv\rho_{L(R)\uparrow}=\rho_{L(R)\downarrow}$. As in the previous section, we assume the resonance level to be deeply inside the band, $E_F^R\ll E_1\ll E_F^L$. If, in addition, $E_1+U\ll E_F^L$, the θ-function in the singular parts of the integrals in (3.3) can be replaced by one. In the opposite case, $E_1+U\gg E_F^L$, the corresponding singular part is zero.

Proceeding this way with the other equations of the system (3.2), we finally obtain

$$(E+i\Gamma_L)\tilde{b}_0(E)=i, \tag{3.5a}$$

$$(E+E_l-E_1+i\Gamma_L'/2+i\Gamma_R/2)\tilde{b}_{\uparrow l}(E)-\Omega_l\tilde{b}_0(E)=0, \tag{3.5b}$$

$$(E+E_l-E_r+i\Gamma_L)\tilde{b}_{lr}(E)-\Omega_r\tilde{b}_{\uparrow l}(E)=0, \tag{3.5c}$$

$$(E+E_l+E_{l'}-2E_1-U+i\Gamma_R')\tilde{b}_{\uparrow\downarrow ll'}(E)-\Omega_l\tilde{b}_{\downarrow l'}(E) + \Omega_{l'}\tilde{b}_{\uparrow l}(E)=0, \tag{3.5d}$$

. . . .

Equations (3.5) can be transformed into equations for the density matrix of the ''device'' by using the method of the previous section. Since the algebra remains essentially the same, we give only the final equations for the diagonal density-matrix elements $\sigma_{aa}^{(n)}(t)$, $\sigma_{bb\uparrow}^{(n)}(t)$, $\sigma_{bb\downarrow}^{(n)}(t)$, and $\sigma_{cc}^{(n)}(t)$. These are the probabilities of finding (a) no electrons inside the well; (b) one electron with spin up (down) inside the well, and (c) two electrons inside the well, respectively. The index n denotes the number of electrons accumulated in the collector. We obtain

$$\dot{\sigma}_{aa}^{(n)}=-2\Gamma_L\sigma_{aa}^{(n)}+\Gamma_R\sigma_{bb\uparrow}^{(n-1)}+\Gamma_R\sigma_{bb\downarrow}^{(n-1)}, \tag{3.6a}$$

$$\dot{\sigma}_{bb\uparrow}^{(n)}=-(\Gamma_L'+\Gamma_R)\sigma_{bb\uparrow}^{(n)}+\Gamma_L\sigma_{aa}^{(n)}+\Gamma_R'\sigma_{cc}^{(n-1)}, \tag{3.6b}$$

$$\dot{\sigma}_{bb\downarrow}^{(n)}=-(\Gamma_L'+\Gamma_R)\sigma_{bb\downarrow}^{(n)}+\Gamma_L\sigma_{aa}^{(n)}+\Gamma_R'\sigma_{cc}^{(n-1)}, \tag{3.6c}$$

$$\dot{\sigma}_{cc}^{(n)}=-2\Gamma_R'\sigma_{cc}^{(n)}+\Gamma_L'\sigma_{bb\uparrow}^{(n)}+\Gamma_L'\sigma_{bb\downarrow}^{(n)}. \tag{3.6d}$$

These rate equations look like a generalization of the rate equations (2.12), if one allows the well to be occupied by two electrons. The Coulomb repulsion leads merely to a modification of the corresponding rates $\Gamma\to\Gamma'$, due to increase of the two-electron energy.

Summing up the partial probabilities we obtain for the total probabilities, $\sigma(t)=\Sigma_n\sigma^{(n)}(t)$, the following equations:

$$\dot{\sigma}_{aa}=-2\Gamma_L\sigma_{aa}+\Gamma_R\sigma_{bb\uparrow}+\Gamma_R\sigma_{bb\downarrow}, \tag{3.7a}$$

$$\dot{\sigma}_{bb\uparrow}=-(\Gamma_L'+\Gamma_R)\sigma_{bb\uparrow}+\Gamma_L\sigma_{aa}+\Gamma_R'\sigma_{cc}, \tag{3.7b}$$

$$\dot{\sigma}_{bb\downarrow}=-(\Gamma_L'+\Gamma_R)\sigma_{bb\downarrow}+\Gamma_L\sigma_{aa}+\Gamma_R'\sigma_{cc}, \tag{3.7c}$$

$$\dot{\sigma}_{cc}=-2\Gamma_R'\sigma_{cc}+\Gamma_L'\sigma_{bb\uparrow}+\Gamma_L'\sigma_{bb\downarrow}, \tag{3.7d}$$

and for the current

$$I(t)=\sum_n n[\dot{\sigma}^{(n)}(t)]=e\Gamma_R[\sigma_{bb\uparrow}(t)+\sigma_{bb\downarrow}(t)]+2e\Gamma_R'\sigma_{cc}(t). \tag{3.8}$$

Equations (3.7), (3.8) can be solved most easily for a dc, $I=I(t\to\infty)$. In this case, $\dot{\sigma}=0$, and Eqs. (3.7a)–(3.7d) turn into the system of linear algebraic equations. One also finds from Eq. (3.7) that $\sigma_{aa}+\sigma_{bb\uparrow}+\sigma_{bb\downarrow}+\sigma_{cc}=1$. The latter implies that dc does not depend on the initial conditions. Finally, we obtain

$$I/e=\frac{2\Gamma_L\Gamma_R'(\Gamma_L'+\Gamma_R)}{\Gamma_L\Gamma_L'+2\Gamma_L\Gamma_R'+\Gamma_R\Gamma_R'}. \tag{3.9}$$

If $E_1\ll E_F^L\ll E_1+U$, one finds from Eq. (3.3) that $\Gamma_L'=0$, so that the state with two electrons inside the well is not available. In this case, one obtains from Eq. (3.9) for the dc,

$$I/e=\frac{2\Gamma_L\Gamma_R}{2\Gamma_L+\Gamma_R}. \tag{3.10}$$

It is interesting to note that this result is different from Eq. (2.16), although in both cases only one electron can occupy the well. However, if the Coulomb repulsion effect is small, i.e., $\Gamma_{L,R}'=\Gamma_{L,R}$, Eq. (3.9) does produce the same result as Eq. (2.16), provided the density of states is doubled due to the spin degrees of freedom.

One can also consider the case when the Fermi level in the right reservoir E_F^R lies above the resonance level E_1, but below E_1+U, so that $\Gamma_R=0$, Eq. (3.3). Then the resonant transitions of electrons from the left to the right reservoirs can go only through the state with two electrons inside the well. Using Eq. (3.9), one finds for the dc,

$$I/e=\frac{2\Gamma_L'\Gamma_R'}{\Gamma_L'+2\Gamma_R'}, \tag{3.11}$$

which coincides with the result found by Glazman and Matveev.[4]

IV. DOUBLE-WELL STRUCTURE

A. Noninteracting electrons

Now we turn to the coherent case of resonant tunneling. Let us consider the coupled-well structure, shown in Fig. 2. We assume that both levels $E_{1,2}$ are inside the band, i.e., $E_F^R\ll E_1,E_2\ll E_F^L$. In order to make our derivation as clear as possible, we begin with the case of no spin degrees of freedom and no Coulomb interaction. The tunneling Hamiltonian for this system is

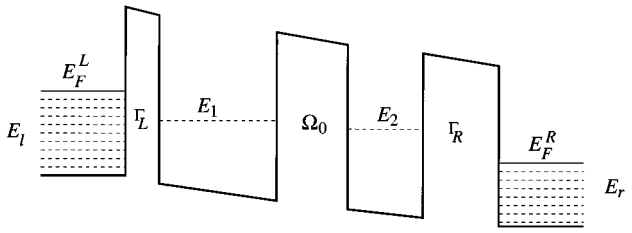

FIG. 2. Resonant transport through a double-well structure.

$$\mathcal{H}=\sum_l E_i a_l^\dagger a_l+E_1a_1^\dagger a_1+E_2a_2^\dagger a_2+\sum_r E_r a_r^\dagger a_r+\Omega_0(a_1^\dagger a_2+a_2^\dagger a_1)+\sum_l \Omega_l(a_l^\dagger a_1+a_1^\dagger a_l)+\sum_r \Omega_r(a_r^\dagger a_2+a_2^\dagger a_r), \tag{4.1}$$

where $a_{1,2}^\dagger, a_{1,2}$ are creation and annihilation operators for an electron in the first or the second well, respectively. All the other notations are taken from Sec. II. The many-body wave function describing this system can be written in the occupation number representation as

$$|\Psi(t)\rangle=\Big[b_0(t)+\sum_l b_{1l}(t)a_1^\dagger a_l+\sum_{l,r} b_{lr}(t)a_r^\dagger a_l+\sum_l b_{2l}(t)a_2^\dagger a_l+\sum_{ll'} b_{12ll'}(t)a_1^\dagger a_2^\dagger a_l a_{l'}+\sum_{l<l',r} b_{1ll'r}(t)a_1^\dagger a_r^\dagger a_l a_{l'}+\cdots\Big]|0\rangle. \tag{4.2}$$

Substituting Eq. (4.2) into the Shrödinger equation with the Hamiltonian (4.1) and performing the Laplace transform, we obtain an infinite set of the coupled equations for the amplitudes $\tilde{b}(t)$:

$$E\tilde{b}_0(E)-\sum_l \Omega_l\tilde{b}_{1l}(E)=i, \tag{4.3a}$$

$$(E+E_l-E_1)\tilde{b}_{1l}(E)-\Omega_l\tilde{b}_0(E)-\Omega_0\tilde{b}_{2l}(E)=0, \tag{4.3b}$$

$$(E+E_l-E_2)\tilde{b}_{2l}(E)-\Omega_0\tilde{b}_{1l}(E)-\sum_{l'} \Omega_{l'}\tilde{b}_{12ll'}(E)-\sum_r \Omega_r\tilde{b}_{rl}(E)=0, \tag{4.3c}$$

$$(E+E_l+E_{l'}-E_1-E_2)\tilde{b}_{12ll'}(E)-\Omega_{l'}\tilde{b}_{2l}(E)+\Omega_l\tilde{b}_{2l'}(E)-\sum_r \Omega_r\tilde{b}_{1ll'r}(E)=0, \tag{4.3d}$$

. . . .

Using exactly the same procedure as in the previous sections, Eq. (2.5), we transform Eqs. (4.3) into the following set of equations:

$$(E+i\Gamma_L/2)\tilde{b}_0(E)=i, \tag{4.4a}$$

$$(E+E_l-E_1)\tilde{b}_{1l}(E)-\Omega_l\tilde{b}_0(E)-\Omega_0\tilde{b}_{2l}(E)=0, \tag{4.4b}$$

$$(E+E_l-E_2+i\Gamma_L/2+i\Gamma_R/2)\tilde{b}_{2l}(E)-\Omega_0\tilde{b}_{1l}(E)=0, \tag{4.4c}$$

$$(E+E_l+E_{l'}-E_1-E_2+i\Gamma_R/2)\tilde{b}_{12ll'}(E)-\Omega_{l'}\tilde{b}_{2l}(E)+\Omega_l\tilde{b}_{l'r}(E)=0, \tag{4.4d}$$

$$\cdots .$$

The amplitudes $b(t)$ determine the density submatrix of the system, $\sigma_{ij}^{(n)}$, in the corresponding Fock space: (a) — the levels $E_{1,2}$ are empty, (b) — the level E_1 is occupied, (c) — the level E_2 is occupied, (d) — both levels $E_{1,2}$ are occupied; the index n denotes the number of electrons in the collector. The matrix elements of the density matrix of the ''device'' can be written as

$$\sigma_{aa}=\sum_n \sigma_{aa}^{(n)}\equiv|b_0(t)|^2+\sum_{l,r}|b_{lr}(t)|^2+\sum_{l<l',r<r'}|b_{ll'rr'}(t)|^2+\cdots, \tag{4.5a}$$

$$\sigma_{bb}=\sum_n \sigma_{bb}^{(n)}\equiv\sum_l|b_{1l}(t)|^2+\sum_{l<l',r}|b_{1ll'r}(t)|^2+\sum_{l<l'<l'',r<r'}|b_{1ll'l''rr'}(t)|^2+\cdots, \tag{4.5b}$$

$$\sigma_{cc}=\sum_n \sigma_{cc}^{(n)}\equiv\sum_l|b_{2l}(t)|^2+\sum_{l<l',r}|b_{2ll'r}(t)|^2+\sum_{l<l'<l'',r<r'}|b_{2ll'l''rr'}(t)|^2+\cdots, \tag{4.5c}$$

$$\sigma_{dd}=\sum_n \sigma_{dd}^{(n)}\equiv\sum_{l<l'}|b_{12ll'}(t)|^2+\sum_{l<l'<l''<l''',r<r'}|b_{12ll'l''l'''rr'}(t)|^2+\cdots, \tag{4.5d}$$

$$\sigma_{bc}=\sum_n \sigma_{bc}^{(n)}\equiv\sum_l b_{1l}(t)b_{2l}^*(t)+\sum_{l<l',r}b_{1ll'r}(t)b_{2ll'r}^*(t)+\cdots. \tag{4.5e}$$

Now we transform Eqs. (4.4) into differential equations for $\sigma^{(n)}(t)$. Consider, for instance, the term $\sigma_{bb}^{(0)}=\Sigma_l|b_{1l}(t)|^2$, Eq. (4.5b), where the amplitudes b_{1l} are determined by Eq. (4.4b). Multiplying Eq. (4.4b) by $\tilde{b}_{1l}^*(E')$ and subtracting the complex conjugate equation with $E\leftrightarrow E'$, we find

$$\sum_l (E'-E)\tilde{b}_{1l}(E)\tilde{b}_{1l}^*(E')-\sum_l \Omega_l[\tilde{b}_0^*(E')\tilde{b}_{1l}(E)-\tilde{b}_0(E)\tilde{b}_{1l}^*(E')]-\Omega_0\sum_l[\tilde{b}_{2l}^*(E')\tilde{b}_{1l}(E)-\tilde{b}_{2l}(E)\tilde{b}_{1l}^*(E')]=0. \tag{4.6}$$

After applying the inverse Laplace transform, Eq. (2.9), the first term in this equation becomes $-i\dot{\sigma}_{bb}^{(0)}(t)$. Next, substituting

$$\tilde{b}_{1l}(E)=\frac{\Omega_l\tilde{b}_0(E)+\Omega_0\tilde{b}_{2l}(E)}{E+E_l-E_1} \tag{4.7}$$

from Eq. (4.4b) into the second term of Eq. (4.6), and replacing the sum by an integral over E_l, we reduce this term to $i\Gamma_L\tilde{b}_0(E)\tilde{b}_0^*(E')$. After the inverse Laplace transform it becomes $i\Gamma_L\sigma_{aa}^{(0)}(t)$. Notice that the ''cross term,'' $\propto\Omega_0\Omega_l\tilde{b}_0\tilde{b}_{2l}$, does not contribute to the integral over E_l, since the poles of the integrand in the E_l variable lie on one side of the integration contour [cf. the second term of Eq. (2.5)]. The third term of Eq. (4.6) turns out to be $\Omega_0[\sigma_{bc}^{(0)}(t)-\sigma_{cb}^{(0)}(t)]$, after the inverse Laplace transform. Finally, we obtain a differential equation for the density submatrix element $\sigma_{bb}^{(0)}$,

$$\dot{\sigma}_{bb}^{(0)}(t)=\Gamma_L\sigma_{aa}^{(0)}+i\Omega_0(\sigma_{bc}^{(0)}-\sigma_{cb}^{(0)}). \tag{4.8}$$

In contrast to the rate equations of the previous sections, the diagonal matrix element σ_{bb} is coupled with the off-diagonal density-matrix element σ_{bc}.

The corresponding differential equation for σ_{bc} can be easily obtained by multiplying Eq. (4.4b) by $\tilde{b}_{2l}^*(E')$ with the subsequent subtraction of the complex conjugated Eq. (4.4c), multiplied by $\tilde{b}_{1l}$. Afterwords, by integrating over E_l, we obtain

$$\dot{\sigma}_{bc}^{(0)}=i(E_2-E_1)\sigma_{bc}^{(0)}+i\Omega_0(\sigma_{bb}^{(0)}-\sigma_{cc}^{(0)})-\tfrac{1}{2}(\Gamma_L+\Gamma_R)\sigma_{bc}^{(0)}. \tag{4.9}$$

Eventually, we arrive to the following set of equations for $\sigma^{(n)}$:

$$\dot{\sigma}_{aa}^{(n)}=-\Gamma_L\sigma_{aa}^{(n)}+\Gamma_R\sigma_{cc}^{(n-1)}, \tag{4.10a}$$

$$\dot{\sigma}_{bb}^{(n)}=\Gamma_L\sigma_{aa}^{(n)}+\Gamma_R\sigma_{dd}^{(n-1)}+i\Omega_0(\sigma_{bc}^{(n)}-\sigma_{cb}^{(n)}), \tag{4.10b}$$

$$\dot{\sigma}_{cc}^{(n)}=-\Gamma_R\sigma_{cc}^{(n)}-\Gamma_L\sigma_{cc}^{(n)}-i\Omega_0(\sigma_{bc}^{(n)}-\sigma_{cb}^{(n)}), \tag{4.10c}$$

$$\dot{\sigma}_{dd}^{(n)}=-\Gamma_R\sigma_{dd}^{(n)}+\Gamma_L\sigma_{cc}^{(n)}, \tag{4.10d}$$

$$\dot{\sigma}_{bc}^{(n)}=i(E_2-E_1)\sigma_{bc}^{(n)}+i\Omega_0(\sigma_{bb}^{(n)}-\sigma_{cc}^{(n)})-\tfrac{1}{2}(\Gamma_L+\Gamma_R)\sigma_{bc}^{(n)}. \tag{4.10e}$$

Using Eqs. (4.10), we can find the charge accumulated in the collector, $N_R(t)$, and subsequently, the total current, $e\dot{N}(t)$, as given by

$$I(t)/e=\dot{N}(t)=\sum_n n[\dot{\sigma}_{aa}^{(n)}(t)+\dot{\sigma}_{bb}^{(n)}(t)+\dot{\sigma}_{cc}^{(n)}(t)+\dot{\sigma}_{dd}^{(n)}(t)]$$

$$=\Gamma_R[\sigma_{cc}(t)+\sigma_{dd}(t)]. \tag{4.11}$$

As in the previous examples, the current is proportional to the total probability of finding an electron in the well adjacent to the right reservoir. The off-diagonal elements of the density matrix do not appear in Eq. (4.11).

Summing up over n in Eqs. (4.10), we obtain the system of differential equations for the density-matrix elements of the device,

$$\dot{\sigma}_{aa}=-\Gamma_L\sigma_{aa}+\Gamma_R\sigma_{cc}, \tag{4.12a}$$

$$\dot{\sigma}_{bb}=\Gamma_L\sigma_{aa}+\Gamma_R\sigma_{dd}+i\Omega_0(\sigma_{bc}-\sigma_{cb}), \tag{4.12b}$$

$$\dot{\sigma}_{cc}=-\Gamma_R\sigma_{cc}-\Gamma_L\sigma_{cc}-i\Omega_0(\sigma_{bc}-\sigma_{cb}), \tag{4.12c}$$

$$\dot{\sigma}_{dd}=-\Gamma_R\sigma_{dd}+\Gamma_L\sigma_{cc}, \tag{4.12d}$$

$$\dot{\sigma}_{bc}=i(E_2-E_1)\sigma_{bc}+i\Omega_0(\sigma_{bb}-\sigma_{cc})-\tfrac{1}{2}(\Gamma_L+\Gamma_R)\sigma_{bc}, \tag{4.12e}$$

[Eqs. (4.12)] resemble the optical Bloch equations.[11] Note that the coupling with the reservoirs produces purely negative contribution into the *nondiagonal* matrix element's dynamic equation, Eq. (4.12e), thus causing damping of this matrix element.

Equations (4.12a)–(4.12e) are solved most easily for the stationary current, $I=I(t\to\infty)$. Using $\sigma_{aa}+\sigma_{bb}+\sigma_{cc}+\sigma_{dd}=1$, we obtain

$$I/e=\left(\frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}\right)\frac{\Omega_0^2}{\Omega_0^2+\Gamma_L\Gamma_R/4+\epsilon^2\Gamma_L\Gamma_R/(\Gamma_L+\Gamma_R)^2}, \tag{4.13}$$

where $\epsilon=E_2-E_1$. This result was obtained earlier in Refs. 12,13 in the framework of one-electron approach, and in Ref. 14 by using rate equations written in the eigenstate basis of the double-well Hamiltonian.[14]

B. Coulomb blockade

The extension of the rate equations (4.12) for the case of spin and Coulomb interaction is done exactly in the same way as in Sec. III. Here, also, the rate equations for the device density matrix are obtained only for $E_{1,2}+U$ inside or outside the band, but not close to the band edges ($E_F^R\ll E_{1,2}+U\ll E_F^L$ or $E_{1,2}+U\gg E_F^L$). Eventually we arrive at the rate equations of type Eqs. (4.12), but with the number of the available states of the device changed due to additional (spin) degrees of freedom and Coulomb blockade restrictions. The Coulomb repulsion manifests itself also in a modification of the transition amplitude Ω and the rates Γ's, Eq. (3.4).

In the case of large Coulomb repulsion, some of electron states of the device are outside the band (the Coulomb blockade). As a result, the number of the equations is reduced. Consider, for instance, the situation where the Coulomb interaction U of two electrons in the same well so large that $E_{1,2}+U\gg E_F^L$, but the Coulomb repulsion of two electrons in different wells, $\overline{U}$, is much smaller, so that $E_{1,2}+\overline{U}\ll E_F^L$. Then the state of two electrons in the same well is not available, but two electrons can occupy different wells. In this case, the rate equations for the corresponding density-matrix elements of the device are

$$\dot{\sigma}_{aa}=-2\Gamma_L\sigma_{aa}+\Gamma_R(\sigma_{cc\uparrow}+\sigma_{cc\downarrow}), \tag{4.14a}$$

$$\dot{\sigma}_{bb\uparrow}=\Gamma_L\sigma_{aa}+\Gamma_R'(\sigma_{dd\uparrow\uparrow}+\sigma_{dd\uparrow\downarrow})+i\Omega_0(\sigma_{bc\uparrow}-\sigma_{cb\uparrow}), \tag{4.14b}$$

$$\dot{\sigma}_{cc\uparrow}=-\Gamma_R\sigma_{cc\uparrow}-2\Gamma_L'\sigma_{cc\uparrow}-i\Omega_0(\sigma_{bc\uparrow}-\sigma_{cb\uparrow}), \tag{4.14c}$$

$$\dot{\sigma}_{dd\uparrow\uparrow}=-\Gamma_R'\sigma_{dd\uparrow\uparrow}+\Gamma_L'\sigma_{cc\uparrow}, \tag{4.14d}$$

$$\dot{\sigma}_{bc\uparrow}=i(E_2-E_1)\sigma_{bc\uparrow}+i\Omega_0(\sigma_{bb\uparrow}-\sigma_{cc\uparrow})-\tfrac{1}{2}(2\Gamma_L'+\Gamma_R)\sigma_{bc\uparrow}, \tag{4.14e}$$

where $\Gamma_{L(R)}'=2\pi\rho_{L(R)}(E_1+\overline{U})|\Omega_{L(R)}(E_1+\overline{U})|^2$. Here, to be brief, we wrote only the equations for the ''spin up'' component of the density matrix. The same equations are obtained for the ''spin down'' components of the density matrix. The total current is

$$I/e=\Gamma_R(\sigma_{cc\uparrow}+\sigma_{cc\downarrow})+\Gamma_R'(\sigma_{dd\uparrow\uparrow}+\sigma_{dd\uparrow\downarrow}+\sigma_{dd\downarrow\uparrow}+\sigma_{dd\downarrow\downarrow}). \tag{4.15}$$

It is quite clear that the ''spin up'' and ''spin down'' components of the density matrix are equal, i.e., $\sigma_{bb\uparrow}=\sigma_{bb\downarrow}=\sigma_{bb}$, the same holding for σ_{cc}, σ_{dd} components. Therefore, Eqs. (4.14) and (4.15) can be rewritten as

$$\dot{\sigma}_{aa}=-2\Gamma_L\sigma_{aa}+2\Gamma_R\sigma_{cc}, \tag{4.16a}$$

$$\dot{\sigma}_{bb}=\Gamma_L\sigma_{aa}+2\Gamma_R'\sigma_{dd}+i\Omega_0(\sigma_{bc}-\sigma_{cb}), \tag{4.16b}$$

$$\dot{\sigma}_{cc}=-\Gamma_R\sigma_{cc}-2\Gamma_L'\sigma_{cc}-i\Omega_0(\sigma_{bc}-\sigma_{cb}), \tag{4.16c}$$

$$\dot{\sigma}_{dd}=-\Gamma_R'\sigma_{dd}+\Gamma_L'\sigma_{cc}, \tag{4.16d}$$

$$\dot{\sigma}_{bc}=i(E_2-E_1)\sigma_{bc}+i\Omega_0(\sigma_{bb}-\sigma_{cc})-\tfrac{1}{2}(2\Gamma_L'+\Gamma_R)\sigma_{bc}, \tag{4.16e}$$

and

$$I/e=2\Gamma_R\sigma_{cc}+4\Gamma_R'\sigma_{dd}. \tag{4.17}$$

Using $\sigma_{aa}+2\sigma_{bb}+2\sigma_{cc}+4\sigma_{dd}=1$, we obtain for the dc

$$I/e=\left(\frac{2\Gamma_L\Gamma_R'}{2\Gamma_L'+\Gamma_R}\right)\frac{\Omega_0^2}{4\Omega_0^2\dfrac{\Gamma_L\Gamma_L'+\Gamma_L\Gamma_R'+\Gamma_R\Gamma_R'/4}{(2\Gamma_L'+\Gamma_R)^2}+\dfrac{\Gamma_L\Gamma_R'}{2}+\epsilon^2\dfrac{2\Gamma_L\Gamma_R'}{(2\Gamma_L'+\Gamma_R)^2}}, \tag{4.18}$$

where $\epsilon = E_2 - E_1$. Notice that the current (4.18) differs from that given by Eq. (4.13) even for $\Gamma_L' = \Gamma_L$ and $\Gamma_R' = \Gamma_R$, despite the fact that in both cases only one electron can occupy each of the wells.

It is interesting to compare our result with that of Stoof and Nazarov[15] for the case of strong Coulomb repulsion between two electrons in different wells ($E_{1,2} + U \gg E_F^L$), where only one electron can be found inside the system. It corresponds to $\Gamma_L' = 0$. In this case, the dc current given by Eq. (4.18) is

$$I/e = \frac{\Gamma_R \Omega_0^2}{\Omega_0^2(2 + \Gamma_R/2\Gamma_L) + \Gamma_R^2/4 + \epsilon^2}. \tag{4.19}$$

This result is slightly different from that obtained by Stoof and Nazarov (by the factor two in front of Γ_L). The difference stems from the account of spin components in the rate equations, which has not been done in Ref. 15.

V. INELASTIC PROCESSES

As an example of a system with coherent tunneling accompanied by inelastic scattering, let us consider the coupled-dot structure shown in Fig. 3. In this system, a resonant current flows due to inelastic transition from the upper to the lower level in the left well. For simplicity, we restrict ourselves to noninteracting spinless electrons. The Coulomb interaction and the spin effects can be accounted for precisely in the same way as in the previous sections, namely, by allowing for states with doubly occupied levels (excluding states violating Coulomb restrictions) and modifying transition amplitudes and inelastic rates.

The tunneling Hamiltonian of the system has the following structure:

$$\begin{aligned}\mathcal{H} = &\sum_l E_l a_l^\dagger a_l + E_1 a_1^\dagger a_1 + E_2 a_2^\dagger a_2 + E_3 a_3^\dagger a_3 + \sum_\alpha E_\alpha^{\rm ph} c_\alpha^\dagger c_\alpha \\ &+ \sum_r E_r a_r^\dagger a_r + \Omega_0 (a_2^\dagger a_3 + a_3^\dagger a_2) + \sum_l \Omega_l (a_l^\dagger a_1 + a_1^\dagger a_l) \\ &+ \sum_\alpha \Omega_\alpha^{\rm ph} (a_2^\dagger a_1 c_\alpha^\dagger + a_1^\dagger a_2 c_\alpha) + \sum_r \Omega_r (a_r^\dagger a_3 + a_3^\dagger a_r).\end{aligned} \tag{5.1}$$

Here, the subscript α enumerates the states in the phonon bath and $\Omega_\alpha^{\rm ph}$ is the corresponding coupling. The many-particle time-dependent wave function of the system is

$$\begin{aligned}|\Psi(t)\rangle = \Bigg[&b_0(t) + \sum_l b_{1l}(t) a_1^\dagger a_l + \sum_{l,\alpha} b_{2l\alpha}(t) a_2^\dagger a_l c_\alpha^\dagger \\ &+ \sum_{l,\alpha} b_{3l\alpha}(t) a_3^\dagger a_l c_\alpha^\dagger + \sum_{l<l',\alpha} b_{12ll'\alpha}(t) a_1^\dagger a_2^\dagger a_l a_{l'} c_\alpha^\dagger \\ &+ \sum_{l<l',\alpha} b_{13ll'\alpha}(t) a_1^\dagger a_3^\dagger a_l a_{l'} c_\alpha^\dagger + \cdots \Bigg] |0\rangle.\end{aligned} \tag{5.2}$$

Repeating the procedure of the previous sections, we find the following set of equations for the Laplace transformed amplitudes, $\tilde{b}(E)$:

$$(E + i\Gamma_L/2)\tilde{b}_0 = i, \tag{5.3a}$$

$$(E + E_l - E_1 + i\Gamma_{\rm in}/2)\tilde{b}_{1l} - \Omega_l \tilde{b}_0 = 0, \tag{5.3b}$$

$$(E + E_l - E_\alpha - E_2 + i\Gamma_L/2)\tilde{b}_{2l\alpha} - \Omega_\alpha^{\rm ph}\tilde{b}_{1l} - \Omega_0 \tilde{b}_{3l\alpha} = 0, \tag{5.3c}$$

$$(E + E_l - E_\alpha - E_3 + i\Gamma_L/2 + i\Gamma_R/2)\tilde{b}_{3l\alpha} - \Omega_0 \tilde{b}_{2l\alpha} = 0, \tag{5.3d}$$

$$\begin{aligned}(E + E_l + E_{l'} - E_1 - E_2 - E_\alpha)\tilde{b}_{12ll'\alpha} - \Omega_{l'}\tilde{b}_{2l\alpha} + \Omega_l \tilde{b}_{2l'\alpha} \\ - \Omega_0 \tilde{b}_{13ll'\alpha} = 0,\end{aligned} \tag{5.3e}$$

$$\begin{aligned}(E + E_l + E_{l'} - E_1 - E_3 - E_\alpha + i\Gamma_{\rm in}/2 + i\Gamma_R/2)\tilde{b}_{13ll'\alpha} \\ - \Omega_0 \tilde{b}_{12ll'\alpha} - \Omega_{l'}\tilde{b}_{3l\alpha} + \Omega_l \tilde{b}_{3l'\alpha} = 0,\end{aligned} \tag{5.3f}$$

. . . .

where $\Gamma_{\rm in} = 2\pi\rho_{\rm ph}|\Omega^{\rm ph}|^2$ is the partial width of the level E_1 due to phonon emission and $\rho_{\rm ph}$ is the density of phonon states.

The density matrix elements of the device is $\sigma_{ij}(t) = \Sigma_n \sigma_{ij}^{(n)}(t)$, where $\sigma_{ij}^{(n)}(t)$, are related to the amplitudes $\tilde{b}(E)$ via Eq. (2.9). All possible states electron states of the device are shown in Fig. 4. Using the previous section procedure for *diagonal* matrix elements, we obtain master equations analogous to Eq. (4.12), in which transitions between isolated levels E_2 and E_3 take place through the coupling with nondiagonal matrix elements. These equations have the appearance of the optical Bloch equation.[11] However, the master equation for the *nondiagonal* matrix element, σ_{ef}, contains an additional term. Therefore, we present the derivation of the master equations for ''coherences'' σ_{ef} and σ_{cd} in some detail. Consider, for example, the nondiagonal density submatrix elements $\sigma_{cd}^{(0)} = \Sigma_{l,\alpha} b_{2l\alpha}(t) b_{3l\alpha}^*(t)$ and $\sigma_{ef}^{(0)} = \Sigma_{l<l',\alpha} b_{12ll'\alpha}(t) b_{13ll'\alpha}^*(t)$. The differential equation for $\sigma_{cd}^{(0)}(t)$ can be obtained by multiplying Eq. (5.3c) by $\tilde{b}_{3l\alpha}^*(E')$, with subsequent subtraction of the complex conjugated Eq. (5.3d), multiplied by $\tilde{b}_{2l\alpha}(E)$. Then using Eq. (2.9), we obtain

$$\begin{aligned}\dot{\sigma}_{cd}^{(0)} = &i(E_3 - E_2)\sigma_{cd}^{(0)} + i\Omega_0(\sigma_{cc}^{(0)} - \sigma_{dd}^{(0)}) \\ &- \tfrac{1}{2}(2\Gamma_L + \Gamma_R)\sigma_{cd}^{(0)}.\end{aligned} \tag{5.4}$$

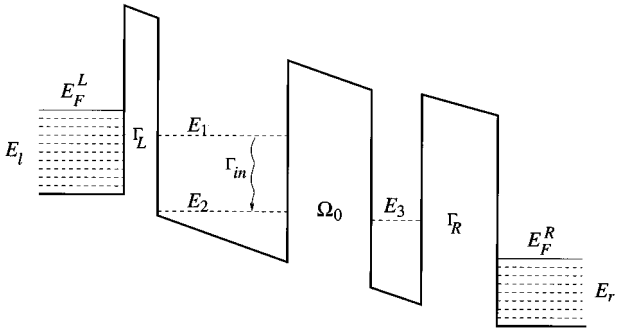

FIG. 3. Resonant transport through a double-well structure in the presence of inelastic process.

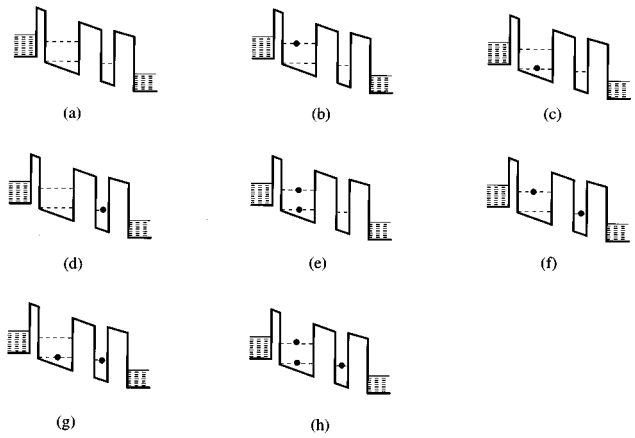

FIG. 4. All possible electron states of the device, shown in Fig. 3: (a) —all the levels $E_{1,2,3}$ are empty; (b) — the upper level, E_1, is occupied; (c) — the lower level, E_2, is occupied; (d) — the level E_3 is occupied; (e) — the levels E_1 and E_2 are occupied; (f) — the levels E_1 and E_3 are occupied; (g) — the levels E_2 and E_3 are occupied; (h) — all the levels $E_{1,2,3}$ are occupied.

Similarly, multiplying Eq. (5.3e) by $\tilde{b}^*_{13ll'\alpha}(E')$ and Eq. (5.3f) by $\tilde{b}_{12ll'\alpha}(E)$, we find the differential equation for $\sigma^{(0)}_{ef}(t)$,

$$\dot{\sigma}^{(0)}_{ef}=i(E_3-E_2)\sigma^{(0)}_{ef}+i\Omega_0(\sigma^{(0)}_{ee}-\sigma^{(0)}_{ff}) - \tfrac{1}{2}(\Gamma_{\rm in}+\Gamma_R)\sigma^{(0)}_{ef}-i\Delta, \tag{5.5}$$

where

$$\Delta=\sum_{l<l',\alpha}\int\frac{dE\,dE'}{4\pi^2}[\tilde{b}^*_{13ll'\alpha}(E')\Omega_{l'}\tilde{b}_{2l\alpha}(E) -\tilde{b}^*_{13ll'\alpha}(E')\Omega_l\tilde{b}_{2l'\alpha}(E)-\tilde{b}_{12ll'\alpha}(E)\Omega_{l'}\tilde{b}^*_{3l\alpha}(E') +\tilde{b}_{12ll'\alpha}(E)\Omega_l\tilde{b}^*_{3l'\alpha}(E')]e^{i(E'-E)t}. \tag{5.6}$$

Substituting the amplitudes $\tilde{b}_{12ll'\alpha}$ from Eq. (5.3e) and $\tilde{b}^*_{13ll'\alpha}$ from Eq. (5.3f) into Eq. (5.6), and replacing the sum over $l(l')$ by the corresponding integral, we find $-i\Delta=\Gamma_L\sigma^{(0)}_{cd}$. It implies that the nondiagonal density matrix σ_{ef} given by Eq. (5.5), is coupled with σ_{cd} via a single-electron transition from the emitter to the left well. Such a term does not appear in the Bloch equations, which deal with two-level systems.

Summing up over n in the rate equations for the density submatrix $\sigma^{(n)}_{ij}(t)$, we obtain the set of rate equations for the density-matrix of the device

$$\dot{\sigma}_{aa}=-\Gamma_L\sigma_{aa}+\Gamma_R\sigma_{dd}, \tag{5.7a}$$

$$\dot{\sigma}_{bb}=\Gamma_L\sigma_{aa}-\Gamma_{\rm in}\sigma_{bb}+\Gamma_R\sigma_{ff}, \tag{5.7b}$$

$$\dot{\sigma}_{cc}=\Gamma_{\rm in}\sigma_{bb}+i\Omega(\sigma_{cd}-\sigma_{dc})+\Gamma_R\sigma_{gg}-\Gamma_L\sigma_{cc}, \tag{5.7c}$$

$$\dot{\sigma}_{dd}=-\Gamma_R\sigma_{dd}+i\Omega(\sigma_{dc}-\sigma_{cd})-\Gamma_L\sigma_{dd}, \tag{5.7d}$$

$$\dot{\sigma}_{ee}=\Gamma_L\sigma_{cc}+i\Omega(\sigma_{ef}-\sigma_{fe})+\Gamma_R\sigma_{hh}, \tag{5.7e}$$

$$\dot{\sigma}_{ff}=\Gamma_L\sigma_{dd}-\Gamma_R\sigma_{ff}+i\Omega(\sigma_{fe}-\sigma_{ef})-\Gamma_{\rm in}\sigma_{ff}, \tag{5.7f}$$

$$\dot{\sigma}_{gg}=\Gamma_{\rm in}\sigma_{ff}-\Gamma_R\sigma_{gg}-\Gamma_L\sigma_{gg}, \tag{5.7g}$$

$$\dot{\sigma}_{hh}=\Gamma_L\sigma_{gg}-\Gamma_R\sigma_{hh}, \tag{5.7h}$$

$$\dot{\sigma}_{cd}=i(E_3-E_2)\sigma_{cd}+i\Omega(\sigma_{cc}-\sigma_{dd})-1/2(2\Gamma_L+\Gamma_R)\sigma_{cd}, \tag{5.7i}$$

$$\dot{\sigma}_{ef}=i(E_3-E_2)\sigma_{ef}+i\Omega(\sigma_{ee}-\sigma_{ff})-1/2(\Gamma_{\rm in}+\Gamma_R)\sigma_{ef} +\Gamma_L\sigma_{cd}, \tag{5.7j}$$

and the resonant current flowing through this system is $I/e=\Gamma_R[\sigma_{dd}+\sigma_{ff}+\sigma_{gg}+\sigma_{hh}]$.

VI. GENERAL CASE

Now utilizing the results obtained in the previous sections, we can write the rate equations for the general case. These equations describing the time evolution of the density matrix $\sigma_{ab}(t)$ of the device are as follows:

$$\dot{\sigma}_{aa}=i\sum_{b(\neq a)}\Omega_{ab}(\sigma_{ab}-\sigma_{ba})-\sigma_{aa}\sum_{d(\neq a)}\Gamma_{a\to d} +\sum_{c(\neq a)}\sigma_{cc}\Gamma_{c\to a}, \tag{6.1a}$$

$$\dot{\sigma}_{ab}=i(E_b-E_a)\sigma_{ab} +i\left(\sum_{b'(\neq b)}\sigma_{ab'}\Omega_{b'b}-\sum_{a'(\neq a)}\Omega_{aa'}\sigma_{a'b}\right) -\frac{1}{2}\sigma_{ab}\left(\sum_{d(\neq a)}\Gamma_{a\to d}+\sum_{d(\neq b)}\Gamma_{b\to d}\right) +\frac{1}{2}\sum_{a'b'\neq ab}\sigma_{a'b'}(\Gamma_{a'\to a}+\Gamma_{b'\to b}), \tag{6.1b}$$

where Ω_{ab} denote the couplings between nonorthogonal isolated states, as, for instance, between the levels in adjacent wells, and $\sigma_{ba}=\sigma^*_{ab}$. The width $\Gamma_{a\to b}$ is the probability per unit time for the system to make a transition from the state $|a\rangle$ to the state $|b\rangle$ of the device, due to the tunneling to (or from) the reservoirs, or due to interaction with the phonon bath, or any other interaction, generated by a continuum state medium. Notice that Eq. (6.1a) for diagonal elements has a classical rate equation form, except for the first term. This term describes transitions between isolated states through the coupling with nondiagonal terms. Therefore, it is responsible for coherent (quantum) effects in the transport.

The nondiagonal matrix elements are described by Eq. (6.1b), which resembles the corresponding Bloch equation, supplemented with an additional term. The latter appears whenever a *one-electron* transition converts the state $|a'\rangle$ into $|a\rangle$ *and* the state $|b'\rangle$ into $|b\rangle$. The positive sign of the additional term calls forth a suspicion that Eq. (6.1b) might have unbounded solutions. This is not the case, however, since any positive contribution from the additional term in the equation for $\dot{\sigma}_{ab}$ has its negative counterpart in the equation for $\dot{\sigma}_{a'b'}$, which corresponds to the conversion

$(a'b')\rightarrow(ab)$ and originates from the third term in the rhs of Eq. (6.1b). Moreover, the negative contributions, corresponding to the conversions $(ab)\rightarrow(a'b)$ and $(ab)\rightarrow(ab')$ have no positive counterparts. Therefore, the coupling with continuum leads to negative total balance, and hence, to the damping of nondiagonal matrix elements.

The current through the mesoscopic device is the time derivative of the total charge accumulated in the collector. We find that the current is totally determined through the *diagonal* elements of the density matrix of the device by the following relation:

$$I(t)=e\sum_{c}\ \sigma_{cc}(t)\Gamma_{R}^{(c)}, \tag{6.2}$$

where $|c\rangle$ are the occupied states in the well adjacent to the collector, and $\Gamma_{R}^{(c)}$ is the partial width of the state $|c\rangle$, due to tunneling to the collector.

Although the nondiagonal density-matrix elements do not enter explicitly in Eq. (6.2), they are coupled with diagonal matrix elements in the rate equations [the first term in (6.1a)], and therefore influence the resonant current. The coupling with nondiagonal elements always appears in the rate equation, whenever a carrier jumps from one to another *isolated* states inside the device. In the absence of such transition as, for instance, in resonant tunneling through a single well, the diagonal and nondiagonal matrix elements are decoupled and the evolution of diagonal density-matrix elements is described by the *classical* rate equation.

Hence, the distinction between isolated and continuum states becomes very essential in the description of quantum transport. At first sight, it may seem that in a real situation such a distinction can hardly be carried out, since there are no pure isolated states. For instance, a single-electron state inside the device is always coupled with the continuum states of phonons. However, the corresponding density of states would display peaks in energy dependence, and they can be considered as isolated states. Indeed, if we have written equations like Eqs. (2.5), (3.3), etc., for such a system, the contribution from these peaks in the integrals over continuum states would generate a coupling with nondiagonal density-matrix elements in the rate equations, just as in a transition between two isolated states, Eqs. (6.1).

As an example of the application of Eq. (6.1) in the case of strong Coulomb blockade, we consider the system shown in Fig. 5. The wells may represent two coupled dots. An electron tunnels from the emitter to the first well, and then to the second well into the upper level E_2. After that, it can either relax inelastically into the lower level E_3 due to interaction with the phonon bath, and then tunnel into the collector, or tunnel out directly into the collector. Here, $\Gamma_{\rm in}$ and Γ_R' are the partial widths of the upper level, E_2, due to coupling to the phonon reservoir and the collector, respectively, and Γ_R is the width of the level E_3, due to coupling to the collector. Let us assume that the Coulomb blockade prevents the system from being occupied by two electrons, even in different wells. Then there are four possible states of the device (a) — all the levels $E_{1,2,3}$ are empty; (b) — the level E_1 is occupied; (c) — the level E_2 is occupied; (d) — the level E_3 is occupied. It is clear that the density-matrix elements for an electron with spin up and spin down inside the system are equal, $\sigma_{bb\uparrow}=\sigma_{bb\downarrow}=\sigma_{bb}$, and the same holds for σ_{cc} and σ_{dd}. Hence, Eqs. (6.1) can be written in this case as

$$\dot{\sigma}_{aa}=-2\Gamma_L\sigma_{aa}+2\Gamma_R'\sigma_{cc}+2\Gamma_R\sigma_{dd}, \tag{6.3a}$$

$$\dot{\sigma}_{bb}=i\Omega_0(\sigma_{bc}-\sigma_{cb})+\Gamma_L\sigma_{aa}, \tag{6.3b}$$

$$\dot{\sigma}_{cc}=-i\Omega_0(\sigma_{bc}-\sigma_{cb})-(\Gamma_R'+\Gamma_{\rm in})\sigma_{cc}, \tag{6.3c}$$

$$\dot{\sigma}_{dd}=-\Gamma_R\sigma_{dd}+\Gamma_{\rm in}\sigma_{cc}, \tag{6.3d}$$

$$\dot{\sigma}_{bc}=i(E_2-E_1)\sigma_{bc}+i\Omega_0(\sigma_{bb}-\sigma_{cc})-\frac{1}{2}(\Gamma_R'+\Gamma_{\rm in})\sigma_{bc}, \tag{6.3e}$$

and the dc I, Eq. (6.2), is given by

$$I/e=2\sigma_{cc}\Gamma_R'+2\sigma_{dd}\Gamma_R. \tag{6.4}$$

Using $\sigma_{aa}+2\sigma_{bb}+2\sigma_{cc}+2\sigma_{dd}=1$, Eqs. (6.3) can be easily solved for $t\rightarrow\infty$, yielding for the dc

$$I/e=\left(\frac{2\Gamma_L\Gamma_R}{\Gamma_{\rm in}+\Gamma_R'}\right)\frac{\Omega_0^2}{\Omega_0^2\dfrac{2\Gamma_{\rm in}\Gamma_L+\Gamma_{\rm in}\Gamma_R+4\Gamma_L\Gamma_R+\Gamma_R\Gamma_R'}{(\Gamma_{\rm in}+\Gamma_R')^2}+\dfrac{\Gamma_L\Gamma_R}{2}+\epsilon^2\dfrac{2\Gamma_L\Gamma_R}{(\Gamma_{\rm in}+\Gamma_R')^2}}. \tag{6.5}$$

This result shows a very peculiar dependence of the dc of the inelastic width $\Gamma_{\rm in}$. One could expect, at least for $\Gamma_R'\sim\Gamma_R$, that the current should increase when $\Gamma_{\rm in}$ grows. However, as follows from Eq. (6.3), the current $I\rightarrow 0$ for $\Gamma_{\rm in}\rightarrow\infty$ (cf. with another example in Ref. 10). In fact, such an unexpected behavior of the dc would always take place in the presence of coherent transitions between isolated states in carrier transport. For instance, it can be traced even in a more simple case of the resonant tunneling through a double-well structure, Eq. (4.19). One finds that $I\rightarrow 0$ when $\Gamma_R\rightarrow\infty$. This phenomenon can be understood by analyzing Eq. (6.1b) for nondiagonal density-matrix elements. In contrast with the rate equation for diagonal matrix elements, Eq. (6.1a), the coupling with continuum states always leads to damping of nondiagonal matrix elements. Since the transport through isolated states goes only via nondiagonal density-matrix ele-

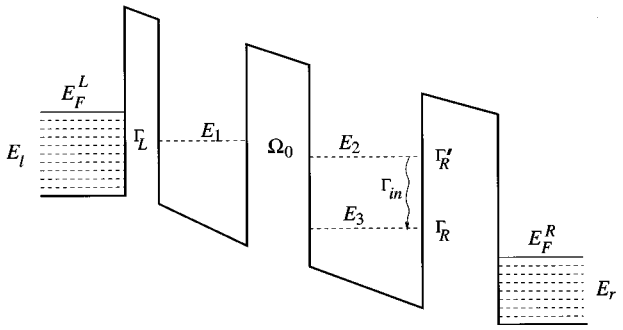

FIG. 5. Resonant transport through a double-well structure in the presence of inelastic process with strong Coulomb blockade effects.

ments, Eq. (6.1a), the total current would always decrease with the growth of the corresponding partial widths.

VII. SUMMARY

In this paper, we have studied quantum transport in mesoscopic systems (quantum dots) containing a finite number of isolated quantum states. Starting with the many-particle wave function in the occupation number representation, and integrating out the continuum states, we have found the equations of motion for the density submatrix of the system. These equations have a form of the master (rate) equations for diagonal density-matrix element. But in addition, nondiagonal density-matrix elements, responsible for transitions between isolated quantum states, appear in these equations. If, however, these transitions are generated by a continuum states medium, the diagonal and nondiagonal density-matrix elements become decoupled, and the quantum transport is described by classical rate equations.

It follows from our derivation that the reduction of many-body Schrödinger equation to the modified rate equations for density submatrix of the device can be performed only if two conditions are met: first, the energy states of the system which carry the resonant transport must be inside the bias, $E_F^L - E_F^R$; second, the width of these states is much smaller than the bias. If the second condition is satisfied, but the resonant levels of the device are close to band edges, our rate equations cannot be derived. Yet, the method still can be used for a dc. However, when the bias is less than the level width, the continuum states of the reservoir cannot be integrated out in the manner of Sec. II, and our method cannot be applied.

We have compared some of our results with results that were obtained earlier in the literature. For example, for the resonant tunneling through a single dot, we obtained the same result as Glazman and Matveev.[4] In the case of resonant tunneling through double-dot structure, we found simple analytical expression for a dc under a condition of strong Coulomb repulsion inside the dots, when no more than one electron can occupy the dots. The obtained expression is very close to that found in Refs. 9 and 15 in a phenomenological rate equation approach.

Of course, the quantum transport in multidot structures can be treated by different methods, which are not necessarily the rate equations. For instance, the multidimensional Landauer approach[16] has been used to study the resistance resonances in multiple-dot structures.[17] However, charging effects have not been included. In fact, their account is rather complicated in the framework of Landauer approach. Also the nonequilibrium Green's function method[18] has been used to study multibarrier resonant tunneling, again without charging effects.[19] The charging can be taken into account via direct diagonalization of the multidot Hamiltonian. It has been done for double-dot[20] and multiple-dot[21] systems by assuming weak coupling to the leads. Yet, this treatment is mainly numerical, and the inelastic scattering is accounted for phenomenologically. In contrast, the quantum rate equations method allows in many cases the analytical treatment of the problem. It also proves to be technically much simpler than the other approaches. An even more important advantage of our treatment is that the effects of charging, inelastic scattering, and coupling with the leads are included from the very beginning.

As an application of our equations, we considered a more complicated case of the resonant tunneling in a coupled-dot system, where the inelastic process takes place in the course of transport. It was found that the resonant current decreases with the growth of the inelastic width. We found that this anomalous behavior always emerges whenever coherent transitions are accompanied by inelastic processes.

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