A theory of tunneling through a quantum dot is presented which enables us to study combined effects of Coulomb blockade and discrete energy spectrum of the dot. The expression of tunneling current is derived from the Keldysh Green’s function method, and is shown to automatically satisfy the conservation at DC current of both junctions.

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Over the past decade, the Coulomb blockade of tunneling has attracted growing interest mainly because of its possible applications in single-electron electronics. In view of ongoing advances in microfabrication techniques of semiconductor devices whose discrete energy-level structures are prominent, it seems urgent to develop a general theory of tunneling which allows us to analyze combined effects of Coulomb blockade and discrete energy-level spectrum of the quantum dot. While a number of articles study the combined effects, in a usual perturbative treatment, the current conservation has been satisfied by adjusting a fitting parameter such as a electrochemical potential of the island. By generalizing the Keldysh equation developed by Caroli et al., we obtain an expression for the \( I-V \) characteristics such that the currents at the left and right junctions satisfy the conservation of DC current. We also find that the half-width of the resonant peak (written by \( \Gamma_{nn'} \) below) is strongly modulated by the Coulomb interaction.

The system consists of two tunnel junctions with capacitances \( C_L \) and \( C_R \), and a gate capacitor \( C_g \) connected to the central island. The Hamiltonian consists of the electronic part \( \hat{H}_E \), the transfer part \( \hat{H}_T \), and the part \( \hat{H}_{EM} \) that describes the electromagnetic (EM) environment surrounding the junctions. The electronic part consists of electrode and island parts,

\[
\hat{H}_E = \sum_{k, \alpha \in L, R} E_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} + \sum_{m} \left[ E_m \delta_{mn} \hat{d}_m \hat{d}_m + V_{mn}^\mathrm{imp} \hat{d}_m \hat{d}_n \right],
\]

where \( \alpha \) represents a set of parameters that, together with wave vectors \( \mathbf{k} \), completely specify the electronic state of the left (L) or right (R) electrode, and \( m, n \) specify the energy levels of the central island. The symbol \( \delta_{mn} \) denotes the Kronecker’s delta and \( V_{mn}^\text{imp} \) describe matrix elements of impurity scatterings in the island. The transfer part is described by

\[
\hat{H}_T = \sum_{n\kappa_0 \in L, R} \left[ V_{n\kappa_0}(t) \hat{c}_{\kappa_0}^\dagger e^{i\phi_{\kappa_0}} \hat{d}_n + \text{h.c.} \right],
\]

where \( \phi_{\kappa_0} \) are the phase operators which are canonically conjugate to the charge operators \( \hat{Q}_{\kappa} \) on the junctions, satisfying the commutation relations \([\hat{\phi}_{\kappa}, \hat{Q}_{\beta}] = i e \delta_{\alpha \beta} \). The EM part is described by

\[
\hat{H}_{EM} = \frac{\hat{Q}_L^2}{2C_L} + \frac{\hat{Q}_R^2}{2C_R} + \frac{\hat{Q}_g^2}{2C_g} - \hat{Q}_LV - \hat{Q}_gV_g + H(\{\hat{\phi}_{\kappa}\})
\]

\[
= \frac{(\hat{Q}_L - C_0V)^2}{2C_L} + \frac{(\hat{Q}_R - C_0V)^2}{2C_R} + \frac{\hat{Q}_g^2}{2C_g} + H(\{\hat{\phi}_{\kappa}\}) + \text{const.,}
\]

where \( C_0 \equiv C_L + C_R \), \( C_S \equiv C_L + C_R + C_g \), \( C_\Sigma = C_L C_g / (C_L + C_g) \), and \( H(\{\hat{\phi}_{\kappa}\}) \) describes the phase part of the Hamiltonian whose concrete form depends on the external circuit. In the second line of Eq. (1), new operators \( \hat{q}_L \) and \( \hat{q}_R \) are introduced such that

\[
\frac{\hat{Q}_L}{C_L} = \frac{C_R + C_g}{C_S} \frac{\hat{q}}{C_0} + \frac{i \hat{q}}{} - C_0 \frac{V_g}{C_0},
\]

\[
\frac{\hat{Q}_R}{C_R} = \frac{C_L + C_g}{C_S} \frac{\hat{q}}{C_0} - \frac{i \hat{q}}{} + C_0 \frac{V_g}{C_0},
\]

\[
\frac{\hat{Q}_g}{C_g} = -\frac{C_L + C_g}{C_S} \frac{\hat{q}}{C_0} + \frac{i \hat{q}}{} + C_0 \frac{V_g}{C_0} + V_g.
\]

The commutation relations for the new operators are given by \( [\hat{\psi}, \hat{q}] = i e \) and \( [\hat{\psi}, \hat{Q}] = i e \), where

\[
\hat{\theta}_L = \hat{\psi} + \kappa_L \hat{\phi}, \quad \hat{\theta}_R = -\hat{\psi} + \kappa_R \hat{\phi}
\]

(2)

with \( \kappa_L \equiv C_R / (C_L + C_R) \) and \( \kappa_R \equiv C_L / (C_L + C_R) \). The current at junction \( \alpha (=L \text{ or } R) \) is given by

\[
J_{\alpha}(t) = (-1)^{\beta} \frac{2e}{h} \text{Re} \left\{ \sum_{n\kappa_0} V_{n\kappa_0}(t) \tilde{G}_{n\kappa_0}^<(t, t) \right\},
\]

(3)

where \( \beta = 0 \) for the left junction and \( \beta = 1 \) for the right junction and \( \tilde{G}_{n\kappa_0}^<(t, t') \equiv i(e_{n\kappa_0}(t) e^{-i\phi_{\kappa_0}(t')} \hat{d}_n(t')) \) is an analytic continuation of the contour-ordered Green’s function \( G_{n\kappa_0}^<(\tau, \tau') \) which is defined in the interaction representation by

\[
\tilde{G}_{n\kappa_0}^<<(\tau, \tau') \equiv i(T_C e_{n\kappa_0}(\tau') e^{-i\phi_{\kappa_0}(\tau')} \hat{d}_n(\tau) \times \exp \left( \frac{1}{\hbar} \int_{\tau}^{\tau'} \hat{H}_T(\tau_1) d\tau_1 \right) \bigg|_{\tau = \tau'}),
\]

(4)
where $T_C$ is the contour-ordering operator. We assume that electrons in the left and right electrodes are noninteracting. Then the only nonvanishing terms in Eq. (3) are those in which $\tilde{c}_\alpha^\dagger (\tau)$ is contracted with $\tilde{c}_\alpha (\tau_1)$ in the exponential term.

$$\tilde{G}_{n_k}(\tau, \tau') = \int \frac{d\tau}{\hbar} \sum_m V^*_m (\tau_2) \langle T_C \{ \tilde{c}_\alpha^\dagger (\tau) \tilde{c}_\alpha (\tau_2) \} \rangle,$$

where $\tilde{G}_{n_k}(\tau, \tau')$ is the Green’s function of the central island, and $\tilde{c}_\alpha^\dagger (\tau)$ and $\tilde{c}_\alpha (\tau_2)$ are given in terms of $\tilde{g}_{\alpha}(t_0, t_2) \equiv i\langle \tilde{c}_\alpha^\dagger (t_2) \tilde{c}_\alpha (t_1) \rangle$ as $\tilde{g}_{\alpha}(t_1, t_2) = \int 2\sigma_r, t \tilde{g}_{\alpha}(t_1, t_2) = \theta(t_2 - t_1)\tilde{g}_{\alpha}(t_1, t_2) \tilde{P}^\alpha_{\alpha}(t_1, t_2) = \tilde{g}_{\alpha}(t_1, t_2) \tilde{P}^\alpha_{\alpha}(t_1, t_2).$

The third term describes effects of scattering:

$$\Sigma^<_{s_n t_n} (t_1, t_2) = \sum_{k, m} \frac{V^*_m (\tau_1) V^*_n (\tau_2)}{\hbar^2} G^<_{n_k} (t_1, t_2) P^<_{\alpha} (t_1, t_2),$$

and the fourth term describes effects of tunneling:

$$\Sigma^<_{s_n t_n} (t_1, t_2) = \sum_{k, m} \frac{V^*_m (\tau_1) V^*_n (\tau_2)}{\hbar^2} G^<_{n_k} (t_1, t_2) P^<_{\alpha} (t_1, t_2).$$
\[ \Lambda_n(\epsilon)^2 + \eta_n^2 = \pi \delta(\epsilon - E_n - V_d + \Lambda_n(\epsilon)). \]
If \( \Sigma^{>\alpha}\!(t) = \sum_{\kappa\alpha} \Gamma_{\kappa n\alpha}(t) g_{\kappa n}(t) P_{\alpha}^<\!(t)/2\pi \), Eq. \((13)\) is cast into
\[ J_\alpha = (-1)^3 \frac{e}{\hbar^2} \int_0^\infty \frac{d\epsilon}{2\pi} \left( G_n^>(\epsilon) \Sigma^{>\alpha}_{\kappa n}(\epsilon) - G_n^<\!(\epsilon) \Sigma^{\alpha\kappa}_{\kappa n}(\epsilon) \right). \]
(14)

Because \( \Gamma_{n\alpha}(\epsilon) = \sum_{\alpha} (\Sigma^{\alpha\kappa}_{\kappa n}(\epsilon) - \Sigma^{\kappa\alpha}_{\alpha n}(\epsilon)) = 0 \) means that \( \Sigma_{\kappa n}(\epsilon) = \Sigma^{\kappa\alpha}_{\alpha n}(\epsilon) = 0 \) [note that each term in Eq. \((12)\) is non-negative], the current disappears when \( \Gamma_{n\alpha}(\epsilon) = 0 \). Thus the free part can be neglected in the expression of current. In a usual resonant tunneling problem, \( \Gamma_n = \Gamma_L + \Gamma_R \) (width at half maximum: constant), so \( \eta \) in the denominator can be neglected anyway.

With \( A_{n m}(\epsilon) = \Im[\Gamma_{n m}(\epsilon) - \Gamma_{m n}(\epsilon)] \), \( \hbar \Theta_{n m}(\epsilon) \equiv \Gamma_{n m}(\epsilon) G_{n m}^\alpha(\epsilon) / A_{n m}(\epsilon) \), \( J_L \) in the absence of scattering can be cast into the following form,
\[ J_L = \frac{e}{\hbar} \int_0^\infty \frac{d\epsilon}{2\pi} \sum_{k k' n m n m} \frac{V_{k n}^\alpha(\epsilon) V_{m k'}^\alpha(\epsilon) V_{n m k' k}(\epsilon) V_{n m k' k}(\epsilon)}{\eta^2} A_{n m}(\epsilon) \Theta_{n m}(\epsilon) \times \left\{ f_L(E_{k L}) (f_R(E_{k R}) - 1) P_{\alpha}^<\!(\epsilon - E_{k L}) P_{\alpha}^\geq\!(\epsilon - E_{k R}) - (f_L(E_{k L}) - 1) f_R(E_{k R}) P_{\alpha}^\geq\!(\epsilon - E_{k L}) P_{\alpha}^\geq\!(\epsilon - E_{k R}) \right\}. \]

This is the central result of this paper. In the absence of the charging effects, i.e., \( P_{\alpha}^<\!(\epsilon - \epsilon') = \delta(\epsilon - \epsilon') \), \( J_L \) is reduced to the familiar expression of resonant tunneling \((12)\). When \( \Sigma_{\kappa n} = \delta_{\kappa n} \Sigma_{\kappa n}^{\alpha\beta} \), all Green’s functions are diagonalized. This corresponds, e.g., to a situation in which energy levels in the island are mutually uncorrelated during the tunneling process. Then \( A_{n m}(\epsilon) \) reduces to
\[ A_n(\epsilon) = \frac{\hbar \Gamma_n(\epsilon)}{\epsilon - (E_n + V_d) - \Lambda_n(\epsilon)^2 + [\Gamma_n(\epsilon)]^2 / 4}, \]
and \( \Theta_n(\epsilon) \) reduces to \( \Gamma_n(\epsilon)^{-1} \).

From Eq. \((2)\), we see that \( P_{\alpha}^<\! \) can be divided into two parts:
\[ P_{\alpha}^<\!(t_1, t_2) = \langle e^{-i\epsilon_1 \varphi(\gamma)} e^{i\epsilon_2 \varphi(\gamma)} \rangle (\varphi_1 = 1 \text{ and } \varphi_2 = -1) \]
where the first factor describes influence of the electrodynamic environment (i.e., the external circuit) \((3)\), and the second factor describes quantum fluctuations of the island charge. Using the relation \( \langle m | e^{-i\gamma \varphi(\gamma)} e^{i\gamma \varphi(\gamma)} | m \rangle = e^{-i[1 + 2\gamma(m - \bar{n})]t} \), where \( \bar{n} \equiv (C_g V + C_g V_g)/e, \gamma \) is an arbitrary constant \((3)\), and \[ m \] is the charge eigenstate of the island with charge \( ce_m \), we obtain
\[ \langle e^{-i\gamma \varphi(\gamma)} e^{i\gamma \varphi(\gamma)} \rangle = \sum_{[m]} e^{-\beta U(m - \bar{n})} / e^{-i[1 + 2\gamma(m - \bar{n})]t}, \]
where \( U \equiv e^2/2C_S \) and \( c \equiv \sum_{[m]} e^{-\beta U(m - \bar{n})} \), and \[ [m] \] runs over \( 1, 2, \cdots, 2N \), where \( N \) is the number of doubly degenerate energy levels. Fourier transforming this in the high-impedance limit gives
\[ P_{\alpha}^<\!(\epsilon) = \sum_{[m]} e^{-\beta U(m - \bar{n})} / 2\pi \hbar \Delta(\epsilon \mp E_{\alpha}^m \pm \kappa_n^2 E_{C_S}), \]
where \( E_{\alpha}^m \equiv U(1 \pm 2|m - \bar{n}|) \), and \( E_{C_S} = e^2/2C_S \).

Before we discuss the main consequences of Eq. \((13)\), let us discuss the relationship of our theory to the ‘orthodox theory’ of double junctions \((14)\). In the orthodox theory, the tunneling rate is assumed to be small, and tunneling processes at the left and right junctions are treated separately by assuming that electrons on the island are always at thermal equilibrium. To ensure this, we assume that inelastic scattering in the island is large and that tunneling is weak so that \( 2\pi h/|V_{k n}(\epsilon) V_{n' k}(\epsilon)| \ll h/2\tau_n \ll E_F \), where \( E_F \) is the Fermi energy of the central electrode. Equation \((14)\) can then be shown to reduce to the corresponding formula in the orthodox theory. In fact, under these assumptions, we have \( \Im[\Gamma_{k n}(\epsilon)]^{-1} \sim \pm h/2\tau_n \) and \( \Sigma^{>\alpha}\! \) may be approximated as \( G_0^{>\alpha}\! \) because near \( \epsilon \sim E_F \) we have \( \Im[\Gamma_{k n}(\epsilon)]^{-1} \). Thus, with appropriate identification of parameters, our formulation reduces to that of Ref. \((14)\).
In the following discussions, we consider the case in which the self-energy is diagonal \([i.e., \epsilon \equiv 0]\) \((i.e., \epsilon \equiv 0)\), and \( \Gamma_{nn' k}(\epsilon) \) does not depend on \( n, n' \) and \( k \), namely, \( \Gamma_{nn' k}(\epsilon) = \Gamma_{n k}(\epsilon) \) and \( C_g \to 0 \) and \( V_d = C_L/C_S V + V_g \).

Figures \((2)\) and \((3)\) show the \( I-V \) characteristics and the \( I-V_g \) characteristics, when the charging energy \( U \equiv e^2/2C_S \) is much greater than the discrete energy-level spacing \( \Delta E_n \). From the relation \( \Gamma_{n k}(\epsilon) = 2\pi D_k(\epsilon)|V_{k n}(\epsilon)|^2 \), resistances \( R_\alpha(\alpha = L, R) \) can be evaluated to be \( R_{\alpha}/R_K = (\Gamma_{\alpha}(\epsilon) D_k(E_F))^{-1} \), where \( R_K \) is the resistance quantum \( h/e^2 = 25.8k\Omega \) and \( D_k(E_F) \) is the DOS of the island at the Fermi energy. The resistances are estimated to be \( R_{\alpha}/R_K \sim 40(\text{weak tunneling}) \) when \( D_k(E_F)E_F \sim 1. \)

Figures \((2)\) shows the \( I-V \) characteristics in which \( \Delta E_n \sim 25\text{meV} \) larger than the elementary charging energy \( U = 0 \) or \( 10\text{meV} \). Here we assume \( \Gamma_{n k}(\epsilon) = \sqrt{\epsilon/E_F} \) for the energy dependence of the density of state (DOS) \( D_k(\epsilon) \) of the electrodes on the \( I-V \) characteristics. In the absence of the Coulomb interaction, i.e., \( U = 0 \), equally-spaced resonant tunneling peaks are seen. The Coulomb interaction deforms this \( I-V \) characteristic in a manner depending on the strength of the interaction and temperature. As the Coulomb interaction increases, the deformation of the peaks becomes more pronounced, and some peaks are suppressed by large Coulomb gaps. At \( T = 100K \) with \( U = 10\text{meV} \), the resonant peaks are thermally blurred. The dips at \( 0.2 \text{ eV} \) and \( 0.4 \text{ eV} \) appear where original resonant peaks overlap with Coulomb gaps. Our results shows that the complex \( I-V \) characteristics appear due to combined effects of Coulomb blockade and resonant tunneling in the quantum dot.

In conclusion, we have studied combined effects of Coulomb blockade and resonant tunneling through a
double-barrier system by using the Keldysh equation. A general expression of the $I-V$ characteristics is obtained which automatically satisfies the conservation of DC currents at both junctions. We found that, in a resonant-tunneling-dominated regime, some of resonant tunneling peaks are suppressed due to the charging effects.

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FIG. 1. $I-V$ characteristics in the continuum limit for two different gate voltages $V_{g}=0$ and -0.5eV and two temperatures $T=4.2$ and 30K, where $E_{F}=0.2eV$, $U=5meV$, $\Gamma_{L}=5meV$, $\Gamma_{R}=0.1meV$.