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Nonlinear resonant tunneling through doubly degenerate local state and strong electron-phonon interaction

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In an approach of low transparency of the barrier the tunneling of electrons through doubly degenerate local state has been considered with allowance for the Coulomb and electron-phonon interactions. It is shown that in the case of weak electron-phonon and strong electron-electron interactions the dependence of tunneling current on the applied voltage has a step-like character at low temperature. The threshold value of the current was measured for small applied bias. The bistable state of the tunneling current is possible in the region of large bias. In the case of strong electron-phonon and weak electron-electron interactions, the threshold of tunneling current can be bistable. This result is a direct consequence of the electron pairing in local states.

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Introduction

It is well know that electron transport through quantum low-dimensional structures in the ballistic regime is very sensitive to certain resonance conditions [1–4]. This circumstance can be used for effective driving of the tunneling process. One of the most frequently used objects to study this phenomenon is double-barrier resonant tunneling structure (DBRTS), which consists of two potential barriers surrounding a potential well (the quantum well). Peculiarity of such a system is the charge accumulation in interbarrier space. Therefore, many-particle effects can play an important role. For instance, the dynamic charge accumulation within a quantum well leads to an electrostatic feedback mechanism that shifts the resonance energy. Under some conditions, this can result in the appearance of nonlinear effects such as intrinsic bistability [5,6], self-oscillations [7,8], Hamiltonian chaos [9], dissipative chaos [10], and other effects. These phenomena assume the presence of electronic states in the quantum well. In the case of a local state this is not valid. However, as it has been shown in Refs. 11 and 12, a doubly degenerate local state is sufficient for nonlinearity of resonant tunneling and the appearance of intrinsic bistability. There is, however, another problem. The strong electron-phonon interaction is possible for the local state [13,14] that can essentially change the tunneling nonlinearity. In particular, it can lead to effective electron-electron attraction and appearance of the electron pairing.

In the present paper we consider this problem for the case of double-degenerated electronic state where an accumulation up to four electrons in the local state is possible. Taking into account interaction between electrons and electron-phonon interaction can lead to a number of properties characteristic of nonlinear tunneling, including the appearance of step-like current-voltage curves and the bistability of threshold tunneling. Detailed consideration is restricted to one-dimensional case of resonant tunneling. The study of fluctuations shows that they can be virtually suppressed [15] in such a structure. The later is typical of double level systems.

1. Hamiltonian of the system

We consider a model of tunneling with a double-degenerate local state in the barrier. The energy profile of this structure is shown in Fig. 1. Electrons are assumed to interact with one another through the Coulomb potential and phonon field in the local state. The Hamiltonian describing the electrons in this system can be written as follows:

$$H = H_0 + H_W + H_T \,. \qquad (1)$$

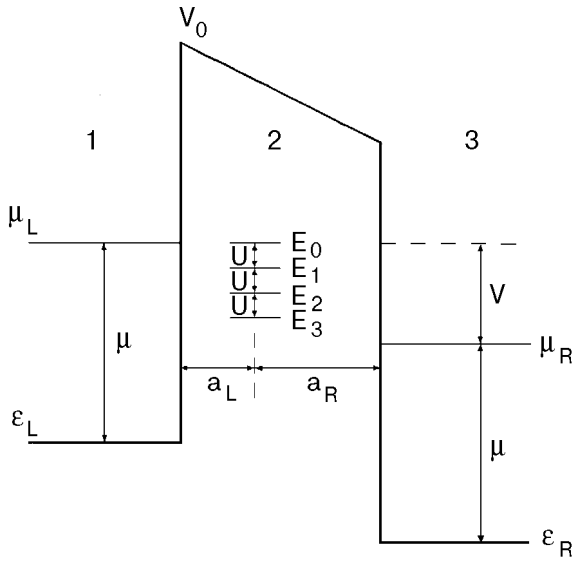

Fig. 1 Energy profile under applied voltage V of a barrier structure with localized energy levels.

The first term of the Hamiltonian

$$H_0 = \sum_{k\sigma} \varepsilon_L(k) a^+_{k\sigma} a_{k\sigma} + \sum_{p\sigma} \varepsilon_R(p)\, a^+_{p\sigma}\, a_{p\sigma} \qquad (2)$$

describes electrons in the left electrode (emitter) and in the right electrode (collector) (regions *1* and *3* in Fig. 1). Here $a^+_{k\sigma}$ ($a_{k\sigma}$) and $a^+_{p\sigma}$ ($a_{p\sigma}$) are the creation (annihilation) operators, respectively; $\varepsilon_L(k) = \varepsilon_L + \hbar^2k^2/2m_L$ is the energy of electrons in the emitter, $\hbar k$ and m_L are their quasi-momentum and effective mass, respectively, and σ is the electron spin. In the collector (with an external potential V applied across the barrier), $\varepsilon_R(k) = \hbar^2k^2/2m_R + \varepsilon_R - V$, where m_R is the effective mass.

In Eq. (1) the Hamiltonian H_W describes electrons and their interactions in a local state (region *2* in Fig. 1). We consider the case where the local state is doubly degenerate. Then H_W can be written as follows:

$$H_W = \sum_{\alpha} E_0\, a^+_\alpha a_\alpha + \sum_i \hbar\omega_i b^+_i b_i +$$

$$+ \sum_{\alpha i} \varphi_{\alpha i}\, a^+_\alpha a_\alpha (b_i + b^+_i) + \frac{1}{2} \sum_{\alpha_1 \neq \alpha_2} V_{\alpha_1\alpha_2} a^+_{\alpha_1} a^+_{\alpha_2} a_{\alpha_2} a_{\alpha_1} . \qquad (3)$$

Here a^+_α (a_α) are the creation (annihilation) operators for electrons in the local state, $\alpha = (l, \sigma)$, σ is the spin number, and l is the quantum state number which takes values 1 or 2. The energy of the local state, taking into account the applied bias, is written as follows: $\overline{E}_0 = \varepsilon_0 - \gamma V$, where ε_0 is the energy of the local state, and γ is the coefficient; $\gamma = a_L/a$, $a = a_L + a_R$, a_L and a_R are the distances of the local state from the left and right borders of the barrier, respectively, and $V_{\alpha_1\alpha_2}$ is a matrix element describing the electron interaction in the local state. For simplicity, we approximate it by the positive constant $V_{\alpha_1\alpha_2} = U_c$, which corresponds to repulsion, b^+_i (b_i) are the creation (annihilation) operators for phonons of the ith mode ($\hbar\omega_i$ is their energy), and $\varphi_{i\alpha}$ is the matrix element of the electron-phonon interaction for local states. The explicit form of such interaction is not important for our goals. It can be an interaction with the acoustic, optical or local vibration modes (see Ref. 14, for example).

The Hamiltonian H_T in Eq. (1) describes the tunneling transition of electrons through the barrier and has the conventional form [16]:

$$H_T = \sum_{k\alpha} T_{k\alpha} a^+_{k\sigma} a_\alpha + \sum_{\alpha p} T_{p\alpha} a^+_{p\sigma} a_\alpha + \sum_{kp} T_{kp} a^+_k a_p + \text{c.c.}, \qquad (4)$$

where $T_{k\alpha}$ and $T_{p\alpha}$ are the matrix elements of the tunneling transition to the local states from the left and right electrodes, respectively, and T_{kp} is the matrix element for direct tunneling transition from the emitter to the collector. In general, the matrix elements depend on the applied bias.

2. Density of states

Before considering the density of states it is convenient to transform the Hamiltonian H_W using the unitary transformation

$$S = \exp\left\{ - \sum_{i\alpha} \frac{\varphi^*_{\alpha i}}{\hbar\omega_i} a^+_\alpha a_\alpha (b_i - b^+_i) \right\} . \qquad (5)$$

We can thus write H_W in the form

$$\tilde{H}_W = \sum_{\alpha} E_0 a^+_\alpha a_\alpha + \sum_i \hbar\omega_i b^+_i b_i + \frac{1}{2} \sum_{\alpha_1 \neq \alpha_2} U a^+_{\alpha_1} a^+_{\alpha_2} a_{\alpha_2} a_{\alpha_1}, \qquad (6)$$

where

$$U = U_c - \sum_i \frac{|\varphi_i|^2}{\hbar\omega_i} , \qquad E_0 = \varepsilon_0 - \gamma V - \sum_i \frac{|\varphi_i|^2}{\hbar\omega_i} .$$

For the Hamiltonian H_T we obtain

$$\tilde{H}_T = \sum_{k\alpha} T_{k\alpha} S_b a^+_{k\sigma} a_\alpha + \sum_{\alpha p} T_{p\alpha} S_b a^+_{p\sigma} a_\alpha + \sum_{kp} T_{kp} a^+_k a_p + \text{c.c.}, \tag{7}$$

where

$$S_b = \exp\left\{ - \sum_i \frac{\varphi^*_{\alpha i}}{\hbar\omega_i} (b_i - b_i^+) \right\} .$$

Next we restrict the analysis to the case of electron tunneling without radiation and absorption of phonons. After averaging Hamiltonians (6) and (7) over the phonon states we obtain

$$H_w = \sum_\alpha E_0 a^+_\alpha a_\alpha + \frac{1}{2} \sum_{\alpha_1 \neq \alpha_2} U a^+_{\alpha_1} a^+_{\alpha_2} a_{\alpha_2} a_{\alpha_1} , \tag{8}$$

$$H_t = \sum_{k\alpha} \tilde{T}_{k\alpha} a^+_{k\sigma} a_\alpha + \sum_{\alpha p} \tilde{T}_{p\alpha} a^+_{p\sigma} a_\alpha + \sum_{kp} T_{kp} a^+_k a_p + \text{c.c.}, \tag{9}$$

where

$$\tilde{T}_{p\alpha} = T_{p\alpha} \exp\left\{ - \sum_i \left| \frac{\varphi_{\alpha i}}{\hbar\omega_i} \right|^2 \left(n_i + \frac{1}{2} \right) \right\} , \tag{10}$$

$$n_i = \left[\exp\left(\frac{\hbar\omega_i}{k_B T} \right) - 1 \right]^{-1} . \tag{11}$$

The density of states $\rho(E)$ of local levels can be determined with the help of Fourier transform of the retarded Green's function $G(\alpha, \alpha, E)$

$$\rho(E) = - \frac{1}{\pi} \sum_\alpha \text{Im}\, G(\alpha, \alpha, E) , \tag{12}$$

where

$$G(\alpha, \alpha, t) = - i\theta(t) \langle [a^+_\alpha(t), a_\alpha(0)]_+ \rangle \tag{13}$$

and $\theta(t)$ is a Heaviside unit step function.

Using the Hamiltonian H_w, the Green's function can be calculated explicitly. For example, for the state α we obtain

$$G(\alpha, \alpha, E) = \frac{1}{E' - E_0} \times$$

$$\times \left\{ 1 + \sum_{m=1}^{3} \sum_{\substack{\alpha_1, \ldots, \alpha_m \neq \alpha \\ \alpha_1 \neq \alpha_2 \neq \ldots \alpha_m}} \prod_{m_1=1}^{m} n_{\alpha_{m_1}} \frac{U}{E' - E_0 - m_1 U} \right\} , \tag{14}$$

where $E' = E + i\eta$ in the limit $\eta \to +0$. Here $n_\alpha = \langle a^+_\alpha a_\alpha \rangle$ are average values of the occupation numbers of the αth state. The Green's function has poles at $E_m = E_0 + mU$, where $m = 0, 1, 2, 3$. The electron-phonon interaction and the electron-electron interaction therefore lead to a splitting of the local degenerated states. New states are separated by the value U. In this case, however, U may also take negative values. Using Eq. (7), we can calculate the density of states ρ for the local states in the barrier. These states depend on the occupation numbers of states n_α, which are functions of the applied voltage. This is the reason behind the nonlinearity of the tunneling current.

3. Occupation numbers

When the constant external voltage is applied to the system, a nonequilibrium steady-state distribution of electrons sets in. It is assumed that the electron distribution functions in the electrodes are at equilibrium because of their large spatial extent, but their chemical potentials change. The latter are connected through the relation $\mu_L - \mu_R = V$ (where μ_L and μ_R are the chemical potentials of the emitter and the collector, respectively). The electron distribution function $g(E)$ in the local state is essentially nonequilibrium. It can be determined from the condition of equality of the tunneling current through the emitter and the collector [16,17]

$$g(E) = \frac{1}{\Gamma(E)} [\Gamma_L(E) f_L(E) + \Gamma_R(E) f_R(E)] , \tag{15}$$

where

$$\Gamma(E) = \Gamma_L(E) + \Gamma_R(E) ,$$

$$\Gamma_L(E) = \sum_k |T_{k\alpha}|^2 \delta[E - \varepsilon_L(k)] , \tag{16}$$

$$\Gamma_R(E) = \sum_p |T_{p\alpha}|^2 \delta[E - \varepsilon_R(p)] ,$$

$f_L(E)$ and $f_R(E)$ are electron distribution functions in the emitter and the collector, respectively. The occupancy of local states in the barrier can be determined with the help of the expression [18]

$$n_\alpha = -\frac{1}{\pi}\int dE\; g(E)\;\mathrm{Im}\; G(\alpha,\alpha,E)\;. \qquad (17)$$

As follows from (7), the expression for n_α does not depend on the index α. Therefore, the mean values of the occupation numbers are also independent of the number of the quantum state, and we can assume that $n_\alpha = n$. Thus, we finally obtain

$$n = F(n)\;, \qquad (18)$$

where

$$F(n) = \sum_{m=0}^{3} C_3^m g_m (1-n)^{3-m} n^m\;,\quad C_3^m = \frac{3!}{m!(3-m)!}\;.$$

The functions $g_m = g(E_m)$ determine the occupancy of new states. Thus, Eq. (18) is a cubic equation for the occupation numbers n. In general, this equation can have three solutions in the interval $0 \le n \le 1$. According to Eq. (11), for $g_m = g$ we obtain $n = g$. The equation admits three solutions when $g_0 = g_1 = 0$, i.e., if the two states are vacant. These solutions have the form

$$n_1 = 0\;,$$

$$n_{2,3} = -\frac{3}{2}\frac{g_2}{g_3 - 3g_2} \pm \left(\frac{9g_2^2 + 4(g_3 - 3g_2)}{4(g_3 - 3g_2)^2}\right)^{1/2}\;. \qquad (19)$$

According to the condition $0 < n < 1$, expression (19) leads to

$$0 < \frac{3g_2}{3g_2 - g_3} < 2\;, \qquad (20)$$

$$9g_2^2 - 4(3g_2 - g_3) > 0\;.$$

These inequalities (15) are compatible when

$$g_2 \ge \frac{2}{3}\left(1 + \sqrt{1 - g_3}\right)\;,\quad g_3 > 3/4\;. \qquad (21)$$

Thus, Eq. (18) has three solutions when the values of g_1 and g_3 are close to unity. The two solutions n_1 and n_3 are stable, while the third one n_2 is unstable. The stable states correspond to the cases in which the local state does not contain electrons or contains four electrons occupying two upper levels. The latter is possible since the system is essentially out of equilibrium.

Matrix elements for tunneling in the one-dimensional case are given in the Appendix by Eqs. (A.1) and (A.2). The functions $\Gamma_L(E)$ and $\Gamma_R(E)$ can be approximated by the value

$$\Gamma_{L,R} = \alpha_{L,R}\sqrt{E - \varepsilon_{L,R}(0)}\;. \qquad (22)$$

Here α_L and α_R are the proportionality factors for the emitter and the collector, respectively:

$$\alpha_L = \frac{m_L V_L^2 B(0,\, a_L\,;\, E)}{4\pi m E_s \sqrt{V_0 - \varepsilon_0}\,(V_0 - \varepsilon_L)}\;,$$

$$\alpha_R = \frac{m_R V_R^2 B(a_L\,,\, a;\, E)}{4\pi m E_s \sqrt{V_0 - \varepsilon_0}\,(V_L - \varepsilon_R)}\;,$$

and

$$E_s = \frac{\hbar^2}{2ma^2}\;.$$

Substituting (22) into (15) and taking into account that

$$f_{L,R} = \left[\exp\left(\frac{E - \mu_{L,R}}{k_B T}\right) + 1\right]^{-1}\;, \qquad (23)$$

where k_B is Boltzman constant, and T is temperature, we obtain the expression for the electron

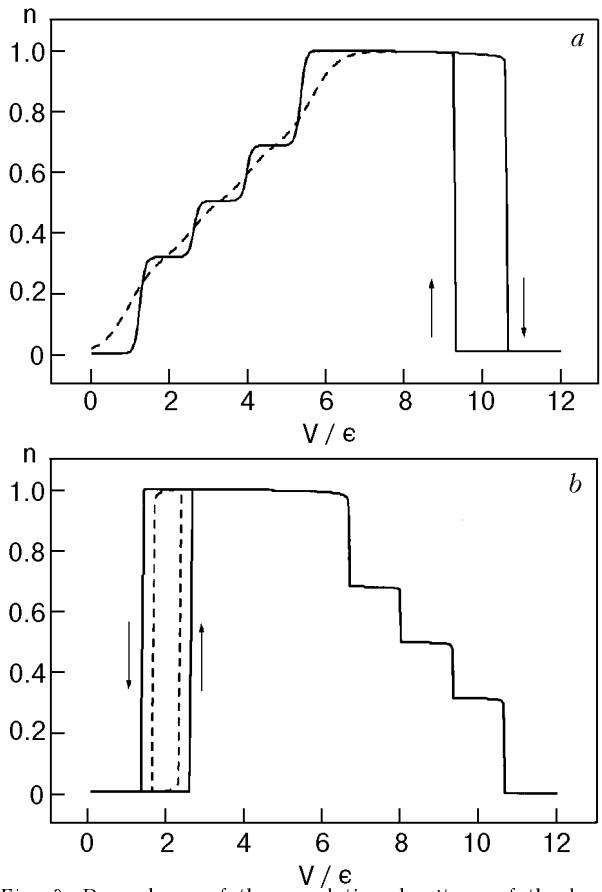

Fig. 2. Dependence of the population density n of the local state on the applied voltage V for $U/\epsilon = 0.2$ (*a*) and -0.2 (*b*). Solid line is for $k_B T = 0.01$; dashed line is for $k_B T = 0.05$.

distribution function g_m. For more detailed investigation of the properties of Eq. (18) we will consider the same particular cases.

a. The case of $U > 0$

A plot of the dependence of the occupancy n on the applied voltage obtained by solving Eq. (18) at low temperatures ($k_B T/\epsilon = 0.01$ and 0.05) and the parameters $m_L/m_R = 1$, $\gamma = 0.5$, $\varepsilon_0/\epsilon = 1.6$, and $U/\epsilon = 0.2$ are represented in Fig. 2,*a*. Here ϵ is a normalizing constant of the order of magnitude μ. It follows that with increase in the applied voltage, the occupancy of the local state increases stepwize due to consecutive occupation of split states. Above the critical value V_2, the occupation drops abruptly to zero due to the departure of the local states from resonance. If the voltage is lowered below V_2, a jump in the occupation number is observed at a lower value of the voltage V_1. Thus, the voltage range from V_1 to V_2 contains a bistability region, which is connected with the removal of electrons from the lower levels and with their attachment to the upper split states.

b. The case of $U < 0$

In this case the dependence of the occupancy n on the applied voltage is more complicated. This dependence is shown in Fig. 2,*b* at $U = -0.2$. It follows that, with increase in the applied voltage, the occupancy of the local state abruptly jumps to one above the critical value V_2. If the voltage is lowered below V_2, the occupation drops abruptly to zero at a lower value of the voltage V_1. Thus, there is a voltage range from V_1 to V_2 that contains a bistable region. The voltage interval $(V_2 - V_1)$ decreases with an increase in temperature. Such character of bistability is a consequence of the negative value of U.

4. Tunneling current

In the case of a constant applied voltage the tunneling current through the double-barrier structure can be calculated in various ways (see for example, Refs. 17 and 19). The following simple expression was obtained for this quantity:

$$J_{cd} = \frac{e}{\hbar}\int dE\,\frac{\Gamma_L(E)\Gamma_R(E)}{\Gamma(E)}\,[f_L(E) - f_R(E)]\,\rho(E) +$$

$$+\frac{e}{\hbar}\int dE\,P(E)\,[f_L(E) - f_R(E)]\,, \qquad (24)$$

where e is the electron charge. The second term in Eq. (24) is caused by the direct tunneling of electrons from the emitter to the collector. The transparency coefficient $P(E)$ is defined as follows:

$$P(E) = \sum_{kp} |T_{kp}|^2 \delta[E - \varepsilon_L(k)]\delta[E - \varepsilon_R(p)]\,,$$

where T_{kp} is given by Eq. (A.3) in the Appendix. For a low barrier transparency, $\Gamma << U$, the density of states ρ can be calculated using formulas (12) and (14), which give

$$\rho(E) = \sum_{m=0}^{3} C_3^m (1-n)^{3-m} n^m \delta(E - E_m)\,. \qquad (25)$$

Equation (24) then becomes

$$J_{cd} = \frac{e}{\hbar}\sum_{m=0}^{3}\frac{\Gamma_R(E_m)\Gamma_L(E_m)}{\Gamma(E_m)}\,\{f_L(E_m) - f_R(E_m)\}\times$$

$$\times (1-n)^{3-m} n^m C_3^m + \frac{e}{\hbar}\int dE\,P(E)\,[f_L(E) - f_R(E)]\,. \qquad (26)$$

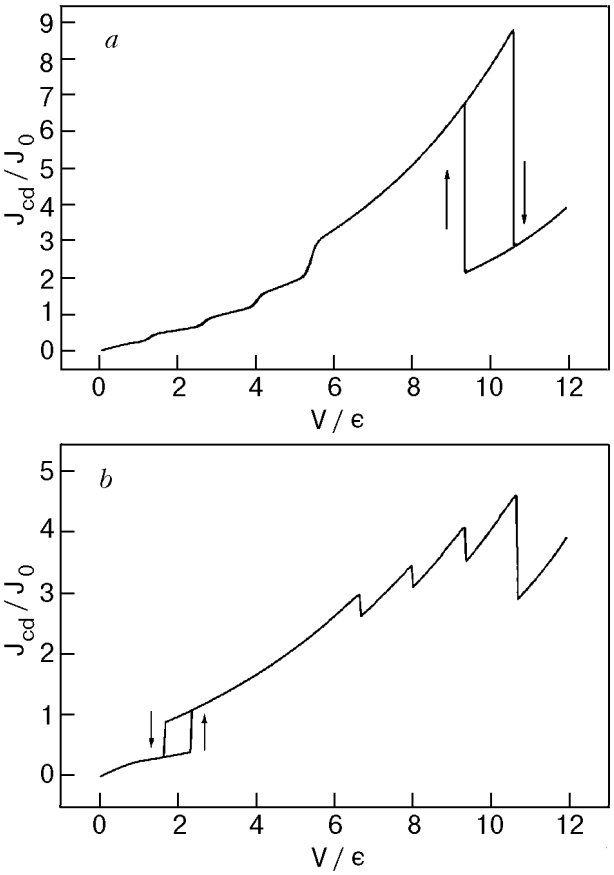

Fig. 3. Dependence of the tunneling current J_{cd}/J_0, where $J_0 = e\mu\cdot 10^{-4}/\hbar$ on the applied voltage V for $U/\epsilon = 0.2$ (*a*) and -0.2 (*b*).

The results of numerical calculations of $J_{cd}(V)$ for the same parameters as those used for constructing the curves in Fig. 2 for different values of temperature are shown in Fig. 3. A bistability of the tunneling current is due to the filling of electrons in the upper energy levels of the splitting state. The toothed shape of the current in Fig. 3,*b*, is due to the departure of the local states from resonance.

Conclusions

Thus, the electron-electron and electron-phonon interactions in the local degenerate state result in the conductance oscillations of the tunneling system. The later is connected with the splitting of electron states by the Coulomb or electron-phonon interactions. The value of splitting defines a period of the conductance oscillations. The step-like shape of the current-voltage curve and its threshold character have some analogy with an effect of single-electron tunneling [19] when $U > 0$. The bistability takes place in the interval of negative differential conductance. The sign of U determines the chape of the current-voltage characteristics. In the case of a strong electron-phonon interaction ($U < 0$) the bistability takes place in the interval of positive differential conductance. Such peculiarity is due to the pairing of two electrons with opposite spins in local states.

An important feature of the present model is its stability with respect to the fluctuations. A simple consideration of the fluctuations of the occupation numbers of the local states results in

$$\langle \delta n^2 \rangle = \langle (\hat{n} - n)^2 \rangle = n(1 - n) \ . \qquad (27)$$

In the region of bistability, n takes values in the vicinity of unity or zero. At these values $\sqrt{\langle \delta n^2 \rangle} << n$. However, in the region of the current steps the fluctuations are comparable with the charge value. This conclusion was confirmed experimentally [20]. With increase in the temperature, the steps quickly smooth out due to the smoothing of the Fermi distribution functions. The region of their existence is limited by temperature $k_B T << U$. The temperature dependence of the bistability is due to the change in the functions g_m, which are not so sensitive to temperature. The bistability disappears when max $g(E) \le 3/4$, which can be achieved at sufficiently high temperatures comparable to μ. In the range of these temperatures one can ignore the spin dependence and the situation becomes similar to the one considered in Ref. 5. When $U < 0$, increasing the temperature leads to suppression of the bistability.

Appendix

When a constant voltage is applied to the system, the wave function of an electron in the barrier can be found in the WKB approximation

$$\psi_k(x) = \frac{1}{\sqrt{L}} B(0, x; \varepsilon_L(k)) \ ,$$

$$\psi_p(x) = \frac{1}{\sqrt{R}} B(x, a; \varepsilon_R(p)) \ ,$$

$$\psi_\alpha(x) = \frac{1}{\sqrt{r}} \begin{cases} B(x, a_L ; \varepsilon_\alpha) & \text{if } x < a_L \\ B(a_L , x; \varepsilon_\alpha) & \text{if } x > a_L \end{cases} ,$$

where

$$B(x_1 , x_2 ; E) = \exp \left\{ - \int_{x_1}^{x_2} \frac{dx}{\hbar} \sqrt{2m(V(x) - E)} \right\} ,$$

L and R are the collector and emitter regions, respectively, and r is the radius of the local state. It is assumed that $r << a_L , a_R$. Under the condition that $E = \varepsilon_L(k) = \varepsilon_R(p) = \varepsilon_\alpha$ is the energy of the tunneling electron, the matrix elements $T_{\alpha k}$, $T_{\alpha p}$, and T_{kp} are

$$T_{k\alpha} = \int_0^{a_L} \psi_k^*(x) V(x) \psi_\alpha(x) \, dx = \bar{V}_L B(0, a_L ; E) \frac{a_L}{\sqrt{a_r L}} , \qquad (A.1)$$

$$T_{p\alpha} = \int_{a_L}^{a} \psi_p^*(x) V(x) \psi_\alpha(x) \, dx = \bar{V}_R B(a_L , a; E) \frac{a_R}{\sqrt{a_r L}} , \qquad (A.2)$$

$$T_{kp} = \int_0^{a} \psi_k^*(x) V(x) \psi_p(x) \, dx = \bar{V} B(0, a; E) \frac{a}{\sqrt{RL}} , \qquad (A.3)$$

where $\bar{V}_L$, $\bar{V}_R$, and $\bar{V}$ are the average values of $V(x)$

$$\bar{V} = \frac{1}{a}\int_0^a V(x)\,dx\ ,$$

$$\bar{V}_L = \frac{1}{a_L}\int_0^{a_L} V(x)\,dx\ ,$$

$$\bar{V}_R = \frac{1}{a_R}\int_{a_L}^{a} V(x)\,dx\ .$$

When $V(x)$ is a linear function of x and the applied voltage V

$$V(x) = V_0 - V\,\frac{x}{a_R + a_L}\ ,$$

$B(x_1\ ,\ x_2\ ;\ E)$ can be written in the form

$$B(x_1\ ,\ x_2\ ;\ E) = \begin{cases} \exp\{Z(x_1) - Z(x_2)\} & \text{if}\quad x_2 < x_0 \\ \exp\{Z(x_1)\} & \text{if}\quad x_2 > x_0 \end{cases}\ ,$$

where

$$x_0 = \frac{x_2 - x_1}{V}\left\{V(x_1) + \frac{x_1 V}{x_2 - x_1} - E\right\}\ ,$$

$$Z(x) = -\,\frac{2(x_0 - x)^{2/3}}{3}\left[\frac{2Vm}{\hbar(x_2 - x_1)}\right]^{1/2}\ .$$

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