An Approach to Quantum Transport Based on Reduced Hierarchy Equations of Motion

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The quantum dissipative dynamics of a tunneling process through double barrier structures is investigated on the basis of a rigorous treatment for the first time. We employ a Caldeira-Leggett Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(q;t) + \sum_j \left[\frac{\hat{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left(\hat{x}_j - \frac{c_j \hat{q}}{m_j \omega_j^2} \right)^2 \right]$$

with an effective potential calculated self-consistently, accounting for the electron distribution. The heat bath can be characterized by the spectral distribution function, defined by $J(\omega) = m\zeta\gamma^2\omega / \pi(\gamma^2 + \omega^2)$,where γ is the reciprocal of the correlation time of the noise induced by phonons and ζ is the electron-phonon coupling strengt. With this Hamiltonian, we employ reduced hierarchy equations of motion (HEOM) approach, which can deal with non-Markovian and non-perturbative system-bath interactions at finite temperature $\beta = 1/kT$ without approximation [1,2]. In the Wigner form the HEOM is expressed as [2-4]

$$\dot{W}^{(n)}_{j_1,\cdots,j_K}(t) = -\left[\hat{L} + \hat{\Xi}' + n\gamma + \sum_{k=1}^{K} j_k \nu_k \right] W^{(n)}_{j_1,\cdots,j_K}(t)$$

$$+ \frac{\partial}{\partial p} \left[W^{(n+1)}_{j_1,\cdots,j_K}(t) + \sum_{k=1}^{K} W^{(n)}_{j_1,\cdots,(j_k+1),\cdots j_K}(t) \right]$$

$$+ n\gamma \hat{\Theta}_0 W^{(n-1)}_{j_1,\cdots,j_K}(t) + \sum_{k=1}^{K} j_k \nu_k \hat{\Theta}_k W^{(n)}_{j_1,\cdots,(j_k-1),\cdots j_K}(t)$$

In the HEOM, the reduced density operator is expressed in the auxiliary hierarchy density matrix elements $W^{(n)}_{j_1,\cdots,j_K}$ with the cutoff $n + \sum_{k=1}^{K} j_k \gg \omega_c / \min(\gamma, 1/\beta\hbar)$, where the index n and j_k arises from the hierarchal expansion of noise correlation time and the kth Matsubara frequency $\nu_k \equiv 2\pi k / \beta\hbar$ and $-\hat{L}$ is quantum Liouvillian (time scale $\approx 1/\omega_c$). Other operatorswith ($c_k \equiv 2\gamma^2 / (\nu_k^2 - \gamma^2)$) are

$$\hat{\Xi}' = -\frac{m\zeta}{\beta} \left[1 - \frac{\beta\hbar\gamma}{2} \cot\left(\frac{\beta\hbar\gamma}{2} \right) - \sum_{k=1}^{K} c_k \right] \frac{\partial^2}{\partial p^2},$$

$$\hat{\Theta}_0 = \zeta \left[p + \frac{\beta\hbar\gamma}{2} \cot\left(\frac{\beta\hbar\gamma}{2} \right) \right], \quad \hat{\Theta}_k = \frac{m c_k \zeta}{\beta} \frac{\partial}{\partial p}.$$

Hysteresis and both single and double plateau-like behavior are observed in the negative differential resistance (NDR) region. We find two distinct types of current oscillations, with large and small oscillation amplitudes, respectively, in some parts of the plateau in the NDR region. The results of eigenstates analysis indicate that the first type is caused by a transition between ground tunneling states and adjacent excited states in the emitter basin, while the second type is caused by a transition between intermediate tunneling states and higher states. These two types of oscillation also appear differently in the Wigner space, with one exhibiting two piston engine-like motion and the other exhibiting tornado-like motion (Figs.4-5).

REFERENCES

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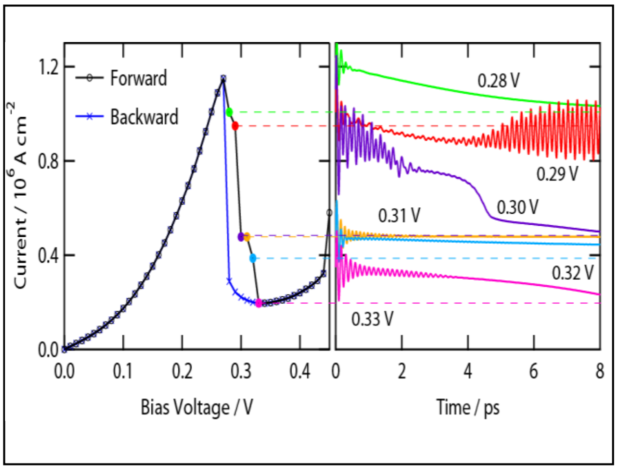

Fig. 1. The I-V characteristics and steady current.

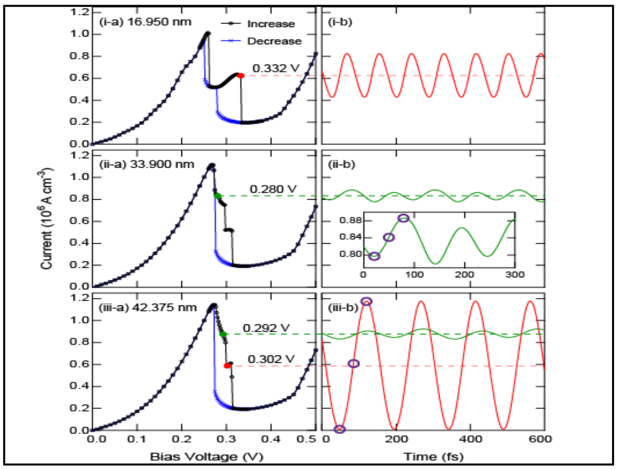

Fig. 2. The I-V characteristics for different contact region size.

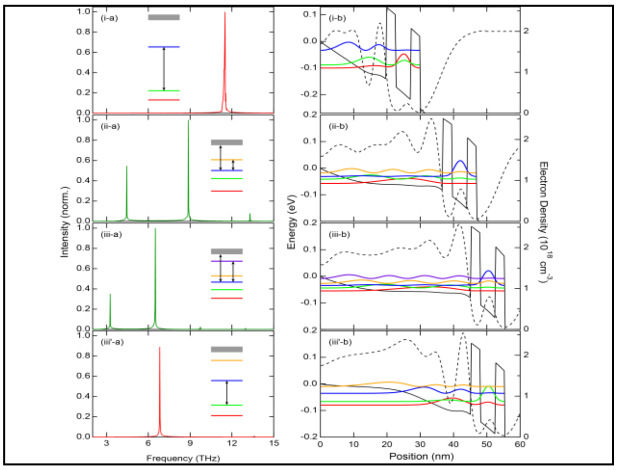

Fig. 3. The spectral distributions and the effective potential for the large (red) and small (green) oscillations in fig.2 (b).

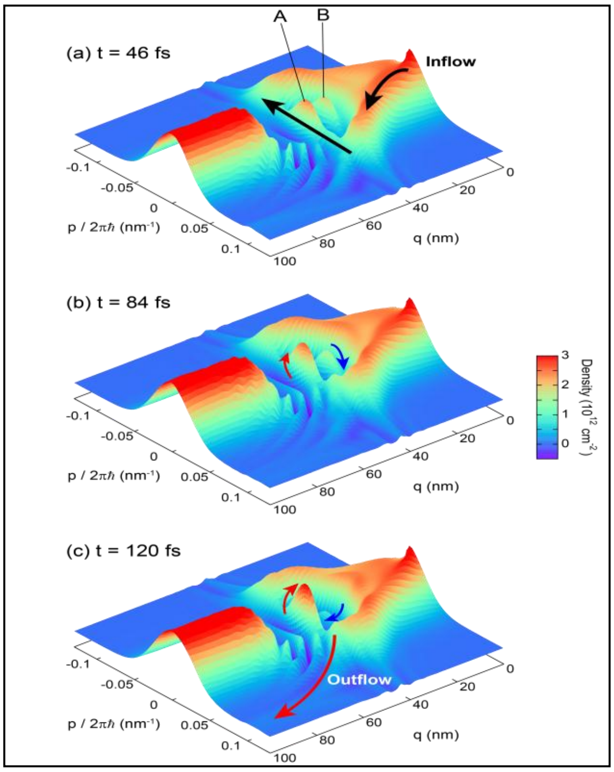

Fig.4. The snapshots of the Wigner distribution for small oscillation case(green curve) at the times marked in Fig.2(ii-b).

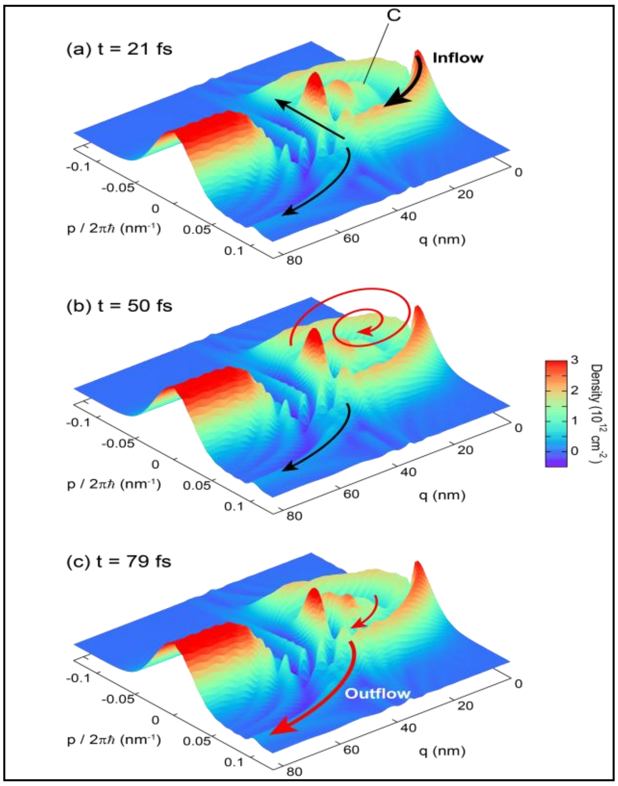

Fig.5. The snapshots of the Wigner distribution for large oscillation case (red curves) at the times marked in Fig.2(iii-b).