Dephasing of electrons in the Aharonov–Bohm interferometer with a single-molecular vibrational junction

Wenxi Lai, Yunhui Xing and Zhongshui Ma

School of Physics, Peking University, Beijing 100871, People's Republic of China

E-mail: wxlai@pku.edu.cn

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Abstract
Phase relaxation of electrons transferring through an electromechanical transistor is studied using the Aharonov–Bohm interferometer. Using the quantum master equation approach, the phase properties of an electron are numerically analyzed based on the interference fringes. The coherence of the electron is partially destroyed by its scattering on excited levels of the local nanomechanical oscillator. The transmission amplitudes with respect to two adjacent mechanical vibrational levels have a phase difference of $\pi$. The character of the $\pi$ phase shift depends on the oscillator frequency only and is robust over a wide range of values of the applied voltage, tunneling length and damping rate of the mechanical oscillator.

1. Introduction

Discrete quantum states and coherent electronic transport are two important properties of mesoscopic conductors. In a recent experiment on a single-molecule C$_{60}$ transistor, current steps due to the quantum behavior of nanomechanical motion were observed [1]. In the subsequent years, electron transport through mechanically vibrating junctions has become a subject of great interest. Such systems have been fabricated quite recently using a gold nanoparticle oscillator [2]. Further fascinating features of the electromechanical systems have been predicted using theoretical approaches, such as negative differential conductance [3, 4], the shuttling effect [5, 6], super- and sub-Poissonian Fano factors [7–10], and spintronic transport [11–13], etc.

By applying an Aharonov–Bohm (AB) interferometer with a quantum dot (QD) embedded in one arm, the coherence of electron tunneling through the QD has been studied in experiments [14–16]. These experiments show that a fixed QD supports coherent transport and causes a phase shift to an electron. When a QD is allowed to mechanically oscillate around its equilibrium point, an electron transferring through the dot would be accompanied by random absorption or emission of phonons. The phase property in the vibration-assisted electron tunneling is still an open and interesting question. The vibrational motion in the system can be modeled to a good approximation as a monochromatic oscillator. It is different from thermal fluctuating bosonic baths, which cause decoherence to the local electronic states of charge [17, 18] and spin [19, 20]. As recently reported, a single vibrational mode of a QD array enhances electron transport and partially preserves its phase information [21]. It is worth mentioning that the coherent transport of electrons in QDs is also sensitive to spin flip, electron–electron interactions and external detectors [22–30].

In this work, we shall investigate dephasing of electrons induced by electromechanical vibration in a single-molecular transistor. It is implemented by embedding a harmonically movable QD in one (target) arm of the AB interferometer and locating a fixed QD in the other (reference) arm. The reason for using the QD in the reference arm is that the phase shift corresponding to each discrete level of the mechanical oscillator can be observed by changing the gate voltage of the reference QD. Previous research close to our topic of interest is the which-path detector of charge using a cantilever [31, 32]. This detector is based on dot–cantilever coupling, which causes remarkable dephasing of the electrons. In their model, the dot–lead coupling does not depend on the oscillator position, whereas the position dependence of the coupling is considered in our system, since
it is significant for the electromechanical shuttle junction [2, 5]. In our previous report, we derived a fully quantum mechanical master equation to describe the electromechanical system [10]. In the equation we considered both diagonal and off-diagonal density matrix elements for the states of vibrational levels, and revealed that the off-diagonal terms give important contributions to the electronic current. Here, we shall develop this approach to describe the influence of the electromechanical system on the AB interference. To obtain knowledge of the phase properties of electron scattering on the vibrational junction, interference fringes as a function of an external magnetic flux through the AB ring will be analyzed with respect to various parameters. In the following, this paper will discuss how the coherence of an electron in the AB ring is suppressed due to excitation of the vibrational mode in the transport process. The suppression becomes more serious when one increases the bias voltage or decreases the oscillator damping rate. It is shown that by moving the energy level of the reference QD, a global phase shift in the transmission amplitude can be observed from the change of interference fringes. The transmission amplitudes corresponding to two neighboring resonant levels of the molecular junction are off-phase by $\pi$. This phase difference causes destructive interference on propagating waves and destroys the coherence of the electron.

This paper is organized as follows: in section 2, we derive the master equation for the model of the AB interferometer with a single-molecular transistor in one arm. In section 3, the method of our numerical calculation is introduced. In section 4, we present solutions for various parameters. The influence of the electromechanical system on the interference fringes is analyzed. In addition, the phase shifts of electronic propagating waves through the resonating QD will be illustrated. Finally, conclusions are given in section 5.

2. Model and equation of motion

The schematic structure of our AB interferometer is illustrated in figure 1. It contains two single-level QDs coupled to two electronic leads in parallel. One of them, with energy $\epsilon_1$ (QD1), is fixed in the upper arm and the other, with energy $\epsilon_2$ (QD2), is located in the lower arm. The two arms and the electrodes enclose a magnetic flux $\Phi$ passing through the loop-plane. The QD2 is assumed to be bounded in a harmonic potential. The QD1 in the upper arm provides a reference path. We consider both inter- and intra-dot Coulomb blockade limits in order to make sure that electrons propagate through the two-path interferometer one by one. The spin degree of freedom is not involved in our approach. The Hamiltonian can be written in the form

$$H = H_{leads} + H_{dots} + H_{mech} + H_{tun},$$

where

$$H_{leads} = \sum_{k,j=\text{u},r} \xi_{jk} d^\dagger_{jk} d_{jk},$$

(2)

describes the noninteracting electrons in the left ($y = l$) and right ($y = r$) leads. $d^\dagger_{jk}$ and $d_{jk}$ are creation and annihilation operators of electrons with momentum $k$ and energy $\xi_{jk}$. In the Hamiltonian

$$H_{dots} = \epsilon_1 c_1^\dagger c_1 + (\epsilon_2 - \hbar \Omega (a^\dagger + a)) c_2^\dagger c_2,$$

(3)

$c_i$ ($c_i^\dagger$) is the creation (annihilation) operator of QDi ($i = 1, 2$). Here, the last term is the work undertaken by the charged QD2 when it moves a distance $x_0(a^\dagger + a)$ in an external electric field $V/d$. The coupling coefficient is given by $\Omega = eVx_0/\hbar d$, with the bias voltage $V$ and effective distance $d$ between the two electrodes. $e$ is the absolute value of the electron charge and $x_0$ is the zero-point position uncertainty $\sqrt{\hbar/2m_0}$ of the oscillator with frequency $\omega_0$ and effective mass $m$. The nanomechanical vibration is treated in the quantum regime as

$$H_{mech} = \hbar \omega_0 a^\dagger a + \sum_k h\omega_k b_k^\dagger b_k + \sum_k \hbar (gb_k^\dagger a + \text{h.c.}).$$

(4)

$a$ ($a^\dagger$) and $b_k$ ($b_k^\dagger$) are annihilation (creation) operators for the vibrational mode and its thermal bath, respectively. $\omega_0$ denotes the frequency of mode $k$ in the thermal bath, which is coupled to the oscillator with a coefficient $g$. Tunneling through the two QDs is represented by

$$H_{tun} = \hbar \sum_{k,j=\text{u},r} (T_{2y} e^{-i\Phi/4} e^{\frac{\varphi}{\lambda}} d^\dagger_{jk} c_2 + \text{h.c.})$$

$$+ \hbar \sum_{k,j=\text{u},r} (T_{1y} e^{i\Phi/4} d^\dagger_{jk} c_1 + \text{h.c.}).$$

(5)

The tunneling amplitudes between the two leads and QD1 are given by $T_{1y} e^{i\Phi/4} (S_{r(t)} = -1 (+1))$ and its complex conjugate, where the phase $\phi$ is related to the magnetic flux $\Phi = 2\pi \Phi/\Phi_0$, with the flux quantum $\Phi_0 = \hbar/e$. The tunneling amplitude with respect to QD2 is written as $T_{2y} e^{-i\Phi/4} e^{\frac{\varphi}{\lambda}}$, which exponentially depends on the position of the oscillator. The parameter $\alpha$ is an inverse ratio of the tunneling length $\lambda$, given by $\alpha = x_0/\lambda$.

We describe the interference process using the quantum master equation. This is an extension from the equation given in our earlier publication, where a more detailed derivation can be found [10]. The state of the total configuration is described by the density matrix $\rho_T(t)$, which satisfies the Liouville–von Neumann equation

$$i\hbar \dot{\rho}_T(t) = [H(t), \rho_T(t)].$$

(6)
Both of the electronic leads and the thermal bath are assumed to be in equilibrium at all times and described by the time-independent equilibrium density matrices $\rho_L$ and $\rho_B$, respectively. Assuming the initial state as $\rho(t=0) = \rho(0)\rho_B\rho_B$, we can write the state at time $t$ in the form $\rho(t) = \rho(0)\rho_B\rho_B$ under the Born approximation. $\rho(t)$ is the reduced density matrix of the system, which consists of the two QDs and the mechanical oscillator. Iterating equation (6) in the interaction picture to the second order and performing a trace over the leads ($T_{\text{Rh}}$) and the bath ($T_{\text{Rb}}$) variables, we obtain the master equation for the reduced density matrix of the system in the Markov approximation as

$$\dot{\rho}^t = \rho_0^t + \rho_1^t + \rho_2^t + \rho_{12}^t + \rho_d^t.$$  (7)

On the right hand side of equation (7), $\rho_0^t$ denotes the evolution term of the system in which QD2 is coupled to the harmonic oscillator. $\rho_1^t$ describes the contribution from direct tunneling by QD1 in the absence of QD2. $\rho_2^t$ is just the right hand side of the master equation in our previous work [10], representing the contribution from vibration-assisted transfer through QD2 alone. $\rho_{12}^t$ is the coherent term for the transfer involving the two dots and $\rho_d^t$ accounts for dissipation of the vibrational mode. Explicit expressions of these terms read

$$\rho_0^t = \frac{i}{\hbar}[\epsilon_1 c_1^\dagger c_1 + h_{00} a_1 a_1 + (\epsilon_2 - \hbar \Omega(a_1 + a_1)) c_2^\dagger c_2, \rho^t],$$  (8)

$$\rho_1^t = \frac{1}{2} \sum_{l,r} [\Sigma_{1ll}^m(0, 0, 1)(2c_1^\dagger \rho c_1 - c_1^\dagger \rho c_1 - \rho^t c_1^\dagger c_1)] + \Sigma_{100}(0, 0, 1)(2c_1^\dagger \rho c_1 - c_1^\dagger \rho c_1 - c_1^\dagger c_1 - c_1^\dagger c_1 tint),$$  (9)

$$\rho_2^t = \frac{1}{2} \sum_{y=1}^{2n} \sum_{m, n, m_1, m_2, n_1, n_2} (S_2^2)^{m_1+n_1+m_2+n_2} \frac{1}{m_1 n_1 m_2! n_2!}$$

$$\times \left[ A_{m_1 m_2}^+ \rho A_{n_1 n_2}^+ - A_{m_1 m_2}^- \rho A_{n_1 n_2}^- \right] \frac{1}{2} \epsilon_1 c_1^\dagger c_1$$

$$+ \left[ A_{m_1 m_2}^+ \rho A_{n_1 n_2}^+ - A_{m_1 m_2}^- \rho A_{n_1 n_2}^- \right] \frac{1}{2} \epsilon_2 c_2^\dagger c_2,$$  (10)

$$\rho_{12}^t = \frac{1}{2} \epsilon_1 \epsilon_2 \sum_{y=1}^{2n} \sum_{m, n} (S_2^2)^{m+n} \frac{1}{m! n!}$$

$$\times \left[ A_{m_1 m_2}^+ \rho A_{n_1 n_2}^+ - A_{m_1 m_2}^- \rho A_{n_1 n_2}^- \right] \frac{1}{2} \epsilon_1 c_1^\dagger c_1$$

$$+ \left[ A_{m_1 m_2}^+ \rho A_{n_1 n_2}^+ - A_{m_1 m_2}^- \rho A_{n_1 n_2}^- \right] \frac{1}{2} \epsilon_2 c_2^\dagger c_2 [\text{h.c.}],$$  (11)

and

$$\rho_d^t = \Sigma^{\text{in}} D[a^\dagger] \rho^t + \Sigma^{\text{out}} D[a] \rho^t.$$  (12)

The degrees of freedom in the electronic leads and the thermal bath are assumed to be continuous, with densities of states $N_q(\xi_q)$ and $D(\omega_a)$, respectively. In the above equations, the coefficients corresponding to particles hopping into or out of the system are composed of integrals over these reservoir variables via

$$\Sigma^{\text{in}}_{ji}(m_1, n_1, z) = \int d\xi_k \Gamma_{ji}(\xi_k) f_i(\xi_k)$$

$$\times \delta(\xi_k - \epsilon_z - (m_1 - n_1) \hbar \omega_0),$$

$$\Sigma^{\text{out}}_{ji}(m_1, n_1, z) = \int d\xi_k \Gamma_{ji}(\xi_k)(1 - f_i(\xi_k))$$

$$\times \delta(\xi_k - \epsilon_z - (m_1 - n_1) \hbar \omega_0),$$

$$\Sigma^{\text{in}} = \int d\omega_k \gamma(\omega_k) n_B(\omega_k) \delta(\omega_k - \omega_0),$$

and

$$\Sigma^{\text{out}} = \int d\omega_k \gamma(\omega_k)(1 + n_B(\omega_k)) \delta(\omega_k - \omega_0).$$

Here, $\Gamma_{ji}(\xi_k) = 2\pi N_q(\xi_k) T_{ji} T_{ji}, \gamma(\omega_k) = 2\pi D(\omega_k)|\gamma|^2$ and $i, j = 1, 2$. We have the Fermi–Dirac distribution function in lead $y$, $f_i(\xi_k) = [e^{(\xi_k - \mu_y)/k_B T} + 1]^{-1}$ and the Bose–Einstein distribution function of the thermal bath, $n_B(\omega_k) = (e^{(h\omega_k/k_B T)} - 1)^{-1}$, where $T$ is temperature and $k_B$ is the Boltzmann constant. In the above equation we have defined $A_{mn}^- = c_2(a_i^\dagger m(a_i^\dagger)^\dagger)^{m} (a_i^\dagger)^{n}$, $A_{mn}^+ = c_1(a_i^\dagger m(a_i^\dagger)^\dagger)^{m} (a_i)^{n}$, where $A_{mn}^+ (A_{mn}^-)$ describes that an electron hops into (out of) QD2 accompanied by the creation of $m$ phonons and the annihilation of $n$ phonons. $\nu$, $\nu^t = \nu + (1 + S_y)/2$ and $\nu^t = \nu - (1 + S_y)/2$ indicate the number of electrons accumulated in the right lead. They are achieved by the following way: $T_{\text{Rh}}(d_{iR}^\dagger d_{iR})$ and $T_{\text{Rb}}(d_{iR} d_{iR}^\dagger)$ contain different information about the number of electrons in the right lead when the number is not infinite. Assuming $n$ electrons are in the right lead, then the number of electrons in this lead can be expressed by $\rho^t f_i(\xi_k) = \rho T_{\text{Rh}}(d_{iR}^\dagger d_{iR})$ and $\rho^{i+1} f_i(\xi_k) = \rho T_{\text{Rb}}(d_{iR} d_{iR}^\dagger)$. In the same way, we have $\rho^{i+1} f_i(\xi_k) = \rho T_{\text{Rh}}(d_{iR}^\dagger d_{iR})$. The density matrix satisfies $\sum_{\rho} \rho^t = \rho$. The above method is equivalent to the counting procedure in the many-body Schrodinger equation [33], representing how many particles arrive at the collector. $D[a] \rho^t$ is a super-operator acting on the density matrix $\rho^t$ as $D[a] \rho^t = a^\dagger a \rho^t - (a^\dagger a \rho^t + \rho^t a^\dagger a)/2$.  

3. Numerical treatment and current formula

In this section, we give a brief introduction to our mathematical approach. We pay attention to the character of stationary transport. Therefore, the electron transmission can be conveniently described by the rate of electrons collected in the right lead. The system current is calculated according to the formula [34]

$$I = -e \sum_{\nu=0}^{\infty} \nu \hat{P}^\nu.$$  (13)

Here, $\nu = T_{\text{mech}}[T_{\text{char}}(\rho^t)]$ is the probability of $\nu$ electrons arriving at the right lead. The trace $T_{\text{mech}}$ is taken over the variables of the mechanical oscillator and $T_{\text{char}}$ is taken over the degrees of freedom of electron occupation in the QDs. For the following numerical treatment, we consider the wide band approximation and apply energy-independent
transmission rates \( \Gamma_{ijy} = 2\pi N_{ijy} T_{ij} \) \((i, j = 1, 2 \text{ and } y = l, r)\) and the damping rate \( \gamma = 2\pi D|g|^2 \). We assume \( \Gamma_{12r} \) and \( \Gamma_{12l} \) are real and satisfy \( \Gamma_{12r} = \Gamma_{12l} = \sqrt{\Gamma_{12r} \Gamma_{12l}} \). The chemical potentials for the left and right electrodes are set to be \( \mu_l = eV/2 \) and \( \mu_r = -eV/2 \), respectively.

The Fock state will be applied for the representation of the master equation. Thus, the Hilbert space of the system is generated by the composite basis \(|00\rangle, |01\rangle, |10\rangle, |11\rangle \otimes |0\rangle, |1\rangle, \ldots, |n\rangle, \ldots\rangle\), where \( \otimes \) means direct product. The state \(|ij\rangle \) represents \( i \) electrons in QD1 and \( j \) electrons in QD2. \(|n\rangle\rangle\) is the eigenstate of the nth excited level of the mechanical oscillator. In the Hilbert space, the system density matrix elements are written as \( \rho_{ijkl, mn} = \langle\langle m | \otimes \langle j | \rho | k | \otimes | n \rangle\rangle \), where \( i, j, k, l = 0, 1 \) and \( m, n = 0, 1, 2, \ldots \). For any two given vibrational states \(|n\rangle\rangle, |m\rangle\rangle \) we have 16 density matrix elements \( \rho_{ijkl, mn} (i, j, k, l = 0, 1) \) in terms of the electronic states. However, just six of them are enough to describe the transport process, since they can constitute a closed equation set for the system dynamics. These matrix elements are \( \rho_{ijij, mn} \) and \( \rho_{jiij, mn} (i, j = 0, 1) \).

For the case of strong inter-dot Coulomb interactions, we assume that the state of two-electron occupation is not inside the transport window. In other words, the bias voltage is so low that only one electron passes the system at any time. As a consequence, the process involving the state \( \rho_{1111, mn} \) is not contained in our equations [33]. Substituting equation (7) into equation (13), we reach the following expression for the current

\[
I = I_1 + I_2 + I_3, \tag{14}
\]

where

\[
I_1 = e\text{Tr}_{\text{mech}}[\Sigma_{ijkl}^{\text{out}}(0, 0, 1)\rho_{1010} - \Sigma_{ijkl}^{\text{in}}(0, 0, 1)\rho_{0000}]. \tag{15}
\]

\[
I_2 = \frac{e^2 \alpha^2}{2} \sum_{m_1, n_1, m_2, n_2} (a^m_{n_1} + n_1 + m_2 + n_2) \times \text{Tr}_{\text{mech}}[\Sigma_{ijkl}^{\text{out}}(m_1, n_1, 1)\langle m_1 | \langle n_1 | \rho_{1010} \rangle | n_1 \rangle | m_1 \rangle | m_1 \rangle | m_2 | \langle m_2 | | n_2 \rangle | m_2 |] \\
+ (a^m_{n_1} a^m_{n_2} a^m_{n_1} a^m_{n_2} a^m_{n_1} a^m_{n_2} a^m_{n_1} a^m_{n_2}) \rho_{0010} \\
- \Sigma_{ijkl}^{\text{in}}(m_1, n_1, 1)\langle m_1 | \langle n_1 | \rho_{1010} \rangle | n_1 \rangle | m_1 \rangle | m_1 \rangle | m_2 | \langle m_2 | | n_2 \rangle | m_2 |] \\
+ (a^m_{n_1} a^m_{n_2} a^m_{n_1} a^m_{n_2} a^m_{n_1} a^m_{n_2} a^m_{n_1} a^m_{n_2}) \rho_{0000}]. \tag{16}
\]

\[
I_3 = \frac{e^2 \alpha^2}{2} \sum_{m_1, n_1, m_2, n_2} (a^m_{n_1} + n_1 + m_2 + n_2) \times \text{Tr}_{\text{mech}}[e^{-\alpha^2/2} \Sigma_{ijkl}^{\text{out}}(0, 0, 1)\langle a^m_{n_1} a^n_{n_2} \rangle \rho_{1010} + \text{h.c.}]. \tag{17}
\]

Here, \( I_1 \) is the current through QD1 alone and \( I_2 \) is the current across the electromechanical junction in the absence of the reference arm. In fact, it is the same as the current directly derived from the master equation of the single-molecular junction [10]. Also, \( I_3 \) is the interference part in terms of the off-diagonal density matrix for the electronic states. The values of density matrix elements are achieved by solving equation (7) under the condition \( \dot{\rho} = 0 \). We project the equation in the basis of the Hilbert space as

\[
\langle m | | ij + 1 | q_1 + q_2 + q_12 + q_21 | ij | n\rangle = 0, \tag{18}
\]

\[
\langle m | | ij + 1 | q_1 + q_2 + q_12 + q_21 | ij | n\rangle = 0. \tag{19}
\]
The visibility is not very high even at the regime \( \gamma > \omega_0 \), which is no longer clearly enhanced for a damping rate decreased in the case of a high damping rate. The visibility observed, as shown in figure 3(b). It is not difficult to see that the coherence of the electron wave is influenced by the electromechanical vibrations. Using the same method of balancing the current amplitudes in the two paths, we give three more examples in figure 2 for different parameters: low bias voltage \( eV = 3\hbar\omega_0 \) (red dotted line), high damping rate \( \gamma = 0.3\omega_0 \) (green dashed line) and small tunneling length \( \alpha = \omega_0/\lambda = 0.3 \) (blue dot-dashed line), all of which weaken the effect of the vibrational mode. As a result, interference fluctuations are enhanced.

Figure 2 shows the minimum and maximum values of the interference pattern do not shift remarkably as the different parameters are varied. Using this feature, the visibility of the current can be calculated easily by making the substitutions \( I_{\text{max}} \simeq I(\phi = 0) \) and \( I_{\text{min}} \simeq I(\phi = \pi) \). This works under the conditions \( \epsilon_1 = \epsilon_2 = 0 \) and \( \Omega \ll \omega_0 \). The visibility of the interference fringes is given by the formula \( \text{Visibility} = (I_{\text{max}} - I_{\text{min}})/(I_{\text{max}} + I_{\text{min}}) \). In figure 3(a), the substantial influence of the bias voltage on the interference visibility can be seen. For very low voltages, \( eV < 2\hbar\omega_0 \), there is no excited level contained in the transport window \( (eV) \) and the visibility is close to unity. When the applied voltage is close to zero, the corresponding current almost vanishes. This causes a small drop in visibility near zero voltage. The excited states of the mechanical oscillator play an important role in the phase relaxation of electrons. Increasing the bias voltage, excited levels of the vibrational mode are involved in the transport, which suppresses the visibility. For low voltages, a few discrete states of the vibration contribute to the transport and the visibility displays a step profile. The mechanical oscillation is naturally coupled to the thermal bath and it has an intrinsic lifetime which is the inverse of the damping rate \( \gamma \). On raising the damping rate, a visibility increase can be observed, as shown in figure 3(b). It is not difficult to see that the contribution from the mechanical motion would be decreased in the case of a high damping rate. The visibility is no longer clearly enhanced for a damping rate \( \gamma > 0.2\omega_0 \). This is in accord with the transition of the electromechanical system from the so-called shuttling regime into the tunneling regime \([6, 7]\). The visibility is still not very high even at the quality factor \( \omega_0/\gamma < 1 \). It implies, for the large damping rate, that coherence of electron does not depend significantly on the intrinsic lifetime of the mechanical oscillator. In fact, the interference pattern is essentially affected by the strength of electron–phonon interaction, which is determined by the parameter \( \alpha = \omega_0/\lambda \). In figure 3(c), the visibility versus the coupling strength \( \alpha \) is plotted. For a given oscillator with mass \( m \) and frequency \( \omega_0 \), the zero-point uncertainty \( \omega_0 \) is fixed, and the coupling strength is mainly related to the tunneling length \( \lambda \). For infinite large tunneling length \( \lambda \to \infty \) we have \( \alpha \to 0 \). In this case, \( \phi_2 \) in equation (7) is close to the form of \( \phi_1 \) and the effect of vibration in \( \phi_2 \) and \( \phi_{12} \) tends towards disappearing. As a consequence, tunneling between the two electrodes and QD2 is almost independent of the dot displacement. Therefore, we find that the visibility is close to unity, as illustrated in figure 3(c).

In general, the large current induced by the vibrational junction is the reason for the reduction in visibility in the AB ring. For instance, when one takes the same bare tunneling rates for the two paths as shown in figure 3, the probability of an electron passing the target arm is much greater than that of the electron propagating through the reference arm. There is another probable reason for the weak interference, namely phase shift of the electron waves, which this is also our main interest in the present paper. The propagation of an electron wave through the vibrational junction gives rise to many scattering excited states. Especially at a sufficiently high applied voltage, the electron is the superposition of a large number of single-particle excited modes associated with the electron–phonon interaction. These excited states are characterized by the phase acquired through the absorption and emission of phonons. One can expect that scattering in the region of positive phase shifts occurs symmetrically in the region of negative phase shifts. As a consequence, the interference of all the scattering waves does not exhibit a global phase shift between the two paths. This property is valid for the same dot levels, \( \epsilon_1 = \epsilon_2 \) and weak charge-field coupling \( \hbar\Omega \). In section 4.2 we will discuss the case \( \epsilon_1 \neq \epsilon_2 \). The influence of the charge-field coupling on the electron coherence has been previously considered in a similar system \([31, 32]\).
4.2. Coherent phase shift

As we mentioned above, there is no global phase shift when an electron is propagating through the single-dot electromechanical system. But it does not mean that there is no phase shift when one component of the electron wave transports through any individual level of the system. In order to observe the phase change of a propagating electron wave through the target system, we change the gate voltage to observe the phase change of a propagating electron transports through any individual level of the system. In order to observe the phase change of a propagating electron wave through the target system, we change the gate voltage to observe the phase change of a propagating electron transports through any individual level of the system. In order to observe the phase change of a propagating electron wave through the target system, we change the gate voltage to observe the phase change of a propagating electron transports through any individual level of the system. 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position-dependent tunneling causes an inelastic process, which improves the decay of the oscillating QD and broadens the energy levels of the system [38].

From figure 2, we know that the changes in the applied voltage, the electron–phonon coupling $\alpha$ and the damping rate of the oscillator do not induce a global phase shift in the AB interferometer. Therefore, the definitive phase relation showing a $\pi$ difference between two adjacent levels is independent of these parameters so long as they are properly taken such that the discrete levels of the mechanical vibration effectively contribute to the electron transport. On one hand, the applied voltage should be large enough so that at least one excited level of the oscillator is included in the transport window. On the other hand, the voltage should not be too large, so that the feature of discrete levels involved in the tunneling is obviously manifested. In fact, the phase shift is related just to the unit quanta of the mechanical oscillator as shown in figure 5.

According to the above analysis, the neighboring resonant levels in the molecular vibrational junction are off-phase by $\pi$. It is the character of a one-dimensional quantum system which is considered in our model. Since, in a one-dimensional system, the upper energy level has one more wavefunction node than the lower energy level, each node changes the phase of the transmission amplitude by $\pi$. This property may not be true if the system is not strictly one-dimensional [39]. In the experiment on an AB interferometer where a fixed QD is embedded in one of the arms, the phase behaviors are the same for all resonant levels of the QD [14–16]. Namely, all the resonant levels are in phase. It is different from present effect found in the electromechanical system, where all the vibrational levels are coherently correlated with a definitive phase difference of $\pi$. The phase shift varies from zero to any large value, depending on the net number of phonons involved in the electron tunneling.

The reason for the reduced visibility mentioned earlier becomes clearer now. Actually, an electron takes all the channels of the discrete vibrational levels which are involved in the transport process. Therefore, interference not only occurs between the propagating waves in the two paths, but also occurs among the waves taking different channels of the vibrational junction. As we analyzed above, any two neighboring channels have a phase difference of $\pi$. The wavefunctions taking different vibrational levels destructively interfere because of the phase differences. This is the reason for phase relaxation in the AB interference due to the vibrational junction (see figure 2). It has been shown in double-QD two-electron AB interference that two components of conductance oscillations with the same amplitudes cancel each other due to their phase difference of $\pi$ [40]. Since the two components of the conductance are the same in amplitude, the final conductance disappears in their system. In the present case, the electron occupation probabilities on different energy levels of the electromechanical system are not the same. Therefore, there is a net current remaining in the system, but it is not fully coherent. In fact, the interference between the different channels is also reflected in the direct transmission of charge through the electromechanical system [10]. The current calculated from the scheme considering both diagonal and off-diagonal density matrix elements of the system is significantly lower than that obtained by the approach in which only diagonal terms are taken into account. This current suppression is related to destructive interference between different transport channels.

5. Conclusions

Electrons propagating through the single-molecular vibrational junction are dephased. This is caused by electron scattering on the excited levels of the vibrational mode. However, the interference fringes of the AB interferometer are not completely destroyed by the nanoelectromechanical system. The visibility is sensitive to the applied voltage, the oscillator damping rate and the tunneling length. The transmission amplitudes corresponding to channels of the vibrational resonant levels are coherently correlated via any neighboring channels having a definitive phase difference of $\pi$. Because of the phase shifts between the resonant levels in the electromechanical junction, different branches of the transmission waves destructively interfere with each other. As a consequence, the electron tunneling through the system appears not to be fully coherent. The character of the phase difference of $\pi$ is robust with respect to wide ranges of bias voltage, tunneling length and vibrational mode lifetime. It depends just on the frequency of the mechanical oscillator. This work will provide guidance for the experimental observation of dephasing in electron transport through a vibrational molecular junction and phonon-assisted conductors.

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