Phonon-induced quantum interference in electron transmission through a one-dimensional system

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We investigate the influence of electron-phonon (EP) scattering on conductance of a finite one-dimensional system by solving Schrödinger equation for EP states. At zero temperature the conductance as a function of gate voltage exhibits both slow and fast oscillations, owing to the quantum interference between channels for the EP states. By introducing disorder the regular oscillations are replaced by white-noise fluctuations. With increasing the temperature both the slow and fast oscillations are gradually smeared. The relaxation of phonon components in the EP states by coupling with the environment is also discussed. The results provide a natural explanation for recent experimental observations of quantum interference in carbon nanotubes in which EP scattering is important.

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Owing to the advances in technology, in recent years it is possible to fabricate one-dimensional (1D) or quasi-1D systems with their widths in nanometer scales. Carbon nanotubes, quantum wires, and quantum point contacts are examples of these systems.[1–3] The transport properties are of particular importance for their possible applications. The conductance of ballistic 1D or quasi-1D systems embedded between two leads is quantized in units of $2e^2/h$.[4] This behavior, however, can be significantly changed when there exists scattering for the motion of electrons resulting in the mean free path shorter than the system length. For 1D or quasi-1D systems there are three important mechanisms causing the scattering, (1) impurities or disorder in the system, (2) electron-electron interaction, and (3) electron-phonon (EP) scattering. By introducing the disorder Anderson localization occurs for all states in 1D systems at the thermodynamical limit.[5] The electron-electron interaction may change the behavior of Fermi liquid in a 1D system.[6] The effects of EP scattering are twofold: it can reduce the conductance by scattering the electrons out of their initial orbits, but in some cases (such as in systems with disorder) it may enhance the conductance by providing phonon-assistant tunneling paths. Recently, the effect of EP scattering in the 0.7 anomaly of quantum point contacts was theoretically studied.[7]

In this paper we investigate the effect of EP scattering on conductance of a finite 1D system by solving Schrödinger equation of the coupled EP system. It is found that the EP scattering can induce a special type of quantum interference (QI) for EP states, manifested by slow and fast oscillations of the conductance with respect to the gate voltage. This is contrary to the knowledge that EP scattering is inelastic and always destroys the QI. The results provide a natural explanation of slow and fast oscillations of conductance observed in nanotubes.[8]

We consider the following Hamiltonian in the 1D system:

$$H = H_e + H_{ph} + H_{e\text{-}ph}, \tag{1}$$

where the electron part is written in a tight-binding form

$$H_e = \sum_i (\varepsilon_i + V_i) C_i^\dagger C_i + \sum_i (t_0 C_i^\dagger C_{i+1} + \text{H.c.}),$$

the part for the phonon modes within the chain is

$$H_{ph} = \sum_q \hbar\omega_q a_q^\dagger a_q,$$

and the EP interaction is

$$H_{e\text{-}ph} = \sum_{i\in B} \sum_q (\lambda_q C_i^\dagger C_i a_q + \text{H.c.}).$$

Here, $C_i^\dagger$ and $a_q^\dagger$ are creation operators for electron at site i and for phonon of the qth mode in the chain, ϵ_i and t_0 are the site energy and the nearest-neighbor hopping integral for electrons, respectively. V_i is the additional potential at site i controlled by the gate voltage. $\hbar\omega_q$ is the phonon energy in mode q, and λ_q characterizes the EP coupling strength. The tight-binding Hamiltonian is used to reproduce the 1D dispersion relation of a system by choosing the parameters, and the sites stand for discretization points. In a pure chain all ε_i's are equal and set to be the energy zero, while in a disordered system they are uniformly distributed in range $[-w/2, w/2]$, with w being the strength of disorder. We are interested in finite area B where the phonon modes locate and the EP interaction for tunneling electrons occurs. The interaction strength is dependent on the phonon energy $\hbar\omega_q$ and can be written as[9] $\lambda_q = c_0/\hbar\omega_q$, with c_0 depending on density, dielectric constant, system size, and average strain. The hopping integral t_0 can be estimated from the effective mass of the conduction band.

Due to the finite size of B, the wave vector of 1D phonon modes is discretized, $q_j = q_0 j/n$, with n being the total number of included modes and $j = 1, \ldots, n$. We are interested in only those modes that are more isolated in segment B and more strongly interacting with the tunneling electron, so n may be less than the number of all vibration modes in B. For acoustic modes we use a uniform frequency distribution for these modes, $\omega_j = j\omega_0$ with ω_0 being the frequency spacing. Because $t_0 \gg \lambda_q$ and the considered length of B is only in the mesoscopic range, the average number of phonons stimulated by an electron during its transmission through area B is

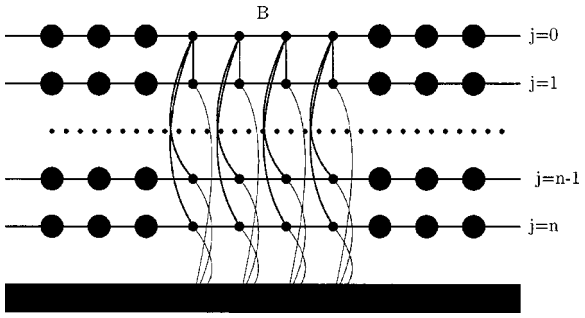

FIG. 1. Equivalent one-electron network illustrating Schrödinger equations. The vertical coordinate of sites represents the phonon states, while the horizontal coordinate is for the position of electron. The bonds in the network stand for the nonzero off-diagonal elements in the Hamiltonian. The black band at the bottom stands for the bath with hot phonons, and the thin links represent the leaking of the 1D phonons to the bath.

much less than 1. So we do not need to include multiphonon processes in the EP scattering. The wave function of the combined electron-phonon system can be written as a superposition

$$|\Psi\rangle = \sum_i \sum_{j=0}^{n} b_{i,j} C_i^\dagger |0\rangle \otimes \phi_j, \tag{2}$$

where $|0\rangle$ denotes the vacuum, ϕ_0 is the zero-phonon state, $\phi_{j\neq 0} = a_j^\dagger |0\rangle$ is the state with one phonon in mode j. Usually this is an EP state and the coefficients $b_{i,j}$'s obey the Schrödinger equations,

$$[\epsilon_i + V_i + (1-\delta_{j,0})\hbar j\omega_0] b_{i,j} + t_0(b_{i+1,j} + b_{i-1,j}) = E b_{i,j} \quad \text{for } i \notin B,$$

and

$$[\epsilon_i + V_i + (1-\delta_{j,0})\hbar j\omega_0] b_{i,j} + t_0(b_{i+1,j} + b_{i-1,j}) + \delta_{j,0} \sum_{j'=1}^{n} \lambda_{q_{j'}} b_{i,j'} + (1-\delta_{j,0})\lambda_{q_j} b_{i,0} = E b_{i,j} \quad \text{for } i \in B. \tag{3}$$

The 1D phonon modes in B may be coupled to 3D phonon modes in the environment so that the phonon components in EP states can decay into the bath in a relaxation time. To include this decaying process, we consider the coupling between the 1D phonons and the bath,

$$H_{ph\text{-}bath} = \sum_{q,r} \eta_{qr} (\sqrt{m_q^{(a)}(m_r^{(X)}+1)} X_r^\dagger a_q + \sqrt{m_r^{(X)}(m_q^{(a)}+1)} a_q^\dagger X_r), \tag{4}$$

where $X_r^\dagger$ is creation operator for the rth mode in the bath, $m_q^{(a)}$ and $m_r^{(X)}$ are numbers of phonons in corresponding modes, and η_{qr} is the coupling strength. The 3D phonons in the bath always obey the statistics of equilibrium, but the 1D phonons in segment B can be out of the equilibrium due to the stimulation of the tunneling electrons. Owing to the coupling of Eq. (4), the 1D phonons in B will eventually decay into the equilibrium. This decay process, however, could not be completed during the tunneling of an electron if segment B is short enough. The relaxation time of 1D phonons is $\tau_1 = \hbar/\eta_{qr} M$ with M being the average number of environment modes coupled to each 1D mode. For $\eta_{qr} = 3\times 10^{-6} t_0$, $M = 180$ and $t_0 = 1$ eV, one has $\tau_1 = 1$ ps. The transmission time τ_2 is estimated from $\hbar L/t_0 a k_F$, with L being the length of B, a the lattice spacing, and k_F the Fermi wave vector. For $L \sim 10$ nm, $\tau_2 \sim 0.1$ ps, shorter than τ_1 by an order of magnitude. In this case the EP coupling may create new effects which cannot be accounted for from theories based on equilibrium distribution of phonons.

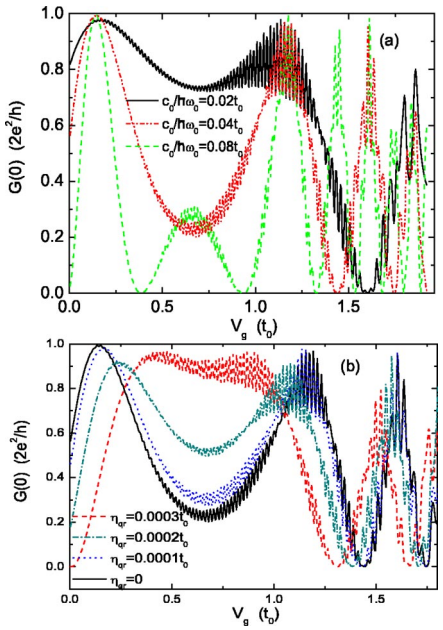

FIG. 2. (Color online) Zero-temperature conductance $G(0)$ as a function of gate voltage V_g without (a) and with (b) the leaking of 1D phonons. The length of region B is 1200 lattice spacings, the energy spacing between 1D phonon modes is $\hbar\omega_0 = 0.0008 t_0$, the chemical potential $\mu = 0.66 t_0$, $w = 0$ and the number of included 1D modes is $n = 20$. For (b), $c_0/\hbar\omega_0 = 0.04 t_0$ and the number of included environment phonon modes is 180 with energies distributed between 0 and $0.01 t_0$.

By including the coupling of Eq. (4), the phonons in states Eq. (2) can leak to the bath, so new terms, $\Sigma_{i,r} b_{i,r} C_i^\dagger X_r^\dagger |0\rangle$, should be added in this superposition. On the left-hand side of Eq. (3) new terms, $(1-\delta_{j,0})\Sigma_r \eta_{q_j,r} b_{i,r}$, are added. New equations for $b_{i,r}$ are similar to Eq. (3) but with frequencies of environment modes and coupling to the 1D modes. The equations can be illustrated by an equivalent one-electron network shown in Fig. 1. Below we will check the effect of the relaxation of 1D phonons by including $H_{ph-\text{bath}}$ in the calculation of Fig. 2(b). In the other calculations $H_{ph-\text{bath}}$ is not included as we focus on the effect of the coupling between the electron and the 1D modes.

We suppose that B is linked to the left and right leads. If an incident electron wave with unity amplitude and energy ϵ is injected from the left and the phonon state in region B is ϕ_j, the coefficients of the wave function outside region B can be written as

$$b_{i,j'} = \begin{cases} \delta_{j,j'}e^{iki} + r_{jj'}e^{-ik_{jj'}i} & \text{for } i \text{ on the left-hand side of } B, \\ t_{jj'}e^{ik_{jj'}i} & \text{for } i \text{ on the right-hand side of } B, \end{cases} \tag{5}$$

where j' denotes the phonon states in both the B region and the 3D bath, k is the wave vector of the incident electron satisfying $\epsilon = 2t_0 \cos k$, and $k_{jj'}$, determined by $\epsilon_{jj'} - \epsilon \equiv 2t_0(\cos k_{jj'} - \cos k) = \hbar(j - j')\omega_0$, denotes the wave vector of electron outside region B after the inelastic scattering. Correspondingly, this scattering causes the change of the electron energy from ϵ to $\epsilon_{jj'}$ and the change of the phonon state from ϕ_j to $\phi_{j'}$. Here, $r_{jj'}$ and $t_{jj'}$ are the corresponding reflection and transmission amplitudes, respectively, with phonon state $\phi_{j'}$ left in B or in the bath. Under a small bias voltage V_b the current through region B can be calculated as

$$I = \frac{2e}{h}\sum_k \sum_{jj'} \frac{|t_{jj'}|^2 |\sin k_{jj'}| F_j(T)}{|\sin k|} \times \left\{ f\left(\epsilon, \frac{eV_b}{2}, T\right)\left[1 - f\left(\epsilon_{jj'}, -\frac{eV_b}{2}, T\right)\right] - f\left(\epsilon, -\frac{eV_b}{2}, T\right)\left[1 - f\left(\epsilon_{jj'}, \frac{eV_b}{2}, T\right)\right]\right\}, \tag{6}$$

where $F_j(T)$ is the probability of phonon state being ϕ_j at temperature T, and $f(\epsilon, \pm eV_b/2, T)$ is the Fermi statistical factor on the left-hand (right-hand) side under the bias,

$$f\left(\epsilon, \pm \frac{eV_b}{2}, T\right) = \frac{1}{\exp\left(\dfrac{\epsilon - \mu \pm eV_b/2}{k_B T}\right) + 1},$$

with μ being the chemical potential. By taking limitation $V_b \to 0$, one obtains the dc conductance

$$G(T) = -\frac{2e^2}{h}\int d\epsilon \sum_{jj'} \frac{|t_{jj'}|^2 |\sin k_{jj'}| F_j(T)}{|\sin k|} \times \left\{ \frac{\partial f(\epsilon, 0, T)}{\partial \epsilon}[1 - f(\epsilon_{jj'}, 0, T)] + f(\epsilon, 0, T)\frac{\partial f(\epsilon_{jj'}, 0, T)}{\partial \epsilon}\right\}. \tag{7}$$

Probability $F_j(T)$ obeys the thermal statistics of phonons. As only phonon states $\{\phi_j\}$ with $j = 0, 1, 2, \ldots, n$ are included, so

$$F_j(T) = \frac{1}{Z}\exp\left(-\frac{\hbar j \omega_0}{k_B T}\right), \tag{8}$$

with $Z = \Sigma_{j=0}^{n} \exp(-\hbar j \omega_0 / k_B T)$.

At $T = 0$, $F_j(0) = \delta_{j,0}$ and we have

$$G(0) = \frac{2e^2}{h}|t_{00}|^2_{\epsilon=\mu}. \tag{9}$$

This means that at $T = 0$ the conductance is only determined by the transmission from the left zero-phonon channel to the right zero-phonon channel for electron at the Fermi level. However, this does not mean the zero effect of EP scattering as t_{00} still depends on the scattering within region B.

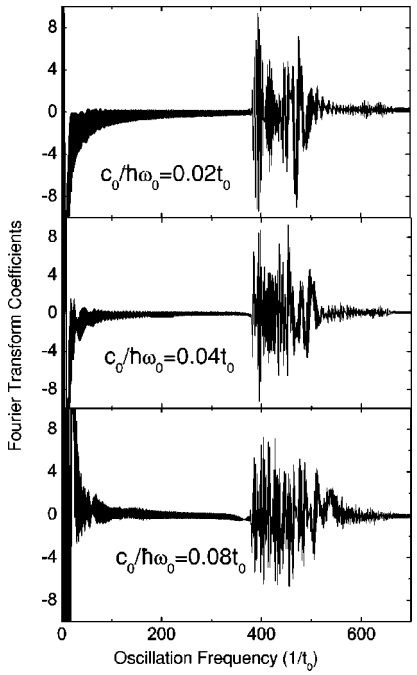

FIG. 3. Fourier transformation of three curves in Fig. 2(a).

In Fig. 2, we plot the zero-temperature conductance as a function of the gate voltage for a pure chain with finite length of B and various EP coupling strengths. The gate voltage is applied only on region B. In (a) the phonon-bath coupling is not included. By introducing the EP interaction both slow and fast oscillations of $G(0)$ appear in varying the gate voltage. This type of oscillation has already been observed in the measurements of low-temperature conductance through carbon nanotubes.[8] They are attributed to the QI within region B illustrated in Fig. 1. Although the EP interaction usually causes decoherence of electron states, the EP state, as a whole, can be coherent, and QI occurs if there exist more than one channels for such state. The EP coupling by itself provides the multiple internal channels within region B as can be seen from Fig. 1. In (b) we investigate the effect of relaxation of phonons in EP states by increasing the phonon-bath coupling. The largest value of η_{qr} corresponds the case of $\tau_2 < \tau_1$. It can be seen that the relaxation suppresses the slow oscillations, but has little effect on the fast oscillations. We also can see that the relaxation effect is negligible if τ_1 is in the order of its typical value, 1 ps.

In order to analyze the components in the slow and fast oscillations, in Fig. 3 we plot the Fourier transformations for curves in Fig. 2(a). Two groups of frequencies, corresponding to the slow and fast oscillations, are evident. Such a structure is robust against the change of parameters, such as ω_0, c_0, n, and L. By increasing the EP coupling, the group near the zero frequency is slightly widened, corresponding to the increase of the components with relatively higher frequencies in the slow oscillations. In fact, the structure of network in Fig. 1 provides the basic mechanism for these two groups of oscillation frequencies: the presence of mul-

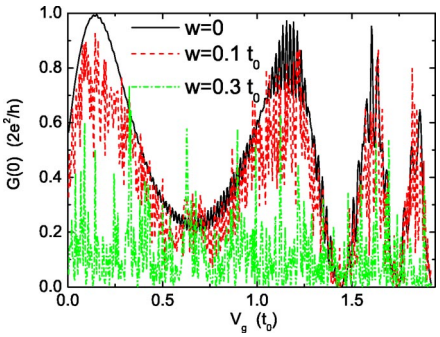

FIG. 4. (Color online) $G(0)$ as a function of gate voltage V_g in chains with different degrees of disorder. Other parameters are the same as those in Fig. 3.

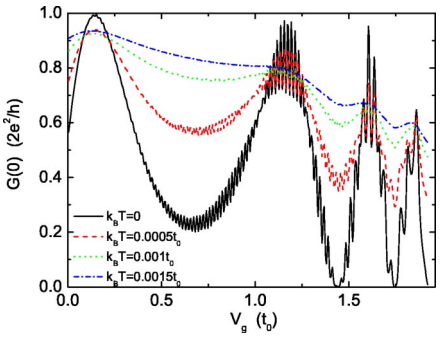

FIG. 5. (Color online) Conductance $G(T)$ as a function of gate voltage V_g in a pure chain. $c_0/\hbar\omega_0=0.04t_0$, and the other parameters are the same as those in Fig. 2(a).

tiple channels in region B gives rise to the interference between them which creates the slow oscillations, meanwhile the finite length of each channel leads to discrete resonances (quantum size effect) corresponding to the fast oscillations in the $G(0)-V_g$ curves. If we eliminate the coupling between channels by partial diagonalization, the obtained energy differences between decoupled channels are in the order of EP coupling strength. These energy differences are much smaller than the resonant energies, and are related to the low-frequency group of oscillations. This is the reason why increasing the EP coupling can enhance frequencies of slow oscillations, meanwhile has almost no effect on the fast oscillations.

The effect of disorder is displayed in Fig. 4 where the $G(0)-V_g$ curves are shown for different strengths of disorder. By introducing the disorder, at first the fast oscillations, then the slow oscillations, are replaced by the white-noise fluctuations typical for disordered systems. It can be seen that the necessary disorder for destruction of the regular oscillations is certainly weak, indicating the frangibility of the QI induced by the EP interaction. This means that the purity of 1D system is a necessary condition for observing such interference.

The conductance $G(T)$ as a function of V_g for different temperatures is shown in Fig. 5. At finite temperatures the transmission amplitude $t_{jj'}$ with $j\neq 0$ also have contributions to the transport. By raising the temperature, both the slow and fast oscillations are smoothed. At higher temperatures the phonon states in the EP states are closer to the thermal equilibrium due to the inclusion of more channels on both sides in Fig. 1, and in turn the quantum coherence of the EP state cannot be kept during the transmission of electrons. This eliminates the effect of QI. Such a temperature dependence of slow and fast oscillations is in good consistence with the experimental measurements.[8]

As a summary, we investigate the effect of the EP interaction on the transport of electrons through a 1D system of mesoscopic length. It is shown that the quantum interference can be induced by the EP interaction provided that the EP states are quantum-mechanically coherent during the tunneling of electrons through the region. This interference is exhibited from the fast and slow oscillations of the conductance with respect to the gate voltage. Such characteristics are robust against the changes of the size of the system and the strength of the interaction, but can be easily eliminated by introducing the disorder and raising the temperature due to the destruction of the coherence. The obtained results provide a natural explanation for the observation of fast and slow oscillations of conductance in quasi-1D systems.

ACKNOWLEDGMENTS

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