Solid State Communications 150 (2010) 799–803

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Bias-dependent bandwidth of the conductance in the presence of electron–phonon interaction

Ying-Tsan Tang *, Kao-Chin Lin, Der-San Chuu

Department of Electrophysics, National Chiao Tung University, Hsinchu, 30013, Taiwan

ARTICLE INFO

Article history:
Received 31 August 2009
Accepted 7 January 2010
by S. Tarucha
Available online 13 January 2010

Keywords:
C. Tunneling
C. Electron–phonon interactions
C. Electronic transport

ABSTRACT

We study the electronic transport in the presence of electron–phonon interaction (EPI) for a molecular electronic device. Instead of mean field approximation (MFA), the related phonon correlation function is conducted with the Langreth theorem (LT). We present formal expressions for the bandwidth of the electron's spectral function in the central region of the devices, such as quantum dot (QD), or single molecular transistor (SMT). Our results show that the out-tunneling rate depends on the energy, bias voltage and the phonon field. Besides, the predicted conductance map, behaving as a function of bias voltage and the gate voltage, gets blurred at the high bias voltage region. These EPI effects are consistent with the experimental observations in the EPI transport experiment.

1. Introduction

As the trend of miniaturization of electronic devices continues, the molecular device has been explored in recent years [1]. In the molecular device, one of the particular interests in studying the physics of these devices, is the coupling of the charge states to the vibration or configurational modes of the molecule. The electronic transport in the presence of electron–phonon interaction (EPI transport) becomes an important topic in the nano-mechanical device system and has been investigated experimentally by a number of groups on a single molecular transistor system [2–7] as well as on a semiconductor quantum dot system [3,8]. Some of which were reported that single molecular transistors are strongly influenced by a single vibrational mode. In Ref. [2], Park et al. show that such mechanical device can be realized by applying a C_{60} molecule against the gold surface, where a single vibrational mode was associated with the oscillation of the C_{60} in the confining well created by the van der Waals force, and the motion of C_{60} is excited by the tunneling electrons. Later a similar current step phenomena was observed by embedding a quantum dot in a suspended GaAs/AlGaAs membrane [8]. Theoretically, EPI induces satellite peaks of phonon sidebands (PSDs) to occur in a spectral function and yields the corresponding phonon sideband conductance (PSDC) [9]. The nth PSDC can be observed at $eV_b = \widetilde{\varepsilon}_0 \pm eV_g \pm n\omega_0$, where $\widetilde{\varepsilon}_0$ is the renormalized resonant energy of the QD (or SMT) due to EPI, n is a positive number, V_g is the gate voltage and V_b is the applied bias ($V_b = (\mu_L - \mu_R)/e$, μ_α is the chemical potential of lead α). Note that PSDC does not emerge till the applied bias voltage (eV_b) exceeds the energy of a phonon. Hence $e|V_b| \geq \omega_0$ is the necessary condition for the occurrence of PSDC [10] and the transport window is controlled by V_b. We find that the bandwidth will increase with the bias voltage. As a result, the conductance map, behaving as a function of the bias voltage (V_b) and gate voltage (V_g), blurs at the larger bias region. In the current–voltage measurement research, shot noise provides additional and important information about the particle fluctuation. According to Ref. [9], the shot noise can be calculated once the tunneling coefficient is found out. Since the tunneling coefficient is highly dependent on the jumping rate of the electron transportation, the explicit analysis of the tunneling rate (bandwidth) on the noise becomes an important issue, and a few results are just beginning to emerge [11]. Before that, in this work we illustrate how the current and the tunneling rate can be performed correctly with the nonequilibrium Green function approach.

2. Model and theoretical tools

In this paper, we consider the electron transport between the leads and the central region, e.g. a single resonant QD or SMT, in which the electron interacts with the phonon field. The Hamiltonian of the system can be defined as [1]:

$$H = H_{\text{cen}} + H_{\text{lead}} + H_T, \tag{1}$$

$$\begin{aligned} H_{\text{cen}} &= (\varepsilon_0 - \Delta)d^+d + \omega_0 b^+ b \\ &\equiv \widetilde{\varepsilon}_0 d^+ d + \omega_0 b^+ b, \end{aligned} \tag{2}$$

$$H_{\text{lead}} = \sum_{k_\alpha, \alpha \in L,R} \varepsilon_{k_\alpha} c^+_{k_\alpha} c_{k_\alpha}, \tag{3}$$

* Corresponding author. Tel.: +886 921095165.
E-mail addresses: yingtsan.tang@gmail.com (Y.-T. Tang), kaochin.lin@gmail.com (K.-C. Lin).

0038-1098/$ – see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ssc.2010.01.007

$$H_T = \sum_{k_\alpha, \alpha \in L,R} V_{k_\alpha} c_{k_\alpha}^{+} dX + h.c, \tag{4}$$

where

$$X \equiv \exp\left[-\frac{\lambda}{\omega_0}(b^{+} + b)\right], \tag{5}$$

$$\Delta \equiv \lambda^2/\omega_0. \tag{6}$$

The operators $d^{+}(d)$ and $c_{k_\alpha}^{+}(c_{k_\alpha})$ are the creation (annihilation) operators of electron in the QD (or SMT) and α lead, respectively. The operator $b^{+}(b)$ is the creation (annihilation) operator of the phonon. $\widetilde{\varepsilon}_0 \equiv (\varepsilon_0 - \Delta)$ is the renormalized energy of the QD (or SMT), ε_0 is the bare dot level energy, Δ is the energy shift due to the EPI, and ε_{k_α} is the energy of the electron in α lead. The coupling strength of EPI is denoted by λ and the tunneling matrix element between the QD (SMT) and the α lead is defined as V_{k_α}. In addition, we briefly outline the Keldysh Green's function and the Langreth theorem. The Keldysh Green's function is a useful and convenient tool for solving kinetic equation under non-equilibrium condition, e.g. the finite bias system. Usually the contour-ordered Green's function maintains the perturbation theory. The retarded (advanced) Green's function brings the information about spectral structure, such as density of state or a scattering (decay) rate. The lesser (greater) Green's function ($G^{<(>)}$) is associated with the occupation number or the current. For an interacting system, the contour-ordered Green's function can be expanded with a systematic perturbation method, e.g. Dyson expansion or the equation of motion, whereas the time variables inside the kinetic equation are with a complex argument. In order to obtain the physics quantities (in terms of $G^{r(a)}$ and $G^{<(>)}$) in a real time axis, it's necessary to replace the contour integrals by real time integrals. This procedure is called the analytic continuation or the Langreth theorem. A convenient table for the analytic continuation (the Langreth rules) is listed in Table 4.1 of [12].

The technique of the Keldysh Green function on charge transportation was developed by Jauho, Wingreen and Meir (JWM's transport formula) [13] and is widely used to calculate the transport problem in nanostructure systems. In JWM's formula, the system is divided into the lead region and the central region (interacting region). The electronic current flowing from the lead $\alpha(\in L, R)$ into the central region (i.e. the incoming current J_{in}) is directly proportional to the product of the Fermi function of the α lead, $f_\alpha(\omega)$, the in-tunneling rate, $\Gamma_{in}^{\alpha}(\omega)$, and the spectral function of the central region $A(\omega)(= -2\,\mathrm{Im}\,G^r(\omega))$. The electronic current flowing out of the central region into the α lead (i.e. the out-going current J_{out}) is directly proportional to the product of the particle occupation in the central region and the out-tunneling rate $\Gamma_{out}^{\alpha}(\omega)$. Thus, the current can be calculated once the Keldysh Green function of the central region is determined. Note that, the out-tunneling rate should equal the decay rate of the particle in the central region (i.e. the bandwidth of the spectral function) due to the tunneling process (i.e. the imaginary part of the tunneling self-energy). However, in the original JWM's formula, the out-tunneling rate depends only on the properties of the tunneling barrier and is independent of the interaction (such as EPI) that occurs in the central area [9,13]. In addition, $\Gamma_{out}^{\alpha}(\omega)$ is assumed to be a constant under the wideband approximation. Therefore, the out-going current resulting from the earlier JWM's formula brings incomplete information about the system. That is, when one associates the tunneling process with the interaction in the central region, the out-tunneling rate needs to be recalculated. In Eq. (4), it is obvious that the phonon participates in the tunneling processes via $X(X^{+})$, and the effect of the phonon field operator should be applied into the tunneling self-energy of the central region. As a result, the corresponding out-tunneling rate is affected by the phonon field with EPI. Since EPI does not take place in the leads, the decay rate of the electron there, i.e. the in-tunneling rate, will not be affected.

3. Method

To apply JWM's formula to the transport problem, the Keldysh Green function for the case of EPI must be evaluated first. At the earlier stages, the interacting retarded Green function $G^r(t)$ of the electron in the QD (or SMT) was approximated with the product of the dressed electronic retarded Green function $\overline{G}^r(t)$ and the expectation value of the phonon correlation function, which is $\langle X(t)X^{+}(0)\rangle = \exp[-\Phi(t)]$, i.e. $G^r(t) = \overline{G}^r(t)\exp[-\Phi(t)]$. The phonon correlation function $\langle X(t)X^{+}(0)\rangle$ was regarded as a scalar value with the mean field approximation (MFA) [9,13]. This decoupling approximation, however, was aimed to work only at high temperatures [14]. Besides, the results based on this approximation also predict that PSDC occurs in the equilibrium situation, i.e. the case of the zero bias voltage. This consequence is clearly inconsistent with the experimental observations [2,3]. The main reason for these erroneous predictions comes from the ill treatment of the phonon correlation function [14]. In Ref. [14] a skillful improvement of MFA is suggested by Chen et al. There, the EPI lesser (greater) Green function $\overline{G}^{\lessgtr}(t)$ is approximated as the product of the electronic lesser (greater) Green function $G^{\lessgtr}(t)$ and the phonon part quantity $\exp[\mp\Phi(-t)]$, i.e. $\overline{G}^{\lessgtr}(t) = G^{<(>)}(t)\exp[\mp\Phi(-t)]$. Moreover, the tunneling matrix elements $\overline{V}_{k_\alpha}$ are approximated as a scalar number, i.e. $\overline{V}_{k_\alpha} = V_{k_\alpha}\langle X\rangle$ for calculating the tunneling rate [14]. As a result, the inconsistent PSDC disappears for $V_b = 0$, in agreement with the experiments [2]. Note that although the peak's position of the PSDC in Ref. [14] agrees with the observation in the lab, the bandwidth of the PSDC in Ref. [14] is independent of bias voltage, which disagrees with the blurred conductance pattern at the large bias region. Besides, the above treatment for the phonon correlation function $\langle X(t)X^{+}(0)\rangle$ or the phonon operators X (or X^{+}) as scalar is inappropriate. Since $X(t)$ and $X^{+}(t)$ are operators, the phonon correlation $\langle X(t)X^{+}(0)\rangle$ should be regarded as part of the Green function and follow with the analytic continuation [13]. That is, when the total Green function is in the form of the product of the electronic Green function and the phonon correlation function, the entire Keldysh Green function needs calculating by the Langreth theorem (LT) [13]. The Keldysh EPI Green function with LT is then explored as follows.

4. Green function formalism

Before calculating the tunneling current in the presence of EPI, it should be noted that either the equation-of-motion or Dyson equation is manipulated in terms of the contour order Green function and the expectation value for phonon correlation function $\langle X^{+}(t')X(t)\rangle$ (or $\langle X(t)X^{+}(t')\rangle$) should be regarded as the lesser (or greater) phonon Green function first. According to Eq. (10) and Eq. (11) in Ref. [13], the current flowing from the left lead to the central region can be written by:

$$\begin{aligned} J_L(t) &= \frac{2}{\hbar}\mathrm{Re}\sum_{k,\alpha\in L} V_{k\alpha} G_{d,k\alpha}^{<}(t,t) \\ &= \frac{2e}{\hbar}\mathrm{Re}\left\{\int_c dt_1 G_{(dd)}^{c}(t,t_1)\Sigma_{T,L}^{c}(t_1,t')\right\}^{<}|_{t'\to t}\,, \end{aligned} \tag{7}$$

where, a useful contour order self-energy of the electron due to the tunneling process can be defined as

$$\Sigma_{T,\alpha}^{c}(t,t') = \sum_{k_\alpha} \left|V_{k_\alpha}\right|^2 F^{+c}(t-t') g_{k_\alpha}^{c}(t-t'), \tag{8}$$

$F^{+c}(t-t') \equiv \left\langle T_C X^{+}(t)X(t')\right\rangle$ and $g_{k_\alpha}^{c}(t-t') \equiv \left\langle T_C c_{k_\alpha}(t)\, c_{k\alpha}^{+}(t')\right\rangle$ represent the contour order phonon correlation function

and the contour order Green function of the electron in α lead, respectively. Note that the retarded self-energy in the presence of EPI must be calculated in terms of lesser and greater Green functions before the expectation value $\langle X(t)X^+(t')\rangle$ is imported from Ref. [6]. According to the Langreth theorem, the retarded self-energy of the electron in QD(SMT) is:

$$\begin{aligned}\Sigma^r_{T,\alpha}(\omega) &= F.T.\left\{\theta(t-t')\left[\Sigma^>_{T,\alpha}(t-t') - \Sigma^<_{T,\alpha}(t-t')\right]\right\} \\ &= F.T.\left\{\sum_{k_\alpha}\left|V_{k_\alpha}\right|^2\theta(t-t')\right. \\ &\quad\left.\times\left[F^{+>}(t-t')g^>_{k_\alpha}(t-t') - F^{+<}(t-t')g^<_{k_\alpha}(t-t')\right]\right\}, \quad (9)\end{aligned}$$

where $F^{+>}(t-t') \equiv \langle X^+(t')X(t)\rangle$ and $F^{+<}(t-t') \equiv \langle X(t)X^+(t')\rangle$ represent the greater/lesser Green function of the phonons respectively, and $g^{<(>)}_{k_\alpha}(t-t')$ is the lesser (greater) Green function of the electron in the lead α. After Fourier transformation, the retarded and the lesser self-energies of the electron can be expressed as:

$$\begin{aligned}\Sigma^r_\alpha(\omega) &= \sum_{n,k}\left[p_n\frac{V^*_{k_\alpha}V_{k_\alpha}}{\omega+n\omega_0-\varepsilon_{k_\alpha}+i\delta}f^<_\alpha(\varepsilon_{k_\alpha})\right. \\ &\quad\left.+p_{-n}\frac{V^*_{k_\alpha}V_{k_\alpha}}{\omega+n\omega_0-\varepsilon_{k_\alpha}+i\delta}f^>_\alpha(\varepsilon_{k_\alpha})\right], \quad (10)\\ \Sigma^<_\alpha(\omega) &= \sum_{n,k}V^*_{k_\alpha}V_{k_\alpha}p_n g^<_{k_\alpha}(\omega+n\omega_0) \\ &= i\sum_n p_n\Gamma_\alpha(\omega+n\omega_0)f^<_\alpha(\omega+n\omega_0), \quad (11)\end{aligned}$$

where $f^<_\alpha(\varepsilon_{k_\alpha}) \equiv f_\alpha(\varepsilon_{k_\alpha})$ is the Fermi function of the lead α and $f^>_\alpha(\varepsilon_{k_\alpha}) \equiv 1-f_\alpha(\varepsilon_{k_\alpha})$. Γ_α represents the tunneling rate of the electron in the system without EPI. Besides, the interacting electronic retarded Green function can be derived as $G^r(\omega) = \left[\omega-(\varepsilon_0-\Delta)-\Sigma^r_\alpha(\omega)\right]^{-1}$ [13]. Note that the retarded self-energy of the electron expressed in Eq. (10) is a similar form as the one reported in Ref. [15]. The factor p_n denotes the weighting factor of the interaction between the electron and n phonons. At a finite temperature, $p_n = e^{-g(2N_0+1)}e^{n\omega_0/2k_BT}I_n(2g\sqrt{N_0(N_0+1)})$. N_0 is the Bose function, $g = (\lambda/\omega_0)^2$ and $I_n(z)$ denotes the Bessel function with a complex argument.

Regarding the steady state lesser Green function, this can be calculated by the continuous condition for the steady state, i.e. $\left\langle\dot{N}\right\rangle = -i\langle\partial G^</\partial t\rangle = 0$. As a result, the lesser (greater) Green function is evaluated as [16]:

$$\begin{aligned}&G^{<(>)}(\omega) \\ &= \frac{\pm i\sum_{n,\alpha}p_{\pm n}\Gamma_\alpha(\omega+n\omega_0)f^{<(>)}_\alpha(\omega+n\omega_0)}{\sum_{n,\alpha}\left[p_n\Gamma_\alpha(\omega+n\omega_0)f^<_\alpha(\omega+n\omega_0)+p_{-n}\Gamma_\alpha(\omega+n\omega_0)f^>_\alpha(\omega+n\omega_0)\right]}A(\omega). \quad (12)\end{aligned}$$

5. EPI current formula

In Eq. (10), the imaginary part of the retarded self-energy interprets the decay rate of the electron in central region, and it depends on the energy, temperature, chemical potential of the leads and the phonon field. The expected out-tunneling rate in the presence of EPI is not a constant, so that the early JWM's transport formula cannot be used directly. Following the deriving processes from Ref. [13], we conclude that the transport formula for the presence of EPI reads

$$\begin{aligned}J_\alpha &= \frac{e}{\hbar}\int\frac{d\omega}{2\pi}\sum_{n=-\infty}^{\infty}Tr\left\{f_\alpha(\omega)\Gamma^\alpha_{in}(\omega)p_nA(\omega-n\omega_0)\right. \\ &\quad\left.+i\left[\Gamma^{\alpha<}_{n,out}(\omega)+\Gamma^{\alpha>}_{n,out}(\omega)\right]G^<(\omega-n\omega_0)\right\}, \quad (13)\end{aligned}$$

with

$$\Gamma^{\alpha<}_{n,out}(\omega) = p_n\Gamma^\alpha f_\alpha(\omega), \quad (14)$$

$$\Gamma^{\alpha>}_{n,out}(\omega) = p_{-n}\Gamma^\alpha(1-f_\alpha(\omega)), \quad (15)$$

$$\Gamma^\alpha_{in}(\omega) \equiv \Gamma^\alpha, \quad (16)$$

and the calculation for the spectral function ($A(\omega) = -2\,\mathrm{Im}\,G^r(\omega)$) reads

$$A(\omega) = \frac{\sum_{n,\alpha}\left[p_n\Gamma^\alpha(\omega+n\omega_0)f^<_\alpha(\omega+n\omega_0)+p_{-n}\Gamma^\alpha(\omega+n\omega_0)f^>_\alpha(\omega+n\omega_0)\right]}{|\omega-(\varepsilon_0-\Delta)-\Sigma^r(\omega)|^2}.$$

The first term in the RHS in Eq. (13) represents the electron flux in the α lead flowing into the nth PSD of the central region J_{in}. The summation of each phonon sideband's spectral function multiplied by p_n guarantees the integration with all energies equal to the unity. $\Gamma^{\alpha\gtrless}_{n,out}(\omega)$ represents the decay rate for an electron jumping out of the nth PSD of the system into the lead α via different channels. Comparing Eqs. (10), (11), (14) and (15), we find that the out-tunneling rate $\Gamma^\alpha_{out}(\omega)$ is equal to the imaginary part of the retarded tunneling self-energy of the particle, i.e. the bandwidth of the spectral function due to the tunneling process. This is an important result, different from the one shown in Ref [14], in which $\Gamma^\alpha_{out}(\omega)$ always characterizes with a constant tunneling rate $p_0\Gamma^\alpha$, with $p_0 = e^{-g(2N_0+1)}$. The second term on the RHS in Eq. (13) describes the out-tunneling current J_{out}, where the electron in the central region tunnels out of the central region via two channels. The first (second) term of the out-tunneling current, i.e. $G^<(\omega-n\omega_0)\Gamma^{\alpha<}_{n,out}(\omega)$ ($G^<(\omega-n\omega_0)\Gamma^{\alpha>}_{n,out}(\omega)$) represents the electron occupying the phonon sideband with absorbing n ($n \in$ *positive*) or emitting n ($n \in$ *negative*) phonon tunnels into the lead α, in which the energy is lower (higher) than the Fermi energy of the lead. Note that the electron in the lead does not interact with the phonon field, which results in the in-tunneling rate $\Gamma^\alpha_{in}(\omega)$, behaving exactly the same as the bare tunneling rate. Finally, with the retarded, lesser Green functions and the EPI transport formula as derived above, we find the current $J(=J_L=-J_R)$ satisfies the requirement of the continuity equation. Therefore, the EPI transport formula Eq. (13) is meaningful and available.

6. Results

In order to compare our spectral function (with LT method) with the one discussed by Chen et al. [14] (with an improved MFA method), we plot the total system's spectral function $A^{(tot)}(\omega) = \sum_n p_nA(\omega-n\omega_0)$ for three different energy levels. The spectral function for the central region near $V_b = 0$ is depicted in Fig. 1(a). Clearly, the results obtained with the LT method (in blue curve) are quite different from those obtained with the MFA method (in red curve) [14]. According to the MFA technique in Ref. [14], the satellite peaks' position of spectral function are strongly dependent on the difference between the resonant energy and chemical potential of the leads. In the case of $\widetilde{\varepsilon}_0 > (<)\mu_\alpha$, i.e. empty (occupied) state of the QD (or SMT), only the $|n|$th ($-|n|$th) PSD of the spectral function appears (see Fig. 1(a) Up/Down). When $\widetilde{\varepsilon}_0 = \mu_\alpha$, a pair of mirror-symmetric PSDs occur in the position of $|n|$ *th* and $-|n|$th bosonic modes with respect to $\widetilde{\varepsilon}_0$ (see Fig. 1(a) Medium) and no peaks can emerge within $\omega < e|V_b|$. That is, the PSDs provide channels for charge transportation only when $e|V_b| \geq \omega_0$. However, the PSDs do not depend on the relative

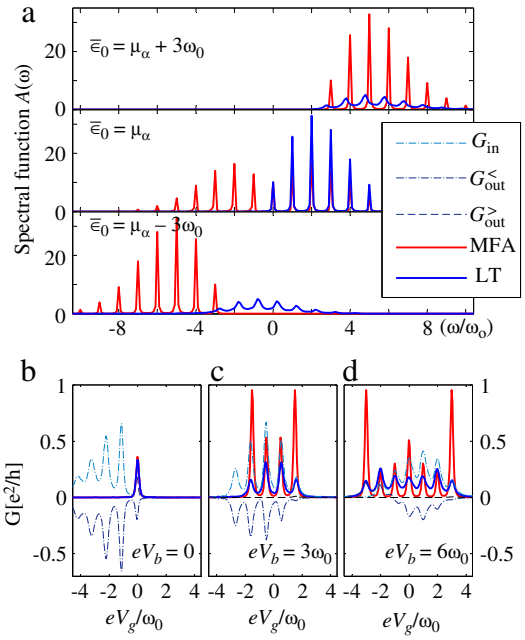

Fig. 1. (a) The spectral function of the strong EPI system v.s. energy ω for different energy levels for $\widetilde{\varepsilon}_0$. The chemical potential in the leads are fixed at $\mu_L = -\mu_R = 0.1\omega_0$. The parameters used are $\Gamma_L = \Gamma_R = 0.4\omega_0$, $k_BT = 0.05\omega_0$, $\lambda = 1.6\omega_0$. (b) The conductance as a function of gate voltage for different bias voltages as indicated. In addition to the parameters given above, we choose a Lorentzian cut-off at $E_C = 100$ in the integral calculation [15]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

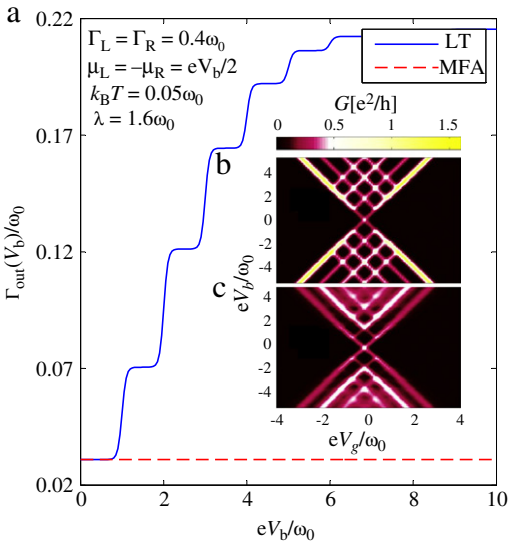

Fig. 2. (a) The out-tunneling rate $\Gamma^\alpha_{out}(\omega = V_b/2)$ v.s bias voltage. (b) The maps of differential conductance as a function of gate and bias voltage is calculated with MFA's approach and (c) is worked with the Langreth theorem.

position between $\widetilde{\varepsilon}_0$ and μ_α in the results obtained with the LT method. The operations of $\widetilde{\varepsilon}_0$ and μ_α only affect the magnitude of the spectral function without changing the number of satellite peaks. As a result, the charge transportation is irrespective of the relative position between $\widetilde{\varepsilon}_0$ and μ_α. Note that the envelope of the PSDs which are skewed toward the positive value of n results from the weighting factor p_n. Such an asymmetric scheme implies the insignificance of the $-|n|$th PSDs at low temperatures [14].

Fig. 1(b), (c) and (d) show the calculated conductance versus the gate voltage for various bias voltage V_b with the LT method (blue curve) and with the MFA technique (red curve). We find that a higher bias voltage yields a wider bandwidth of PSDC as one utilizes the LT technique, but it remains unchanged for the MFA calculation. The PSDC reproduces the same curve as depicted with the MFA approach for $V_b = 0$ (equilibrium case, Fig. 1(b)), i.e. $\sum_n(\Gamma^{\alpha<}_{n,out} + \Gamma^{\alpha>}_{n,out}) \to p_0\Gamma^\alpha$, which implies the significance of bias dependence in the out-tunneling rate of our calculation. Although both methods result from different spectral function when changing the bias voltage, they result in an symmetric shape as a function of V_g. We can analyze branches of conductance from the definition: $G_{in(out)} = \partial J_{in(out)}/\partial V_b$, where G_{in} shows the conductance corresponding to the in-tunneling current, and it implies the profile of the spectral function in the central region. $G^<_{out}$ and $G^>_{out}$ are the conductances corresponding to the out-tunneling current with the out-tunneling rates $\Gamma^{\alpha<}_{n,out}(\omega)$ and $\Gamma^{\alpha>}_{n,out}(\omega)$, respectively. Note in the case of $V_b = 0$, the PSDC of G_{in} and $G^<_{out}$ eliminate each other and the remaining PSDCs turn to zero for $e|V_g| > \omega_0$ (Fig. 1(b)). For $e|V_b| \geq \omega_0$, the conductance also results from the analogous cancellation of the G_{in} and $G^<_{out}$ and it further dominates the symmetric behavior of the conductance (Fig. 1(c) and (d)). For example, the spectral functions in Fig. 1(b) are asymmetric due to the phonons, which yields the asymmetric type of G_{in}. However, after the cancellation of G_{in} and $G^<_{out}$, the total conductance becomes surprisingly symmetric about $V_g = 0$, as the same symmetric form as reported in Ref. [14]. In addition to explaining the symmetric mechanism of the conductance, we next examine the staircase change of broadening in the following section.

Since the conductance is defined by the change of current with respect to the bias voltage, the bandwidth of the conductance is thus related to the bandwidth of the spectral function near the chemical potential of the leads. Fig. 2(a) shows the calculated bandwidth $\Gamma^\alpha_{out}(\omega = eV_b/2)$ versus the bias voltage with the LT method (blue curve) and the MFA method (red line). We can see that the out-tunneling rate $\Gamma^\alpha_{out}(\omega = eV_b/2)$ of the LT behaves like a staircase, whereas the MFA method produces a flat line. In the LT results, Γ^α_{out} increases abruptly in the neighborhood of $eV_b = n\omega_0$ and the plateau is generated around $eV_b = (n+1)\omega_0/2$. The abrupt increment in the $\Gamma^\alpha_{out}(eV_b/2)$ results from the opening of an additional channel via the PSD when the bias voltage exceeds a phonon energy. As a result, the increasing bias voltage yields a quantized-incremental broadening of PSD in the spectral function and the conductance gets blurred at the larger bias region (see also Fig. 1(b) Medium, Right). Note that the LT result is exactly the same as the MFA ($\Gamma^\alpha_{out} = \Gamma^\alpha p_0$) when $eV_b < \omega_0$, This is because only the state with $n \to 0$ is allowed for charge transportation, and it further brings about the identical bandwidth for the conductance as mentioned above (see Fig. 1(b)). Fig. 2(b) and (c) illustrate the plot of the conductance map as a function of V_b and V_g with the interacting Keldysh Green function calculated with the MFA method [14] and with the LT method, separately. Fig. 2(b) and (c) represent the same peaks' position of PSDC and they both show the only and oth PSDC at $V_b = 0$. However, Fig. 2(c) further depicts that the conductance becomes blurred with a large bias voltage, which differs from the majority of theoretical predictions [9,14] but it agrees with the experimental observations [2–5,7].

7. Conclusion

We introduce an appropriate scheme based on the framework of the Langreth theorem to calculate the electron–phonon interaction (EPI) Keldysh Green function for EPI transport problem. Since the process of the electron tunneling out of the central regime is related with EPI, the out-tunneling rate is dependent on the phonon field, energy and the chemical potential of the

leads. Owing to this, a modified JWM's formula is presented for calculating the transport problem in the presence of EPI. In this work, we found that the satellite peaks' position of the conductance (PSDC) agrees with the other theoretical study, e.g. MFA [14] and the experimental observation. However, our results further show that the out-tunneling rate can be increased in a staircase way with the bias voltage. As a result, the larger the bias voltage, the wider the bandwidth of the conductance becomes and this conductance map gets blurred when it is displayed with a function of gate voltage and the bias voltage. This is consistent with the experimental results. Finally we bring up few issues raised by this work, but not yet resolved. One important research is to utilize the analytic continuation of the LT for calculating the noise spectrum $S(\omega)$, in particular to the case of a strong EPI. The second is to explore the crossover condition of negative conductance and investigate the influence of temperature on the conductance and the noise, especially at low temperature. The third issue is to bridge the connection between the broadening bandwidth of the conductance with the LT Green function method and the never-broadening bandwidth of the conductance in the standard Master equation [17,18]. Work in the first direction is now in progress.

The authors gratefully appreciate the discussion with Prof. Dr. M. F. Lin and Prof. H. C. Kan, and are thankful for the support of the NSC-DAAD Sandwich Program under the grant number 96-2911-I-009-025-2 and the National Science Council, Taiwan under the grant number NSC 97-2112-M-009 -004.

References

[1] M. Galperin, M.A. Ratner, A. Nitzan, J. Phys. Condens. Matter 19 (2007) 103201.
[2] H. Park, J. Park, A.K.L. Lim, E.H. Anderson, A.P. Alivisatos, P.L. McEuen, Nature 407 (2000) 57.
[3] R. Leturcq, C. Stampfer, K. Inderbitzin, L. Durrer, C. Hierold, E. Mariani, M.G. Schultz, F. von Oppen, K. Ensslin, Nature Phys. 5 (2009) 327–331.
[4] L.H. Yu, D. Natelson, Nano Lett. 4 (2004) 79.
[5] S. Sapmaz, P. Jarillo-Herrero, J. König, C. Dekker, L.P. Kouwenhoven, H.S.J. van der Zant, Phys. Rev. B 71 (2005) 153402.
[6] G.D. Mahan, Many Particle Physics, Plenum, New York, 1981, (Sec. 5.5B).
[7] S. Sapmaz, P. Jarillo-Herrero, Y.M. Blanter, C. Dekker, H.S.J. van der Zant, Phys. Rev. Lett. 96 (2006) 026801.
[8] E.M. Weig, R.H. Blick, T. Brandes, J. Kirschbaum, W. Wegscheider, M. Bichler, J.P. Kotthaus, Phys. Rev. Lett. 92 (2004) 046804.
[9] J.-X. Zhu, A.V. Balatsky, Phys. Rev. B 63 (2003) 165326.
[10] M. Galperin, A. Nitzan, M.A. Ratner, Phys. Rev. B 73 (2006) 045314.
[11] F.M. Souza, A.P. Jauho, J.C. Egues, Phys. Rev. B 78 (2008) 155303.
[12] H. Haug, A.P. Jauho, Quantum Kinetics in Transport and Optics of Semiconductors, 2nd edition, Springer, 2007.
[13] A.P. Jauho, N.S. Wingreen, Y. Meir, Phys. Rev. B 50 (1994) 5528.
[14] Z.Z. Chen, R. Lu, B.F. Zhu, Phys. Rev. B 71 (2005) 165324.
[15] J. König, H. Schoeller, G. Schön, Phys. Rev. Lett. 76 (1996) 1715–1718.
[16] K.C. Lin, D.S. Chuu, Phys. Rev. B 72 (2005) 125314.
[17] A. Mitra, I. Aleiner, A.J. Millis, Phys. Rev. B 69 (2004) 245302.
[18] M. Esposito, M. Galperin, Phys. Rev. B 79 (2009) 205303.