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Cooling effect of thermal bias on a current-carrying nanodevice

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ABSTRACT

We investigate the heat generation in a quantum dot (QD) coupled to two normal leads with different temperatures. It is found that heat in the QD can be conducted efficiently away through electron–phonon interaction in the QD when the QD is coupled stronger to colder lead than to the hotter one. As temperature of the colder lead is close to zero, the current through the QD peaks at the very QD level position, where the heat generation is zero, which helps to keep the stability of a working nanodevice. Then an ideal condition for nanodevice operation can be found.

The heat generation in nanoscale devices has attracted increasing attention in recent years due to the miniaturization of electronic devices. For heat generation in a solid-state device, the electron–phonon interaction (EPI) is the main cause. An electron tunnels into the device and left with diminished energy, with the loss energy being transferred to the ionic degree of freedom through the EPI. Even though the characteristic size of a nanodevice is smaller than the electronic coherence length, the heat generation is still substantial owning to the huge density of current-carrying electrons. Such local heating has been observed experimentally by Huang et al. [1,2] and Schulze et al. [3] by measuring the bond rupture force of individual molecule junctions and by measuring the electron current required to thermally decompose the fullerene cage. The temperature increase is relevant for a nanoscale device, because such temperature increase may affect the normal behavior of devices [2].

In the past decade, studies have been carried out to investigate local heating in nanoscale junctions [4–17]. Sun et al. [4–7] researched the current-induced heat generation in a QD containing EPI. They found that the heat generation is not proportional to the current for a fixed voltage bias and a threshold bias voltage V_{onset} is required to generate heat at low temperature. These characteristics are unique properties of nanosystems, absent in macroscopic systems. Chen et al. [13] reported the first-principles calculations of local heating in nanojunctions, and they obtained that if the external bias V is below V_{onset}, heating can still be noticeable when the background temperature is on the order of approximately $e(V_{onset} - V)/\kappa_B$ (where e is electron charge and κ_B is the Bolzman constant). They also reported that for various alkanethiols sandwiched between metal electrodes, the local temperature of the alkanethiols is relatively sensitive to their length [14]. When examining a vibrating free junction, Entin-Wohlman et al. found the phonon population of the junction is determined by bias voltage [15]. Experimentally, Huang et al. [1] discovered that the effective local temperature of a molecular junction varies with the applied bias voltage and the molecular length. Similar phenomenon was also observed by Ioffe et al. [16]. Cahill et al. [17] measured the local temperature of a carbon nanotube, and found it varying with the distance along and across the nanotube.

Lately, increasing attention has been paid to the idea of local cooling of nanojunctions [18]. R. D'Agosta et al. [19] predicted that at sufficiently large biases, the electron heating effect lowers the effective temperature of the ionic degrees of freedom in a nanostructure. This prediction has been confirmed experimentally [1,16]. McEniry et al. [20] studied a model system consisting of an adatom bonded to an atom wire. They found the vibrational energy of such a system may decrease under bias due to the anti-resonance in the transmission function. Galperin et al. [21–23] obtained that current-induced vibrational cooling can be realized for a nanojunction, containing EPI, when the junction is properly voltage biased that phonon absorption is favored over phonon emission. A two-terminal junction can be cooled under applied bias when it couples more strongly to the cold side, the high-voltage side, than to the other [21]. Apparently, the bias voltage plays an important role in the cooling effect mentioned above. In this paper, instead of

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discussing the influence of bias voltage on cooling effect, we study the local cooling in a nanojunction resulting from thermal bias.

In order to stress the effect of thermal bias, we ignore the electron–electron interaction in the nanodevice and model the system as simple as possible. Consider a lead-quantum dot (QD)-lead system, where the QD has one electronic energy level that is coupled to a local single-phonon mode. The Hamiltonian of this system is (hereafter $e, \hbar = 1$)

$$H = \epsilon_d d^\dagger d + \lambda\left(a^\dagger + a\right) d^\dagger d + \omega_0 a^\dagger a + \sum_{k,\alpha} \varepsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} + \sum_{k,\alpha}\left(V_\alpha c_{k\alpha}^\dagger d + V_\alpha^* d^\dagger c_{k\alpha}\right). \tag{1}$$

Here, the first three terms represent the Hamiltonian for the QD, with ω_0 the phonon frequency and λ the coupling strength between the electrons and the phonons in the QD. $d^\dagger$ and $a^\dagger$ create an electron and a phonon, respectively, in the QD. The last two terms describe the electronic reservoirs ($\alpha = L, R$ represents the left and right lead respectively) and the electronic coupling between the QD and the leads, with V_α the coupling strength. The same Hamiltonian has been used to investigate the thermoelectric transport through a molecular bridge [24].

The heat generation Q in the QD per unit time at time t is $Q(t) = \langle dE_{ph}(t)/dt\rangle$, where $E_{ph}(t) = \omega_0 a^\dagger(t) a(t)$. With the equation-of-motion technique, we get [4]

$$Q = \omega_0 \lambda^2 \left[2N_{ph}\,\mathrm{Im}\, G_{AA}^r(\omega_0) + iG_{AA}^<(\omega_0)\right], \tag{2}$$

where, the G_{AA}^r and $G_{AA}^<$ are the retarded and lesser components of the electronic two-particle Green's functions for the QD and governed by the Hamiltonian in Eq. (1). In order to solve these two-particle Green's functions, we need to make a unitary transformation $\bar{H} = UHU^\dagger$, with the unitary operator $U = \exp\{(\lambda/\omega_0)(a^\dagger - a) d^\dagger d\}$. After some algebra, we obtain

$$\bar{H} = \bar{\epsilon}_d d^\dagger d + \omega_0 a^\dagger a + \sum_{k,\alpha} \varepsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} + \sum_{k,\alpha}\left(\bar{V}_\alpha c_{k\alpha}^\dagger d + \bar{V}_\alpha^\dagger d^\dagger c_{k\alpha}\right), \tag{3}$$

where, $\bar{\epsilon}_d = \epsilon_d - \lambda^2/\omega_0$ and $\bar{V}_\alpha = V_\alpha X$, with $X = \exp\{-(\lambda/\omega_0) \times (a^\dagger - a)\}$. When replacing the X approximately with its expectation value $\langle X\rangle = \exp\{-(\lambda/\omega_0)^2 (N_{ph} + 1/2)\}$, the EPI is decoupled and then the Q can be given in terms of the electronic single-particle Green's functions for the QD in the frame of $\bar{H}$. This approximation has been used in previous works [4–6] and is only valid when $V_\alpha \ll \lambda$.

In terms of the single-particle Green's functions governed by the Hamiltonian $\bar{H}$, the Q is now given by [4–6]

$$Q = \frac{\omega_0 \lambda^2}{\bar{\Gamma}^2} \int \frac{d\omega}{2\pi} \left\{ \bar{\Gamma}_L \bar{\Gamma}_R (f_L - f_R)(\bar{f}_L - \bar{f}_R) + 2\bar{\Gamma} \sum_\alpha (N_{e\alpha} - N_{ph}) \bar{\Gamma}_\alpha (\bar{f}_\alpha - f_\alpha) \right\} \times \mathrm{Im}\, \bar{G}^r(\omega)\, \mathrm{Im}\, \bar{G}^r(\omega - \omega_0). \tag{4}$$

Here, $\bar{\Gamma} = (\bar{\Gamma}_L + \bar{\Gamma}_R)/2$ and $\bar{\Gamma}_\alpha = \Gamma_\alpha \langle X\rangle^2$ ($\alpha = L, R$), with $\Gamma_\alpha = 2\pi \sum_k |V_\alpha|^2 \delta(\omega - \varepsilon_{k\alpha})$ being the linewidth function and assumed to be independent of energy ω. $N_x = 1/[\exp(\omega_0/\kappa_B T_x) - 1]$, with T_x the temperature of lead α (when $x = e\alpha$) or of the phonon bath (when $x = ph$). f_α and $\bar{f}_\alpha$ represent $f_\alpha(\omega)$ and $f_\alpha(\omega - \omega_0)$ respectively, and $f_\alpha(\omega) = 1/\{\exp[(\omega - \mu_\alpha)/\kappa_B T_\alpha] + 1\}$ is the Fermi distribution function in the lead α. $\bar{G}^r(\omega) = 1/(\omega - \bar{\epsilon}_d + i\bar{\Gamma})$ is the retarded component of the electronic Green's function for the QD.

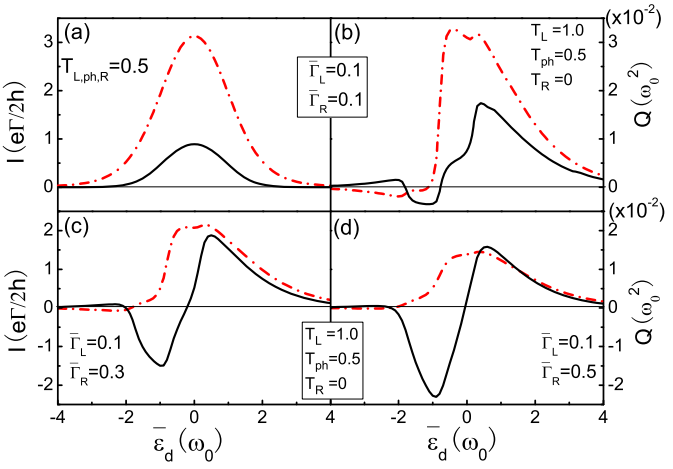

Fig. 1. (Color online.) The heat generation Q (thick solid line) and the current I (dash dot line) as a function of the effective QD level $\bar{\epsilon}_d$, with the left and right chemical potentials, in unit of ω_0, $\mu_{L,R} = \pm 0.8$ and the strength of EPI $\lambda = 0.6$.

Previous research works have shown that the relation of $Q \propto I$ (I the current flowing through the QD) fails in nanosystems [4–6, 25]. Therefore it is significant to give the current [26],

$$I = \frac{ie}{2h} \int d\omega \left\{ (f_L \Gamma_L - f_R \Gamma_R) \sum_n L_n \bar{G}^>(\omega - n\omega_0) + \left\{(1 - f_L)\Gamma_L - (1 - f_R)\Gamma_R\right\} \sum_n L_n \bar{G}^<(\omega + n\omega_0) \right\}. \tag{5}$$

In Eq. (5), $L_n \equiv e^x e^y I_n(2(\lambda/\omega_0)^2 \sqrt{N_{ph}(N_{ph}+1)})$, with $x = -(\lambda/\omega_0)^2(2N_{ph} + 1)$, $y = n\omega_0/(2\kappa_B T_{ph})$ and $I_n(z)$ the n-th Bessel function of complex argument. $\bar{G}^{<,>}(\omega)$ are the lesser and greater Green's functions governed by $\bar{H}$, and are obtained as $\bar{G}^<(\omega) = i\sum_\alpha \bar{\Gamma}_\alpha f_\alpha/[(\omega - \bar{\epsilon}_d)^2 + \bar{\Gamma}^2]$, $\bar{G}^>(\omega) = -i\sum_\alpha \bar{\Gamma}_\alpha (1 - f_\alpha)/[(\omega - \bar{\epsilon}_d)^2 + \bar{\Gamma}^2]$.

In the following numerical calculation, we set the phonon frequency $\omega_0 = 1$ as the energy unit. Generally, an electron can tunnel elastically through the QD, an electron of energy ω in one lead arrives at the other lead and enters an empty state of the same energy ω. The process of emitting (or absorbing) a phonon can take place when there are an occupied state at ω and an empty one at $\omega - \omega_0$ (or at $\omega + \omega_0$).

Fig. 1 shows the Q and I as a function of the effective QD level $\bar{\epsilon}_d$, with the chemical potentials of the left and right leads $\mu_{L,R} = \pm 0.8$ and the strength of EPI $\lambda = 0.6$. One can see in Fig. 1(a) that the Q is always positive when the phonon bath and leads have the same temperature, $T_{L,ph,R} = 0.5$, and the Q and I reach their peak values at the same level position. As we lower the temperature of the right lead to zero, $T_R = 0$, and at the same time increase T_L to 1.0, negative Q arises for some QD level position, as seen in Fig. 1(b), indicating that energy is transferred from phonon bath to electronic reservoirs, i.e., heat in the QD is conducted away. In Figs. 1(a) and 1(b), the QD is coupled symmetrically to both leads, $\bar{\Gamma}_L = \bar{\Gamma}_R = 0.1$. If we strengthen coupling to the colder one, the right one, then the magnitude and the energy range of negative Q increase, as seen in Fig. 1(c), $\bar{\Gamma}_R = 0.3$, and Fig. 1(d), $\bar{\Gamma}_R = 0.5$. What's more, the zero heat generation locates at the very level position where the current peaks. The ideal working condition for a nanodevice. The vanishing heat generation helps to keep a nanodevice in a constant temperature and then in a steady working state. If the current through the QD is induced solely by the voltage bias, in the absence of thermal bias, the Q is always positive [4,5].