

Coupled electron and phonon transport in one-dimensional atomic junctions

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Employing the nonequilibrium Green's function method, we develop a fully quantum mechanical model to study the coupled electron-phonon transport in one-dimensional atomic junctions connecting to one-dimensional leads. This model enables us to study the electronic and phononic transport on an equal footing. We derive the electrical and energy currents of the coupled electron-phonon system and present a self-consistent picture of energy exchange between them. As an application, we study the heat dissipation in current-carrying atomic junctions with metallic and semiconductor leads. We find that the inclusion of phonon transport is important in determining the heat dissipation and temperature change of the atomic junctions.

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I. INTRODUCTION

The electronic transport and phononic transport in meso- and nanostructures have attracted a great deal of interest in the past two decades, although their development is not so parallel sometimes. These structures display important quantum effects due to the confinement in one or more directions.¹ The quantized electrical conductance² was observed much earlier than that of the thermal conductance³ mainly due to the difficulty in measuring thermal transport properties. Electrons and phonons are not two isolated systems. Their interactions are important for both electronic and phononic transport. With the development of both fields, there arises the requirement to study the coupled electron-phonon transport from time to time. When studying electron transport problems, one usually assumes that electrons interact with some phonon bath where the phonons are in their thermal equilibrium state characterized by the Bose distribution. This simple assumption is not able to give satisfactory results in some cases where the phonons are driven out of equilibrium by the electrons. This is especially true in places where the thermal conductance is low or the phonon relaxation is slow.^{4,5} To take into account the nonequilibrium phonon effect, one usually introduces into the electronic transport formalism some phenomenological parameters that describe the phonon relaxation process. In engineering applications, as the size of the electronic devices decreases to nanoscale, the heat dissipation and conduction in these structures become critical issues, which may influence the electronic properties dramatically.⁶ Only studying the electronic transport is not enough in these cases. On the other hand, heat transport in one-dimensional (1D) structures has received considerable attention recently.⁶⁻⁸ Fourier's law of heat conduction is no longer valid in many 1D systems. The microscopic origins of the macroscopic Fourier's law remain one of the most frustrating problems in nonequilibrium statistical mechanics. Since the electrons and phonons both contribute to the heat conduction, their relative roles in many nanostructures are still not clear. Especially in semiconductors, which one carries the majority of the thermal current is not a trivial problem. To answer these questions, we need some general models, which take into account the electron and phonon transport, and their mutual interactions.

Theoretically, although the development of electronic transport in 1D structures has been very striking, that of the

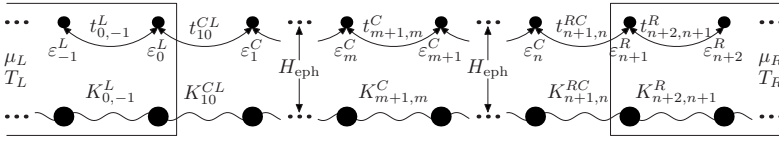
phononic transport is relatively slow. Classical molecular dynamics (MD) and the Boltzmann-Peierls equation are the widely used methods in phononic transport. The MD method is not accurate below the Debye temperature, while the Boltzmann-Peierls equation cannot be used in nanostructures without translational invariance. In both cases, the quantum effect becomes important.¹ Only recently, the nonequilibrium Green's function method,⁹⁻¹² which has been widely used to study the electronic transport, has been applied to study the quantum phononic transport.¹³⁻¹⁷ As far as we know, the study of the coupled electronic and phononic transport in nanostructures is rare.¹⁸⁻²² In this paper, using the nonequilibrium Green's function method, we study the coupled electronic and phononic transport in 1D atomic junctions connecting with 1D leads. The formalism is similar to that of Ref. 18, where the authors analyzed the heat generation in current-carrying molecular systems from the electronic transport point of view. Here, we study the heat generation from both the electron and the phonon points of view and present a self-consistent picture of energy exchange between them. We also go beyond the wideband approximation in Ref. 18 and study the heat generation in atomic junctions with semiconductor leads. In our model, the electron subsystem is described by a single-orbital tight-binding Hamiltonian, and the phonon subsystem is described in a harmonic approximation. We assume that the electron-phonon interaction is not strong so that the mean-field treatment is valid. The strong-interaction case is the scope of future work.

The rest of the paper is organized as follows. In Sec. II, we introduce the 1D model system and derive expressions for the electrical and energy currents of the coupled electron-phonon system. In Sec. III, we show the heat generation in one- and two-atom structures connecting with different leads. Section IV is the conclusion. In Appendixes A and B, we give some technical details of our derivation.

II. COUPLED ELECTRONIC AND PHONONIC TRANSPORT

A. Hamiltonian

Our model system is an infinite 1D atomic chain, as shown in Fig. 1. The electrons and atoms are only allowed to move in the longitudinal direction. We treat the atoms as



coupled harmonic oscillators and take into account their nearest neighbor interactions up to the second order. We assume that there is only one single electronic state for each atom and take into account hopping transitions between the nearest states. This corresponds to a single-orbital tight-binding model. Also, we assume that there is only one spin state for each orbital. Following Caroli,²³ we divide the whole system into one central region and two semi-infinite leads, which act as electrical and thermal baths (Fig. 1). The Hamiltonian of the whole system is

$$H = \sum_{\alpha=L,C,R;\beta=e,ph} H_{\beta}^{\alpha} + \sum_{\alpha=L,R;\beta=e,ph} (H_{\beta}^{\alpha C} + H_{\beta}^{C\alpha}) + H_{eph}. \quad (1)$$

The electron-phonon interaction Hamiltonian H_{eph} is nonzero only in the central region. The electron Hamiltonian reads

$$H_e^{\alpha} = \sum_i \epsilon_i^{\alpha} c_i^{\dagger} c_i^{\alpha} + \sum_{|i-j|=1} t_{ij}^{\alpha} c_i^{\dagger} c_j^{\alpha}, \quad (2)$$

where $c_i^{\dagger\alpha}$ and c_i^{α} are the electron creation and annihilation operators. ϵ_i^{α} is the electron onsite energy and t_{ij}^{α} is the hopping energy between adjacent states. i and j run over the sites in the α region. The coupling Hamiltonian with the leads is

$$H_e^{LC} = \sum_{ij} t_{ij}^{LC} c_i^{\dagger L} c_j^C, \quad (3)$$

and

$$H_e^{CR} = \sum_{ij} t_{ij}^{CR} c_i^{\dagger C} c_j^R. \quad (4)$$

H_e^{CL} and H_e^{RC} have similar expressions. We also have $t^{\alpha C} = t^{C\alpha\dagger}$, $\alpha=L,R$. For our 1D tight-binding model, $t^{\alpha C}$ has only one nonzero element. If we label the central atoms with indices 1 to n , as shown in Fig. 1, the nonzero elements will be t_{01}^{LC} , t_{10}^{CL} , $t_{n+1,n}^{RC}$, and $t_{n,n+1}^{CR}$.

The phonon Hamiltonian is

$$H_{ph}^{\alpha} = \frac{1}{2} \sum_i \dot{u}_i^{\alpha} \dot{u}_i^{\alpha} + \frac{1}{2} \sum_{|i-j|=0,1} u_i^{\alpha} K_{ij}^{\alpha} u_j^{\alpha}, \quad (5)$$

where u_i^{α} and $\dot{u}_i^{\alpha}$ are the mass-renormalized atom displacement and momentum operator. $K_{ii}^{\alpha} = 2K_0^{\alpha}/m_i^{\alpha}$ and $K_{ij}^{\alpha} = -K_0^{\alpha}/\sqrt{m_i^{\alpha}m_j^{\alpha}}$ ($i \neq j$). Here, K_0^{α} is the spring constant and m_i^{α} is the mass of the i th atom in the α region. Like the electrons, the coupling Hamiltonians with the leads are

$$H_{ph}^{LC} = \frac{1}{2} \sum_{ij} u_i^L K_{ij}^{LC} u_j^C \quad (6)$$

and

FIG. 1. Schematic diagram of the 1D coupled electron-phonon system and the parameters used in the model. The big dots in the bottom line represent atoms, while the small dots in the upper line represent electron states. They are coupled via the electron-phonon interaction.

$$H_{ph}^{CR} = \frac{1}{2} \sum_{ij} u_i^C K_{ij}^{CR} u_j^R. \quad (7)$$

We also have $K^{C\alpha} = K^{\alpha C\dagger}$. The nonzero elements are K_{01}^{LC} , K_{10}^{CL} , $K_{n+1,n}^{RC}$, and $K_{n,n+1}^{CR}$.

The electron-phonon interaction is included within the adiabatic Born-Oppenheimer approximation. First, the electron subsystem is solved with all the atoms in their equilibrium positions. Then, the isolated phonon subsystem is considered. After that, the electron-phonon interaction is turned on by allowing the atoms to oscillate around their equilibrium positions. Within this picture, the electron-phonon interaction is¹¹

$$H_{eph} = \sum_{i,j,k} M_{ij}^k c_i^{\dagger} c_j u_k. \quad (8)$$

The interaction matrix element is $M_{ij}^k = \langle i | \frac{\partial H_e}{\partial u_k} | j \rangle$. All the operators in Eq. (8) are in the central region, so we omitted the superscript C . In our model, the electron operators are in the second quantization, those that of the phonons are in the first quantization.

B. Green's functions

The nonequilibrium Green's function method for the electronic transport is discussed in Refs. 9–12 and that for the phononic transport in Refs. 13–17. Here, we concentrate on the electron-phonon interactions. The definition of the electron contour-order Green's function is $G_{jk}(\tau, \tau') = -i \langle \mathcal{T} \{ c_j(\tau) c_k^{\dagger}(\tau') \} \rangle$ and the phonon counterpart is $D_{jk}(\tau, \tau') = -i \langle \mathcal{T} \{ u_j(\tau) u_k(\tau') \} \rangle$. Here, τ is time on the Keldysh contour and $\mathcal{T} \{ \dots \}$ is the contour-order operator. We set $\hbar=1$ throughout the formulas. Without the electron-phonon interaction, the isolated electron and phonon problem can be solved exactly. We denote these Green's functions as $G_0(\tau, \tau')$ and $D_0(\tau, \tau')$, respectively. In our case, it is convenient to write the Hamiltonians as matrices and work in the energy space. The electron retarded and advanced Green's functions are $G_0^r(\epsilon) = G_0^{a\dagger}(\epsilon) = [(\epsilon + i\eta)I - H_e^C - \Sigma_L^r(\epsilon) - \Sigma_R^r(\epsilon)]^{-1}$. I is an identity matrix and $\eta \rightarrow 0^+$. The retarded self-energy $\Sigma_{\alpha}^r = t^{C\alpha} g_{\alpha}^r t^{\alpha C}$ is due to the interactions with the lead α . The retarded Green's function of the semi-infinite lead g_{α}^r can be obtained analytically (Appendix A). The “less than” Green's function is given by $G_0^< = G_0^r(\Sigma_L^< + \Sigma_R^<) G_0^a$, where $\Sigma_{\alpha}^< = -f_{\alpha}^e(\Sigma_{\alpha}^r - \Sigma_{\alpha}^a)$. f_{α}^e is the Fermi-Dirac distribution. The phonon retarded and advanced Green's functions are²⁴ $D_0^r(\omega) = D_0^{a\dagger}(\omega) = [(\omega + i\eta)^2 I - K^C - \Pi_L^r(\omega) - \Pi_R^r(\omega)]^{-1}$. The lead retarded self-energy is $\Pi_{\alpha}^r(\omega) = K^{C\alpha} d_{\alpha}^r(\omega) K^{\alpha C}$. d_{α}^r also has an analytical expression (Appendix A). The phonon less than Green's function is $D_0^< = D_0^r(\Pi_L^< + \Pi_R^<) D_0^a$, where $\Pi_{\alpha}^< = f_{\alpha}^{ph}(\Pi_{\alpha}^r - \Pi_{\alpha}^a)$. f_{α}^{ph} is the Bose distribution function.

Knowing the bare electron and phonon Green's functions G_0 and D_0 , we can include their interaction as a perturbation. Following the standard procedure of the nonequilibrium Green's function method, we can express this interaction as self-energies. The full Green's functions are obtained from the Dyson equation, e.g., for electrons, $G^{r,a} = G_0^{r,a} + G_0^{r,a} \Sigma_{\text{eph}}^{r,a} G^{r,a}$, and $G^< = G^r \Sigma_t^< G^a$. $\Sigma_t^< = \Sigma_{\text{eph}}^< + \Sigma_L^< + \Sigma_R^<$ is the total self-energy. Keeping the lowest nonzero order (the second order) of the self-energies, we have two (Hartree- and Fock-like) terms for the electrons and one polarization term for the phonons. This is the so-called Born approximation (BA).¹¹ The Fock self-energies are

$$\Sigma_{mn}^{F,<}(\varepsilon) = iM_{mi}^k \int G_{0ij}^<(\varepsilon - \omega) D_{0kl}^<(\omega) \frac{d\omega}{2\pi} M_{jn}^l \quad (9)$$

and

$$\begin{aligned} \Sigma_{mn}^{F,r}(\varepsilon) = iM_{mi}^k \int \frac{d\omega}{2\pi} [G_{0ij}^r(\varepsilon - \omega) D_{0kl}^<(\omega) \\ + G_{0ij}^<(\varepsilon - \omega) D_{0kl}^r(\omega) + G_{0ij}^r(\varepsilon - \omega) D_{0kl}^r(\omega)] M_{jn}^l. \end{aligned} \quad (10)$$

The less than Hartree self-energy is zero, and the retarded one is

$$\Sigma_{mn}^{H,r} = -iM_{mn}^i D_{0ij}^r(\omega' = 0) M_{kl}^j \int G_{0lk}^<(\varepsilon) \frac{d\varepsilon}{2\pi}. \quad (11)$$

This term is a constant for all energies, which represents a static potential due to the presence of phonons. The self-energies for the phonons are

$$\Pi_{mn}^<(\omega) = -iM_{lk}^m \int \frac{d\varepsilon}{2\pi} G_{0ki}^<(\varepsilon) G_{0jl}^>(\varepsilon - \omega) M_{ij}^n \quad (12)$$

and

$$\begin{aligned} \Pi_{mn}^r(\omega) = -iM_{lk}^m \int \frac{d\varepsilon}{2\pi} [G_{0ki}^r(\varepsilon) G_{0jl}^<(\varepsilon - \omega) \\ + G_{0ki}^<(\varepsilon) G_{0jl}^a(\varepsilon - \omega)] M_{ij}^n. \end{aligned} \quad (13)$$

In Eqs. (9)–(13), sum over repeated indices is assumed. The self-consistent Born approximation (SCBA) is obtained by replacing all the bare Green's functions G_0 and D_0 in Eqs. (9)–(13) with the full G and D .¹¹ In Appendix B, we show that the SCBA fulfills the electrical and energy current conservation, while BA fails.

C. Electrical and energy currents

The electrical and energy currents can be expressed by the Green's functions. The electrical current out of the lead α is^{11,25}

$$J_\alpha = e \int \frac{d\varepsilon}{2\pi} \text{Tr}\{G^>(\varepsilon) \Sigma_\alpha^<(\varepsilon) - G^<(\varepsilon) \Sigma_\alpha^>(\varepsilon)\}. \quad (14)$$

The electron energy current is

$$J_\alpha^{\text{E,e}} = \int \frac{d\varepsilon}{2\pi} \varepsilon \text{Tr}\{G^>(\varepsilon) \Sigma_\alpha^<(\varepsilon) - G^<(\varepsilon) \Sigma_\alpha^>(\varepsilon)\}. \quad (15)$$

The electron heat current is obtained from Eqs. (14) and (15) as $J_\alpha^{\text{h,e}} = J_\alpha^{\text{E,e}} - \mu_\alpha J_\alpha / e$. μ_α is the lead chemical potential. The derivation of the phonon energy current runs parallel with that of the electrons,¹⁷

$$J_\alpha^{\text{E,ph}} = - \int \frac{d\omega}{4\pi} \omega \text{Tr}\{D^>(\omega) \Pi_\alpha^<(\omega) - D^<(\omega) \Pi_\alpha^>(\omega)\}. \quad (16)$$

For phonons, the energy current is the same as the heat current. When there is no electron-phonon interaction, the electron energy current is conserved throughout the structure. So is the phonon energy current. In the presence of such an interaction, only the total energy current is conserved due to the energy exchange between them. The phonons do not carry charges, so in both cases, the electrical current is conserved. Since we cannot get the exact self-energies in most cases, we need some approximations. Properly defined self-energies should fulfill the electrical and energy current conservation,

$$\sum_\alpha J_\alpha = 0, \quad (17)$$

$$\sum_\alpha (J_\alpha^{\text{E,e}} + J_\alpha^{\text{E,ph}}) = 0, \quad (18)$$

where α runs over all the leads. We justify that the SCBA fulfills these conservation laws, while the BA fails to conserve the energy current (Appendix B). Provided that we satisfy these conservation laws, we can write the electrical and energy currents in symmetric forms. The electrical current is

$$J = e \int \frac{d\varepsilon}{2\pi} \tilde{T}^e(\varepsilon) [f_L^e(\varepsilon) - f_R^e(\varepsilon)]. \quad (19)$$

The transmission coefficient reads

$$\begin{aligned} \tilde{T}^e = \text{Tr} \left\{ \frac{1}{2} \left[G^r \left(\Gamma_L + \frac{1}{2} \Gamma_{\text{eph}} - S^e \right) G^a \Gamma_R \right. \right. \\ \left. \left. + G^r \Gamma_L G^a \left(\Gamma_R + \frac{1}{2} \Gamma_{\text{eph}} + S^e \right) \right] \right\}, \end{aligned} \quad (20)$$

where S^e is

$$S^e = \frac{\frac{1}{2}(f_R^e + f_L^e) \Gamma_{\text{eph}} + i \Sigma_{\text{eph}}^<}{f_L^e - f_R^e}. \quad (21)$$

$\Gamma_\alpha = i(\Sigma_\alpha^r - \Sigma_\alpha^a)$, where $\alpha = L, R$ is the electron level-width function. $\Gamma_{\text{eph}} = i(\Sigma_{\text{eph}}^r - \Sigma_{\text{eph}}^a)$ is due to the electron-phonon interaction. The total energy current is

$$J^E = \int \frac{d\varepsilon}{2\pi} \varepsilon \left\{ \tilde{T}^e(\varepsilon) [f_L^e(\varepsilon) - f_R^e(\varepsilon)] - \frac{1}{2} \tilde{T}^{\text{ph}}(\varepsilon) [f_L^{\text{ph}}(\varepsilon) - f_R^{\text{ph}}(\varepsilon)] \right\}. \quad (22)$$

The phonon transmission coefficient is

$$\tilde{T}^{\text{ph}} = \text{Tr} \left\{ \frac{1}{2} \left[D^r \left(\Lambda_L + \frac{1}{2} \Lambda_{\text{eph}} - S^{\text{ph}} \right) D^a \Lambda_R + D^r \Lambda_L D^a \left(\Lambda_R + \frac{1}{2} \Lambda_{\text{eph}} + S^{\text{ph}} \right) \right] \right\}, \quad (23)$$

where S^{ph} is

$$S^{\text{ph}} = \frac{\frac{1}{2} (f_R^{\text{ph}} + f_L^{\text{ph}}) \Lambda_{\text{eph}} - i \Pi_{\text{eph}}^<}{f_L^{\text{ph}} - f_R^{\text{ph}}}. \quad (24)$$

$\Lambda_\alpha = i(\Pi_\alpha^r - \Pi_\alpha^a)$ is the phonon level-width function. $\Lambda_{\text{eph}} = i(\Pi_{\text{eph}}^r - \Pi_{\text{eph}}^a)$ is due to the electron-phonon interaction. Equations (19)–(24) are the generalization of the Caroli formula²³ to include the electron-phonon interaction.

III. HEAT GENERATION IN CURRENT-CARRYING ONE-DIMENSIONAL ATOMIC JUNCTIONS

As an application of the formalism in Sec. II, we study the heat dissipation in current-carrying 1D atomic junctions. In the presence of potential difference between the two leads, there will be electrical current flowing between them. When the electrons pass the central region, there is an energy exchange between the electron and phonon systems. This is only a small part of the generated Joule heat, most of which is dissipated into the leads. However, this small fraction may still make the atom temperature higher than that of the leads. This influences the transport properties of the atomic junction and even leads to junction breakup.^{26,27} According to Appendix B, the heat generation is given by [Eq. (B9)]

$$Q = i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{2\pi} \omega [G_{nm}^>(\varepsilon) M_{mi}^k D_{kl}^<(\omega) G_{ij}^<(\varepsilon - \omega) M_{jn}^l]. \quad (25)$$

Before presenting our results, we first discuss how our model is related to available ones and show some general features of the local heating effect that have been mentioned in previous studies.

A. General features and relation with other approaches

Different models have been used to study the local heating effect in atomic junctions.^{18,26–42} Horsfield *et al.* compared different classical, semiclassical, and quantum mechanical models.^{31–33} Within the framework of MD, they developed the correlated electron-ion dynamics method to take into account the correlations between the electron and the nuclei dynamics and the energy transfer between them. This approach goes beyond the perturbative treatment, includes the anharmonicity inherently, and contains the screening effect. It also reproduces the Fermi golden rule (FGR)

results for the energy exchange between electrons and nuclei. The FGR method is equivalent to the BA in our Green's function approach. We can generalize the FGR to include all orders of perturbation and solve the problem by matching the many body problem into a single electron problem with many scattering channels.^{34,35} However, this approach is only valid near equilibrium.³⁵ Furthermore, it assumes that the phonon subsystem is in equilibrium, so it cannot be used to study the nonequilibrium phononic transport. Many Green's function and/or density functional theory based approaches are able to include the electron-phonon interaction and the phonon subsystem at the SCBA level.^{19,37,39,40,42} These approaches are more accurate than our model calculation. The advantage of our approach is that we treat the phonon subsystem in real space, instead of the normal mode used in most approaches. The inclusion of phonon anharmonicity is convenient within the real space representation.¹⁷ Furthermore, the leads in our model can serve as both electron and phonon baths. This enables us to study the coupled nonequilibrium electronic and phononic transport. Although our formalism is similar to that of Ref. 18, there, the authors studied the local heating effect from the electronic transport point of view. We present a self-consistent picture for the two viewpoints and show that under SCBA, they give exactly the same result (Appendix B). We also go beyond the wideband limit in Ref. 18 by introducing 1D electron and phonon baths (Appendix A), which can be metal or semiconductor depending on the parameters. This enables us to study more effects that are not studied in Ref. 18.

As expected, our model reproduces the well-known inelastic tunneling features presented in the literature. For a perfect conducting channel, we observed the differential conductance drop due to electron-phonon interaction.^{20,39,42} For weak coupling with the leads, we observed phonon-assisted tunneling peaks. These serve as important checks of our formalism. Now, we turn to the heat generation in these atomic structures. Figure 2 compares results from different equations for the heat generation in a single-atom structure ($n=1$ in Fig. 1). The parameters used in the calculation are stated in the figure caption. With these parameters, the electron energy band is in the range $-1 \leq \varepsilon \leq 1$ eV. The chemical potential of each lead is zero in equilibrium. The phonon energy is approximately $\omega=0.05$ eV. In all the results presented in this paper, the lead temperature is $T=4.2$ K and the electron-phonon coupling matrix $M=0.08$ eV/(Å amu^{1/2}). The cutoff energy of the electron system is 2.1 eV and the phonon system is 0.2 eV. The energy spacing is discretized into grids of 1 meV. Equation (B5) gives the energy decrease of the electron system, while Eq. (B8) gives the energy increase of the phonon system. Numerical results from Eqs. (B5) and (B8) under SCBA have some slight discrepancy. This is due to numerical inaccuracies. We also show results from BA since it is equivalent to the FGR approach in Ref. 32. The lowest order perturbation method cannot conserve energy. The electron and phonon results show large discrepancy. We note that although Eqs. (B5) and (B7) are equivalent, the numerical result from Eq. (B5) is unstable in many cases. The reason is that the energy exchange between the electron and the phonon system is only a small fraction of the total electrical energy current. Equation (B5) is the dif-

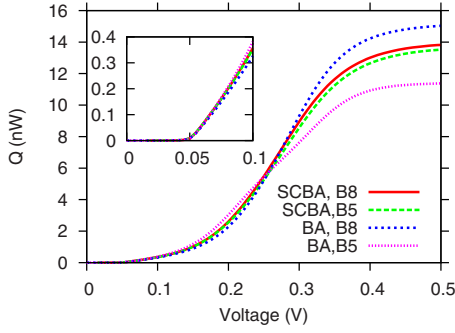


FIG. 2. (Color online) Comparison of different methods to compute the heat generation in a single-atom structure. The four curves correspond to results from Eqs. (B5) and (B8) under BA and SCBA, respectively. If we label this single atom as index 1, its electronic on-site energy is written as $\varepsilon_1^C = 0.1$ eV. The on-site energy of the leads is $\varepsilon^L = \varepsilon^R = 0$ eV. The hopping energy is $t_{ij}^L = t_{ij}^R = 0.5$ eV. The nonzero electronic coupling with the lead is $t_{10}^C = t_{21}^C = 0.1$ eV. The matrix element of the single atom is $K_{11}^L = K_{11}^R = 0.654$ eV/(Å² amu). The spring constant between the lead atoms is $K_{ij}^L = K_{ij}^R = 0.654$ eV/(Å² amu). The nonzero atomic coupling with the leads is $K_{10}^{CL} = K_{21}^{RC} = 0.127$ eV/(Å² amu).

ference between two large numbers, so our numerical integration has to be accurate enough to get a reasonable result.³⁷ On the contrary, Eq. (25) is much more stable since we know the difference analytically. All the results presented below use this equation.

Figure 2 also shows some general features of heat generation in atomic junctions. We can see two threshold values. The first one corresponds to the onset of phonon emission. Due to the almost zero phonon occupation at low temperatures, only when the applied voltage is larger than the phonon energy can the phonon emission be turned on. The second threshold value corresponds to the alignment of the lead chemical potential with the electron on-site energy $eV = 2\varepsilon_0$. These two threshold behaviors may be smoothed out when the coupling with the leads gets stronger. The atomic coupling with the leads cause broadening of the first threshold behavior, while the electronic coupling is responsible for that of the second.

B. Effect of coupling with leads

The electron-lead coupling not only leads to the electron level broadening but also influences the electron tunneling time. The larger this coupling, the less time electrons spend in the central region. In Fig. 3, we show the heat generation and the atom temperature for a single-atom structure under different electronic coupling strengths. The definition of temperature is ambiguous in nanostructures.⁶ Here, we use the method proposed in Ref. 18. We can only see one threshold behavior at about 0.2 V, which is smoothed out when the coupling is larger than 0.2 eV. The temperature and the heat generation show similar trends. The saturation voltage of heat generation increases with the increase of the electron-lead coupling. This is due to the coupling induced atomic level broadening. The decrease of the heat generation and temperature with increasing electron-lead coupling can be

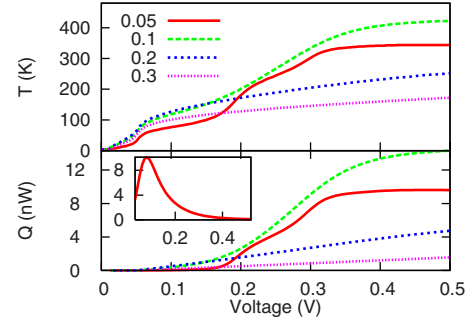


FIG. 3. (Color online) Heat generation Q and the atom temperature T under different electron coupling strengths $t_{10}^{CL} = t_{21}^{RC} = 0.05, 0.1, 0.2$, and 0.3 eV. Other parameters are the same as Fig. 2. The inset shows the heat generation as a function of electron coupling strength at an applied bias $V = 0.3$ V.

easily understood. The larger this coupling, the less time electrons spend at the central atom. Since the electron-phonon interaction takes place there, the heat generation decreases. We also show the heat generation as a function of electron-lead coupling in the inset of the lower panel. The applied voltage is 0.3 V. On one side, when the coupling is too small, few electrons can tunnel through the atom. The heat generation is small. On the other side, when the coupling is very large, the electron tunneling process is too quick for the phonons to interact with the electrons. The heat generation is also small. It has a maximum value at some moderate coupling strength. This is different from the electrical current, which increases monotonously with the increase of coupling strength.

The atom-lead coupling determines how well the generated heat can be conducted into the surrounding leads. One of the important reasons why we are interested in the heat generation in nanostructures is that it may lead to temperature increase and even structure breakup. To study the temperature change, we need to take into account not only the heat generation but also the heat conduction into the leads. In the simplest one-atom structure, the heat conductance is mainly determined by the atom-lead coupling. Our model includes this intrinsically. Figure 4 shows the heat generation and the atom temperature as a function of atom-lead coupling under different biases. In the case of a perfect junction, the heat generation reaches its maximum value, while the atom temperature is the lowest. The reason is that the perfect junction has the best heat conductance. When the atom-lead coupling is weak, the heat generation is small. However, the poor heat conductance can still result in a much higher temperature than the surrounding leads. We also show the heat conductance as a function of atom-lead coupling in the inset of the upper panel, which shows a sharp peak at resonance. The atom-lead coupling also influences the electronic current profile. Our model calculation reproduces the result that heating of the phonon subsystem may increase the electron-phonon scattering rates and lead to the electronic current decrease or negative differential conductance.^{4,5}

In Fig. 5, we show the heat generation of a two-atom structure ($n=2$ in Fig. 1). The central region has two identical atoms. Interaction between them leads to two discrete

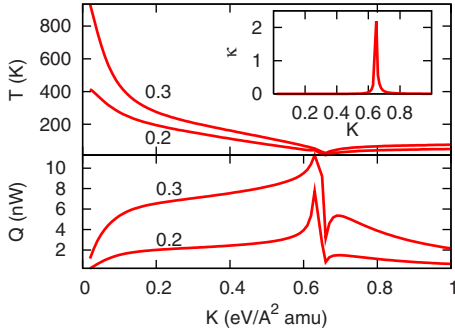


FIG. 4. (Color online) Heat generation Q and the atom temperature T as a function of the atom-lead coupling $K_{10}^{CL}=K_{21}^{RC}=K$ at $V=0.2$ and 0.3 V. Other parameters are the same with Fig. 2. The inset shows the thermal conductance κ as a function of K . The unit is 1×10^{-12} W/K.

energy levels. One is at 0 eV and the other at 0.4 eV. When the electrical coupling between the leads and the central region is small (0.1 eV), in addition to the threshold behavior at $eV=\omega$, there are two ladders corresponding to the phonon-assisted resonant tunneling across the two electrical levels. If the electrical coupling gets larger (0.2 eV), the two ladders broaden out. Again, this is attributed to the coupling induced level broadening. The heat generation for the two-atom structure is much larger than that of a single-atom structure. The more the electrical levels, the larger the electrical current and heat generation. It is worth noting that for multiatom structures, the distribution of the electrostatic potential may influence the results significantly.⁴¹ In the above calculation, we assume that the two electrical levels do not change with the applied bias and that we can tune their positions via a gate voltage.

C. Effect of a semiconductor lead

If one of the metallic leads is replaced by a semiconductor, there will be some new features in the electrical current

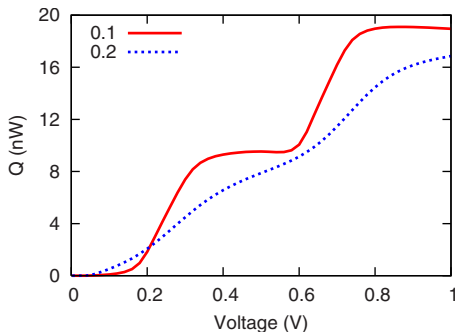


FIG. 5. (Color online) Heat generation Q as a function of applied voltage for a two-atom structure. The two-atom on-site energy is $\varepsilon^C=0.2$ eV, the hopping energy is $t^C=0.1$ eV, and the spring constant is $K^C=0.654$ eV/(Å² amu). The two leads are identical. The electron on-site energy is $\varepsilon^L=\varepsilon^R=0$ and the hopping energy is $t^L=t^R=0.5$ eV. Their spring constants are the same as the central region. The nonzero couplings with the leads are $K_{10}^{CL}=K_{32}^{RC}=0.327$ eV/(Å² amu) and $t_{10}^{CL}=t_{32}^{RC}=0.1$ eV (solid) and 0.2 eV (dashed), respectively.

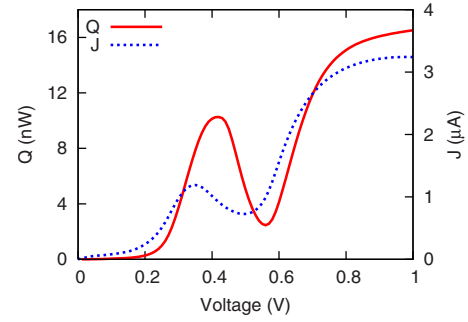


FIG. 6. (Color online) Heat generation Q and electrical current J as a function of applied voltage for a single-atom structure. The left lead is a semiconductor. Its alternating on-site energies are -0.2 and -0.1 eV. The chemical potential is $\mu^L=0.05$ eV higher than the conduction band bottom, which corresponds to n -type doping. Other parameters are $K_{10}^{CL}=K_{21}^{RC}=0.4$ eV/(Å² amu), $t_{10}^{CL}=t_{21}^{RC}=0.1$ eV, $\varepsilon_1^C=0.1$ eV, $K_{11}^C=0.654$ eV/(Å² amu), $\varepsilon^R=-0.05$ eV, $t^L=t^R=0.5$ eV, and $K^L=K^R=0.654$ eV/(Å² amu).

and the heat generation. In our simple model, we can alternate the electron on-site energies between two values to mimic a simple semiconductor (Appendix A). In Fig. 6, we show the heat generation and the electrical current for such kind of structure. The alternating on-site energies of the left lead are -0.1 and -0.2 eV. This produces an energy band gap of 0.1 eV. Other parameters are given in the figure caption. We can see that there appears negative differential conductivity in the current-voltage characteristics due to the semiconductor band gap. This qualitatively agrees with the experimental⁴³ and first-principles⁴⁴ studies. The heat generation curve is slightly different. In addition to its threshold behavior, the peak and valley positions are also different. The electrical current has a peak when the chemical potential of the lead is aligned with the central electrical level, while the peak of the heat generation shifts to the right by one phonon energy. This corresponds to the phonon-assisted resonant tunneling. The current and the heat generation decrease when the single electrical level is within the band gap of the left lead. The peak-to-valley ratio depends on the coupling with the semiconductor lead. In the limit of small band gap and large coupling, we recover the metallic lead results.

IV. CONCLUSION

We studied the coupled electron and phonon transport in 1D atomic junctions in the weak electron-phonon interaction regime. Based on the nonequilibrium Green's function method, we derived the electrical and energy currents of the coupled electron-phonon system and the energy exchange between them. We showed that the SCBA conserves the energy current. Using this formalism, we studied the heat generation in one- and two-atom structures coupling with different leads under a broad range of parameters. Especially, we studied the influence of the thermal transport properties on the heat generation and atom temperature of the central region. The results on semiconductor leads agree qualitatively with the experimental and first-principles studies. This model

can be easily extended to study more realistic structures such as molecular transport junctions and metallic nanowires. The electron phonon Hamiltonians, their interaction, and lead-coupling matrices can all be obtained from first-principles calculations.^{17,39,45} The surface Green's functions for bulk leads can be computed by the recursive method.^{17,45} It is also possible to include the electron-electron and the phonon-phonon interactions.^{14,17}

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APPENDIX A: SURFACE GREEN'S FUNCTIONS OF THE ONE-DIMENSIONAL LEAD

In this appendix, we show that for the 1D tight-binding model, the lead self-energies can be expressed analytically.¹⁷ The electron and phonon self-energies are similar in their form. Here, we take electrons as an example and give the phonon results directly. We assume that the on-site energies of the electrons alternate between ε_1 and ε_2 . The hopping energy is $t_{ij}^\alpha = t_0$. If $\varepsilon_1 = \varepsilon_2$, we get a continuum band. This corresponds to a metallic lead. If they are not equal, we get two bands with a band gap. We can take the lower as the valence band (VB) and the upper as the conduction band (CB). We use this method to mimic a semiconductor lead. In this case, the semi-infinite lead has two electron states in each period. In the tight-binding model, only the left- (right) most state of the central region is coupled to the left (right) lead. So, we only need to know the surface Green's function, e.g., for the left lead, it is $g_0 = g_{00}^r$. We assume that the retarded Green's function is

$$g_{ij}^r = \begin{cases} c_1 \lambda^{i-j} & \text{state 1} \\ c_2 \lambda^{i-j} & \text{state 2.} \end{cases} \quad (\text{A1})$$

Substituting it into the definition of the retarded Green's functions $[(\varepsilon + i\eta)I - H]g^r = I$, we have

$$-t_0 c_1 + (\varepsilon + i\eta - \varepsilon_2)c_2 - t_0 c_1 \lambda = 0, \quad (\text{A2})$$

$$-t_0 c_2 + (\varepsilon + i\eta - \varepsilon_1)c_1 \lambda - t_0 c_2 \lambda = 0. \quad (\text{A3})$$

From Eqs. (A2) and (A3), we get an equation for λ ,

$$\lambda^2 + \left[2 - \frac{(\varepsilon + i\eta - \varepsilon_1)(\varepsilon + i\eta - \varepsilon_2)}{t_0^2} \right] \lambda + 1 = 0. \quad (\text{A4})$$

The condition that Eq. (A4) has traveling wave solutions gives the dispersion relation

$$\frac{(\varepsilon_1 + \varepsilon_2) - \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 16t_0^2}}{2} \leq \varepsilon \leq \varepsilon_1 \quad (\text{VB}),$$

$$\varepsilon_2 \leq \varepsilon \leq \frac{(\varepsilon_1 + \varepsilon_2) + \sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 16t_0^2}}{2} \quad (\text{CB}). \quad (\text{A5})$$

We assume that $\varepsilon_1 \leq \varepsilon_2$ without loss of generality. The energy band gap is $\varepsilon_2 - \varepsilon_1$. If they are equal, the two bands

merge into one, which corresponds to a metallic lead.

For the surface Green's function of the left lead, we also have

$$(\varepsilon + i\eta - \varepsilon_1)c_1 - t_0 c_2 = 1. \quad (\text{A6})$$

From Eqs. (A2) and (A6), we get

$$g_0 = \begin{cases} \frac{\varepsilon + i\eta - \varepsilon_2}{(1 + \lambda)t_0^2} & (\text{VB}) \\ \frac{\varepsilon + i\eta - \varepsilon_1}{(1 + \lambda)t_0^2} & (\text{CB}). \end{cases} \quad (\text{A7})$$

$|\lambda| \geq 1$ is one of the roots of Eq. (A4). The surface Green's function of the right lead is identical.

We can also alternate the atom masses to generate a phonon band gap. In our model, the mass change will modify the renormalized spring constants. The diagonal elements of the dynamical matrix will be two alternating values $K_{ii}^\alpha = 2k_1$ or $2k_2$, while the off-diagonal elements will be a single value $K_{ij}^\alpha = -\sqrt{k_1 k_2}$, where $|i - j| = 1$. If we assume that $k_2 \geq k_1$, the acoustic band (AB) is $0 < \omega^2 < 2k_1$ and the optical band (OB) $2k_2 < \omega^2 < 2(k_1 + k_2)$. The surface Green's function is

$$d_0 = \begin{cases} \frac{\Omega_2}{(1 + \lambda)k_1 k_2} & (\text{AB}) \\ \frac{\Omega_1}{(1 + \lambda)k_1 k_2} & (\text{OB}), \end{cases} \quad (\text{A8})$$

where $\Omega_n = (\omega + i\eta)^2 - 2k_n$. $|\lambda| \geq 1$ is one of the roots of

$$\lambda^2 + \left(2 - \frac{\Omega_1 \Omega_2}{k_1 k_2} \right) \lambda + 1 = 0. \quad (\text{A9})$$

In all the simulation results of the present paper, the two spring constants are equal ($k_1 = k_2$), which correspond to a single continuum phonon band. The electron on-site energies are also equal ($\varepsilon_1 = \varepsilon_2$) except in Fig. 6, where we set $\varepsilon_1 = -0.2$ eV and $\varepsilon_2 = -0.1$ eV to mimic a semiconductor lead.

APPENDIX B: ENERGY CURRENT CONSERVATION

In this appendix, we justify that the SCBA satisfies the energy current conservation. The justification of the electrical current conservation is given in Refs. 42 and 46. What we need to prove is that

$$\sum_{\alpha} (J_{\alpha}^{\text{E,e}} + J_{\alpha}^{\text{E,ph}}) = 0. \quad (\text{B1})$$

The electron part is

$$\sum_{\alpha} J_{\alpha}^{\text{E,e}} = \sum_{\alpha} \int \frac{d\varepsilon}{2\pi} \varepsilon \text{Tr}\{G^>(\varepsilon)\Sigma_{\alpha}^<(\varepsilon) - G^<(\varepsilon)\Sigma_{\alpha}^>(\varepsilon)\}. \quad (\text{B2})$$

Using the important relation^{39,46}

$$\text{Tr}\{G^>\Sigma_t^< - G^<\Sigma_t^>\} = 0, \quad (\text{B3})$$

we get

$$\sum_{\alpha} J_{\alpha}^{E,e} = - \int \frac{d\varepsilon}{2\pi} \varepsilon \text{Tr}\{G^{>}(\varepsilon)\Sigma_{\text{eph}}^{<}(\varepsilon) - G^{<}(\varepsilon)\Sigma_{\text{eph}}^{>}(\varepsilon)\}. \quad (\text{B4})$$

The Hartree term does not contribute to the current directly. It is just like a static potential which only modifies the Green's function. Substituting the Fock self-energy into Eq. (B4), we have

$$\begin{aligned} -Q &= \sum_{\alpha} J_{\alpha}^{E,e} \\ &= -i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{2\pi} \varepsilon [G_{nm}^{>}(\varepsilon)M_{mi}^k D_{kl}^{<}(\omega)G_{ij}^{<}(\varepsilon - \omega)M_{jn}^l \\ &\quad - G_{nm}^{<}(\varepsilon)M_{mi}^k D_{kl}^{>}(\omega)G_{ij}^{>}(\varepsilon - \omega)M_{jn}^l]. \end{aligned} \quad (\text{B5})$$

Sum over all the indices is assumed. The heat generation Q is the energy decrease of the electron system, which should also be the energy increase of the phonon system. Replacing ω by $-\omega$, using the symmetric properties of the phonon Green's functions,¹⁷ replacing ε by $\varepsilon - \omega$, and finally changing dummy variables, we get

$$\begin{aligned} &i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{2\pi} \varepsilon [G_{nm}^{<}(\varepsilon)M_{mi}^k D_{kl}^{>}(\omega)G_{ij}^{>}(\varepsilon - \omega)M_{jn}^l] \\ &= i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{2\pi} \varepsilon [G_{nm}^{<}(\varepsilon)M_{mi}^k D_{kl}^{>}(-\omega)G_{ij}^{>}(\varepsilon + \omega)M_{jn}^l] \\ &= i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{2\pi} (\varepsilon - \omega) [G_{nm}^{<}(\varepsilon - \omega)M_{mi}^k D_{lk}^{<}(\omega)G_{ij}^{>}(\varepsilon)M_{jn}^l] \\ &= i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{2\pi} (\varepsilon - \omega) [G_{nm}^{>}(\varepsilon)M_{mi}^k D_{kl}^{<}(\omega)G_{ij}^{<}(\varepsilon - \omega)M_{jn}^l]. \end{aligned} \quad (\text{B6})$$

Substituting Eq. (B6) back into Eq. (B5), we get

$$\begin{aligned} -Q &= \sum_{\alpha} J_{\alpha}^{E,e} \\ &= -i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{2\pi} \omega [G_{nm}^{>}(\varepsilon)M_{mi}^k D_{kl}^{<}(\omega)G_{ij}^{<}(\varepsilon - \omega)M_{jn}^l] \\ &\quad \neq 0. \end{aligned} \quad (\text{B7})$$

For the phonon energy current, we have

$$\begin{aligned} Q &= \sum_{\alpha} J_{\alpha}^{E,\text{ph}} \\ &= i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{4\pi} \omega [D_{nm}^{>}(\omega)M_{lk}^m G_{ki}^{<}(\varepsilon)G_{jl}^{>}(\varepsilon - \omega)M_{ij}^n \\ &\quad - D_{nm}^{<}(\omega)M_{lk}^m G_{ki}^{>}(\varepsilon)G_{jl}^{<}(\varepsilon - \omega)M_{ij}^n]. \end{aligned} \quad (\text{B8})$$

Following the same procedure as electrons, finally, we get

$$\begin{aligned} Q &= \sum_{\alpha} J_{\alpha}^{E,\text{ph}} \\ &= i \int \frac{d\varepsilon}{2\pi} \int \frac{d\omega}{2\pi} \omega [G_{nm}^{>}(\varepsilon)M_{mi}^k D_{kl}^{<}(\omega)G_{ij}^{<}(\varepsilon - \omega)M_{jn}^l] \neq 0. \end{aligned} \quad (\text{B9})$$

So, we still have

$$\sum_{\alpha} (J_{\alpha}^{E,e} + J_{\alpha}^{E,\text{ph}}) = 0. \quad (\text{B10})$$

Equations (B7) and (B9) give the energy exchange between the electron and the phonon system, which is also the heat generation of the atomic junction. Replacing $D^{<}$, $G^{<}$ by $D_0^{<}$, $G_0^{<}$ in Eq. (B7) and $G^{>}$, $G^{<}$ by $G_0^{>}$, $G_0^{<}$ in Eq. (B9), we get the results under BA. We can find that the energy increase of the phonons does not equal the energy decrease of the electrons under BA.

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