Interfacial thermal transport in atomic junctions

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We study ballistic interfacial thermal transport across atomic junctions. Exact expressions for phonon transmission coefficients are derived for thermal transport in one-junction and two-junction chains, and verified by numerical calculation based on a nonequilibrium Green’s function method. For a single-junction case, we find that the phonon transmission coefficient typically decreases monotonically with increasing frequency. However, in the range between equal frequency spectrum and equal acoustic impedance, it increases first then decreases, which explains why the Kapitza resistance calculated from the acoustic mismatch model is far larger than the experimental values at low temperatures. The junction thermal conductance reaches a maximum when the interfacial coupling equals the harmonic average of the spring constants of the two semi-infinite chains. For three-dimensional junctions, in the weak coupling limit, we find that the conductance is proportional to the square of the interfacial coupling, while for intermediate coupling strength the conductance is approximately proportional to the interfacial coupling strength. For two-junction chains, the transmission coefficient oscillates with the frequency due to interference effects. The oscillations between the two envelop lines can be understood analytically, thus providing guidelines in designing phonon frequency filters.

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I. INTRODUCTION

In the past decade there has been a significant research focus on thermal transport in microscale. Several conceptual thermal devices, such as thermal rectifiers/diodes, thermal transistors, thermal logical gates, and thermal memory3–5, have been proposed, which, in principle, make it possible to control heat due to phonons and process information with phonons. The issue of quantum thermal transport in nanostructures was also addressed.6–14 In this context, the critical information is in phonon transmission coefficients that in quasi-one-dimensional atomic models can be calculated by transfer matrix methods15–18. However, the evaluation of the transfer matrix may be numerically unstable, particularly when the system size becomes large. Alternatively, nonequilibrium Green’s function (NEGF) method is an efficient way to calculate the transmission coefficient.11 Unfortunately, both of these two methods are numerical in nature and do not give analytical expressions.

For thermal transport and control, the interfacial thermal scattering process is becoming increasingly important, especially in practical devices. Two theories, acoustic mismatch model and the diffuse mismatch model, have been proposed to study the mechanism of the thermal interfacial resistance. However, both models offer limited accuracy in nanoscale interfacial resistance predictions14 because they neglect atomic details of actual interfaces. A scattering boundary method within the lattice dynamic approach was first proposed by Lumpkin and Saslow to study the Kapitza conductance in a one-dimensional (1D) lattice, and was then applied to calculate the Kapitza resistance in two- and three-dimensional (3D) lattices.16,17 This method can predict thermal interfacial conductance between heterogeneous materials with full consideration of the atomic structures in the interface. Recently, this method was applied to study the ballistic thermal transport in nanotube junctions, spin chains, and honeycomb lattice ribbons.

In this paper we give an explicit analytical expression of transmission coefficient obtained through the scattering boundary method, and use it to study the interfacial thermal transport across atomic junctions. First, in Sec. II we introduce a model in which two semi-infinite 1D atomic chains are coupled either via a point junction or an extended junction region. By using the boundary scattering method we derive the exact expressions for phonon transmission coefficients for thermal transport in one-junction and two-junction chains in Sec. III. The role of various parameters on the junction conductance is analyzed and discussed in Sec. IV. In section IV we also estimate the interfacial conductance between two 3D solids. In Sec. V we introduce briefly the NEGF method, and use it to verify the results from analytical formulae for the thermal transport in our model. A short summary is presented in Sec. VI.

II. MODEL

The one-dimensional atomic chain consists of three parts: two semi-infinite leads and an center region (see
FIG. 1: (color online) A schematic representation of the 1D atomic chain model. The size of the center part is $N_C = 8$. The left and right regions are two semi-infinite harmonic atomic chains at different temperatures $T_L$ and $T_R$. The three parts are coupled by harmonic springs with constant strength $k_{12}$ and $k_{23}$; all of which are harmonic chains with mass and spring constant as $m_1, k_1$, $m_2, k_2$ and $m_3, k_3$, respectively.

The two leads are in equilibrium at different temperatures $T_L$ and $T_R$. The three parts are coupled by harmonic springs with constant strength $k_{12}$ and $k_{23}$; all of which are harmonic chains with mass and spring constants $m_1, k_1$, $m_2, k_2$ and $m_3, k_3$, respectively. So the total Hamiltonian can be written as

$$H = \sum_{\alpha=1,2,3} H_{\alpha} + \frac{1}{2} k_{12} (x_{1,1} - x_{2,1})^2 + \frac{1}{2} k_{23} (x_{2,N_c} - x_{3,1})^2; \quad (1)$$

where,

$$H_{\alpha} = \sum_{i=1}^{N_\alpha} \frac{1}{2} m_\alpha x_{\alpha,i}^2 + \sum_{i=1}^{N_\alpha-1} \frac{1}{2} k_\alpha(x_{\alpha,i} - x_{\alpha,i+1})^2. \quad (2)$$

Where $x_{\alpha,i}$ is the relative displacement of $i$-th atom in $\alpha$-th part. If there is no center part, that is, the two semi-infinite leads connected directly by $k_{12}$, then by setting $\alpha = 1, 2$ and $k_{23} = 0$ in Eq. (1), we can obtain the corresponding Hamiltonian. For the semi-infinite leads, $N_\alpha = \infty$.

**III. ANALYTICAL SOLUTION FROM THE SCATTERING BOUNDARY METHOD**

Heat current flowing from left to right through a junction connecting two leads kept at different equilibrium heat-bath temperatures $T_L$ and $T_R$ is given by the Landauer formula

$$I = \frac{1}{2\pi} \int_0^\infty \hbar \omega \left[ f_L(\omega) - f_R(\omega) \right] T[\omega] d\omega, \quad (3)$$

which allows us to develop the junction conductance formula

$$\sigma = \frac{1}{2\pi} \int_0^\infty d\omega \ h_\omega T[\omega] \frac{\partial f(\omega)}{\partial T}, \quad (4)$$

here, $f_{L,R} = \{\exp[\hbar \omega/(k_B T_{L,R})] - 1\}^{-1}$ is the Bose-Einstein distribution for phonons, and $T[\omega]$ is the frequency dependent transmission coefficient. Therefore, the key step for the thermal transport characterization is to calculate the transmission coefficients.

We first consider a point-junction case, that is, two semi-infinite harmonic chains connected by a spring with constant strength $k_{12}$. We assume a wave solution transmitting from the left lead to the right lead. We label the atoms as $-\infty, \cdots, -1, 0, 1, 2, \cdots, +\infty$. Atoms 0 and 1 are connected by $k_{12}$ spring. An incident wave from left is assumed as $x_I = \lambda_1^L e^{-i\omega t}$. When it arrives at the interface, it will be partially reflected and partially transmitted. The reflected wave amplitude is

$$x_R = r_{12} \lambda_1^L e^{-i\omega t}$$

and the transmission wave can be written as $x_T = t_{12} \lambda_1^L e^{-i\omega t}$. So at each atom we have

$$x_{-1} = (\lambda_1^{-1} + r_{12} \lambda_1) e^{-i\omega t}, \quad x_0 = (1 + r_{12}) e^{-i\omega t}, \quad x_1 = t_{12} e^{-i\omega t}, \quad x_2 = t_{12} \lambda_2 e^{-i\omega t}, \cdots$$

where, $\lambda_j = e^{i q_j a_j}$, $q_j$ is the wave vector, $a_j$ is the interatomic spacing. For the atom in the $j-th$ part, we can have the equation of motion as

$$m_j \frac{d^2 x_{j,n}}{dt^2} = k_j (x_{j,n+1} - x_{j,n}) + k_j (x_{j,n} - x_{j,n-1}), \quad (5)$$

each wave transport separately and satisfies such equation. Thus $\lambda_j$ satisfies the dispersion relation of the corresponding lead as

$$\omega^2 m_j = -k_j \lambda_j^{-1} + 2 k_j - k_j \lambda_j. \quad (6)$$

The quadratic equation has two roots. Which one should we choose? Replacing $\omega$ with $\omega + i \eta$, $\eta = 0^+$, none of the eigenvalues $\lambda$ will have modulus exactly 1. We find for the traveling waves

$$|\lambda| = 1 - \frac{\alpha}{2}$$

thus the forward moving waves with group velocity $v > 0$ have $|\lambda| < 1$. Therefore we should take the one with $|\lambda| < 1$ of the two roots which are given as

$$\lambda_j = \frac{-h_j \pm \sqrt{h_j^2 - 4}}{2}, \quad h_j = \frac{m_j}{k_j} (\omega + i \eta)^2 \quad (2).$$

From the scattering boundary method, the coefficients $r_{12}, t_{12}$ can be obtained from the continuity condition at the interface as:

$$\omega^2 m_1 x_0 = -k_1 x_{-1} + (k_1 + k_{12}) x_0 - k_{12} x_1; \quad (9)$$

$$\omega^2 m_2 x_1 = -k_{12} x_0 + (k_2 + k_{12}) x_1 - k_{12} x_2. \quad (10)$$

Finally we can get the transmission coefficient as

$$T[\omega] = 1 - |r_{12}|^2 = 1 - |r_{21}|^2, \quad (11)$$

here,

$$r_{ij} = \frac{k_i (\lambda_j - 1/\lambda_j) (k_j - k_{ij} - k_j/\lambda_j)}{(k_i - k_{ij} - k_i/\lambda_j) (k_j - k_{ij} - k_j/\lambda_j) - k_{ij}^2} - 1. \quad (12)$$

Of course, we can also use $t_{12}$ to express $T[\omega]$ as $m_{12} v_{12}^2/a^2 |t_{12}|^2$, here the group velocity $v_i = \frac{d\omega}{d\eta_i}$ =
\frac{a_1}{2} \sqrt{\frac{4k_i}{m_i} - \omega^2}, which is derived from the dispersion relation given by Eq. (8). Thus, the transmission coefficient can also be expressed as

\[ T[\omega] = \frac{\sqrt{4k_2m_2 - \omega^2m_i^2}}{\sqrt{4k_1m_1 - \omega^2m_i^2}} |t_{12}|^2, \]  

where \[ t_{ij} = \frac{-k_{ij}k_i(\lambda_i - 1/\lambda_i)}{(k_i - k_{ij} - k_i/\lambda_i)(k_j - k_{ij} - k_j/\lambda_j) - k_{ij}^2}. \]  

For the long-wave limit, that is, \( \omega = 0^+ \), we get \( r_{ij} = \frac{\sqrt{\kappa_i}}{\sqrt{\kappa_j} + \sqrt{\kappa_j}} \); and the transmission is

\[ T[0^+] = \frac{4\sqrt{k_1m_1k_2m_2}}{(\sqrt{k_1m_1} + \sqrt{k_2m_2})^2}. \]  

This result is consistent with the one obtained for the acoustic mismatch model, i.e., \( T = \frac{Z_2}{(Z_1 + Z_2)^2} \). Where the acoustic impedance is \( Z_i = \rho_i v_i = (m_i/\alpha_i)v_i \), and \( Z_i(\omega = 0^+) = \sqrt{\kappa_i}v_i \). We note that in acoustic mismatch model the transmission coefficient is frequency independent, and in reality it only applies in the limit of low frequency/long wavelengths. In this case the phonon sees the interface only as a discontinuity between two semi-infinite media and the transmission does not depend on the coupling spring strength \( k_{ij} \). If the two leads have the same acoustic impedance for long wave limit, then \( T[0^+] = 1 \); otherwise \( T[0^+] < 1 \).

For a two-junction case, which is shown in Fig. 1 the transmission wave will be reflected and transmitted by the second boundary, leading to multiple reflections. Finally the total transmitted wave function is obtained as a superposition of multiple reflections and transmissions, resulting in the transmission coefficient through the center part

\[ T[\omega] = \frac{(1 - |r_{12}|^2)(1 - |r_{23}|^2)}{|1 - r_{23}r_{21}|^2(\lambda_2^{-1}N_2)^2}, \]  

here \( r_{ij} \) and \( \lambda_i \) are determined by Eq. (12) and Eq. (8); \( N_2 \) is the number of atoms in the center atomic chain. From this expression, we can find that the transmission coefficient oscillates with frequency, and is between the envelope lines of maximum and minimum transmission, which are \( T_{\text{max}}[\omega] = (1 - |r_{12}|^2)(1 - |r_{23}|^2)/(|1 - r_{23}r_{21}|^2) \) for constructive interference and \( T_{\text{min}}[\omega] = (1 - |r_{12}|^2)(1 - |r_{23}|^2)/(|1 + r_{23}r_{21}|)^2 \) for destructive interference.

IV. RESULTS AND DISCUSSIONS

A. Thermal transport in 1D one-junction chains

In Sec. III we have derived the analytical expressions for the phonon transmission coefficient for point-junction and extended-junction (two point junction) cases Eq. (11), Eq. (12) and Eq. (10) by using the scattering boundary method. Using these analytical expressions, we analyze the role of various parameters on the thermal transport in one- and two-point junctions.

Figure 2 shows the transmission coefficient as a function of frequency for a different interface spring constant \( k_{12} \) for the point-junction model. The maximum frequency at which the transmission coefficient is above zero is equal to the minimum of \( 2\sqrt{k_1/m_1} \) and \( 2\sqrt{k_2/m_2} \). In Fig. 2(a), the two semi-infinite atomic chains have the same mass and spring constant. When the inter-
face coupling $k_{12}$ equals to that of the chains, the transmission is equal to one in the whole frequency domain, because of the homogeneity of the chain structure. If $k_{12}$ increases or decreases, the transmission coefficient decreases. If we set $k_1/m_1 = k_2/m_2$, the transmission coefficient exhibits similar behavior, the only difference is that the transmission coefficient changes to the value obtained by Eq. (15). In Fig. 2(b), the two semi-infinite atomic chains have different masses and spring constants. The transmission decreases with increased frequency for all the coupling values $k_{12}$. Also, it appears that for a given frequency the transmission is maximized for a $k_{12}$ value residing between $k_1$ and $k_2$. From Eq. (11) and Eq. (12), $T[\omega] = 0$, if $k_{12} = 0$; and $T[\omega]$ has definite value $1 - \left(\frac{k_1(\lambda_1 - 1) - k_2(1 - \lambda_2)}{k_1(1 - \lambda_2) + k_2(1 - \lambda_1)}\right)^2$, if $k_{12} = \infty$.

The maximum transmission concept results in the maximum junction conductance as shown in Fig. 3 With the increasing of $k_{12}$, we find that the conductance will first increase, then arrive at maximum value, and then slightly decrease and at last it will tend to a constant. We find that the maximum transmission or conductance occurs at $k_{12}$ given by

$$k_{12} = k_{12m} = \frac{2k_1k_2}{k_1 + k_2},$$

i.e., when the coupling spring stiffness is equal to the harmonic average of spring connecting atoms in the two semi-infinite chains. In Fig. 4 we show the thermal conductance vs the ratio of $k_{12}/k_{12m}$ in one-junction atomic chain. Here $k_{12m}$ is the harmonic average of the spring constants of the two semi-infinite leads. (a) $k_1 = 1.0, m_1 = m_2 = 1.0$; the solid, dashed, and dotted lines correspond to $k_2 = 0.1, 1.0,$ and 40.0, respectively. (b) $k_1 = 1.0, m_1 = 1.0, k_2 = 10.0$; the solid, dashed, and dotted lines correspond to $m_2 = 0.01, 1.0$, and 100.0, respectively.

FIG. 4: (color online) The thermal conductance vs the ratio of $k_{12}/k_{12m}$ in one-junction atomic chain. Here $k_{12m}$ is the harmonic average of the spring constants of the two semi-infinite leads. (a) $k_1 = 1.0, m_1 = m_2 = 1.0$; the solid, dashed, and dotted lines correspond to $k_2 = 0.1, 1.0,$ and 40.0, respectively. (b) $k_1 = 1.0, m_1 = 1.0, k_2 = 10.0$; the solid, dashed, and dotted lines correspond to $m_2 = 0.01, 1.0$, and 100.0, respectively.

FIG. 5: (color online) The transmission coefficient vs frequency for different mass ratios $m_2/m_1$ at the interface coupling $k_{12m}$. Here, $k_1 = 1.0, k_2 = 3.0, k_{12} = k_{12m} = 1.5$ and $m_1 = 1.0$.

FIG. 6: (color online) The transmission coefficient vs frequency for different interface coupling $k_{12m}$. Here, $k_1 = 1.0, m_1 = 1.0, k_2 = 0.7, m_2 = 0.3$. 
expects that the transmission should be the largest in the long wavelength limit. For highly dissimilar materials, the transmission coefficient in the whole frequency range is much larger than that in the long wave limit $T[\omega = 0^+]=\frac{12h^2}{(2\omega)^2}$, thus the real conductance is far larger than that calculated from the acoustic mismatch model. This result explain why the interfacial resistance calculated from the acoustic mismatch model is far larger than the experimental value measured at low temperatures, where the phonon transport can be regarded as ballistic transport.

In many real interfaces, interface coupling is very weak, that is, the $k_{12}$ is less than $k_{12m}$. So it is desirable to study the thermal transport in atomic chains in the weak coupling limit. Figure 6 shows the transmission coefficient as function of interface coupling. In the weak coupling limit, with the frequency increasing, the transmission decreases rapidly to zero, so the frequency region where phonons are effectively transmitted is very narrow. With interface strength increasing, more and more modes contribute to the transmission and the phonon transmission window widens. If the interface coupling increases further, that is $k_{12}/k_{12m} > 0.1$, out of the weak interface coupling limit, all the phonons contribute to the transmission. The only further change with increasing $k_{12}$ is the actual values of the transmission coefficients increase. In Fig. 7(a), we show the transmission cutoff frequency as function of the interface coupling. Here, we define the cutoff frequency $\omega_{\text{cutoff}}$ at which the transmission $T(\omega_{\text{cutoff}})=0.1T(0^+)$. We find that the cutoff frequency shows linear dependence on interface coupling in the weak coupling limit $k_{12} < 0.1k_{12m}$. If the interface strength increase further, the cutoff frequency is saturated. In Fig. 7(b), we show the transmission as function of interface coupling for several different phonons. We find that in the weak interface coupling region, the transmission is proportional to the square of the interface coupling, which is consistent with the formulas Eq. (13) and Eq. (14). In the weak interface coupling region, for the 1D atomic one-junction chains, it is shown that the thermal conductance is linear with the interface coupling (see Fig. 8). If we strengthen the interface coupling between the two chains, the conductance will be linearly enhanced. For different mismatched chains, the absolute values of the conductance are different, but dependence on the coupling strength is the same.

**B. Thermal transport in 3D single-interface structures**

The thermal conductance Eq. (14) can also be written as:

$$\sigma = \int_0^\infty d\omega \ h\omega T[\omega] \frac{\partial f(\omega)}{\partial T} v(\omega) D(\omega), \quad (18)$$

because of $v(\omega) = \partial \omega / \partial k$ and phonon density of states.
in 1D structure, \( D(\omega) = 1/(2\pi v) \), we can obtain Eq. (4). In order to estimate the behavior of the interfacial thermal transport across interfaces in 3D structures, we only need to change the phonon density of states in the above equation. Because the density of states for 3D structure within the Delye approximation is \( D(\omega) \sim \omega^2 \), therefore we can replace \( \omega \) with \( \omega^3 \) in Eq. (4), the thermal conductance as a function of the coupling strength is shown in Fig. 9. From Fig. 9(a), we find that in the weak interface limit, conductance is proportional to the square of interface coupling, which is consistent with the results from other models, while it is linear dependent on the interface coupling in 1D junctions. This is due to the fact that in 3D low frequency region contributes relatively little to the conductance as the density of states is low there. If the interface coupling increases further, that is \( k_{12}/k_{12m} > 0.1 \), out of the weak interface coupling limit, all the modes contribute to the transmittance, the conductance is no longer proportional to the square of the interface coupling, and the slope continuously decreases. In some intermediate ranges the conductance is approximately proportional to the interfacial coupling (see Fig. 9(b)), which is consistent with the results from molecular simulation approach. For stronger coupling the conductances for the 1D case and 3D one have similar behaviors, the slope of both cases will decrease continuously to be zero at point \( k_{12m} \), where the conductance will be maximized and then decrease slightly to a limiting value.

C. Thermal transport in extended junctions

Now we focus on a case where the junction is extended and involves a center part. The overall behavior of the transmission is the combination of the transmission behavior in single point-junction case and the oscillatory behavior due to phonon interferences arising form multiple scattering. We show the transmission coefficient as a function of frequency of an arbitrary case in Fig. 10(a). Here, the three chain parts have different masses and spring constants, and the interface coupling is not special. From the analytical expression of Eq. (16), we plot curves of the maximum transmission and minimum transmission, \( N_c = 4 \) and \( N_c = 9 \). The transmission oscillates between the envelop lines of maximum and minimum transmission. The maximum transmission line will increase first, and the minimum transmission line will monotonically decrease with frequency. However for interface coupling that is the same with the leads, the two envelop lines will monotonically decrease, which can be seen in Fig. 10(b).

For some special cases, the transmission coefficient in

FIG. 10: (color online) The transmission coefficient of the two-junction atomic chains. Parameters: \( k_1 = 1.0, m_1 = 1.0, k_2 = 0.9, m_2 = 1.6, k_3 = 4.5, m_3 = 2.0 \). The solid, dotted, dashed and shot dashed lines correspond to maximum transmission, minimum transmission, \( N_c = 4 \) and \( N_c = 9 \), respectively. The interface couplings are different: (a) \( k_{12} = 0.3, k_{23} = 0.7 \); (b) \( k_{12} = 1.0, k_{23} = 4.5 \).

FIG. 11: (color online) The transmission coefficient of the two-junction atomic chains. Here, \( k_1 = 1.0, m_1 = 1.0 \). The solid, dotted, dashed and shot dashed lines correspond to maximum transmission, minimum transmission, \( N_c = 4 \) and \( N_c = 9 \), respectively. (a) \( k_2 = 3.0, m_2 = 5.0, k_3 = 1.0, m_3 = 1.0, k_{12} = k_{23} = 1.0 \); (b) \( k_2 = 3.0, m_2 = 1.0, k_3 = 5.0, m_3 = 1.0, k_{12} = k_{12m} = 1.5, k_{23} = k_{23m} = 3.75 \); (c) \( k_2 = 3.0, m_2 = 3.0, k_3 = 5.0, m_3 = 5.0, k_{12} = k_{12m} = 1.5, k_{23} = k_{23m} = 3.75 \).
the frequency domain has interesting phenomena, which are shown in Fig. 11. In Fig. 11(a), the transmission for the case of two identical leads is shown. In this case, the maximum transmission is equal to one, the infinite-long wavelength phonon and the resonance mode can transmit fully through the center part. The minimum transmission is very low, indicating efficient destructive interference. Figure 11(b) shows the transmission when all three parts are different and connected by interface couplings \(k_{12m}\) and \(k_{23m}\). We find that overall trend for the maximum transmission is increasing first, then decreasing. If, in addition, the ratios of \(v_j/m_j\) are different from the ones of the two leads, the oscillatory peak is sharp, and transmission for most of the frequency will tend to zero, only few resonant frequency can be transmitted. This finding provides guidelines for the design of selective frequency filters.

Figure 12: (color online) The maximum and minimum transmission coefficient of the two-junction atomic chains. Here, \(k_1 = 1.0, m_1 = 1.0\). The solid, dashed lines correspond to maximum transmission and minimum transmission \(k_1 = 1.0, m_3 = 1.0\), respectively; the dotted and dash-dotted lines correspond to maximum transmission and minimum transmission \(k_3 = 5.0, m_3 = 5.0\), respectively. The inset shows the transmission coefficient with frequency for different \(k_2\). The solid, dashed, and solid lines correspond to \(k_2 = 0.5, 0.1\), and 0.02 respectively. For all the curves, \(m_2 = k_2\) and \(k_{12} = k_{12m}, k_{23} = k_{23m}\).

Figure 13: (color online) The comparison of the results from scattering boundary method and nonequilibrium Green’s function method for the transmission coefficient in two-junction atomic chains. The square curve and solid line correspond the parameters: \(N_c = 6, k_1 = 1.0, m_1 = 1.0, k_2 = 1.5, m_2 = 1.3, k_3 = 2.0, m_3 = 1.7, k_{12} = 1.3, k_{23} = 0.8\); the circle curve and dashed line correspond the parameters: \(N_c = 13, k_1 = 1.0, m_1 = 1.0, k_2 = 1.5, m_2 = 1.3, k_3 = 4.0, m_3 = 2.7, k_{12} = 1.3, k_{23} = 0.8\). The square and circle curves are the results from nonequilibrium Green’s function method; The solid and dash lines are the results from scattering boundary method.

V. VERIFICATION BY NONEQUILIBRIUM GREEN’S FUNCTION METHOD

The NEGF method is an exact approach to study the ballistic thermal transport through junctions. Following the discussion in Sec. 8 if we use a transformation for the coordinates, \(u_j = \sqrt{m_j} x_j\), which is called the mass-normalized displacement, then the Hamiltonian can be written as

\[
H = \sum_{\alpha=1,2,3} H_\alpha + \sum_{\beta=1,3} U^T \beta V_{\beta,2} U_2.
\]

where \(H_\alpha = \frac{1}{2} (P_\alpha^T P_\alpha + U_\alpha^T K_\alpha U_\alpha)\). \(K_\alpha\) is the mass-normalized spring constant matrix, and \(V_{12} = (V_{21})^T\) is the coupling matrix of the left lead to the central region and similarly for \(V_{23}\) is the coupling matrix of the right lead to the central region. As stated in Ref. 7, the element of the coupling matrix \(V_{ij}\) is equal to \(-i \delta_{ij} / \sqrt{m_i m_j}\), which corresponding to the coupling between the \(i_{th}\) atom in region \(\alpha\) and the \(j_{th}\) atom in region \(\beta\).

We can use the nonequilibrium Green’s function method to study the thermal transport in the atomic chain. We define the contour-ordered Green’s function as

\[
G^{\alpha\beta}(\tau, \tau') = -\frac{i}{\hbar} \langle T \ U_\alpha(\tau) U_\beta(\tau')^T \rangle,
\]

where \(\alpha\) and \(\beta\) refer to the region that the coordinates belong to and \(T\) is the contour-ordering operator. Then
the equations of motion of the Green’s function can be derived. In particular, the retarded Green’s function for the central region in frequency domain is

\[ G'[\omega] = \left[(\omega + i\eta)^2 - K_2 - \Sigma'[\omega]\right]^{-1}. \] (21)

Here, \( \Sigma' = \sum_{\alpha=1,3} \Sigma'_\alpha \), and \( \Sigma_\alpha = V_{2,\alpha} g_\alpha V_{\alpha,2} \) is the self-energy due to interaction with the heat bath, \( g_\alpha' = [(\omega + i\eta)^2 - K_\alpha]^{-1} \). And in the advanced Green’s function \( g_\alpha = (G')^{-1} \), the transmission coefficient can be calculated by the so-called Caroli formula as

\[ T_{\beta\alpha}[\omega] = \text{Tr}(G^r \Sigma_\beta G^a \Gamma_\alpha), \] (22)

where \( \Gamma_\alpha = i(\Sigma'_\alpha[\omega] - \Sigma''_\alpha[\omega]) \).

For single-junction atomic chains, if we regard the two atoms in the interface (atom 0 and atom 1) as the center part, then we can still use the formulae above to study the phonon transmission leading to the exact formula yielding the same result with the one obtained from the scattering boundary method. In Appendix A, We give the analytical proof of this fact.

For two-junction atomic chains, according to the NEGF formulas, we do the numerical calculation and plot the curves of the transmission coefficient as a function of frequency and compare them to the results obtained the scattering boundary method (see Fig. 13). We find that for any arbitrary case, the results from the NEGF method and the scattering boundary method are exactly the same. If there is no many-body interaction, that is, for the ballistic thermal transport the scattering matrix approach and the Green’s function method give the same results. These two methods are equivalent, which has been proved from other points of view in Refs.28,29.

VI. CONCLUSION

In this paper, we study the ballistic interfacial thermal transport in atomic junctions, we give the analytical simple formulae Eq. (11), Eq. (12) and Eq. (16) for the transmission of one-junction and two-junction cases, which are consistent with the results from the NEGF method.

For one-junction case, we find the transmission and conductance are maximized when the interface spring constant equals to the harmonic average of the two spring constants of the leads. At the point near \( k_{12} = k_{12m} \), the transmission \( T[\omega] \) is a constant if \( k_2/m_2 = k_1/m_1 \); if not equal, in the range between \( k_1/m_1 = k_2/m_2 \) and \( k_1 m_1 = k_2 m_2 \), the transmission coefficient increases first then decreases with the increasing of frequency, otherwise the transmission monotonically decreases as the frequency increasing. For weak interface coupling, the cutoff frequency and the interface conductance for 1D chain is linear dependent with the interface coupling strength.

Because of different density of states, we change the formula of conductance to mimic the thermal transport in 3D junctions. In weak interface coupling limit, we find that the conductance is proportional to the square of the interface coupling, which is consistent with the results from other models. The slope of the conductance as function of interfacial coupling strength decreases continuously from two to zero, in certain range of which, the conductance is linear proportional to the interface coupling, which are consistent with the results of other molecular simulations.

For two-junction case, the transmission will oscillate with frequency in the envelop lines of maximum and minimum transmission which are determined by the one-junction picture. The transmission sometimes oscillates between two decreasing envelop lines, sometimes between two increasing envelop curves, or between two constants, etc.

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Appendix A: Analytical proof of the equality of the two methods for one junction

In this appendix we give the analytical proof for the equality of the scattering boundary method and the non-equilibrium Green’s function approach for the one-junction atomic chains.

From the scattering boundary method, we obtain the transmission Eq. (13) and Eq. (14), that is

\[ T[\omega] = \frac{\sqrt{4k_2 m_2 - \omega^2 m_2^2}}{\sqrt{4k_1 m_1 - \omega^2 m_1^2}} \frac{-k_{12} k_1 (1/\lambda_1)}{(k_1 - k_{12} - k_1/\lambda_1)(k_2 - k_{12} - k_2/\lambda_2) - k_{12}^2}, \] (A1)

From the dispersion relation Eq. (9), we can obtain

\[ k_j - k_j/\lambda_j = \omega^2 m_j - k_j(1 - \lambda_j) \] (A2)

\[ k_j^2 |\lambda_j - 1/\lambda_j|^2 = \omega^2 (4k_j m_j - \omega^2 m_j^2) \] (A3)
Using the NEGF formulae, we regard the two atoms in the interface (atom 0 and atom 1) as the center part 0, then the dynamic matrix of the center as

$$K_0 = \begin{pmatrix} \frac{k_{12} + k_{12}}{m_1} & \frac{k_{12}}{m_1} \\ \frac{k_{12}}{m_1 m_2} & \frac{k_{12} + k_{12}}{m_2} \end{pmatrix},$$

(A5)

And the coupling matrices between the leads (parts 1 and 2) and the center (part 0) are $V_{01} = (k_{1}, m_1, 0)^T$ and $V_{02} = (0, k_2, m_2)^T$, and according to Ref. [10], we can obtain the surface Green’s function as

$$g_r = -\frac{m_1 \lambda_i}{k_i},$$

(A6)

here, $i = 1, 2$ corresponds to the left and right lead. Then we can get the self energy ($\Sigma_r = V_{01} g_l V_{10} + V_{02} g_r V_{20}$) as

$$\Sigma_r = \begin{pmatrix} \frac{k_{12} \lambda_1}{m_1} & 0 \\ 0 & \frac{k_{12} \lambda_2}{m_2} \end{pmatrix}.$$  

(A7)

Thus we can calculate the retarded Green’s function of the center $G^r = (\omega^2 I - K_0 - \Sigma_r)^{-1}$, which reads as

$$G^r = \begin{pmatrix} A_1 & B \\ B & A_2 \end{pmatrix}^{-1} = \frac{1}{\Delta} \begin{pmatrix} A_2 & -B \\ -B & A_1 \end{pmatrix},$$

(A8)

here, $I$ is two-dimensional identity matrix and

$$A_i = \omega^2 - \frac{k_i}{m_i} (1 - \lambda_i) - \frac{k_{12}}{m_1};$$

(B)

$$B = \frac{k_{12}}{\sqrt{m_1 m_2}}; \Delta = A_1 A_2 - B^2.$$  

(A10)

The advanced Green’s function $G^a$ equals to $(G^r)^\dagger$. And from the self energy we can get

$$\Gamma_1 = \begin{pmatrix} C_1 & 0 \\ 0 & 0 \end{pmatrix}; \Gamma_2 = \begin{pmatrix} 0 & 0 \\ 0 & C_2 \end{pmatrix},$$

(A11)

here, $C_i = \frac{\omega}{m_i} \sqrt{4k_i m_i - \omega^2 m_i^2}$. Therefore, we can calculate the transmission coefficient from the Caroli formula Eq. (23), at last we obtain

$$T[\omega] = Tr(G^r \Gamma_1 G^a \Gamma_2) = \frac{B^2 C_1 C_2}{\Delta \Delta^*} = \frac{B^2 C_1 C_2}{|A_1 A_2 - B^2|^2},$$

(A12)

Inserting the values of $A_i, B$ and $C_i$, we get exactly the same result with Eq. (A3). Therefore, the results from the scattering boundary method and non-equilibrium Green’s function approach are equivalent.
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