Towards ultrafast cooling through transient phonon currents: A closed-form solution

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We develop a closed-form formula to calculate the transient thermal currents flowing through an arbitrary nanoscale phonon device in response to a sudden thermal switch. Our theory provides a solution to the problem in the far-from-equilibrium nonlinear response regime beyond the wide-band-like approximation and Drude regularization. We present calculations in a one-dimensional monatomic chain with Lorentzian-like thermal baths and show that the transient phonon currents are significantly larger than the long-time-limit steady-state phonon current. From the formula's clear mathematical structure, we also show that the transient oscillation periodicity and relaxation time are determined by the poles of the retarded phonon Green's function. In addition, higher temperatures of the thermal baths and stronger coupling between the baths and the central monatomic chain result in higher transient thermal currents. Our results suggest that ultrafast cooling of nanodevices through transient phonon currents is a promising route.

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I. INTRODUCTION

Thermal transport in low-dimensional systems has aroused lots of interests due to the novel thermal properties, such as quantized thermal conductance [1], breakdown of the classical Fourier's law [2], exceptionally high thermal conductivity [3], intrinsic anisotropy of thermal conductance [4], exotic angular and length dependence of thermal conductance in carbon-based quantum junctions [5–7]. The possibility of building thermal circuits to manipulate information using phonons instead of electrons is also intriguing [8–10].

Previously, researchers have been largely focused on the steady transport properties of phonons [11–14]. However, it is found that time variation introduces new possibilities. For example, ac modulation can be used to enhance thermoelectric performance of noncollinear spin valves [15] and spin transfer torques [16]. Despite considerable research on transient behavior of charge currents [17–24], spin currents [25,26], and heat currents of electrons [27,28], time-dependent behavior of phonon currents remain understudied [29,30]. In 2010, Wang *et al.* studied the transient behavior of a one-dimensional atomic chain under a sudden thermal switch [31]. Later, Tuovinen *et al.* developed a closed-form analytic expression of one-particle reduced density matrix based on the equation of motion in a wide-band-like approximation [32]. Recently, Sandonas *et al.* adopted an auxiliary mode approach to numerically describe time-dependent phonon transport, where a spectral density of the thermal baths with a Drude regularization was assumed [33].

In this work, we derive a closed-form solution for calculating the transient phonon currents under a sudden thermal switch beyond the wide-band-like approximation and Drude regularization. We further investigate a monatomic chain with analytical self-energies of thermal baths, demonstrating that our solution reduces computational complexity significantly. In Sec. II, we present our theory for obtaining the closed-form expression for the transient phonon currents and the simplification over a one-dimensional (1D) atomic chain model. We present and discuss numerical results in Sec. III before concluding in Sec. IV.

II. GENERAL FORMALISM

To calculate the transient thermal currents flowing through an arbitrary nanoscale phonon device, we consider a system consisting of thermal leads (L, R) and a central region (C). The Hamiltonian of the vibrating system can be written as

$$\hat{H} = \hat{H}_L + \hat{H}_R + \hat{H}_C + \hat{V}_{LC} + \hat{V}_{CR}, \tag{1}$$

where $\hat{H}_\alpha (\alpha = L, C, R)$ is the Hamiltonian of region α and $\hat{V}_{CR}$ ($\hat{V}_{CL}$) is the interaction between region C and R (L), respectively. Under the Harmonic approximation, these terms can be written as [34]

$$\hat{H}_{L/R/C} = \sum_{I\in L/R/C} \sum_{\alpha=xyz} \frac{1}{2}\hat{v}_{I\alpha}^2 + \frac{1}{2} \sum_{I,J\in L/R/C} \sum_{\alpha,\beta=xyz} \hat{u}_{I\alpha} D_{I\alpha,J\beta} \hat{u}_{J\beta}, \tag{2}$$

$$\hat{V}_{LC} = \frac{1}{2}\left(\sum_{\substack{I\in L\\ J\in C}} + \sum_{\substack{I\in C\\ J\in L}}\right) \sum_{\alpha,\beta} \hat{u}_{I\alpha} D_{I\alpha,J\beta} \hat{u}_{J\beta}, \tag{3}$$

$$\hat{V}_{CR} = \frac{1}{2}\left(\sum_{\substack{I\in R\\ J\in C}} + \sum_{\substack{I\in C\\ J\in R}}\right) \sum_{\alpha,\beta} \hat{u}_{I\alpha} D_{I\alpha,J\beta} \hat{u}_{J\beta}. \tag{4}$$

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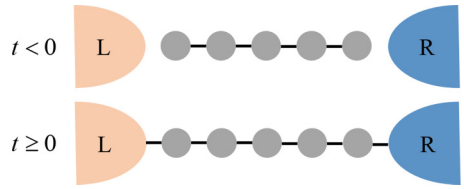

FIG. 1. Schematic plot of a monatomic chain model. Coupling of the central part to the thermal baths are switched on abruptly at $t = 0$.

Here, $\hat{u}_{I\alpha} \equiv \sqrt{M_I}\hat{\eta}_{I\alpha}$ and $\hat{v}_{I\alpha} \equiv \dot{\hat{u}}_{I\alpha} = \hat{p}_{I\alpha}/\sqrt{M_I}$ are mass-weighted displacements and momenta, respectively, of the I^{th} atom along direction α. In addition, $D_{I\alpha,J\beta}$ is the $(I\alpha, J\beta)^{\text{th}}$ element of the dynamical matrix $\mathbf{D}$. $\hat{V}_{LC}$ and $\hat{V}_{CR}$ are absent when $t < 0$. A sudden coupling of two regions can be achieved by establishing a point contact between them. For example, by using a scanning tunneling microscope tip in molecular junctions to induce a bond through proximity, a thermal switch can be realized [31].

The phonon current flowing out of thermal lead L can be written as (see Appendix)

$$J_L(t) = -\hbar \int_{-\infty}^{+\infty} \mathrm{d}t_1 \mathrm{ReTr}\big[\mathbf{G}^r_{CC}(t,t_1)\boldsymbol{\Sigma}^{<,1}_L(t_1,t) + \mathbf{G}^<_{CC}(t,t_1)\boldsymbol{\Sigma}^{a,1}_L(t_1,t)\big], \tag{5}$$

where $\mathbf{G}^r_{CC}$ ($\mathbf{G}^<_{CC}$) is the retarded (lesser) phonon Green's function of the central region, and $\boldsymbol{\Sigma}^{<,1}_L$ ($\boldsymbol{\Sigma}^{a,1}_L$) is the lesser (advanced) type-1 phonon self-energy of thermal lead L ($\gamma = r, a, <, >$):

$$\boldsymbol{\Sigma}^{\gamma,1}_L(t_1,t) \equiv \int \frac{d\omega}{2\pi}\omega \mathbf{D}_{CL}(t_1)\mathbf{g}^\gamma_L(\omega)\mathbf{D}_{LC}(t)e^{-i\omega(t_1-t)}. \tag{6}$$

Note that $\mathbf{g}^\gamma_L(\omega)$ [$\mathbf{g}^\gamma_R(\omega)$] are the phonon Green's functions of the isolated thermal lead L (R), $\mathbf{D}_{CL}$ is the dynamical matrix between the central region and the thermal lead L, and $\mathbf{D}_{LC} = \mathbf{D}^T_{CL}$. Under a sudden connection of thermal bath L, R with the central region at $t = 0$ (Fig. 1), we have the phonon current expressed as

$$J_L(t) = -\frac{\hbar}{2}\int_0^{+\infty} dt_1 \mathrm{Tr}\big[\mathbf{G}^r_{CC}(t,t_1)\boldsymbol{\Sigma}^{<,1}_L(t_1,t) + \mathbf{G}^<_{CC}(t,t_1)\boldsymbol{\Sigma}^{a,1}_L(t_1,t) + \mathrm{H.c.}\big], \tag{7}$$

and the modified type-1 phonon self-energies as ($\gamma = r, a, >, <$)

$$\boldsymbol{\Sigma}^{\gamma,1}_L(t_1,t) = \theta(t_1)\theta(t)\int \frac{d\omega}{2\pi}\omega \mathbf{D}_{CL}\mathbf{g}^\gamma_L(\omega)\mathbf{D}_{LC}e^{-i\omega(t_1-t)}. \tag{8}$$

Here, $\theta(x)$ is the Heaviside step function. Because of the sudden connection at $t = 0$, the self-energies of thermal leads are zero before that. It is reasonable to assume that the sudden thermal switch does not alter the phonon structure of both thermal leads. When both t and t_1 are later than zero, $\boldsymbol{\Sigma}^{\gamma,1}_L(t_1,t) = \boldsymbol{\Sigma}^{\gamma,1}_L(t_1 - t)$ is a function of time difference according to Eq. (8). Therefore, a Fourier transform can be used to obtain

$$\boldsymbol{\Sigma}^{\gamma,1}_{L(R)}(\omega) = \omega\boldsymbol{\Sigma}^\gamma_{L(R)}(\omega), \tag{9}$$

where $\boldsymbol{\Sigma}^\gamma_{L(R)}(\omega) = \mathbf{D}_{CL(R)}\mathbf{g}^\gamma_{L(R)}(\omega)\mathbf{D}_{L(R)C}$.

In the following, we shall omit the subscript "CC" for the Green's functions of the central region such that $\mathbf{G}^{r,a,<} \equiv \mathbf{G}^{r,a,<}_{CC}$.

According to Dyson's equation, the retarded Green's function becomes [35]

$$\mathbf{G}^r(t,t') = \mathbf{G}^r_0(t,t') + \iint_0^{+\infty} dt_1 dt_2 \mathbf{G}^r_0(t,t_1)\boldsymbol{\Sigma}^r(t_1,t_2)\mathbf{G}^r(t_2,\ t'), \quad t,t' > 0, \tag{10}$$

where $\mathbf{G}^\gamma_0$ is the retarded Green's function of the central region when the thermal leads are disconnected from the central region.

Recognizing that self-energies are nonzero when time is later than zero, by the Keldysh equation for the lesser Green's function $\mathbf{G}^<$, we obtain, for $t, t' > 0$,

$$\mathbf{G}^<(t,t') = \mathbf{G}^r(t,0)\mathbf{G}^<_0(0,0)\mathbf{G}^a(0,t') + \iint_0^{+\infty} dt_1 dt_2 \mathbf{G}^r(t,t_1)\boldsymbol{\Sigma}^<(t_1,t_2)\mathbf{G}^a(t_2,\ t'), \tag{11}$$

by noting that self-energies are nonzero when time is later than zero. Here, $\boldsymbol{\Sigma}^\gamma = \boldsymbol{\Sigma}^\gamma_L + \boldsymbol{\Sigma}^\gamma_R$.

Furthermore, by introducing the spectral function as [21]

$$\mathbf{A}(\omega,t) = \int_0^t dt' \mathbf{G}^r(t,t')e^{i\omega(t-t')}, \tag{12}$$

we can rewrite $\mathbf{G}^r$ and $\mathbf{G}^<$ in terms of spectral function $\boldsymbol{A}$ for $t, t' > 0$ as

$$\mathbf{G}^r(t,t') = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\mathbf{A}(\omega,t)e^{-i\omega(t-t')}, \tag{13}$$

and

$$\mathbf{G}^<(t,t') = \mathbf{G}^r(t,0)\mathbf{G}^<_0(0,0)\mathbf{G}^a(0,t') + \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\mathbf{A}(\omega,t)\boldsymbol{\Sigma}^<(\omega)\mathbf{A}^\dagger(\omega,t')e^{-i\omega(t-t')}, \tag{14}$$

respectively. Also, we have [26,36]

$$\mathbf{A}(\omega,t) = \bar{\mathbf{G}}^r(\omega) + \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i}\frac{e^{-i(\omega'-\omega)t}}{\omega - \omega' + i0^+}\bar{\mathbf{G}}^r(\omega'), \tag{15}$$

and

$$\mathbf{G}^r(t,t') = \bar{\mathbf{G}}^r(t-t'), \quad t,t' > 0, \tag{16}$$

where 0^+ is an infinitesimal positive number and $\bar{\mathbf{G}}^r(t-t')$ [$\bar{\mathbf{G}}^r(\omega)$] is the steady-state retarded Green's function (in energy space) where both thermal leads' couplings are present (the long-time limit). Substituting Eq. (14) into Eq. (7),

we have

$$J_L(t) = -\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \mathrm{ReTr}[\hbar\omega \mathbf{A}(\omega,t)\boldsymbol{\Sigma}_L^<(\omega) + \mathbf{A}(\omega,t)\boldsymbol{\Sigma}^<(\omega)\mathbf{B}_L(\omega,t) + \mathbf{G}^r(t,0)\mathbf{G}_0^<(0,0)\bar{\mathbf{G}}^a(\varepsilon)\mathbf{C}_L(\varepsilon)], \tag{17}$$

with

$$\mathbf{B}_\alpha(\omega,t) = -\int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i} \frac{e^{i(\omega'-\omega)t}}{\omega-\omega'+i0^+} \omega' \bar{\mathbf{G}}^a(\omega')\boldsymbol{\Sigma}_\alpha^a(\omega') = \omega\bar{\mathbf{G}}^a(\omega)\boldsymbol{\Sigma}_\alpha^a(\omega) - \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i} \frac{e^{i(\omega'-\omega)t}}{\omega-\omega'-i0^+} \omega' \bar{\mathbf{G}}^a(\omega')\boldsymbol{\Sigma}_\alpha^a(\omega'), \tag{18}$$

and

$$\mathbf{C}_\alpha(\omega) = -\int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i} \omega' \boldsymbol{\Sigma}_\alpha^a(\omega') \frac{e^{i\omega' t}}{\omega-\omega'+i0^+}. \tag{19}$$

Equation (17) is the close-form solution for the transient phonon current under a sudden thermal switch.

For phonon Green's functions, they have the following relations [37]: $\bar{\mathbf{G}}^r(-\omega) = [\bar{\mathbf{G}}^r(\omega)]^*$, $[\bar{\mathbf{G}}^{<,>}(\omega)]^+ = -\bar{\mathbf{G}}^{<,>}(\omega)$, $\mathbf{G}^<(-\omega) = [\mathbf{G}^>(\omega)]^T$, and naturally $\boldsymbol{\Sigma}^{r,a}(-\omega) = [\boldsymbol{\Sigma}^{r,a}(\omega)]^*$ and $\boldsymbol{\Sigma}^<(-\omega) = [\boldsymbol{\Sigma}^>(\omega)]^T$. Thus, we have $\mathbf{A}(-\omega,t) = \mathbf{A}^*(\omega,t)$, $\mathbf{B}_\alpha(-\omega,t) = -\mathbf{B}_\alpha^*(\omega,t)$, and

$$J_\alpha(t) = -\int_0^{+\infty} \frac{d\omega}{2\pi} \mathrm{ReTr}[\hbar\omega \mathbf{A}(\omega,t)(\boldsymbol{\Sigma}_\alpha^< + \boldsymbol{\Sigma}_\alpha^>) + \mathbf{A}(\omega,t)(\boldsymbol{\Sigma}^< + \boldsymbol{\Sigma}^>)\mathbf{B}_\alpha(\omega,t)] \tag{20}$$

for zero occupation of the central region $[\mathbf{G}_0^<(0,0) = 0]$. In Eq. (20), integration is done within $[0, +\infty)$. Recognizing that thermal currents at the right thermal lead can be obtained by simply replacing the quantities of L in $J_L(t)$ with the corresponding quantities of R, we have $\alpha = L, R$ in Eqs. (18)–(20).

Equation (20) obviously consists of two parts: dc and ac components. The dc part corresponds to the steady-state limit when $t \to \infty$. Based on Eq. (20), the dc parts of $\mathbf{A}$ and $\mathbf{B}$ can be extracted as

$$\mathbf{A}_{dc}(\omega,t) = \bar{\mathbf{G}}^r(\omega), \tag{21}$$

$$\mathbf{B}_{\alpha;dc}(\omega,t) = \omega\bar{\mathbf{G}}^a(\omega)\boldsymbol{\Sigma}_\alpha^a(\omega). \tag{22}$$

Accordingly, the dc component of the thermal current can also be calculated as

$$J_{L;dc} = -\frac{1}{2}\int_0^{+\infty} \frac{d\omega}{2\pi} \hbar\omega \mathrm{Tr}\big[(\bar{\mathbf{G}}^r - \bar{\mathbf{G}}^a)(\boldsymbol{\Sigma}_L^< + \boldsymbol{\Sigma}_L^>) + \bar{\mathbf{G}}^r(\boldsymbol{\Sigma}^< + \boldsymbol{\Sigma}^>)\bar{\mathbf{G}}^a\big(\boldsymbol{\Sigma}_L^a - \boldsymbol{\Sigma}_L^r\big)\big] = \int_0^{+\infty} \frac{d\omega}{2\pi} \hbar\omega(f_L - f_R)\mathrm{Tr}(\boldsymbol{\Gamma}_L\bar{\mathbf{G}}^r\boldsymbol{\Gamma}_R\bar{\mathbf{G}}^a), \tag{23}$$

and

$$J_{R;dc} = \int_0^{+\infty} \frac{d\omega}{2\pi} \hbar\omega(f_R - f_L)\mathrm{Tr}(\boldsymbol{\Gamma}_R\bar{\mathbf{G}}^r\boldsymbol{\Gamma}_L\bar{\mathbf{G}}^a), \tag{24}$$

where $\bar{\mathbf{G}}^r - \bar{\mathbf{G}}^a = -i\bar{\mathbf{G}}^r\boldsymbol{\Gamma}\bar{\mathbf{G}}^a$. Equations (23) and (24) recover the results of Landauer-like thermal currents for quasiballistic systems [4,5]. The upper limit for the integrals can be replaced by $\omega_{\max}$, which is the highest eigenfrequency in the phonon spectra.

Combining Eqs. (15), (18), and (20), transient phonon currents can be calculated by using the phonon Green's functions of the central region and the self-energies of both thermal leads. It is worth noting that the forms of self-energies are not restricted to any particular type. Thus, our theory provides a closed-form solution to the transient phonon currents flowing through an arbitrary nanoscale phonon device under a sudden thermal switch in the far-from-equilibrium nonlinear response regime beyond the wide-band-like approximation and Drude regularization.

III. MODEL AND RESULTS

A. Monatomic chain under a thermal switch

Now we shall use a monatomic chain in the central region (Fig. 1) to investigate the transient phonon current under a thermal switch. Such a chain model can be used to present quasi-1D, two-dimensional (2D), and three-dimensional (3D) systems because atomic layers can be treated effectively as sites. Suppose that a monatomic chain with N atoms is sandwiched between two phonon baths, L and R. Connections between the central region and thermal baths are switched on at time $t = 0$. The dynamical matrix of the central region can be written as

$$\mathbf{D}_0 = \frac{1}{2}\omega_0^2 \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}_{N\times N}, \tag{25}$$

which is simply $D_0 = \omega_0^2$ when there is only one atom ($N = 1$) in the central part, implying an isolated oscillation mode of angular frequency ω_0. We begin by presenting results for $N = 1$.

Coupling to thermal baths L, R after $t = 0$ can be introduced through self-energies. The bandwidth function of thermal bath α can be assumed to be a Lorentzian-like lineshape [33,38,39]

$$\Gamma_\alpha(\omega) = \frac{\omega\gamma_\alpha\omega_c^2}{\omega^2 + \omega_c^2}, \tag{26}$$

where ω_c is the cutoff angular frequency for thermal baths L and R. Under the Drude regularization, the self-energies can be determined as [17]

$$\Sigma_\alpha^{r,a}(\omega) = \int \frac{d\varepsilon}{2\pi} \frac{\Gamma_\alpha(\varepsilon)}{\omega - \varepsilon \pm i0^+} = \int \frac{d\varepsilon}{2\pi} \frac{1}{\omega-\varepsilon\pm i0^+} \frac{\varepsilon\gamma_\alpha\omega_c^2}{(\varepsilon+i\omega_c)(\varepsilon-i\omega_c)} = \mp\frac{i}{2}\frac{\gamma_\alpha\omega_c^2}{\omega\pm i\omega_c}. \tag{27}$$

The lesser self-energies due to thermal lead α are

$$\Sigma_\alpha^<(\omega) = -if_{BE;\alpha}(\omega)\Gamma_\alpha(\omega), \tag{28}$$

and

$$\Sigma_\alpha^>(\omega) = -i[f_{BE;\alpha}(\omega)+1]\Gamma_\alpha(\omega), \tag{29}$$

with $f_{BE;\alpha}(\omega) = 1/[\exp(\hbar\omega/k_BT_\alpha)-1]$ is the Bose-Einstein distribution function.

The retarded Green's function at the steady state is

$$\begin{aligned}\bar{G}^r &= \frac{\omega+i\omega_c}{(\omega+i\omega_c)\left[(\omega+i\eta)^2-\omega_0^2\right]+i\gamma\omega_c^2/2} \\ &= \frac{\omega+i\omega_c}{(\omega-\omega_1)(\omega-\omega_2)(\omega-\omega_3)},\end{aligned} \tag{30}$$

where $\gamma = \gamma_L+\gamma_R$ and ω_i $(i=1,2,3)$ are defined through $(\omega+i\omega_c)[(\omega+i\eta)^2-\omega_0^2]+i\gamma\omega_c^2/2 = (\omega-\omega_1)(\omega-\omega_2)(\omega-\omega_3)$.[1] The auxiliary functions $A(\omega,t)$ and $B_\alpha(\omega,t)$ can be calculated according to Eqs. (15) and (18) as

$$A(\omega,t) = \bar{G}^r(\omega) + \sum_{i=1,2,3}\frac{e^{-i(\omega_i-\omega)t}}{\omega_i-\omega}\frac{\omega_i+i\omega_c}{\prod_{k\neq i}(\omega_i-\omega_k)}, \tag{31}$$

and

$$B_\alpha(\omega,t) = \omega\bar{G}^a\Sigma_\alpha^a + \frac{i\gamma_\alpha\omega_c^2}{2}\sum_{i=1,2,3}\frac{\omega_i^* e^{i(\omega_i^*-\omega)t}}{(\omega_i^*-\omega)\prod_{k\neq i}(\omega_i^*-\omega_k^*)}. \tag{32}$$

For $N>1$, $\mathbf{A}(\omega,t)$ and $\mathbf{B}_\alpha(\omega,t)$ can be calculated using numerical integration and subsequently the transient phonon currents can be calculated through Eq. (20).

From the above expression, we can see that there are long-tail oscillations of the transient current. The damping factor lies in the imaginary part of the poles ω_i. Since the poles of the retarded Green's function are located in the lower-half complex plane, the ac part of the transient thermal current has a damping factor and finally approaches the dc limit when $t\to+\infty$.

B. Results and discussion

We present numerical results of the transient thermal current under a thermal switch. Parameters are chosen to be around the order of 1 THz because phonon oscillation is typically around this order. To facilitate presentation, we converted angular frequencies to frequencies. The case with $N=1$ is fully explored and followed by the case with $N>1$.

Figure 2 shows the transient phonon current for a symmetric junction ($\gamma_L=\gamma_R$) after the coupling of the central region to thermal leads are both switched on suddenly at $t=0$. Although the two thermal leads have the same temperature, transient thermal currents begin emerging from $t=0$ onwards. The transient thermal currents are equal in thermal leads L and R in the symmetric junction. $J_\alpha>0$ implies that for $t\geqslant 0$ thermal currents flow out of both thermal leads to the central part. General features of quick growth from zero to a maximum value and slow decay with fast oscillation can

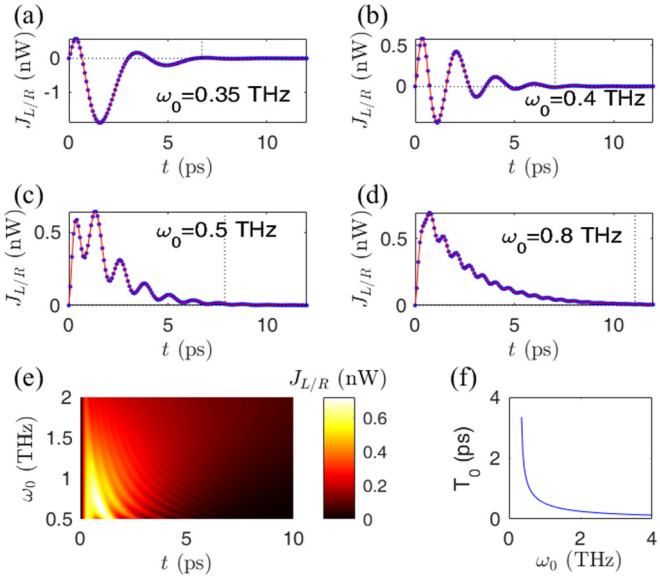

FIG. 2. Transient thermal currents at thermal lead L (blue dotted line) and R (red line) after switching on the coupling between the thermal leads and the central part at $t=0$. Both thermal leads are supposed to be Lorentzian thermal baths in equilibrium and at the temperature of 300 K. Other parameters are set to be $N=1$, $\omega_c=1$ THz, $\gamma_L=\gamma_R=0.1$ THz, $\eta=10^{-7}$ THz. Vertical dotted lines in the figure indicates the relaxation time $\tau_{L/R}$ calculated from Eq. (39).

be seen in Figs. 2(a)–2(d), which is consistent with previous studies [31,32]. When t is long enough, phonon current approaches the steady-state limit, where the net thermal flow is zero due to the equal temperature of the two thermal leads.

As ω_0 increases from 0.35 to 0.8 THz, oscillation frequency increases and the decaying time becomes longer. A contour plot of transient current $J_{L/R}$ as a function of the characteristic frequency of the central part (ω_0) and time t is given in Fig. 2(e). The maximum or minimum value is achieved within $t=2$ ps. In addition, oscillation of the transient thermal currents is reflected in the wavy patterns in the plot, where the oscillation period is roughly the same at a fixed ω_0 and decreases as ω_0 increases. When ω_0 decreases, the transient thermal current vanishes more quickly.

To better understand the transient behavior of the thermal current, we shall make a simple analysis here. From Eqs. (20), (31), and (32), it is indicative that both the decaying and oscillating behavior can be attributed to the poles ω_i of the retarded Green's function G^r since integration over frequency ω smears out the oscillation caused by $e^{\pm i\omega t}$ and leaves the contribution from $e^{\pm i\omega_i t}$. Writing the poles in forms of real and imaginary parts as

$$\omega_i = a_i - ib_i, \quad a_i, b_i\in\mathbb{R}, \tag{33}$$

where $b_i>0$ due to the distribution of poles, we have

$$e^{-i\omega_i t} = e^{-ia_i t-b_i t}, \tag{34}$$

$$e^{i\omega_i^* t} = e^{ia_i t-b_i t}. \tag{35}$$

The integral in Eq. (20) consists of both dc terms and ac terms, which are generated by the ac parts of A, B_α, and AB_α. As a consequence, this integral contains several

[1]When $\gamma<2\omega_0^2/\omega_c$, all poles $(\omega_1,\omega_2,\omega_3)$ distribute in the lower half of the complex plane.

parts that effectively vary with time since the three ac terms correspond to

$$e^{-ia_it-b_it},\ e^{ia_it-b_it},\ \text{and}\ e^{i(a_i-a_j)t-(b_i+b_j)t}. \tag{36}$$

Thus, the oscillation period of the transient phonon current can be estimated using the largest oscillation frequency as

$$T_0 = \frac{2\pi}{\max\{|a_i|, |a_i - a_j|\}_{i,j=1,\ldots,3;i\neq j}}, \tag{37}$$

with ω_i in the unit of rad/s.[2] The imaginary part of ω_i causes decay characterized by the relaxation time τ, which is defined through [32]

$$10\% = \frac{J_\alpha(t=\tau) - J_\alpha(t=+\infty)}{J_\alpha(t=+\infty)}, \tag{38}$$

can be roughly estimated using the smallest decaying factor,

$$\tau_\alpha = \frac{\ln 10}{\min\{b_i\}_{i=1}^3}. \tag{39}$$

Estimations of oscillation period and transient relaxation time agree well with numerical results: the oscillation period given by Eq. (37) when $\omega_0 = 0.35$, 0.4, 0.5, and 0.8 THz is about 3.35, 1.97, 1.24, and 0.66 ps, respectively. The estimated relaxation time $\tau_{L/R}$ is also reasonable as indicated by the vertical dotted lines in Figs. 2(a)–2(d). Furthermore, oscillation period T_0 as a function of ω_0 is obtained using Eq. (37) and plotted in Fig. 2(f). It shows that T_0 decreases dramatically as ω_0 increases. Since the thermal current is transported via the central region, it makes sense that the oscillation period is closely related to ω_0.

When $T_L \neq T_R$, the steady-state thermal current is nonzero. However, due to the aforementioned fact that the oscillation and decaying characters are determined by the poles of G^r, varying the temperatures of thermal baths only causes a shift in thermal currents. As shown in Figs. 3(a) and 3(b), transient currents in thermal leads L and R under a temperature difference of 20 K have the same oscillating period as those with equal-temperature thermal baths in Figs. 2(a) and 2(b). When t is long enough, $J_L(t) = -J_R(t) = J_{dc}$, indicating a steady flow from the high-temperature thermal lead to the low-temperature thermal lead.

When coupling strengths vary, however, profiles of transient thermal currents change significantly. The variation originates from changing the poles of G^r. In Figs. 3(c)–3(d), we plot the time variation of transient currents ω_0 when $T_L = T_R$. Due to different coupling strengths, $\gamma_L = 2\gamma_R$, transient current at thermal lead L is higher than that at R, suggesting that larger coupling guarantees larger phonon flow. In this figure, it is also shown that when t is long enough, $J_L(t) \approx 2J_R(t)$, due to the fact that $\gamma_L = 2\gamma_R$. During the transient process, energy transfers between the thermal leads and the central region. It is thus interesting to investigate how much energy is transferred. We may define the total transferred energy within the transient time τ as

$$W_{\text{trans}} = W_L + W_R, \tag{40}$$

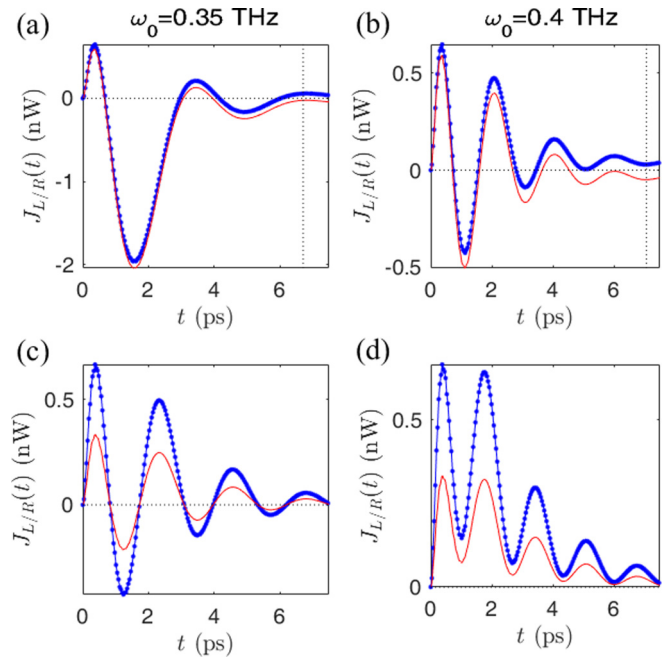

FIG. 3. Transient phonon currents at thermal lead L (thick blue line) and R (thin red line) after switching on the coupling between thermal leads and the central part at $t = 0$ when (a), (b) $T_L = 320$ K, $T_R = 300$ K, $\gamma_L = \gamma_R = 0.1$ THz and (c), (d) $T_L = T_R = 300$ K, $\gamma_L = 2\gamma_R = 0.1$ THz. Other parameters are set as $N = 1$, $\omega_c = 1$ THz, $\eta = 10^{-7}$ THz. ω_0 is 0.35 THz for panels (a) and (c) and 0.4 THz for panels (b) and (d).

with

$$W_\alpha = \int_0^\tau J_\alpha(t)dt, \quad \alpha = L, R, \tag{41}$$

$$\tau = \max(\tau_L, \tau_R). \tag{42}$$

From the definition, W_α is the energy transferred from the lead α to the central region within the transient time τ. One can infer that coupling strength γ_α, oscillation frequency ω_0, and the phonon spectrum of the leads should be pivotal for the energy transfer. For the chosen 1D chain model with Lorentzian-like baths, we may investigate the impact of γ_α and ω_0.

Figure 4(a) shows the total transferred energy as a function of coupling strength $\gamma_{L/R}$ with various oscillating frequency of the central region (ω_0). It is shown that W_{trans} is positive when $\gamma_{L/R}$ is small enough, which means that energies are effectively extracted from the thermal leads to the central region. As the coupling strength increases, W_{trans} decreases quickly and switches its sign at some critical values of $\gamma_{L/R}$, implying that the thermal baths effectively acquire energy from the switching process instead when the coupling strengths are large enough. This abnormal behavior can be attributed to the extra energy added during switch on [31]. It is also shown that for a given coupling strength, increasing the value of ω_0 leads to an increase of W_{trans}, and may even lead to a sign change of W_{trans}. Thus, as long as the coupling strength is small enough, the device acts as a cooling device, where energy is efficiently extracted from the thermal leads to the central region during the transient time.

[2] An extra factor of 2π should be added if ω is in units of THz.

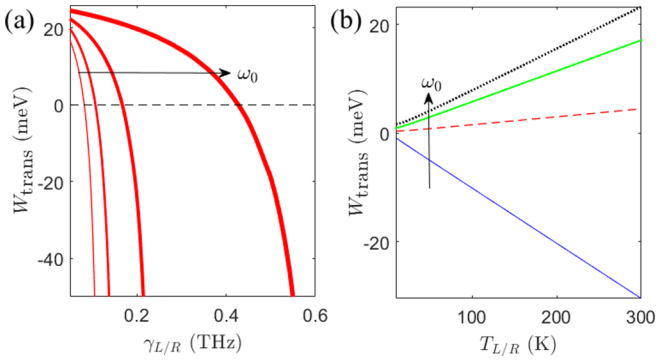

FIG. 4. Transferred energy from the leads to the central dot ($W_{\rm trans} > 0$) or the inverse ($W_{\rm trans} > 0$) during the relaxation time as a function of (a) coupling strength $\gamma_{L/R}$ and (b) temperature with $\omega_0 =$ 0.35, 0.4, 0.5, and 0.8 THz, respectively. Here, $T_L = T_R$ and $\gamma_L = \gamma_R$. Particularly, $T_L = T_R = 300$ K in panel (a) and $\gamma_L = \gamma_R = 0.1$ THz in panel (b).

To examine the influence of temperature, the variation of $W_{\rm trans}$ with temperature $T_{L/R}$ is plotted in Fig. 5(b). For different ω_0, $W_{\rm trans}$ varies linearly with the increase of temperature. In particular, $W_{\rm trans}$ is negative when $\omega_0 =$ 0.35 THz. The reason lies in the fact that the coupling strength $\gamma_{L/R}$ is too big for this case, which is consistent with Fig. 5(a).

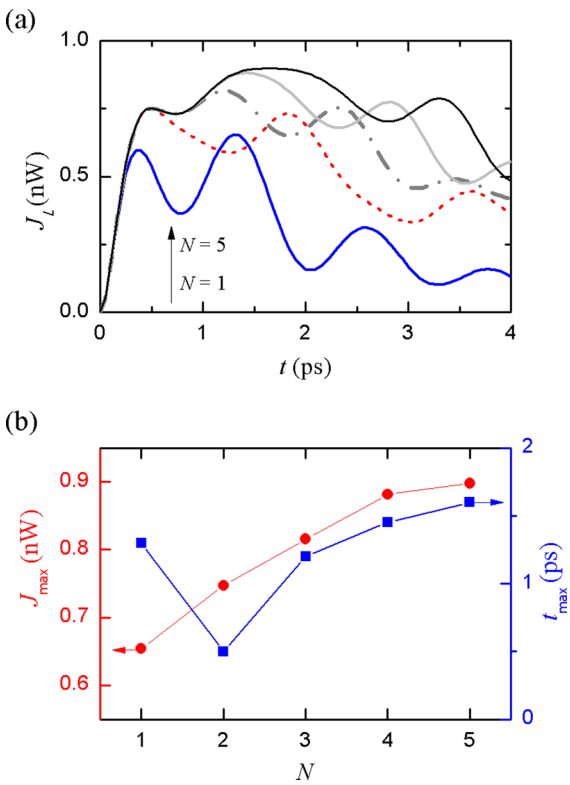

FIG. 5. (a) Transient phonon current at thermal lead L under a thermal switch at $t = 0$ with central atom number $N = 1, \ldots, 5$. (b) The maximum value of $J_L(t)$ after $t = 0$ within 4 ps, $J_{\rm max}$ and the corresponding time $t_{\rm max}$. The other parameters are specified as follows: $\omega_c = 1$ THz, $\omega_0 = 0.5$ THz, $T_L = T_R = 300$ K, $\gamma_L = 2\gamma_R =$ 0.1 THz, $\eta = 10^{-4}$ THz.

We have explored the transient behavior of thermal currents for $N = 1$. Thanks to the analytical results of $A(\omega, t)$ and $B_\alpha(\omega, t)$, the transient behavior and mechanisms are rather clear in this case. However, the number of atoms may also influence the transient behavior. When $N > 1$, analytical results of $\mathbf{A}(\omega, t)$ and $\mathbf{B}_\alpha(\omega, t)$ are not available and numerical calculations can be performed instead.

We calculated the transient phonon current at thermal lead L with elongated central atomic chain and plotted the results in Fig. 5. The patterns of variation of J_L for $1 \leqslant N \leqslant 5$ is similar in the quick increase at the beginning and in the subsequent fluctuations during the transient period. The oscillation of transient thermal current should be also governed by the poles of $\mathbf{G}^r$. Changes in N lead to changes the dimension and also poles of $\mathbf{G}^r$, giving rise to variation of the transient thermal currents. Interestingly, the quick increase of J_L at the beginning is roughly the same for $1 \leqslant N \leqslant 5$. Since the buildup of thermal current is facilitated by the coupling between the thermal leads and the central region, the increase of J_L should be faster for larger coupling strength. The peak value of the transient thermal current is largest at the second peak except for the case of $N = 2$. Nevertheless, the peak value of J_L steadily increases with the number of atoms in the central region. Yet, the increase may saturate eventually with more atoms since a declining trend of the increment can be observed.

Finally, we consider a 1D carbon chain model. Since the force constants between nearest-neighbor carbon atoms is about $k = 60$ eV/Å^2, the eigenfrequency of the central region ω_0 is around 50 THz as estimated from $2\sqrt{k/m_{\rm C}}$, where $m_{\rm C}$ is the atomic mass of carbon atoms. The cutoff frequency of the thermal baths may estimated from the Debye temperature of the carbon systems as $\omega_c \approx 50$ THz. The transient phonon currents under a thermal switch for the 1D carbon chain resembles the one showing in Fig. 2(d) for the case with $\gamma_L = \gamma_R = 0.1\omega_c$, and has a much shorter decaying time of about 0.28 ps. With $\gamma_{L/R}$ properly set, $W_{\rm trans}$ stays positive, which means that energy flows out of both thermal leads. Because of the reasons that the thermal leads are thermal reservoirs and that thermal equilibrium cannot be established instantly, temperatures of both thermal leads are fixed in our model. Thus, thermodynamics cannot be properly treated in our model. For realistic materials, temperature would be lowered essentially as the energy is extracted. Since transient phonon currents can be significantly larger than steady-state phonon currents, the cooling process can be ultrafast.

IV. CONCLUSION

In summary, we have derived a closed-form formula for exploring transient phonon currents under an abrupt thermal switch. For a single atom connected to two Lorentzian baths, the transient current can be obtained through a single integral instead of multiple integrals in previous studies, thereby greatly simplifying the problem and providing a clear picture of the transient phonon currents. Investigation of this simple model shows that similar to electric current, transient phonon current exists even when the two baths have the same temperature. In addition, the transient oscillating behavior and relaxation time are determined by the poles of the retarded

Green's function of the central region: larger ω_0 results in a smaller oscillating period, and the relaxation time can be evaluated by the minimum imaginary part of the poles. For the thermal lead with a higher temperature and stronger coupling to the central region, its transient current is also larger.

Interestingly, when the coupling constant exceeds a critical value, the energy transfer between the thermal leads and the central region changes direction. Thus, under relatively small coupling constant, this device acts as a cooling device, where energy is rapidly subtracted from thermal baths, with the transferred energy during the relaxation time proportional to the average temperature. Our research suggests that generating transient phonon currents is a promising route for cooling nanodevices.

Although self-energies for a phonon system might not be analytic as what we show here, the complex absorbing potential (CAP) method can be further utilized to obtain an analytical expression for the retarded Green's function, locate the positions for poles, and perform integration analytically [27,40].

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APPENDIX: PHONON CURRENTS

For a two-probe L/C/R system, the thermal current flowing across the thermal lead L can be calculated by evaluating the energy change in thermal lead L and expressed as [11]

$$J_L(t) = -\left\langle \frac{d\hat{H}_L}{dt} \right\rangle. \tag{A1}$$

According to Heisenberg equation, the above equation can be further calculated as [34]

$$J_L(t) = \frac{1}{2} \lim_{t' \to t^+} \frac{\partial}{\partial t'} \mathrm{Tr}[i\hbar \mathbf{D}_{LC}(t) \mathbf{G}^<_{CL}(t, t') + \mathrm{H.c.}]. \tag{A2}$$

Here, $\mathbf{D}_{\alpha\beta}(t)$ and $\mathbf{G}^<_{\alpha\beta}(t, t')$ $(\alpha, \beta \in \{L, C, R\})$ are the dynamical matrix and the double-time lesser Green's function between regions α and β.

Further by using the Dyson equation, we have [15]

$$\mathbf{G}_{CL}(\tau, \tau') = \int d\tau_1 \mathbf{G}_{CC}(\tau, \tau_1) \mathbf{D}_{CL}(\tau_1) \mathbf{g}_L(\tau_1, \tau'), \tag{A3}$$

where $\mathbf{g}_\alpha$ is the isolated Green's function for region $\alpha(= L, R)$. Applying continuation rules lead to

$$\mathbf{G}^<_{CL}(t, t') = \int dt_1 \mathbf{G}^r_{CC}(t, t_1) \mathbf{D}_{CL}(t_1) g^<_L(t_1, t') + \int dt_1 \mathbf{G}^<_{CC}(t, t_1) \mathbf{D}_{CL}(t_1) \mathbf{g}^a_L(t_1, t'). \tag{A4}$$

Thus, the thermal current can be expressed in terms of physical quantities of the central region as

$$J_L(t) = \frac{i\hbar}{2} \int dt_1 \lim_{t' \to t^+} \frac{\partial}{\partial t'} \mathrm{Tr}\big[\mathbf{G}^r_{CC}(t, t_1) \mathbf{D}_{CL}(t_1) \times \mathbf{g}^<_L(t_1, t') \mathbf{D}_{LC}(t) + \mathbf{G}^<_{CC}(t, t_1) \mathbf{D}_{CL}(t_1) \times \mathbf{g}^a_L(t_1, t') \mathbf{D}_{LC}(t) + \mathrm{H.c.}\big] \tag{A5}$$

Differentiation of Green's functions with respect to t' is not favorable. During a thermal switch, we may suppose that thermal leads remain intact, which is the fixed-boundary condition [41]. This assumption has been widely adopted for transient phonon currents [31–33]. In this way, $\mathbf{g}_\alpha(t, t')$ is time-translational invariant.

In other words, we neglect the variation in diagonal elements of the surface dynamical matrix during the thermal switch. Then, we can apply Fourier transformation to get $(\gamma = r, a, >, <)$

$$\mathbf{g}^\gamma_L(t_1, t') = \int \frac{d\omega}{2\pi} \mathbf{g}^\gamma_L(\omega) e^{-i\omega(t_1 - t')}. \tag{A6}$$

Correspondingly,

$$\lim_{t' \to t^+} \frac{\partial}{\partial t'} \mathbf{D}_{CL}(t_1) \mathbf{g}^\gamma_L(t_1, t') \mathbf{D}_{LC}(t) = i\boldsymbol{\Sigma}^{\gamma,1}_L(t_1, t), \tag{A7}$$

with

$$\boldsymbol{\Sigma}^{\gamma,1}_L(t_1, t) \equiv \int \frac{d\omega}{2\pi} \omega \mathbf{D}_{CL}(t_1) \mathbf{g}^\gamma_L(\omega) \mathbf{D}_{LC}(t) e^{-i\omega(t_1 - t)}. \tag{A8}$$

Therefore, the general formula for phonon current flowing out of thermal lead L [Eq. (A5)] can be written as

$$\begin{aligned} J_L(t) &= -\frac{\hbar}{2} \int_{-\infty}^{+\infty} dt_1 \mathrm{Tr}\big[\mathbf{G}^r_{CC}(t, t_1) \boldsymbol{\Sigma}^{<,1}_L(t_1, t) + \mathbf{G}^<_{CC}(t, t_1) \boldsymbol{\Sigma}^{a,1}_L(t_1, t) + \mathrm{H.c.}\big] \\ &= -\hbar \int_{-\infty}^{+\infty} \mathrm{d}t_1 \mathrm{ReTr}\big[\mathbf{G}^r_{CC}(t, t_1) \boldsymbol{\Sigma}^{<,1}_L(t_1, t) + \mathbf{G}^<_{CC}(t, t_1) \boldsymbol{\Sigma}^{a,1}_L(t_1, t)\big]. \end{aligned} \tag{A9}$$

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