Heat conduction in quantum harmonic chains with alternate masses and self-consistent thermal reservoirs

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We consider the analytical investigation of the heat current in the steady state of the quantum harmonic chain of oscillators with alternate masses and self-consistent reservoirs. We analyze the thermal conductivity κ and obtain interesting properties: in the high temperature regime, where quantum and classical descriptions coincide, κ does not change with temperature, but it is quite sensitive to the difference between the alternate masses; and contrasting with this behavior, in the low temperature regime, κ becomes an explicit function of the temperature, but its dependence on the masses difference disappears. Our results reinforce the message that quantum effects cannot be neglected in the study of heat conduction in low temperatures.

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I. INTRODUCTION

Despite its fundamental importance for nonequilibrium statistical physics, the complete understanding of the heat conduction from first principles is still an open problem. For example, the derivation of the phenomenological Fourier's law is still unknown, which states that the heat flow is proportional to the local temperature gradient, $\mathbf{J}(x)=-\kappa(T(x))\nabla T(x)$; κ is the thermal conductivity. After years of study (see e.g., [1,2] for reviews), the precise conditions in microscopic models of interacting particles that lead to the macroscopic Fourier's law are still ignored. The detailed investigation of the mechanisms behind the heat conduction (including other questions besides the derivation of the Fourier's law) involves considerable technical difficulties and even contradictions in numerical simulations, a scenario that makes the analysis of simple treatable analytical models a problem of interest (more comments are presented, e.g., in [3,4]).

Recently, the model of the harmonic chain of oscillators with self-consistent stochastic thermal reservoirs at each site has been revisited and rigorously analyzed [5] (this model was previously proposed in [6,7]). The authors prove that the Fourier's law holds in such a model. They still prove that there is a local thermal equilibrium and the heat conductivity κ is a constant (it does not depend on the temperature). In this simple model, the reservoirs at each site describe the anharmonic degrees of freedom present in a more realistic (and much more intricate) interaction. The "self-consistent" condition means that there is no heat flow between an inner reservoir and its site, i.e., the inner reservoirs do not inject energy into the system. The quantum version of this model (proposed in [8]) has been revisited quite recently in [9]. The study of the quantum version is important to understand the behavior of the thermal conductivity in the low temperature regions, where a quantum description may introduce significant changes. In particular, it is shown (for this quantum model [8]) that the thermal conductivity becomes dependent on the temperature.

In the present paper, also with the aim of understanding the properties of the thermal conductivity of simple Hamiltonian models, we consider the quantum chain of harmonic oscillators with reservoirs at each site and study, in detail, the heat flow for the case of particles (oscillators) with different masses (precisely, we take a chain with alternate masses—details ahead). The physical interest of models with unequal masses is well known. We recall, first, a few examples of analytical studies. The one-dimensional (1D) harmonic chain with baths at the boundaries has been rigorously studied a long time ago: first the version with equal masses [10], where it is proved that the heat current J is independent of the system size N (the Fourier's law holds if $J\sim N^{-1}$). In sequel, versions with different masses have been treated in [11,12]. In particular, for a random mass distribution, it is proved that $J\sim N^{-1/2}$ [13]. For the harmonic Fibonacci chain, a model with the sequence of the particle masses given by $\{m_i|i=1,\ldots,N;m_i=m_\alpha \text{ or } m_\beta\}$ according to the Fibonacci sequence, it is shown that $J\sim(\ln N)^{-1}$ [14]. Unfortunately, these models do not obey Fourier's law and the investigation, in such case, is mainly related to the dependence of the heat flow on the system size. Recently, we have analyzed a system with unequal masses and normal conductivity [15]: the harmonic chain with stochastic self-consistent reservoirs and unequal masses. We show that the thermal conductivity does not depend on temperature, but it is quite sensitive to the difference between the masses of the particles. Turning to the models treated by numerical simulations, there are many other problems where the presence of particle with unequal or alternate masses lead to interesting physical results: e.g., a nontrivial steady state is obtained for the two-mass problem in [16]; the relevance of the total momentum conservation for the validity of Fourier's law is investigated in a model with alternate masses in [17]; a strange behavior for Fermi-

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Pasta-Ulam chains with alternate masses in the steady state is numerically shown in [18].

Now, in the present work, we turn to the quantum version of this harmonic chain with self-consistent reservoirs and alternate masses. Using the techniques presented in [9,19], we derive a formula for the thermal conductivity which presents interesting new properties and shows that the quantum effects are quite significant. Besides the explicit dependence on temperature (that does not happen in the classical version, but appears in the quantum model with equal masses), we show that, for very small temperatures, the difference between the masses, which is significant for the conductivity behavior in high temperature, is wiped out. In short, our results emphasize the significance of quantum effects in the low temperature region, which indicates that, in some recent approaches proposed to understand the heat mechanism and involving classical models and the region of $T\to 0$ (see, e.g., [20]), the inclusion of quantum effects may give important corrections.

The rest of the paper is organized as follows. In Sec. II we introduce the model and the expressions for the heat currents. In Sec. III we analyze the steady heat current in the self-consistent condition and derive the expression for the thermal conductivity, which is studied in the low and high temperature regimes in Sec. IV. Section V is devoted to the final comments, and the Appendix to a technical point, namely, the inversion of a tridiagonal matrix.

II. PRELIMINARIES: THE MODEL AND FORMALISM FOR THE STEADY HEAT CURRENT

Now we introduce the model and, briefly, schematize the derivation of the formula for the steady heat current as presented in [9]; there, the authors obtain a formalism to analyze quantum harmonic lattices following a Ford-Kac-Mazur program [21]. In a few words, the approach considers harmonic lattices connected to baths modeled also as mechanical harmonic systems with initial coordinates and momenta distributed according to some statistical distribution. The quantum dynamical equations are solved and the steady properties are obtained by taking stochastic distributions for the initial coordinates of the reservoirs and the limit $t\to\infty$. For clearness, we will use, essentially, the same notation of [9].

We consider a harmonic system which consists of a chain (W) with each site coupled to a bath (B) described also by harmonic interactions. The Hamiltonian of the chain and baths is given by

$$\mathcal{H} = \tfrac{1}{2}\dot{X}^T M \dot{X} + \tfrac{1}{2}X^T \Phi X$$

$$= \mathcal{H}_W + \sum_{i=1}^{N} \mathcal{H}_{B_i} + \sum_{i=1}^{N} \mathcal{V}_{B_i},$$

$$\mathcal{H}_W = \tfrac{1}{2}\dot{X}_W^T M_W \dot{X}_W + \tfrac{1}{2}X_W^T \Phi_W X_W,$$

$$\mathcal{H}_{B_i} = \tfrac{1}{2}\dot{X}_{B_i}^T M_{B_i} \dot{X}_{B_i} + \tfrac{1}{2}X_{B_i}^T \Phi_{B_i} X_{B_i},$$

$$\mathcal{V}_{B_i} = X_W^T V_{B_i} X_{B_i}, \qquad (1)$$

M, M_W, M_{B_i} are diagonal matrices representing masses of the particles in the entire system, chain, and baths, respectively; N is the number of sites in the chain. The symmetric matrices Φ, Φ_W, Φ_{B_i} give the potential quadratic energies, and $\mathcal{V}_{B_i}$ gives the interaction between the ith site of the chain and its bath. $X=[X_1,X_2,\ldots,X_{N_s}]^T$, where X_i is the position operator of the ith particle, N_s is the number of elements in the entire system. We still have $\dot{X}=M^{-1}P$, where P_r is the momentum operator of the rth particle satisfying the commutation relations $[X_r,P_l]=i\hbar\delta_{rl}$. In fact, we will be more specific: we will consider a one-dimensional harmonic chain with

$$\mathcal{H}_W = \sum_{l=1}^{N}\left(\frac{m_l}{2}\dot{X}_l^2 + \frac{m_0}{2}\omega_0^2 X_l^2\right) + \sum_{l=1}^{N+1}\frac{m_0}{2}\omega_c^2 (X_l - X_{l-1})^2, \quad (2)$$

where $m_0\omega_0^2$ is the on-site potential strength constant; $m_0\omega_c^2$ is the interparticle potential strength; m_0 is a constant with unit of mass. We still consider $m_l=m_1$ if l is odd, $m_l=m_2$ if l is even; and we take Dirichlet boundary conditions, i.e., $X_0=X_{N+1}=0$.

The Heisenberg equations (giving the dynamic) for system and baths are

$$M_W \ddot{X}_W = -\Phi_W X_W - \sum_i V_{B_i} X_{B_i},$$

$$M_{B_i}\ddot{X}_{B_i} = -\Phi_{B_i} X_{B_i} - V_{B_i}^T X_W. \qquad (3)$$

The procedure is to treat the equations of the baths as linear inhomogeneous equations. Then, the solutions are plugged back into the equation for the chain, and the initial conditions of the baths are assumed to be distributed according to equilibrium phonon distribution functions (with temperatures properly chosen—details ahead). All the reservoirs are taken to be Ohmic, and the coupling to the reservoirs is given by a dissipation constant γ.

The stationary properties are obtained turning to the equations of motion, taking $t\to\infty$ and $t_0\to-\infty$, and manipulating them by using Fourier transforms. As said, details are presented in [9] and references therein. For the heat current from the lth reservoir into the chain we obtain

$$J_l = \sum_{m=1}^{N}\gamma^2\int_{-\infty}^{\infty} d\omega\,\omega^2 |[G_W^+(\omega)]_{l,m}|^2 \frac{\hbar\omega}{\pi}[f(\omega,T_l) - f(\omega,T_m)], \qquad (4)$$

where

$$G_W^+(\omega) = \left(-\omega^2 M_W + \Phi_W - \sum_l \Sigma_l^+(\omega)\right)^{-1},$$

$$M_W = \begin{pmatrix} m_1 & & & \\ & m_2 & & \\ & & \ddots & \\ & & & m_N \end{pmatrix},$$

$$\Phi_W = m_0\omega_c^2 \begin{pmatrix} 2+\nu^2 & -1 & & \\ -1 & 2+\nu^2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2+\nu^2 \end{pmatrix}, \qquad (5)$$

with $\nu^2 = \omega_0^2/\omega_c^2$. The self-energy matrix has only one nonvanishing element, $(\Sigma_l^+)_{ll} = i\gamma\omega$. The variable ω appears with the Fourier transform

$$\tilde{X}_W(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt X_W(t) e^{i\omega t},$$

etc. And $f(\omega, T_l)$ is the phonon distribution function

$$f(\omega,T_l) = \frac{1}{\exp(\hbar\omega/k_B T_l) - 1}. \qquad (6)$$

To proceed we consider the linear response regime with the temperature difference $\Delta T = |T_1 - T_N| \ll T = (T_1 + T_N)/2$. In this situation, we may simplify the expression for J_l above by expanding the phonon distribution functions (6) about the mean temperature T to get

$$J_l = \gamma^2 \int_{-\infty}^{\infty} d\omega \frac{\hbar\omega^3}{\pi} \partial f(\omega,T)\partial T \sum_{m=1}^{N} |[G_W^+(\omega)]_{l,m}|^2 (T_l - T_m). \qquad (7)$$

For the heat current inside the chain, from the site l to $l+1$, in the linear response limit, we have

$$J_{l,l+1} = -\frac{m_0\omega_c^2\gamma}{\pi}\int_{-\infty}^{\infty} d\omega\omega\left(\frac{\hbar\omega}{2k_BT}\right)^2 \mathrm{cosech}^2\left(\frac{\hbar\omega}{2k_BT}\right) \times \sum_{m=1}^{N} k_B T_m \,\mathrm{Im}\{[G_W^+(\omega)]_{l,m}[G_W^+(\omega)]^*_{l+1,m}\}, \qquad (8)$$

where * denotes the complex conjugate.

III. ANALYSIS OF THE STEADY HEAT CURRENT

To perform a detailed investigation of the steady heat currents of our specific model, according to the preceding section, we need to know the matrix G_W^+ (5) and the temperature profile, which is determined by the self-consistent condition $J_l = 0$ for all inner sites, i.e. there is no heat flow between an inner site and the reservoir connected to it.

To determine $[G_W^+(\omega)]_{l,m}$, we write [see Eq. (5)]

$$G_W^+(\omega) = \frac{Z^{-1}}{m_0\omega_c^2}, \qquad (9)$$

where Z is a tridiagonal (Jacobi) matrix

$$Z = \begin{pmatrix} z_1 & -1 & & & & \\ -1 & z_2 & -1 & & & \\ & -1 & z_3 & -1 & & \\ & & -1 & \ddots & \ddots & \\ & & & \ddots & z_{N-1} & -1 \\ & & & & -1 & z_N \end{pmatrix}, \qquad (10)$$

with

$$z_j(\omega) = \left(2 + \nu^2 - \frac{m_j}{m_0}\frac{\omega^2}{\omega_c^2}\right) - \frac{i\gamma\omega}{m_0\omega_c^2}, \qquad (11)$$

with $m_j = m_1$ for j odd, and $m_j = m_2$ for j even. There is a general procedure to calculate the inverse of a tridiagonal matrix [22]—we present the details for our specific case (10) in the Appendix. We have

$$(Z^{-1})_{lm} = c_{lm}(\mathcal{Z}^{-1})_{lm},$$

$$c_{lm} = \begin{cases} \sqrt{\dfrac{z_2}{z_1}} & \text{if } l \text{ and } m \text{ are odd,} \\ \sqrt{\dfrac{z_1}{z_2}} & \text{if } l \text{ and } m \text{ are even,} \\ 1 & \text{otherwise,} \end{cases} \qquad (12)$$

where $\mathcal{Z}$ is the tridiagonal matrix

$$\mathcal{Z} = \begin{pmatrix} z & -1 & & \\ -1 & z & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & z \end{pmatrix}, \quad z(\omega) = \sqrt{z_1(\omega)z_2(\omega)}, \qquad (13)$$

with inverse

$$(\mathcal{Z}^{-1})_{lm} = \begin{cases} \dfrac{\sinh[(N-m+1)\alpha]\sinh(l\alpha)}{\sinh(\alpha)\sinh[(N+1)\alpha]} & \text{if } m \geq l, \\ \dfrac{\sinh[(N-l+1)\alpha]\sinh(m\alpha)}{\sinh(\alpha)\sinh[(N+1)\alpha]} & \text{if } m < l, \end{cases} \qquad (14)$$

where α is given by

$$e^{\alpha} = \frac{z}{2} \pm \sqrt{\left(\frac{z}{2}\right)^2 - 1}, \quad e^{-\alpha} = \frac{z}{2} \mp \sqrt{\left(\frac{z}{2}\right)^2 - 1}, \qquad (15)$$

i.e., $z = 2\cosh\alpha$. Any of the two roots can be taken in (15). As said, the detailed computation of Z^{-1} is presented in the Appendix.

For points in the bulk of the chain, i.e., far from the boundaries ($N \to \infty$), we have with a simple algebra

$$(G_W^+)_{lm} = \frac{(Z^{-1})_{lm}}{m_0\omega_c^2} \approx \frac{c_{lm}e^{-\alpha|l-m|}}{2m_0\omega_c^2\sinh(\alpha)}, \qquad (16)$$

and we may choose α (15) such that $\mathrm{Re}(\alpha) > 0$. In what follows, we will ignore the points close to the boundaries.

To carry out the analysis of the heat currents, we still need to know the temperature profile: it must be taken such that $J_l=0$ for the inner points l, i.e., to assure the self-consistent condition. For the classical harmonic chain it is rigourously proved [5] that there is a unique profile (the linear one) that leads to the self-consistent condition. As the quantum and classical models coincide at high temperatures, this linear profile is assumed for the quantum version with equal masses in [9]: it is shown that the linear profile leads to $J_l=0$ for the inner points (and it is also reobtained there by numerical simulations). Here we follow the same strategy (a direct derivation of the temperature profile for the quantum models is very intricate): if we turn to the classical model with unequal masses as treated in [15] (i.e., using the techniques developed by us—some of the authors and collaborators [23,24]), we may easily find that the temperature profile for this classical version is the linear one—see the general derivation given by Eqs. (22)–(25) presented in [23], and compare with Eqs. (16)–(18) in [15]. We remark that, in a finite system, close to the boundaries, where the real thermal reservoirs are linked, the temperature profile shall deviate from the linear form (see [9] for more discussions). We also recall that this model involving the self-consistent condition does not allow the inner baths to inject energy into the system, and so, the inner reservoirs shall be understood as a mechanism of phonon scattering (i.e., in some sense they act as the anharmonic degrees of freedom not present in the potential) and not as real thermal reservoirs. It is also worth to recall that all of the situations, and the heat flow in the system, shall change if we leave the self-consistent condition and let the inner reservoirs inject energy into the system—see [25], for example, of systems with strange heat flows. In a recent work [26], a quantum chain system with baths at the boundaries is analyzed and significant boundary effects are presented (see also [27] for other interesting results in quantum chains). But there, the system has a small length and differs very much from our problem: we are in the bulk of the system, far from the boundaries (the length of our chain goes to infinite).

Now, we take the linear temperature profile and show, for our quantum version, that it leads to the self-consistent condition $J_l=0$, for l in the bulk of the chain. Indeed, for l far from the boundaries (and $N\to\infty$), from (7) we essentially have

$$J_l \propto \sum_{m=-\infty}^{\infty}(l-m)|[G_W^{+}(\omega)]_{lm}|^2 = \sum_{m=-\infty}^{\infty}|c_{lm}|^2\frac{|e^{-\alpha|l-m|}|^2}{4m_0^2\omega_c^4\sinh^2\alpha}(l-m).$$

We write $m=l\pm k$, with $k=1,2,\ldots$ (for $k=0$, we have $l-m=0$). Then, in the sum we get

$$\begin{aligned}\mathcal{S}_1 &= \sum_{m=-\infty}^{\infty}|c_{lm}|^2|e^{-\alpha|l-m|}|^2(l-m)\\ &= \sum_{k=1}^{\infty}\{|c_{l,l-k}|^2e^{-2\alpha|l-(l-k)|}[l-(l-k)] + |c_{l,l+k}|^2e^{-2\alpha|l-(l+k)|}[l-(l+k)]\}\\ &= \sum_{k=1}^{\infty}k(|c_{l,l-k}|^2-|c_{l,l+k}|^2)e^{-2\alpha k}=0,\end{aligned}$$

since $c_{l,l-k}=c_{l,l+k}$: see (12) and note that $c_{l,r}=c_{l,r\pm 2}=c_{l,r\pm 2m}$, $\forall l,r,m\in\mathbb{Z}$.

Now we turn to the heat current inside the chain $J_{l,l+1}$. From (8) and (16) we have

$$J_{l,l+1}=\frac{-\gamma}{8m_0\omega_c^2\pi i}\int_{-\infty}^{\infty}d\omega\frac{\omega}{|\sinh\alpha|^2}\left(\frac{\hbar\omega}{2k_BT}\right)^2\operatorname{cosech}^2\left(\frac{\hbar\omega}{2k_BT}\right)\times\sum_m k_BT_m[c_{l,m}c_{l+1,m}^{*}e^{-\alpha|l-m|}e^{-\alpha^{*}|l+1-m|}-\text{c.c.}], \quad (17)$$

where "c.c." means the complex conjugate. We still introduce the linear temperature profile

$$T_m=T_L+\frac{m-1}{N-1}(T_R-T_L)\Rightarrow T_m=T_l+\frac{m-l}{N-1}(T_R-T_L).$$

We write T_R and T_L for the temperatures at the boundaries, instead of T_N and T_1, respectively. With the expression for T_m, we get in the sum (17) terms such as

$$\sum_{m=-\infty}^{\infty}F(l,m)\quad\text{and}\quad\sum_{m=-\infty}^{\infty}(m-l)F(l,m),$$

with $F(l,m)=f(l,m)-f^{*}(l,m)$, where $f(l,m)=c_{l,m}c_{l+1,m}^{*}e^{-\alpha|l-m|}e^{-\alpha^{*}|l+1-m|}$. Again, we consider l far from boundaries and $N\to\infty$. To exploit the symmetry in the exponential, we write

$$\mathcal{S}_2\equiv\sum_{m=-\infty}^{\infty}F(l,m)=\sum_{k=0}^{\infty}[F(l,l-k)+F(l,l+1+k)].$$

To carry out the summation above, we note that we have for k even $c_{l,l-k}=c_{l,l}$, $c_{l+1,l+1+k}=c_{l+1,l+1}$ and $c_{l,l+1+k}=1=c_{l+1,l-k}$. On the other hand, for k odd we have $c_{l,l+1+k}=c_{l,l}$, $c_{l+1,l-k}=c_{l+1,l+1}$, and $c_{l,l-k}=1=c_{l+1,l+1+k}$.

It is convenient to split the sum into the terms with k even and with k odd. We have

$$\mathcal{S}_2=\mathcal{S}_2^{\text{odd}}+\mathcal{S}_2^{\text{even}} = [(c_{l,l}-c_{l+1,l+1})(e^{\alpha}+e^{-\alpha})-\text{c.c.}]\frac{e^{\alpha+\alpha^{*}}}{e^{2(\alpha+\alpha^{*})}-1}.$$

But, if we assume l odd (similar manipulation follows for l even)

$$(c_{l,l}-c_{l+1,l+1})(e^{\alpha}+e^{-\alpha})=(c_{1,1}-c_{2,2})z = \left(\sqrt{\frac{z_2}{z_1}}-\sqrt{\frac{z_1}{z_2}}\right)\sqrt{z_1z_2}=z_2-z_1.$$

And, as we can see from (11), z_2-z_1 is real,

$$z_2-z_1=\frac{m_1-m_2}{m_0}\frac{\omega^2}{\omega_c^2}.$$

That is,

$$\operatorname{Im}[(c_{l,l}-c_{l+1,l+1})(e^{\alpha}+e^{-\alpha})]=0\Rightarrow\mathcal{S}_2=0. \quad (18)$$

Let us analyze $\mathcal{S}_3=\Sigma_{m=-\infty}^{\infty}(m-l)F(l,m)$. As before, we write $m=l-k$ and $m=l+1+k$, with $k\in\{0,1,2,\dots\}$, and split the expression into terms with k even and k odd,

$$\mathcal{S}_3=\sum_{k=0}^{\infty}[(-k)F(l,l-k)+(k+1)F(l,l+1+k)]$$
$$=\sum_{k=0}^{\infty}F(l,l+1+k)+\sum_{k=0}^{\infty}k[F(l,l+1+k)-F(l,l-k)].$$

After a considerable algebrism, we obtain

$$\mathcal{S}_3=-2[(c_{l,l}+c_{l+1,l+1})(e^{\alpha}-e^{-\alpha})-\text{c.c.}]\frac{e^{\alpha+\alpha^*}}{(e^{2(\alpha+\alpha^*)}-1)^2}+[2c_{l,l}e^{-\alpha}-c_{l+1,l+1}(e^{\alpha}-e^{-\alpha})-\text{c.c.}]\frac{e^{\alpha+\alpha^*}}{e^{2(\alpha+\alpha^*)}-1}.$$

To make explicit the symmetry $l\leftrightarrow l+1$, we write for the second term above

$$[2c_{l,l}e^{-\alpha}-c_{l+1,l+1}(e^{\alpha}-e^{-\alpha})-\text{c.c.}]=[(c_{l,l}+c_{l+1,l+1})e^{-\alpha}+c_{l,l}e^{-\alpha}-c_{l+1,l+1}e^{\alpha}]-\text{c.c.}\quad (19)$$

Using that $(c_{l,l}-c_{l+1,l+1})(e^{\alpha}+e^{-\alpha})-\text{c.c.}=0$, from (18), we note that

$$(c_{l,l}e^{\alpha}+c_{l,l}e^{-\alpha}-c_{l+1,l+1}e^{\alpha}-c_{l+1,l+1}e^{-\alpha})-\text{c.c.}=0$$
$$\Rightarrow(c_{l,l}e^{-\alpha}-c_{l+1,l+1}e^{\alpha}-\text{c.c.})=(c_{l+1,l+1}e^{-\alpha}-c_{l,l}e^{\alpha}-\text{c.c.})$$
$$\Rightarrow(c_{l,l}e^{-\alpha}-c_{l+1,l+1}e^{\alpha}-\text{c.c.})$$
$$=\tfrac{1}{2}(c_{l,l}e^{-\alpha}-c_{l+1,l+1}e^{\alpha}+c_{l+1,l+1}e^{-\alpha}-c_{l,l}e^{\alpha}-\text{c.c.}).$$

We rewrite $\mathcal{S}_3$ as

$$\mathcal{S}_3=(c_{l,l}+c_{l+1,l+1})\left\{\frac{-\sinh(\alpha)e^{-(\alpha+\alpha^*)}}{\sinh^2(\alpha+\alpha^*)}+\frac{[e^{-\alpha}-\sinh\alpha]}{2\sinh(\alpha+\alpha^*)}\right\}-\text{c.c.}\quad (20)$$

We remark that, in the particular case of masses $m_1=m_2$, we have $c_{l,l}=c_{l+1,l+1}=1$, and so, after some algebraic manipulations we have

$$\mathcal{S}_3(m_1=m_2)=\frac{\sinh\alpha^*-\sinh\alpha}{4\sinh^2\alpha_R},\quad (21)$$

where $\alpha_R=\text{Re}(\alpha)=(\alpha+\alpha^*)/2$. It leads to the same expression of [9] [see Eq. (5.8) there in], where the case of equal masses was treated.

Finally, turning to the expression (17) for $J_{l,l+1}$, now we have

$$J_{l,l+1}=\left[-\frac{\gamma k_B}{8m_0\omega_c^2\pi i}\int_{-\infty}^{\infty}d\omega\frac{\omega}{|\sinh\alpha|^2}\left(\frac{\hbar\omega}{2k_BT}\right)^2\times\text{cosech}^2\left(\frac{\hbar\omega}{2k_BT}\right)\mathcal{S}_3(\omega)\right]\frac{T_R-T_L}{N-1},\quad (22)$$

with $\mathcal{S}_3(\omega)$ given by (20). In short, the Fourier's law holds with κ given by the expression that multiplies $(T_R-T_L)/(N-1)$ in (22).

In the next section we study the behavior of κ as we change the temperature.

IV. THE EFFECTS OF TEMPERATURE ON THE THERMAL CONDUCTIVITY

We are mainly interested in the region of small temperatures, where the difference between the quantum and the classical description of the model may be significant.

As we have described in the preceding section, the difference in κ for the quantum systems with equal and unequal masses comes essentially from the factor $(c_{l,l}+c_{l+1,l+1})$ that appears in the expression of $\mathcal{S}_3(\omega)$, see (20) and (21). For small temperatures, the main contribution to κ comes from small ω—see Eq. (22) (we give details below). Hence, let us investigate the factor $(c_{l,l}+c_{l+1,l+1})$ for small ω. Recall that

$$c_{l,l}+c_{l+1,l+1}=\sqrt{\frac{z_1}{z_2}}+\sqrt{\frac{z_2}{z_1}}=\frac{z_1+z_2}{z},\quad (23)$$

where z_j is given by (11). Thus, simple manipulations give us

$$z\equiv\sqrt{z_1z_2}=2+\nu^2-\frac{1}{2}\frac{m_1+m_2}{m_0}\frac{\omega^2}{\omega_c^2}-\frac{i\gamma\omega}{m_0\omega_c^2}+O(\omega^3),$$

i.e., up to $O(\omega^2)$, the expression of z becomes that of z_j with $m_j=(m_1+m_2)/2$, i.e., $z=(z_1+z_2)/2$. Hence,

$$c_{l,l}+c_{l+1,l+1}=\frac{z_1+z_2}{z}=2,$$

that is, our κ becomes the same of a system with equal masses, where the particle mass is $(m_1+m_2)/2$. In [9], numerical computations for small T in the quantum chain with equal masses are carried out, and graphics $\kappa\times T$ are plotted (see Figs. 1 and 2 in [9]). We present a brief analytical study which coincides with their results as $T\to 0$. From Eqs. (22) and (20) we get

$$\kappa=\frac{\gamma k_B}{16m_0\omega_c^2\pi i}\int_{-\infty}^{\infty}d\omega\left(\frac{\hbar\omega}{2k_BT}\right)^2\text{cosech}^2\left(\frac{\hbar\omega}{2k_BT}\right)\times\frac{4m_0\omega_c^2 i}{\gamma}\frac{\sin^2\alpha_I\cosh\alpha_R}{\sinh\alpha_R[\cosh^2\alpha_R-\cos^2\alpha_I]},$$

where $\alpha_I=\text{Im}(\alpha)=(\alpha-\alpha^*)/(2i)$. As $T\to 0$, $\text{cosech}^2(\hbar\omega/2k_BT)\approx 4e^{-\hbar|\omega|/k_BT}$, and so

$$\kappa=C_1\int_0^{\infty}d\omega\left(\frac{\hbar\omega}{2k_BT}\right)^2e^{-\hbar\omega/k_BT}\times\frac{\sin^2\alpha_I\cosh\alpha_R}{\sinh\alpha_R(\cosh^2\alpha_R-\cos^2\alpha_I)}$$
$$=C_1\hbar^2\beta^2\int_0^{\infty}d\omega e^{-\hbar\omega\beta}\omega^2f(\omega),\quad (24)$$

where C_1 is a constant depending on m_0, ω_c^2, γ, etc., but not on T; and $\beta=(k_BT)^{-1}$. In what follows, we will use the notation C even for different constants. Now we study the asymptotic behavior of the equation above as $\beta\to\infty$. We follow the procedure given by the Laplace method [28]. It establishes that for a function such as

$$F(\tau) = \int_0^\infty g(t)e^{-\tau h(t)}dt,$$

with $h(t) > h(0)$, $h'(0)=0$, and $h''(0)>0$ (i.e., h with a minimum in $t=0$), the asymptotic behavior of $F(\tau)$ for $\tau\to\infty$ is determined by the minimum of h. In a general case, with $h(t)=h(0)+\frac{1}{2}t^2h''(0)+\cdots$, $g(t)=g(0)+tg'(0)+\cdots$, and simple manipulations, we have

$$F(\tau) \sim g(0)\left(\frac{\pi}{2\tau h''(0)}\right)^{1/2} e^{-\tau h(0)} + e^{-\tau h(0)}O\left(\frac{1}{\tau}\right).$$

If $g(0)=0$, to determine the asymptotic behavior of $F(\tau)$, we take the next term in the expression above, etc. From (24), if we write $\omega=u^2$, we obtain

$$\kappa = C\beta^2\int_0^\infty du e^{-\hbar u^2\beta}u^5 f(u^2). \qquad (25)$$

To examine $f(u^2)$, we need to split the analysis into the cases $\nu\neq 0$ and $\nu=0$. From (11) and $z=2\cosh\alpha$, we have [recalling that our analysis is around $u^2=\omega\approx 0$, the minimum of h in the exponential term in (25)]

$$2\cosh\alpha_R\cos\alpha_I \approx 2+\nu^2 - \frac{\bar{m}}{m_0}\frac{\omega^2}{\omega_c^2} \approx 2+\nu^2,$$

$$2\sinh\alpha_R\sin\alpha_I \approx -\frac{\gamma}{m_0\omega_c^2}\omega,$$

where $\bar{m}=(m_1+m_2)/2$. Therefore, $f(\omega)\approx C\sin^2\alpha_I\approx C\omega^2 = Cu^4$, where C is some constant. Hence,

$$\kappa \approx C\beta^2\int_0^\infty du e^{-u^2\hbar\beta}u^9 = C/\beta^3.$$

That is, for $\nu\neq 0$, we have $\kappa\sim CT^3$.

For $\nu=0$, again from (11) and $z=2\cosh\alpha$, we have

$$2\cosh\alpha_R\cos\alpha_I \approx 2 - \frac{\bar{m}}{m_0}\frac{\omega^2}{\omega_c^2} \approx 2,$$

$$2\sinh\alpha_R\sin\alpha_I \approx -\frac{\gamma}{m_0\omega_c^2}\omega, \Rightarrow \sinh\alpha_R \approx \sin\alpha_I \approx \omega^{1/2}.$$

Recalling the expression for $f(\omega)$,

$$f(\omega) = \frac{\sin^2\alpha_I\cosh\alpha_R}{\sinh\alpha_R[\cosh^2\alpha_R - \cos^2\alpha_I]} \approx \frac{\cosh\alpha_R}{\sinh\alpha_R} \approx \omega^{-1/2}.$$

Therefore,

$$\kappa \approx C\beta^2\int_0^\infty du e^{-u^2\hbar\beta}u^5 f(u^2)$$
$$\approx C\beta^2\int_0^\infty du e^{-u^2\hbar\beta}u^4 = C\beta^2\left(\frac{1}{\beta}\right)^{5/2}.$$

That is, $\kappa\sim CT^{1/2}$, if $\nu=0$. Note that the C in κ involves γ, m_0, $(m_1+m_2)/2$, but not $|m_1-m_2|$, which appears in the expression of κ for the classical version [15]. As the quantum and classical versions shall coincide in the high temperature regime, our previous computations show that considerable changes appear with the temperature in the quantum model. We give more comments ahead.

Let us investigate the high temperature region. From (22), we note that the contribution of large ω for κ goes to zero exponentially fast as ω increases. For bounded ω, we have

$$\lim_{T\to\infty}\left(\frac{\hbar\omega}{2k_BT}\right)^2 \operatorname{cosech}^2\left(\frac{\hbar\omega}{2k_BT}\right) \to 1,$$

and so, as T increases, κ becomes a constant function on T.

In a previous work on the classical harmonic chain with self-consistent stochastic reservoirs and alternate masses [15], using the approach developed in [23,24] and a perturbative analysis, we show that, for weak coupling between the neighbor sites, i.e., for ω_c^2 small, and an interaction with nonzero on-site potential, we have

$$\kappa = (2m_0\omega_c^2)^2\gamma m_1^{-1}m_2^{-1}\Bigg[[\omega_c^2(2+\nu^2)]^2\left(\frac{1}{m_1}-\frac{1}{m_2}\right)^2 + 2\gamma^2\omega_c^2(2+\nu^2)\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\Bigg]^{-1}. \qquad (26)$$

It is interesting to note that, for a huge difference between the masses m_1 and m_2, the behavior of κ is determined by the inverse of the square of the difference of masses. But if $m_1 = m_2$, this behavior becomes related to the inverse of the mass, and not to the inverse of the square of the mass. In other words, κ is more sensitive to changes in the particle masses for the system with alternate masses. As already mentioned, it is also interesting to note that such a behavior is wiped out for the quantum system in a small temperature region, where κ depends on m_1+m_2 only. In short, large T, $\kappa\sim 1/[\text{const}+(m_1-m_2)^2]$; small T, κ does not depend on (m_1-m_2).

A detailed expression for κ in the high temperature region for the quantum chain with alternate masses requires a huge algebrism and we will not present it here. But it is easy to see that κ depends on $(m_1-m_2)^2$: we turn to the factor $c_{l,l} + c_{l+1,l+1} = (z_1+z_2)(z_1z_2)^{-1/2}$ and write

$$z_1+z_2 = 2\bar{z}, \quad \bar{z} \equiv \left(2+\nu^2 - \frac{m_1+m_2}{2m_0}\frac{\omega^2}{\omega_c^2} - i\frac{\gamma\omega}{m_0\omega_c^2}\right),$$

$$\sqrt{z_1z_2} = \left[\left(\bar{z}+\frac{m_2-m_1}{2m_0}\frac{\omega^2}{\omega_c^2}\right)\left(\bar{z}-\frac{m_2-m_1}{2m_0}\frac{\omega^2}{\omega_c^2}\right)\right]^{1/2} = \left\{\left[\bar{z}^2 - \left(\frac{m_2-m_1}{2m_0}\frac{\omega^2}{\omega_c^2}\right)^2\right]\right\}^{1/2},$$

$$\frac{z_1+z_2}{\sqrt{z_1z_2}} = 2\left[1-\left(\frac{m_2-m_1}{2m_0}\frac{\omega^2}{\omega_c^2}\right)^2(\bar{z}^2)^{-1}\right]^{-1/2}.$$

We also recall that, for the simpler case of equal masses, the thermal conductivity for the classical and the quantum models in the high temperature region are the same, as shown in [9] by using the same approach for the heat current of that adopted here.

V. FINAL COMMENTS

In this paper, we consider the investigation of the heat current in the steady state of the quantum harmonic chain of oscillators with alternate masses and self-consistent reservoirs—the anharmonic interactions which lead to a normal thermal conductivity (i.e., to Fourier's law) are represented, in this model, by the reservoirs connected to each site. We use a recently proposed an approach for the study of the heat current [9], and investigate, in detail, the thermal conductivity, presenting analytical results.

Models of unequal masses, as recalled in the introduction, have been used in several works related to the analysis of heat conduction, with important physical information. Here, for this quantum chain of particle with alternate masses, we show interesting properties of the thermal conductivity κ: in the high temperature regime, where the quantum and classical descriptions coincide, κ is constant, i.e., it does not change with temperature, but it is quite sensitive to the difference between the alternate masses (m_1-m_2); however, in the low temperature regime, κ becomes a function of the temperature T ($\kappa \sim CT^3$ for an interaction with on-site potential; otherwise, $\kappa \sim CT^{1/2}$), and more, the dependence on (m_1-m_2) is wiped out. Note that the difference between systems with and without on-site potential is physically expected: the on-site potential inhibits the heat transport, and so, decreases the thermal conductivity.

In a few words, our results reinforce the message that quantum effects cannot be neglected in the study of heat conduction in low temperatures.

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APPENDIX: INVERSE OF THE TRIDIAGONAL MATRIX

We start from the formula for the inverse of a general tridiagonal matrix

$$A = \begin{pmatrix} b_1 & c_1 & 0 & & & 0 \\ a_2 & b_2 & c_2 & & & \\ 0 & a_3 & b_3 & c_3 & & \\ & & a_4 & \ddots & \ddots & \\ & & & \ddots & b_{n-1} & c_{n-1} \\ 0 & & & & a_n & b_n \end{pmatrix}. \tag{A1}$$

In [22] it is proved, for $\phi_{ij}=(A^{-1})_{ij}$, that

$$\phi_{jj} = \left(b_j - a_j c_{j-1}\frac{z_{j-2}}{z_{j-1}} - a_{j+1}c_j \frac{y_{j+2}}{y_{j+1}} \right)^{-1}, \tag{A2}$$

for $j=1,2,\ldots,n$, and

$$\phi_{ij} = \begin{cases} -c_i \dfrac{z_{i-1}}{z_i}\phi_{i+1,j} & \text{if } i<j, \\ -a_i \dfrac{y_{i+1}}{y_i}\phi_{i-1,j} & \text{if } i>j, \end{cases} \tag{A3}$$

where z_j and y_j are defined according the recurrence relations

$$z_i = b_i z_{i-1} - a_i c_{i-1} z_{i-2}, \quad z_0 = 1, \quad z_1 = b_1,$$

$$y_j = b_j y_{j+1} - a_{j+1} c_j y_{j+2}, \quad y_{n+1} = 1, \quad y_n = b_n,$$

with $i=1,2,\ldots,n$, and $j=n-1,n-2,\ldots,1$.

In our specific problem we have $c_i=a_j=-1$, $\forall i,j$; $b_j=b_1$ if j is odd, and $b_j=b_2$ if j is even.

Let us consider first the simpler case $b_j=b$, $\forall j$, related to the problem of equal masses, since we will need it. In this case, we will denote the (A1) matrix by $\mathcal{A}(b)$. Now, the recurrence relations above become

$$z_i = b z_{i-1} - z_{i-2}, \quad z_0 = 1, \quad z_1 = b,$$

$$y_j = b y_{j+1} - y_{j+2}, \quad y_{n+1} = 1, \quad y_n = b.$$

Defining $x_i \equiv y_{n+1-i}$, we have $x_0=y_{n+1}=1$, $x_1=y_n=b$, and $x_i = bx_{i-1}-x_{i-2}$. Thus, the recurrence relation for x_i is the same one of z_i.

Denoting by $\mathcal{D}_j(b)$ the determinant of the $\mathcal{A}(b)$ matrix of size $j\times j$, it is easy to see (e.g., by induction) that $\mathcal{D}_j(b)$ follow the same recurrence relation of z_j, namely, $\mathcal{D}_j(b) = b\mathcal{D}_{j-1}(b)-\mathcal{D}_{j-2}(b)$ [define first $\mathcal{D}_0(b)\equiv 1$]. It follows that, if $b\geqslant 2$, then $\mathcal{D}_j(b)>0$, and so $\mathcal{A}$ is invertible. We have the following:

Lemma 1. For the $n\times n$ matrix $\mathcal{A}(b)$, we have

$$\mathcal{D}_n(b) = \frac{\sinh[(n+1)\alpha]}{\sinh \alpha},$$

where

$$e^{\alpha} = \frac{b \pm \sqrt{b^2-4}}{2}. \tag{A4}$$

Proof. The recurrence relation $\mathcal{D}_n(b)=b\mathcal{D}_{n-1}(b)-\mathcal{D}_{n-2}(b)$ reminds us that a second-order differential equation with constant coefficients $f=bf'-f''$, whose solutions are $e^{\pm\alpha x}$, α to be determined. If we try to write $\mathcal{D}_n(b)$ as $e^{\alpha n}$ and $e^{-\alpha n}$, from the recurrence relation, we obtain the restriction for e^{α} given by the formula (A4) above. Moreover, if we write $\mathcal{D}_n(b)=c_1e^{\alpha n}+c_2e^{-\alpha n}$, with (say, the boundaries condition) $\mathcal{D}_1(b)=b$ and $\mathcal{D}_2(b)=b^2-1$, we find c_1 and c_2 which leads to the formula of the lemma. ■

Theorem 1. Let $\mathcal{A}(b)$ be a $N\times N$ matrix, with $b_j=b\geqslant 2$. Then $\mathcal{A}(b)$ is invertible and

$$(\mathcal{A}^{-1})_{l,m} = \begin{cases} \dfrac{\mathcal{D}_{l-1}\mathcal{D}_{N-m}}{\mathcal{D}_N} & \text{if } m>l, \\ \dfrac{\mathcal{D}_{m-1}\mathcal{D}_{N-l}}{\mathcal{D}_N} & \text{if } m\leqslant l. \end{cases} \tag{A5}$$

Proof. It follows from the general formulas for ϕ_{ij}, (A2) and (A3), restricted to this special case, from the observation that z_j and $\mathcal{D}_j(b)$ have the same recurrence relation, and some algebrism. ■

Now we turn to the case of our interest, the matrix with alternate masses, i.e., $a_i=c_j=-1$ and $b_j=b_1$ if j is odd and $b_j=b_2$ if j is even. We will denote this matrix by $\widetilde{A}(b_1,b_2)$. For simplicity, we will be restricted to the cases of $\widetilde{A}$ in a $N\times N$ matrix, with N odd (then, $b_N=b_1$). Now we have

$$\widetilde{z}_i=b_i\widetilde{z}_{i-1}-\widetilde{z}_{i-2},\quad \widetilde{z}_0=1,\quad \widetilde{z}_1=b_1,$$

$$\widetilde{y}_j=b_j\widetilde{y}_{j+1}-\widetilde{y}_{j+2},\quad \widetilde{y}_{n+1}=1,\quad \widetilde{y}_n=b_1,$$

again with $i=1,2,\ldots,N$, and $j=N-1,N-2,\ldots,1$. For odd N, we have $\widetilde{x}_j\equiv\widetilde{y}_{n+1-j}=\widetilde{z}_j$. It follows then that $\widetilde{D}_j(b_1,b_2)$ [the determinant of a $j\times j$ $\widetilde{A}(b_1,b_2)$ matrix] and $\widetilde{z}_j$ have the same recurrence relation, namely, $\widetilde{D}_k=b_k\widetilde{D}_{k-1}-\widetilde{D}_{k-2}$ (again, we define $\widetilde{D}_0=1$). We can obtain a relation between the determinant of the matrix with alternate masses $\widetilde{D}_k(b_1,b_2)$ and the determinant of the specific matrix with equal masses $\mathcal{D}_k(\sqrt{b_1b_2})$. We have the following lemma.

Lemma 2. We have

$$\widetilde{D}_k(b_1,b_2)=\begin{cases}\sqrt{\dfrac{b_1}{b_2}}\mathcal{D}_k(\sqrt{b_1b_2}) & \text{if } k \text{ is odd},\\ \mathcal{D}_k(\sqrt{b_1b_2}) & \text{if } k \text{ is even}.\end{cases}$$

Proof. It follows by induction and simple manipulations. ■

Finally, let us calculate $\widetilde{A}^{-1}$.

From the formulas (A2) and (A3), and from the recurrence relations, it follows that

$$(\widetilde{A}^{-1})_{ij}=\begin{cases}\dfrac{\widetilde{z}_{i-1}\widetilde{y}_{j+1}}{\widetilde{z}_j\widetilde{y}_{j+1}-\widetilde{z}_{j-1}\widetilde{y}_{j+2}} & \text{if } i<j,\\ \dfrac{\widetilde{z}_{j-1}\widetilde{y}_{i+1}}{\widetilde{z}_{j-1}\widetilde{y}_j-\widetilde{z}_{j-2}\widetilde{y}_{j+1}} & \text{if } i\geqslant j,\end{cases}\tag{A6}$$

and we have the same relations for $(\mathcal{A}^{-1})_{ij}$, but, of course, with its own z_j and y_j terms. We have seen that $\widetilde{z}_j=\widetilde{D}_j$ for $\widetilde{A}$, $z_j=\mathcal{D}_j$ for $\mathcal{A}$, and lemma 2 gives us the relation between $\widetilde{D}_j$ and $\mathcal{D}_j$. Then, using (A5) it is easy to prove the following result.

Theorem 2. We have

$$(\widetilde{A}^{-1})_{ij}=\begin{cases}\sqrt{\dfrac{b_2}{b_1}}(\mathcal{A}^{-1})_{ij} & \text{if } i \text{ and } j \text{ are odd},\\ \sqrt{\dfrac{b_1}{b_2}}(\mathcal{A}^{-1})_{ij} & \text{if } i \text{ and } j \text{ are even},\\ (\mathcal{A}^{-1})_{ij} & \text{otherwise}.\end{cases}\tag{A7}$$

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