Size effects in the long-time quasi-static heat transport

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We consider finite size effects on heat transfer between thermal reservoirs mediated by a quantum system, where the number of modes in each reservoir is finite. Our approach is based on the generalized quantum Langevin equation and the thermal reservoirs are described as ensembles of oscillators within the Drude-Ullersma model. A general expression for the heat current between the thermal reservoirs in the long-time quasi-static regime, when an observation time is of the order of $\Delta^{-1}$ and $\Delta$ is the mode spacing constant of a thermal reservoir, is obtained. The resulting equations that govern the long-time relaxation for the mode temperatures and the average temperatures of the reservoirs are derived and approximate analytical solutions are found. The obtained time dependences of the temperatures and the resulting heat current reveal peculiarities at $t = 2\pi m/\Delta$ with nonnegative integers $m$ and the heat current vanishes non-monotonically when $t \to \infty$. The validity of Fourier’s law for a chain of finite-size macroscopic subsystems is considered. As is shown, for characteristic times of the order of $\Delta^{-1}$ the temperatures of subsystems’ modes deviate from each other and the validity of Fourier’s law cannot be established. In a case when deviations of initial temperatures of the subsystems from their average value are small, $t \to \infty$ asymptotic values for the mode temperatures do not depend on a mode’s number and are the same as if Fourier’s law were valid for all times.

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I. INTRODUCTION

One of the most fundamental pursuits in modern physics is the way heat transfers through microscopic systems (such as nanotubes, molecules, or quantum dots) \[1,2\]. Despite of the recent advances, this study still presents many challenges due to intrinsic non-equilibrium nature of the problem. Beyond a purely academic interest in the problem, research suggests that nanoscale and molecular systems may be good candidates for many technological advances, such as molecular wires, molecular diodes, rectifiers, and switches \[3,4\].

In accordance with empirically established Fourier’s law, the heat flux $\mathbf{J}$ through both fluids and solids is determined by the expression $\mathbf{J} = -\kappa \nabla T(\mathbf{r})$, where the temperature $T$ varies slowly on the microscopic scale and $\kappa$ is the thermal conductivity. Despite the ubiquitous occurrence of this phenomenon, very few rigorous mathematical derivations of this law are known \[5\]. While for three-dimensional generic models Fourier’s law is expected to be true, this law may not be valid for one- and two-dimensional systems \[1\]. The problem acquired nowadays even more attention due to growing interest in energy transfer at the nanoscale and possible use of nanostructures for energy applications \[6–10\].

A recently developed approach to study heat transport at the microscopic level is usually based on the quantum Langevin equation, first considered in Ref. \[11\] for a weakly damped harmonic oscillator. In Ref. \[12,13\], it was used to formulate transport, collective motion, and Brownian motion from a unified, statistical-mechanical point of view. Later, in Refs. \[14–18\], the Langevin equation was used for studying the thermalization of a particle coupled harmonically to a thermal reservoir and other closely-related problems. The developed Langevin approach was generalized in Refs. \[19–22\] in order to explore the steady-state heat current and temperature profiles in chains of harmonic oscillators placed between two thermal baths, which were considered as infinitely large, i.e. having infinitely large number of modes. An important alternative to the Langevin approach is the non-equilibrium Green’s function (NEGF) method. It was developed at first to describe electron transport and calculate the steady-state properties of a finite system connected to reservoirs that are modeled by non-interacting Hamiltonians with infinite degrees of freedom \[23,25\]. Various important quantities, such as currents and local densities, can be obtained using the steady-state density matrix and can be written in terms of the Keldysh Green’s functions \[26\]. Later, the NEGF approach was applied to phonon transport \[27,32\]. However, for non-interacting systems, the Langevin approach reproduces the NEGF results exactly \[1,33\]. Recently, a new method for an exact solution to the Lindblad and Redfield master equations, which can be also considered as an alternative to the quantum Langevin equation, has been developed \[34,35\].

In this paper, we investigate size effects in quasi-static heat transfer between two thermal reservoirs described as a finite collections of quantum harmonic oscillators mediated by a quantum system, which is also considered in the harmonic approximation.

Study of size effects in nano-structured materials occupy an important part of contemporary research. One profound theoretical question is related to the applicability of macroscopic theories when a particle has only few nanometers in size. While study of size and quantum effects and their influence on linear and nonlinear response on electromagnetic fields have a rather long history (see, for example, Refs \[36–40\]), systematic investigation of the role of these effects and its influence on thermal properties of small bodies took part...
only recently. In Refs. [41–43], static thermodynamic properties of nanostructures were investigated. In Ref. [41], using molecular dynamics simulations, the authors analyzed the local structure and vibrational properties of the grain boundary in ultrananocrystal diamond. In Ref. [42], the authors studied the phonon density of states in different nanostructures. They showed that all discontinuities (such as grain boundaries and interfaces) introduce vibrational modes with low frequencies that directly affect the thermal properties of the material, such as the specific heat. In Ref. [43], a Monte-Carlo simulations on order-disorder transition in Pt-Rh nanoparticles were performed in order to study size-dependent trends such as the lowering of the critical ordering temperature and the broadening of the compositional stability range of the ordered phases. Finally, in Ref. [44] the authors revealed the critical role of the on-site pinning potential in establishing quasi-steady-state conditions of heat transport in finite quantum systems.

Our approach is based on the quantum Langevin equation and employs the Drude-Ullersma model for a bath mode spectrum. The developed model allows one to obtain the heat current between the thermal reservoirs and explore the baths’ temperature relaxation in the quasi-static regime when an observation time can be of the order of the “Heisenberg” time $\tau_H \sim \Delta^{-1}$, in which case the discreteness of a reservoir’s energy spectrum becomes resolvable [18, 45].

The paper is organized as follows. The model is introduced in Sec. II, where the generalized Langevin equation is derived and solved. This derivation assumes that the number of modes in the thermal reservoirs is finite. In Sec. III, expressions for the heat current between the baths and equations that govern temperature relaxation of the baths’ modes are derived. An analytical approach for solving the temperature equations, temporal behavior of the heat current, and a question of applicability of Fourier’s law for a chain of finite macroscopic subsystems are considered in Sec. IV. Finally, Sec. V provides brief summary to our research.

II. MODEL

The total Hamiltonian of the system under consideration is similar to that in Refs. [22, 46, 47]:

$$\mathcal{H}_{\text{tot}} = \mathcal{H} + \mathcal{H}_{B1} + \mathcal{H}_{B2} + \mathcal{V}_1 + \mathcal{V}_2.$$  

(1)

Here

$$\mathcal{H} = \frac{p^2}{2m} + \frac{kx^2}{2}$$  

(2)

is the Hamiltonian of the quantum system (the mediator) described as a harmonic oscillator,

$$\mathcal{H}_{B\nu} = \sum_i \left[ \frac{p_{\nu i}^2}{2m_{\nu i}} + \frac{m_{\nu i} \omega_{\nu i}^2 x_{\nu i}^2}{2} \right]$$  

(3)

are the Hamiltonians of the $\nu$th baths ($\nu = 1, 2$), and

$$\mathcal{V}_\nu = -x \sum_i C_{\nu i} x_{\nu i} + x^2 \sum_i \frac{C_{\nu i}^2}{2m_{\nu i} \omega_{\nu i}^2}$$  

(4)

are the Hamiltonians that describe interaction between the mediator and the baths. In Eq. (4), $x$ and $p$ are the displacement and momentum operators and $m$ and $k$ are the particle’s mass and the spring constant, respectively. In Eqs. (3) and (4), $x_{\nu i}$ and $p_{\nu i}$ are the displacement and momentum operators, whereas $m_{\nu i}$ and $\omega_{\nu i}$ are the masses and frequencies of the oscillators for the $i$th mode that belongs to the $\nu$th bath. Finally, $C_{\nu i}$ are the coupling coefficients that describe the interaction between the quantum system and the baths. The last contributions to the right-hand side of (4) are self-interaction terms, which guarantee that $\mathcal{H}_{B\nu} + \mathcal{V}_\nu$ is positively defined for each $\nu$.

Solutions of the Heisenberg equations

$$\dot{x}_{\nu i} = \frac{p_{\nu i}}{m_{\nu i}} \quad \text{and} \quad \dot{p}_{\nu i} = -m_{\nu i} \omega_{\nu i}^2 x_{\nu i} + C_{\nu i} x$$  

(5)

for the baths’ operators can be presented as

$$x_{\nu i}(t) = x_{\nu i}(0) \cos(\omega_{\nu i} t) + \frac{p_{\nu i}(0)}{m_{\nu i} \omega_{\nu i}} \sin(\omega_{\nu i} t) + \frac{C_{\nu i}}{m_{\nu i} \omega_{\nu i}} \int_0^t \sin(\omega_{\nu i}(t-s)) x(s) ds$$  

(6)

and

$$p_{\nu i}(t) = m_{\nu i} \dot{x}_{\nu i}(t) = -m_{\nu i} \omega_{\nu i} x_{\nu i}(0) \sin(\omega_{\nu i} t) + \frac{p_{\nu i}(0) \cos(\omega_{\nu i} t)}{m_{\nu i} \omega_{\nu i}} + C_{\nu i} \int_0^t \cos(\omega_{\nu i}(t-s)) x(s) ds. \quad (7)$$

After substituting (6) into the other dynamic equations

$$\dot{x} = \frac{p}{m} \quad \text{and} \quad \dot{p} = -kx + \sum_{i \nu} C_{\nu i} x_{\nu i} - x \sum_{i \nu} \frac{C_{\nu i}^2}{m_{\nu i} \omega_{\nu i}^2}.$$  

(8)

which describe our quantum system, one obtains the following quantum Langevin equation:

$$m \ddot{x} = -kx(t) + \eta(t) - \int_0^t \gamma(t-s) \dot{x}(s) ds - \gamma(t) x(0), \quad (9)$$

where

$$\eta(t) = \sum_{i \nu} C_{\nu i} \left[ x_{\nu i}(0) \cos(\omega_{\nu i} t) + \frac{p_{\nu i}(0)}{m_{\nu i} \omega_{\nu i}} \sin(\omega_{\nu i} t) \right]$$  

(10)

is the noise that comes from the baths and

$$\gamma(t) = \sum_{i \nu} \frac{C_{\nu i}^2}{m_{\nu i} \omega_{\nu i}^2} \cos(\omega_{\nu i} t)$$  

(11)

is the friction kernel which takes into account the interaction of the quantum particle with both thermal reservoirs.

The Drude-Ullersma model [18, 48, 49] that we employ here assumes that in the absence of the interaction with the quantum system, each bath consists of uniformly spaced modes and introduces the following frequency dependence for the coupling coefficients:

$$\omega_{\nu i} = i \Delta_{\nu i}, \quad C_{\nu i} = \sqrt{\frac{2 \gamma_{\nu i} m_{\nu i} \Delta_{\nu i}}{\pi (\omega_{\nu i}^2 + D_{\nu i}^2)}}$$  

(12)
where \( i = 1, 2, \ldots, N_p \). In Eq. (14), \( \Delta_p \) are the mode spacing constants, \( D_p \) are the characteristic cutoff frequencies qualitatively similar to the Debye frequency, and \( \gamma_p \) are the coupling constants between a given reservoir and the mediator. Hereafter we assume that the heat baths are identical, which means that
\[
X_1 = X_2 \equiv X \quad \text{and} \quad \gamma_1 = \gamma_2 \equiv \gamma/2, \quad (13)
\]
where \( X_p = N_p \), \( \Delta_p \), or \( D_p \). However, unlike in Ref. [47], we consider \( \Delta \) as a small but finite parameter. In this case, the friction kernel \( \Pi \) must be considered as a periodic function with a finite period \( T = 2\pi/\Delta \). Using \( \Pi \), one finds that
\[
\gamma(t) = \gamma D [e^{-D\tau} + e^{-((T-t)D)}] \quad \text{for} \quad 0 \leq t \leq T \quad (14)
\]
and continued periodically with the period \( T \) beyond this interval in accordance with the relation \( \gamma(t + T) = \gamma(t) \). In deriving \( \Pi \), we approximated the finite sum by the corresponding series. Due to the fast convergence of \( \Pi \), the resulting error is small. It also does not change the result qualitatively because the periodicity property is determined by the first harmonic in \( \Pi \).

Equation (9) can be solved by the Laplace transformation [51]:
\[
x(t) = \hat{g}(t)x(0) + \frac{1}{m} \hat{g}(0)p(0) + \frac{1}{m} \int_0^t g(t-s)\eta(s) ds \quad (15)
\]
Detailed derivation of (15) can be found in Refs. [18, 22], where similar problems were considered. Here \( \hat{g} = dg/dt \),
\[
g(t) = L^{-1} \left[ \frac{1}{z^2 + \omega_0^2 + z\hat{\gamma}(z)} \right] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{zt} \frac{dz}{h(z)} \quad (16)
\]
where \( L^{-1} \) is the inverse of the Laplace transform \( L \),
\[
\hat{\gamma}(z) = -\frac{\gamma}{m} L[\gamma(t)] = \frac{D\hat{\gamma}}{1 - e^{-zT}} \times \left( \frac{1 - e^{-(D+z)T}}{D+z} + e^{-D\tau} - e^{-zT} \right) \approx \frac{D\hat{\gamma}}{1 - e^{-zT}} \left( \frac{1}{D+z} + \frac{e^{-zT}}{D-z} \right) \quad \text{with} \quad \hat{\gamma} = \gamma/m, \quad (17)
\]
\( \omega_0 = \sqrt{k/m} \) is the quantum particle’s frequency, and
\[
h(z) = z^2 + \omega_0^2 + \frac{D\hat{\gamma} z}{1 - e^{-zT}} \left( \frac{1}{D+z} + \frac{e^{-zT}}{D-z} \right) \quad \text{with} \quad h(z) = z^2 + \omega_0^2 + \frac{D\hat{\gamma} z}{1 - e^{-zT}} \left( \frac{1}{D+z} + \frac{e^{-zT}}{D-z} \right). \quad (18)
\]
In Eqs. (17) and (18) we neglected \( O[\exp(-DT)] \) terms.

In order to obtain \( g(t) \), one can resort to the Heaviside expansion theorem in accordance with which
\[
g(t) = \sum_{n} e^{z_n t} \frac{1}{h'(z_n)}, \quad h'(z) = \frac{dh(z)}{dz}, \quad (19)
\]
and \( z_n \) are the roots of \( h(z) \). The roots can be found iteratively as expansions over the small parameter \( \Delta \):
\[
z_n = i\omega_n + z_{1n} + z_{2n} + \ldots \equiv i\omega_n + z' \quad (20)
\]
where \( \omega_n = n\Delta \), integer \( n \geq 1 \), and \( z_n' = z_{1n} + z_{2n} + \ldots \). Equation \( h(z_n) = 0 \) can be written as
\[
(1 - e^{-z_n T})(z_n^2 + \omega_0^2) + \hat{\gamma} D z_n \left( \frac{1}{D+z_n} + \frac{e^{-z_n T}}{D-z_n} \right) = 0 \quad (21)
\]
Here we take into account that \( \omega_n T = 2\pi n \) and \( \exp(-iz_n T) = \exp(-iz'_n T) \). Solving (21) with respect to \( \exp(-iz'_n T) \), Eq. (21) can be rewritten as
\[
\exp(-iz'_n T) = \frac{\omega_0^2 + z_{1n}^2 + \hat{\gamma} D z_n (D+z_n)}{\omega_0^2 + z_{1n}^2 - \hat{\gamma} D z_n (D-z_n)}. \quad (22)
\]
Thus, the first correction, \( z_{1n} \), is determined by
\[
\exp(-iz_{1n} T) = \frac{\omega_0^2 - \omega_0^2 + i\hat{\gamma} D \omega_0 (D + i\omega_0)}{\omega_0^2 - \omega_0^2 - i\hat{\gamma} D \omega_0 (D - i\omega_0)}, \quad (23)
\]
where \( z_{1n} \) from the right hand side of (22) is substituted by its zero order approach, \( i\omega_0 \). It gives
\[
z_{1n} = -i\Delta \psi(\omega_n) \equiv -i\Delta \psi_n, \quad (24)
\]
where
\[
\psi(\omega) = \frac{1}{\pi} \arctan \left[ \frac{\hat{\gamma} D^2 \omega}{(\omega_0^2 - \omega^2)(D^2 + \omega^2) + \hat{\gamma} D \omega^2} \right]. \quad (25)
\]
The second correction, \( z_{2n} \), is determined from the same equation (23), where \( z_{1n} \) is substituted by \( z_{1n} + z_{2n} \) on the left hand side of that equation and \( \omega_n \) is substituted by \( \nu_n = \omega_n - \Delta \psi_n \) on the right hand side of (23). As is clear, the resulting equation for \( z_{2n} \) is \( z_{1n} + z_{2n} = -i\Delta \psi(\nu_n) \), or
\[
z_{1n} + z_{2n} = -i\Delta [\psi(\omega_n) - \frac{\partial \psi(\omega_n)}{\partial \omega_n} \Delta \psi_n] + O(\Delta^3)
\]
\[
\approx z_{1n} + i\Delta \hat{\gamma} \frac{\partial \psi(\nu_n)}{\partial \omega_n} \psi_n + O(\Delta^3). \quad (26)
\]
Thus,
\[
z_{2n} = i\Delta^2 \frac{\partial \psi(\nu_n)}{\partial \omega_n} \psi_n = z_{1n} O(\tau \Delta), \quad (27)
\]
where \( \tau \) is a time needed to establish the steady-state heat current. In what follows, we assume that \( \tau \) satisfies inequality
\[
\tau = \max(\gamma^{-1}, \omega_0^{-1}, D^{-1}) < \Delta^{-1}. \quad (28)
\]
In this case, one can neglect \( z_{2n} \) and Eq. (19) gives
\[
g(t) = -\frac{i\hat{\gamma} D^2}{\pi} \sum_{n=-\infty}^{\infty} \frac{\Delta \nu_n e^{i\nu_n t}}{\text{den}(\nu_n)} = \frac{2\hat{\gamma} D^2}{\pi} \sum_{n \geq 1} \frac{\Delta \nu_n \sin(\nu_n t)}{\text{den}(\nu_n)}, \quad (29)
\]
where \( \nu_n = \omega_n - \Delta \psi_n, \text{den}(\nu) = A(\nu) A^*(\nu) \), and
\[
A(\nu) = (D - i\nu)(\omega_0^2 - \nu^2) - i\hat{\gamma} D \nu. \quad (30)
\]
As is clear, \( \text{den}(\nu) \) can be rewritten as
\[
\text{den}(\nu) = (\omega_0^2 - \nu^2)D^2 + \nu^2(\omega_0^2 - \nu^2 + \hat{\gamma}D)^2 = (\nu^2 + \mu_1^2)(\nu^2 + \mu_2^2)(\nu^2 + \mu_3^2),
\]
where \( \mu_{1,2,3} \) are the roots of equation
\[
(D - \mu)(\omega_0^2 + \mu^2) - \hat{\gamma}D\mu = 0
\]
and satisfy an inequality \( \Re(\mu_{1,2,3}) > 0 \).
When \( \Delta \to 0 \), the sum in (29) transforms to the integral
\[
g(t) \equiv g_0(t) = -i\frac{\hat{\gamma}D^2}{\pi} \int_{-\infty}^{\infty} \frac{dv}{\text{den}(\nu)} e^{it\nu}.
\]
Taking into account (31) and closing the integration contour in the upper complex half plane (for \( t > 0 \)), one finds the following (expected) result [18]:
\[
g_0(t) = L^{-1}[\hat{g}(z)] = \sum_{j=1}^{3} g_j e^{-\nu_j t}
\]
where
\[
\hat{g}(z) = \frac{D + z}{(D + z)(z^2 + \omega_0^2) + \hat{\gamma}Dz}
\]
Derivation of (34) is facilitated by noting that
\[
\hat{\gamma}D^2 = \sum_{j=1}^{3} \frac{g_j}{\nu_j^2 + \mu_j^2},
\]
which can be also considered as a definition of the coefficients \( g_j \)’s. Expression (34) has been obtained and used for study fundamental issues of statistical thermodynamics of a quantum particle couple to a heat bath in Ref. [18] when \( D \) is large. We consider here a more general case of the heat transfer between thermal reservoirs when \( D, \omega_0, \text{and} \hat{\gamma} \) can be comparable, but the relation (28) is satisfied with finite \( \Delta \).

III. QUASI-STATIC HEAT BALANCE

As was shown [47], the rate of change of the energy of the given \( \nu \)th thermal reservoir is determined by
\[
\frac{d}{dt} \sum_{i=1}^{N} \left( \frac{p_{\nu i}^2}{2m_{\nu i}} + \frac{m_{\nu i}\omega_{\nu i}^2 x_{\nu i}^2}{2} \right) = -\langle P_{\nu} \rangle,
\]
where the angular brackets denote the ensemble averaging and
\[
\langle P_{\nu} \rangle = -\sum_{i=1}^{N} \frac{C_{\nu i}}{2m_{\nu i}} (p_{\nu i}x + x_{\nu i}p_{\nu i})
\]
is the work that the quantum system performs on the \( \nu \)th bath per unit of time (the power dispersed in the \( \nu \)th bath) [19].

Here \( p_{\nu i} = p_{\nu i}(t), x_{\nu i} = x_{\nu i}(t), \text{and} x = x(t) \) are the solutions (5, 7), and (15), respectively. These solutions, as well as the resulting balance equation (37) are accurate in the frame of the adopted harmonic approximation. Thus, Eq. (37) provides a correct description of the energy balance for any moment \( t \geq 0 \). In the general case, (37) is a complicated equation because it describes both initial transient processes that occur at a microscopic time \( \tau \) as well as a subsequent long-time quasi-static variation of the reservoirs’ temperatures. Our goal here is to consider only the long-time quasi-static relaxation which happens on a much longer scale \( \tau_H \sim \Delta^{-1} \gg \tau \), as was indicated in Ref. [47]. In this regard, we can neglect variations in the baths’ temperatures over time intervals of the order of \( \tau \). In this case, after substitution (7) and (15) into (37), one can also drop all the terms that contain explicitly \( g(t) \) or \( \hat{g}(t) \). Indeed, \( g(t) \) differs noticeably from zero only on the time intervals of the order of \( \tau \) near \( t = n\tau \) where \( n \geq 0 \) is an integer and the corresponding contributions cannot influence the temperature variations. It results in the following expression (see also [47]):

\[
\langle P_{\nu} \rangle \approx -\frac{1}{2m} \sum_{i=1}^{N} C_{\nu i} \cos(\omega_{\nu i}t) \int_{0}^{t} ds g(t - s) \times \\
\langle p_{\nu i}(0)\eta(s) + \eta(s)p_{\nu i}(0) \rangle - m_{\nu i}\omega_{\nu i}\sin(\omega_{\nu i}t) \times \\
\int_{0}^{t} ds g(t - s)\langle x_{\nu i}(0)\eta(s) + \eta(s)x_{\nu i}(0) \rangle + J'_\nu,
\]
where
\[
J'_\nu = -\frac{1}{2m} \sum_{i=1}^{N} C_{\nu i}^{2} \int_{0}^{t} d\tau \cos(\omega_{\nu i}(t - \tau))x(\tau) \times \\
\int_{0}^{t} ds g(t - s) \eta(s) + \\
\int_{0}^{t} ds g(t - s) \eta(s) \int_{0}^{t} d\tau \cos(\omega_{\nu i}(t - \tau))x(\tau).
\]
In the quasi-static (or steady-state) regime, the power acquired by one reservoir is taken from the other, so that \( \langle P_1 \rangle = -\langle P_2 \rangle \).
Thus, we can define the quasi-static heat current in the symmetric form:
\[
J_{th} = \frac{1}{2} \langle P_1 - P_2 \rangle.
\]
If one takes into account (14), \( J'_\nu \) in (39) is canceled out simplifying the following derivation.
In order to find the contributions preceding \( J'_\nu \) in (39), we use the following approach. As was shown in [17, 18], after coupling of a quantum particle to a thermal bath, the whole system comes to equilibrium after a microscopic time \( \tau \). The thermal bath will be comprised of a sum of independent modes having frequencies \( \nu_k = \omega_k - \Delta \psi(\omega_k) \) where \( \psi(\omega_k) \equiv \psi_k \) coincides with (25). We have now two thermal reservoirs at different temperatures. However, one can assume that the influence of the quantum particle on both reservoirs is
small and each reservoir at any moment of time can be characterized by the equilibrium density matrix
\[ \rho_{\nu} = Z_\nu^{-1} e^{-\frac{\hbar}{2} \sum_k \beta_k v_{\nu k} (n_{\nu k} + 1/2)}, \]
where \( n_{\nu k} = n(T_{\nu k}, \nu) \)
\[ Z_\nu = \text{Tr}[e^{-\frac{\hbar}{2} \sum_k \beta_k v_{\nu k} (n_{\nu k} + 1/2)}], \]
and \( \beta_k = 1/k_B T_{\nu k} \), but we allow now (slow) temperature variations for each mode of both reservoirs: \( T_{\nu k} = T_{\nu k}(t) \). Due to this assumption, one can easily find expressions for \( \langle x_{\nu i}(0) \eta(s) + \eta(s) x_{\nu i}(0) \rangle \) and \( \langle p_{\nu i}(0) \eta(s) + \eta(s) p_{\nu i}(0) \rangle \) in [49].

Using the symmetric form [41] of the quasi-static heat current, performing the time integrations, and employing the Drake-Ullersma model, one finds (see the Appendix)
\[ J_{th} = -\frac{\hbar}{2} \sum_{k} \frac{\Delta \nu_k^2}{\nu_k + \Delta^2} G(\nu_k, t)(n_{1 k} - n_{2 k}), \]
where \( n_{\nu k} = n(T_{\nu k}, \nu) = 1/[\exp(h\nu_k/k_B T_{\nu k}) - 1] \) are the phonon occupation numbers for each mode of the respective (\( \nu \)th) thermal reservoir and
\[ G(\nu_k, t) = \int_0^t g(s)\sin(\nu_k s) ds. \]
In the general case, \( g(t) \) is determined by Eq. [29]. In a special case, when the observation time \( t \) is small compared to \( \Delta^{-1} \), the mode temperatures \( T_{\nu k}(t) \) can be considered unchanged during the heat transfer:
\[ T_{\nu k}(t) \approx T_{\nu k}(0) = T_{\nu}. \]
Here \( T_{1,2} \) are the reservoirs’ temperatures before they are interconnected by the quantum particle. We assume that each thermal reservoir was initially in a state of thermal equilibrium with a particular temperature \( T_{\nu} \). Also, if \( \tau \ll t \ll \Delta^{-1} \) (in particular, when \( \Delta \to 0 \)),
\[ G(\nu_k, t) \approx \int_0^t g_0(s)\sin(\nu_k s) ds = \nu_k \sum_{j=1}^{3} \frac{g_j}{\nu_k^2 + \mu_j^2}. \]
In this case, one can also replace the sum in [44] by the corresponding integral over the frequency and the resulting heat current
\[ J_{th}^{(0)} = -\frac{\hbar}{2} \sum_{j=1}^{3} \frac{g_j}{\nu_k^2 + \mu_j^2} \int_0^\infty \frac{d\omega}{\omega} \left[ n(T_{1, \omega}) - n(T_{2, \omega}) \right] \frac{1}{(\Delta^2 + \omega^2)(\mu_j^2 + \omega^2)}, \]
and the corresponding heat conductance
\[ J_{th}^{(0)} / \delta T = \frac{\Delta \nu_k^2}{2\pi(\nu_k^2 + \Delta^2)} G(\nu_k, t) \]
and the corresponding heat conductance \( K = J_{th}^{(0)} / \delta T \) at \( \delta T = T_1 - T_2 \to 0 \) reduce to the respective quantities derived in [47].

In the case when \( \Delta \) satisfies relation [28] but is finite and \( t \sim \Delta^{-1} \), one has to return to Eq. [44]. In accordance with [42], the average energy of the \( \nu \)th thermal reservoir \( \langle E_{\nu} \rangle \) is the sum of the average energies \( \langle E_{\nu k} \rangle \) of its independent oscillator modes and the time derivative of \( \langle E_{\nu} \rangle \) is determined as
\[ \frac{d}{dt} \sum_{k=1}^N \langle E_{\nu k} \rangle = \frac{N}{2} \sum_{k=1}^N \frac{d h \nu_k}{dt} \coth \left( \frac{h \nu_k}{2k_B T_{\nu k}} \right). \]
As follows from [38], [41], and [44], the energy balance for the 1st bath is
\[ \frac{d}{dt} \sum_{k=1}^N \langle E_{1 k} \rangle = -\frac{\hbar}{2} \sum_{k=1}^N \frac{\Delta \nu_k^2}{\nu_k^2 + \Delta^2} [n_{1 k} - n_{2 k}] \]
and is satisfied if each \( (k) \)th mode satisfies its own energy balance equation
\[ \frac{d}{dt} \langle E_{1 k} \rangle = C(\nu_k, T_{1 k}) \frac{\Delta \nu_k^2}{2\pi(\nu_k^2 + \Delta^2)} G(\nu_k, t)[n(T_{1 k}, \nu_k) - n(T_{2 k}, \nu_k)], \]
which determines the temperature \( T_{1 k} \) of the \( k \)th mode. Here \( C(\nu_k, T_{1 k}) \) is the heat capacitance of the \( k \)th mode of the first bath:
\[ C(\nu_k, T_{1 k}) = \frac{k_B}{4} \left( \frac{h \nu_k}{k_B T_{1 k}} \right)^2 \frac{1}{\sinh^2(h \nu_k/2k_B T_{1 k})}. \]
The same equation can be written for the temperature \( T_{2 k} \) of the \( k \)th mode of the of the second thermal reservoir (with the same frequency \( \nu_k \) by interchanging \( T_{1 k} \) and \( T_{2 k} \) in [51]). Figure 1 contains graphical illustration of Eq. [51]. If \( |T_{1 k} - T_{2 k}| \ll (T_{1 k} + T_{2 k})/2 = \bar{T}_k \), [51] can be reduced to
\[ C_k(T_{1 k}) \frac{\Delta \nu_k^2}{2\pi(\nu_k^2 + \Delta^2)} G(\nu_k, t) C_k(T_k)(T_{1 k} - T_{2 k}) \]
or, if one neglects the difference between \( C_k(T_{1 k}) = C(\nu_k, T_{1 k}) \) and \( C(\nu_k, \bar{T}_k) \), which is equivalent to dropping \( O(T_{1 k} - T_{2 k})^2 \) contributions to [53], it results in
\[ \bar{T}_{1 k} = -\frac{\gamma \Delta \nu_k^2}{2\pi(\nu_k^2 + \Delta^2)} G(\nu_k, t)(T_{1 k} - T_{2 k}). \]
Finally, due to the symmetry between the baths that follows from our assumption [13], \( T_{1 k}(t) + T_{2 k}(t) = T_1 + T_2 = 2\bar{T} \).
does not depend on time and (54) can be rewritten as

$$\frac{d}{dt} \delta T_k = -\frac{\gamma_k \Delta \nu_k D^2}{\pi (\nu_k^2 + D^2)} G(\nu_k, t) \delta T_k,$$

(55)

where $\delta T_k \equiv T_{1k} - T_{2k}$. These equations can be solved independently for each $\nu_k$ with the following initial conditions

$$\delta T_k(0) = T_1 - T_2$$

(56)

that are independent on the mode number $k$.

As is clear, the form of Eq. (55) is the same for the classical (high-temperature) and quantum (low-temperature) cases. However, for the classical case,

$$n(T_{1k}, \nu_k) - n(T_{2k}, \nu_k) \approx \frac{k_B}{\hbar \nu_k}(T_{1k} - T_{2k})$$

(57)

and Eq. (55) is accurate (no need for any additional linearizing to produce (53) and (55) from (51)).

One can also define average temperatures $T_{1,2}(t)$ of each bath from the condition that $T_{1,2}(t)$ provide the same total energies of the baths:

$$\sum_{k=1}^{N} \frac{\hbar \nu_k}{2} \coth \frac{\hbar \nu_k}{2k_B T_k(t)} = \sum_{k=1}^{N} \frac{\hbar \nu_k}{2} \coth \frac{\hbar \nu_k}{2k_B T_{\nu}(t)},$$

(58)

where $\nu = 1, 2$. As is clear, $T_\nu(t = 0) = T_\nu$ and $T_1(t) + T_2(t) = T_1 + T_2 = 2T$. (59)

Subtracting Eq. (58) at $\nu = 2$ from Eq. (58) at $\nu = 1$, one finds that

$$\sum_{k=1}^{N} \hbar \nu_k[n(\nu_k, T_{1k}(t)) - n(\nu_k, T_{2k}(t))] = \sum_{k=1}^{N} \hbar \nu_k[n(\nu_k, T_1(t)) - n(\nu_k, T_2(t))].$$

(60)

If $|T_1(t) - T_2(t)| \ll T$, relation (60) results in

$$\sum_{k=1}^{N} C(\nu_k, T_k)(T_{1k} - T_{2k}) = \delta T(t) \sum_{k=1}^{N} C(\nu_k, T),$$

(61)

where $\delta T(t) \equiv T_1(t) - T_2(t)$. Thus, taking into account that $T_k = T$ for each $k$, we find the following expression for $\delta T(t)$:

$$\delta T(t) = \left[ \sum_{k=1}^{N} C(\nu_k, T) \right]^{-1} \sum_{k=1}^{N} C(\nu_k, T) \delta T_k(t).$$

(62)

One can expect that these temperatures $T_{1,2}(t)$ can be established in a case when the baths have small nonlinearities due to phonon-phonon interaction [10], provided that a thermalization time $\tau_{therm}$ for the baths’ modes satisfies the following condition:

$$\tau \ll \tau_{therm} \ll \Delta^{-1}.$$ 

(63)

In this case, $T_{1,2}(t)$ determine the temperatures of the thermal reservoirs. Using (59), one finds

$$T_{1,2}(t) = \frac{1}{2}(T_1 + T_2) \pm \frac{1}{2}\delta T(t).$$

(64)

A. $G$ factor

After substituting (29) into (45), factor $G \equiv G(\nu_k, t)$ (“$G$ factor”) can be expressed as

$$G = \frac{\gamma_k}{\pi} \sum_{n \geq 1} \frac{D^2 \Delta \nu_n}{\text{den}(\nu_n)} \sin(\nu_k - \nu_n)t \left[ \frac{\sin(\nu_k + \nu_n)t}{(\nu_k - \nu_n)} \right].$$

(65)

It is impossible to derive closed forms for $g(t)$ or $G(\nu_k, t)$ because of the frequency shift $\Delta \psi_n$. One can find, however, an approximate analytical expression for $G(\nu_k, t)$ in the following way. For $t \gg \tau$, one can neglect the second contribution in the square brackets in (65) and write

$$G(\nu_k, t) \approx \frac{\gamma_k}{\pi} \frac{D^2}{\text{den}(\nu_k)} \Delta \sin(\nu_k - \nu_n)t.$$ 

(66)

The last sum can be easily found (50) and the result is

$$\sum_{n \geq 1} \frac{\sin(\nu_k - \nu_n)t}{(\nu_k - \nu_n)} = \pi f(\Delta t),$$

(67)

where

$$f(x) = \theta(x) + 2 \sum_{m \geq 1} \theta(x - 2\pi m)$$

(68)

and $\theta(x)$ is Heaviside’s $\theta$-function. Finally, taking into account that $|\Delta \psi_n| \ll \omega_n$ for any $n \geq 1$ and smallness of $\Delta / \omega_0$, (66) can be rewritten as

$$G(\nu_k, t) \approx \frac{\gamma_k}{\pi} \frac{D^2}{\text{den}(\nu_k)} f(\Delta t) \approx \frac{\gamma_k}{\pi} \frac{\omega_0 D^2}{\text{den}(\omega_k)} f(\Delta t).$$

(69)

It is interesting to notice that the same result can be obtained if one simply neglects the frequency shift $\Delta \psi_n$ in (29) and (45), setting $\nu_n \approx \omega_n$ there. In this case, using Eq. (56), taking into account (50),

$$\sum_{n = -\infty}^{\infty} \frac{\Delta \omega_n \sin(\omega_n t)}{\omega_n \pm i\mu_j} = \frac{\pi \sinh[(\pi - \Delta)t]a_j}{\sinh(\pi a_j)},$$

(70)

where $a_j = \mu_j / \Delta$, and neglecting small quantities $|e^{-\mu_j T}|$, one finds that

$$g(t) = \sum_{j=1}^{3} \mu_j e^{-\mu_j t} - e^{-T(0)\mu_j}, \text{ if } 0 \leq t \leq T$$

(71)

and is continued periodically for $t > T$ in accordance with the relation

$$g(t + T) = g(t).$$

(72)

Using (71), (72), and the definition (45) with $\nu_n \approx \omega_n$, one arrives at the same result (59). Strictly speaking, as one can also understand from this alternative derivation, (69) is correct only if $mT + \tau < t < (m + 1)T - \tau$, so, again, our approximation can be applied only if (29) is satisfied.
As is clear from Figs. 2 - 4, formula (69) represents fairly smooth algebraic frequency cutoff, when the bath frequency spectrum does not end exactly at $\omega = D$. The number $N$ of the baths’ modes is finite now and we assumed that

$$N = \frac{\omega_{\text{max}}}{\Delta} \sim \frac{D}{\Delta},$$

(73)

where $\omega_{\text{max}}$ is the maximum frequency in the bath spectrum. When $D \ll \omega_0$, the mediating particle is effectively uncoupled from the baths [47]. It cannot be excited, and, as a consequence, cannot absorb or transfer energy between the thermal reservoirs. For this reason, one can assume that $D \sim \omega_0$ and $\omega_{\text{max}} \gtrsim D$. On the other hand, in order to avoid using too large $N$ in the case of small $\Delta$ (which is needed to satisfy (28)), it is desirable also to have $D \lesssim \omega_0$. Thus, any values for $D$ and $\omega_{\text{max}}$ that satisfy inequality $D \lesssim \omega_0 \lesssim \omega_{\text{max}}$ are acceptable and we choose here $D = \omega_0$. Taking the above observations into account, we choose also $\omega_{\text{max}} = 1.3D$. In this case, in Figs. 2 - 3 and in Fig. 5 we use $\Delta/\omega_0 = 0.01$ and $N = 130$, and in Fig. 4 and Figs. 6 - 7 $\Delta/\omega_0 = 0.001$ and $N = 1300$ are chosen. As our numerical analysis shows, the result of summation in (65) does not depend noticeably on $N$ provided that $N > 1.2D/\Delta$ due to the fast convergence.

In Figs. 2 - 4 $\nu_k = 0.5\omega_0$ and in Fig. 5 $\nu_k = \nu_{\text{res}} \approx \omega_0$. The frequency $\nu_{\text{res}}$ is chosen from a condition that $\nu_{\text{res}}$ minimizes $\text{den}(\nu)$:

$$\frac{d}{d\nu}\text{den}(\nu)|_{\nu=\nu_{\text{res}}} = 0.$$  

(74)

The latter means that the energy exchange between the thermal reservoirs is carried out by the modes that are in “resonance” with the mediating quantum system.

As is clear from Figs. 2 - 4 formula (69) represents fairly well the exact result (65) for $G(\nu_k, t)$ and the accuracy improves proportionally to $\Delta$. Indeed, when $\Delta/\omega_0$ decreases from 0.01 to 0.001, the relative difference between the accurate and approximate results also decreases by approximately ten times. The same results are observed for all other ratios $\nu_k/\nu_{\text{res}} \neq 1$. It is important to notice that deviations of $G(\nu_k, t)$ from its approximate analytical expression are not only small for $\Delta/\omega_0 \lesssim 0.01$ but also appear as oscillations.
that occur on a time scale of the order of $\tau$. In accordance with our assumption, temperature variations are insensitive to these short-scale oscillations, and we have an additional argument by which the latter can be neglected. In these cases, analytical formula (69) can be used for solving equations (55) or (51) for temperature variations.

A reason why our approximation (69) works well can be explained in the following way. As is clear from Eq. (25), $|\psi_k| \leq 1/2$ for all values of its parameters and $|\psi_k| \approx 1/2$ only when $\nu_k \approx \nu_{\text{res}} \approx \omega_0$ and is small otherwise. When $\nu_k \approx \nu_{\text{res}} \approx \omega_0$, Eq. (69) may not be accurate, which is illustrated in Fig. 5. The main reason for this is because the factor $\nu/\text{den}(\nu)$ in (65) changes also sharply with $\nu$ when $\nu \approx \nu_{\text{res}}$ and our approximation (66) can be only qualitatively correct. In this case one cannot use (62) for accurate calculations and must employ (65) for solving the temperature equations. As follows from our numerical analysis, however, the number of $\nu_k$ in the vicinity of $\nu_{\text{res}}$, which makes Eq. (69) inaccurate, is relatively small and decreases with $\Delta$. For example, if $\Delta/\omega_0 = 0.001$ and $\gamma/\omega_0 = 0.5$, $\nu_{\text{res}} = |\nu_{\text{res}}/\Delta| = 1130$ and formula (69) already provides a reasonable accuracy if $|k - \nu_{\text{res}}| \geq 4$.

The step-wise time dependence of $G(\nu_k, t)$, approximated by (69), is due to the finiteness of $\Delta$. Indeed, in the opposite case, when $\Delta \to 0$, we have the steady-state result (47), corresponding to the contribution of the only first term in (68).

As follows from our numerical analysis, the major contribution to $G(\nu_k, t)$ is determined by the first term in the square brackets in (65). It also comes from a region of the frequency spectrum of $g(t)$ close to $\nu_k$ but not only from one frequency $\nu_n = \nu_k$. The contribution from $\nu_n = \nu_k$ is linear in $t$. The other part of the sum in (66) is the periodic function of period $\mathcal{T}$ and is equal to $\pi - \Delta t$ on each time interval $m\mathcal{T} < t < (m + 1)(\pi)$ for $m = 0, 1, 2, \ldots$. Thus, the sum (66) results in the step-wise time dependence determined by (68).

For smaller $\gamma$, $\tau \sim \gamma^{-1}$. In this case, our model will be valid for the proportionally smaller values of $\Delta$ in order to satisfy the inequality (28) and will produce results similar to the ones shown above.

**IV. TEMPERATURE RELAXATION AND FOURIER’S LAW**

As follows from the above analysis, Eq. (69) is accurate for all modes (except $\nu_k = \nu_{\text{res}}$) provided that $\Delta$ is sufficiently small ($\Delta/\omega_0 \lesssim 0.001$ in the considered example). In this case, Eq. (55) can be rewritten as

$$\frac{d}{dt} \delta T_k = - (2m + 1) \mathcal{\Omega}_k \Delta \delta T_k$$

(75)

on each time interval $m\mathcal{T} \leq t \leq (m + 1)\mathcal{T}$, where $m = 0, 1, 2, \ldots$ and

$$\mathcal{\Omega}_k = \frac{(\gamma \omega_k D^2)^2}{\pi (\omega_k^2 + D^2) \text{den}(\omega_k)}.$$ 

(76)

Assuming continuity in the temperature variations and taking into account initial conditions (56), solution of Eq. (75) can be presented as

$$\delta T_k(t) = (T_1 - T_2) e^{-2\pi m^2 \mathcal{\Omega}_k} e^{-(2m + 1) \mathcal{\Omega}_k (\Delta t - 2\pi m)},$$

(77)

where $m = m(t) = |t\Delta/(2\pi)|$ is the integer part of the value inside the square brackets. Using this result, temperature dependencies for the $k$th mode of the $\nu$th thermal reservoir can be presented as

$$T_{1,2k}(t) = \frac{1}{2} (T_1 + T_2) \pm \frac{1}{2} \delta T_k(t).$$

(78)

Figure 6 shows results of application of (77) for several modes. As one finds, the fastest relaxation (leveling of the corresponding temperatures of both reservoirs) occurs when $\omega_k \approx \omega_0$ due to the resonance character of the heat transport at these frequencies (curve (b)). The rate of heat exchange decreases as $|\omega_k - \omega_0|$ increases, as also follows from the figure (curves (a) and (c)). Due to different relaxation rates, $T_{1k}(t)$ (or $T_{2k}(t)$) will all differ when $t \sim \Delta^{-1}$, in accordance with (77) and (78). Thus, neither of the two thermal reservoirs can
be characterized by a single local (in time) temperature \(T_l(t)\) or \(T_2(t)\) if \(t \sim \Delta^{-1}\).

Figure 8 shows time variations of \(\delta T/(T_1 - T_2)\) that represent \(\delta T_k/(T_1 - T_2)\) averaged over the baths’ modes in accordance with Eq. (62) for different values of ratio \(R = \hbar \omega_0/2k_B T\). When \(R \ll 1\) (curve (a)), we have the high-temperature limit (classical case). As our calculations reveal, when \(R\) decreases below 0.1, all such curves approach to \(\delta T_k(t) \approx \sum_{k=1}^{N} \delta T_k(t)\), as is expected. At low temperatures (quantum regime), when \(R\) is large (curve (b)), the temperature relaxation is slow. This is in accordance with the fact that the thermal conductance decreases when \(T\) decreases. Prominent features that appear in Figs. 6 and 7 are the peculiarities that occur at \(t = mT\) with \(m = 1, 2, \ldots\). This is a consequence of the finite values of \(\Delta\) (or \(T = 2\pi/\Delta\), see the comment at the end the previous section).

Finally, Fig. 8 shows the time dependence of the dimensionless heat current \(10^5 J_{th}(t)/\hbar \omega_0^2\), where \(J_{th}(t)\) is determined by (44). The shown time dependences are generic for the considered model. In computing the heat current, we used expression (78) for the temperatures of the baths’ modes and assumed that \(\alpha \equiv (T_1 - T_2)/T\) is small. Here \(T = (T_1 + T_2)/2\) and \(T_{1,2}\) are the initial temperatures of the baths. As our numerical analysis indicates, if \(|\alpha| \ll 0.01\), linearizing of Eq. (51) that gives (55) is well justified and \(J_{th} \sim \alpha\). The factor \(G(\nu_k, t)\), which grows stepwise, is suppressed by the exponentially decaying difference of the phonon occupation numbers for each \(\nu_k\) due to the above result (77), and \(J_{th}(t) \to 0\) when \(t \to \infty\). As we also found (see Fig. 8), when \(\Delta/\omega_0 \approx 0.001\) approximate expression (69) for the \(G\) factor gives essentially the same result for \(J_{th}(t)\) as when the corresponding accurate expression \(65\) is used. Thus, the short-scale oscillations from accurate \(G(\nu_k, t)\) around its approximate value \(69\) average out due to summation in (44) and smooth resulting \(J_{th}(t)\) is determined by \(69\). It must be mentioned that even when \(t \Delta t\) is large, the heat current still can be non-zero if one recovers the contributions to \(J_{th}(t)\) containing explicitly \(g(t)\) or \(\tilde{g}(t)\) (see the text just before Eq. (59)). These contributions, however, are the short-scale oscillations that occur during microscopic times of the order of \(\tau\) near \(t = nT\), where \(n \geq 0\) is an integer. Because \(\tau \ll \Delta^{-1}\), where \(\Delta^{-1}\) is the characteristic time scale in Fig. 8 we did not consider them in this study.

A. Fourier’s law

We consider now a chain of \(P\) macroscopic subsystems coupled by the mediators described by the Hamiltonian (2), which is illustrated in Fig. 9. Each subsystem and coupling are described by the Hamiltonian (3) and interaction (4), respectively, within the framework of the Drude-Ullersma model (12). The extended in this way model reduces to our initial model (3) - (4) when \(P = 2\). Assume that before the connection, all subsystems are prepared in the state of thermal equilibrium having temperatures \(T_{0n} = T_n(0)\), where \(n = 1, 2, \ldots, P\) and \(|T_{0n} - T_{0(n-1)}| \ll T_{0n} = [T_{0n} + T_{0(n-1)}/2].\)

After a short time \(\tau_{P}\) of initial transient processes (we assume that \(\tau_{P} \ll \Delta^{-1}\), one can consider this chain as an example of a system in local thermal equilibrium, consisting of weakly interacting parts (interaction is only due to the mediating quantum systems) having temperatures \(T_{n}\) close to \(T_{0n}\). One can expect that the temperatures at \(t > \tau_{P}\) will change in accordance with Fourier’s law and in the stationary state, achieved when \(t \to \infty\), a uniform temperature distribution will be reached [5]. However, we show here that Fourier’s law cannot be validated in the considered model for \(t \sim \Delta^{-1}\).

Indeed, the energy conservation law can be written in the form similar to Eq. (53) for each mode. In particular, for the first and \(P\)th subsystems they read

\[
C(\omega_k, T_{1k}) \dot{T}_{1k} = -K(\omega_k, T_{2k})(T_{1k} - T_{2k})
\]

and

\[
C(\omega_k, T_{Pk}) \dot{T}_{Pk} = -K(\omega_k, T_{P(T+1)k})(T_{Pk} - T_{(P+1)k})
\]

respectively, and for thenth system, where \(2 \leq n \leq P - 1\), we have

\[
C(\omega_k, T_{nk}) \dot{T}_{nk} = K(\omega_k, T_{(n+1)k})(T_{(n-1)k} - T_{nk}) - K(\omega_k, T_{(n+1)k})(T_{nk} - T_{(n+1)k})
\]

Here

\[
K(\omega_k, T_{nk}) \approx (m + 1/2)\Omega_k \Delta C_k(\omega_k, T_{nk})
\]

FIG. 8: (Color online) Dimensionless thermal current curves when \(\gamma/\omega_0 = 0.5, D/\omega_0 = 1, \Delta/\omega_0 = 0.001, \hbar \omega_0/2k_B T = 1\), and (a) approximation (69) is used; (b) accurate expression (65) is used.

FIG. 9: (Color online) Diagram representation for a chain of nanoparticles (squares) interconnected by the mediating quantum systems (circles).
and $T_{nk} = [T(n-1)k + T_{nk}] / 2$. These equations can be rewritten in the differential form if one introduces a continuous coordinate $x = nd$, where $d$ is the distance between two adjacent subsystems. In this case, (81) can be rewritten as

$$C_k(T_k) \dot{T}_k(x) = K_k(x - d/2)[T_k(x - d) - T_k(x)] - K_k(x + d/2)[T_k(x) - T_k(x + d)],$$  

(83)

which leads to the energy conservation law for each $k$ mode:

$$\dot{C}_k(T_k) \dot{T}_k(x) = \partial_x [\kappa_k(x) \partial_x T_k(x)],$$  

(84)

where $\dot{C}_k = C_k / d$ and $\kappa_k = K_k d$ are the specific heat and thermal conductivity of the $k$th mode of the chain, respectively.

If one considers evolution of the system on a time scale $t \ll \Delta^{-1}$, one can approximate the mode temperatures $T_{nk}$ as $\tilde{T}_n \approx T_0 \approx T_n$ and $\ddot{T}_{nk} \approx \dot{T}_n \approx \ddot{T}_n$ with accuracy $O(\Delta t)$. Here we define a subsystem’s temperature $T_n = T_n(t)$ as $T_{nk}$ averaged over the $k$ modes in accordance to Eq. (62):

$$T_n(t) = \left[ \sum_{k=1}^N C(\nu_k, T_{n0}) \right]^{-1} \sum_{k=1}^N C(\nu_k, T_{nk}) T_{nk}(t).$$  

(85)

With the same accuracy, one can also approximate $C(\omega_k, T_{nk}) \approx C(\omega_k, T_n)$ and $K(\omega_k, T_{nk}) \approx K(\omega_k, T_n)$. Equations (79) - (81) can be rewritten now as

$$C(\omega_k, T_1) \dot{T}_1 = -K(\omega_k, \bar{T}_1)(T_1 - T_2),$$  

(86)

$$C(\omega_k, T_P) \dot{T}_P = -K(\omega_k, \bar{T}_P)(T_P - T_{P-1}),$$  

(87)

and

$$C(\omega_k, T_n) \dot{T}_n = K(\omega_k, \bar{T}_n)[T_{n-1} - T_n] - K(\omega_k, \bar{T}_{n+1})(T_n - T_{n+1}),$$  

(88)

respectively. Summing up each of Eqs. (86) - (88) over all $k$ modes of the system, one arrives at

$$C(T_1) \dot{T}_1 = -K(\bar{T}_2)(T_1 - T_2),$$  

(89)

$$C(T_P) \dot{T}_P = -K(\bar{T}_P)(T_P - T_{P-1}),$$  

(90)

and

$$C_n(T_n) \dot{T}_n = K(\bar{T}_n)(T_{n-1} - T_n) - K(\bar{T}_{n+1})(T_n - T_{n+1}),$$  

(91)

respectively. Here

$$K(\bar{T}_n) = \sum_{k=1}^N K(\omega_k, \bar{T}_n), \quad C(T_n) = \sum_{k=1}^N C(\omega_k, T_n).$$  

(92)

Thus, the above system (89) - (91) is correct if one neglects the contributions of the order of $O(\Delta t)$. In this case, it can be recast in the form of Fourier’s law in the same way as is described above:

$$\dot{C}(T) \dot{T}(x) = \partial_x [\kappa(x) \partial_x T(x)],$$  

(93)

which coincides with Eq. (83) from Ref. [47]. For longer times, when $t \sim \Delta^{-1}$, temperatures of different modes may deviate significantly from each other, as is discussed in the text following Eq. (78). It means that thermal equilibrium in each subsystem shown in Fig. 2 breaks with time and Fourier’s law cannot be validated on the time scale $t \sim \Delta^{-1}$. As we already discussed, a possible way to restore Fourier’s law is to introduce a weak phonon-phonon interaction which may thermalize our subsystems if the condition (63) is satisfied.

It is interesting to notice that in a case when deviations of $T_n$ from their average at $t = 0$ are small, asymptotic values $T_{nk}(t)$ of our system (79) - (81) at $t \rightarrow \infty$ coincide with the corresponding asymptotic values $T_n(t)$ of (89) - (91) as if Fourier’s law were correct at all times $t > \tau_p$. Indeed, assume that

$$\max[T_{0n}] - \min[T_{0n}] \ll \ddot{T} = \frac{1}{P} \sum_{n=1}^P T_{0n},$$  

(94)

In this case, one can approximate

$$C(\omega_k, T_{nk}) \approx C(\omega_k, \bar{T}) = C_k,$$

$$K(\omega_k, T_{nk}) \approx K(\omega_k, \bar{T}) = K_k,$$  

(95)

and the system (79) - (81) can be rewritten as

$$C_k \dot{T}_{1k} = -K_k(T_{1k} - T_{2k}),$$  

(96)

$$C_k \dot{T}_{Pk} = -K_k[T_{Pk} - T_{(P-1)k}],$$  

(97)

and

$$C_k \dot{T}_{nk} = -K_k[2T_{nk} - T_{(n+1)k} - T_{(n-1)k}].$$  

(98)

As one can easily find after summing up Eqs. (96) - (98),

$$\sum_{n=1}^P \ddot{T}_{nk} = 0, \quad \sum_{n=1}^P T_{nk}(t) = C,$$  

(99)

where $C$ is an arbitrary constant. At the same time, as follows already from (79) - (81), $T_{nk}(t)$ reach the following asymptotic at $t \rightarrow \infty$:

$$T_{1k} = T_{2k} = \ldots = T_{Pk} \equiv \bar{T}.$$  

(100)

Thus, using (99) at $t = 0$ and $t = \infty$, one can write

$$\sum_{n=1}^P T_{nk}(0) = C = PT_k, \quad T_k = \bar{T}.$$  

(101)

On the other hand, when (94) is satisfied and if Fourier’s law were correct, one can rewrite system (89) - (91) in the same way:

$$C \ddot{T}_1 = -K(T_1 - T_2), \quad C \ddot{T}_P = -K(T_P - T_{P-1}),$$  

(102)
and
\[ C \dot{T}_n = -K(2T_n - T_{n+1} - T_{n-1}), \quad (103) \]
where
\[ C \approx C(T) \quad \text{and} \quad K \approx K(T). \quad (104) \]
Summing up equations (102) - (103), one finds as before that
\[ \sum_{n=1}^{P} T_n(0) = PT, \quad \text{or} \quad T = \frac{1}{P} \sum_{n=1}^{P} T_n(0) = \bar{T}, \quad (105) \]
where \( T_1 = T_2 = \ldots = T_P \equiv T \) is the asymptotic solution of (89) - (91) when \( t \to \infty \). Thus, the asymptotic for mode temperatures
\[ T_k = T = \bar{T} \quad (106) \]
does not depend on \( k \) and coincides with the asymptotic of (89) - (91), which is a discrete version of Fourier’s law (93).

The chain system discussed above is similar to some extend to chain systems considered in Refs. [52, 53]. In Ref. [52], a weakly coupled chain of many-level identical subsystems is explored. Each subsystem has a band of \( n \sim 1000 \) exited states equally distributed over a bandwidth \( \delta \epsilon \ll \Delta E \), where \( \Delta E \) is the energy gap between the band and a non-degenerate ground state. As was shown, if some conditions on the system Hamiltonian are met (in particular, if \( \lambda \ll \delta \epsilon \ll \Delta E \), where \( \lambda \) is a coupling constant that describes interaction between neighboring subsystems), Fourier’s law can be validated. As was also shown by numerical integrating the Schrödinger equation, no diffusive transport results if these conditions are violated. In Ref. [53], a chain also consisting of identical subsystems \( S_n \) (\( n = 1, 2, \ldots, P \)) is attached by its left-most \( S_1 \) and right-most \( S_N \) subsystems to external environments (very large thermal reservoirs) held at fixed temperatures \( T_L \) and \( T_R \), respectively. It is assumed that there are no interactions in subsystems \( S_n \). As is shown, however, due to the contacts \( S_1 \) and \( S_N \) with the corresponding environments, Fourier’s law can be established in the case of weak enough interaction between \( S_n \)’s. This result is also in accordance with Ref. [54], where Fourier’s law is derived for a general system that satisfies the same conditions as the model (53) does. A model that always exhibits validity of Fourier’s law is the model of self-consistent reservoirs [32, 55, 56]. It is constructed from a harmonic chain of quantum particles placed between two large thermal reservoirs (like in the model [53]) by connecting each quantum particle (subsystem) to a heat bath. Temperatures of these baths are determined by demanding that there is no net heat current between the chain and these reservoirs in the steady-state. The introduction of self-consistent thermal reservoirs introduces dephasing in the system’s dynamics and leads inherently to local equilibrium and onset of Fourier’s law. This is in contrast to the models [52, 53], where the validity of Fourier’s law is not guaranteed depending on the chain Hamiltonian. In particular, it breaks down if the coupling between the subsystems is strong [53].

All these examples, including our chain system, show that the fact that a system is one-dimensional alone does not mean that Fourier’s law is violated. The validity (or violation) of Fourier’s law depends on the Hamiltonian which underlines the type of system’s interactions and their strength.

V. CONCLUSIONS

We have considered the finite-size effects in heat transport between two heat baths mediated by a quantum particle using the generalized quantum Langevin equation. Both heat baths and the quantum system are considered in the harmonic approximation. We derive expressions for the quasi-static heat current for the case when each thermal reservoir comprises of a finite number of modes having a finite mode spacing \( \Delta \). In the limiting case when \( \Delta \to 0 \), the previously obtained expressions for the steady-state heat current and the corresponding heat conductance are restored. The resulting equations that govern long-time (\( t \geq \Delta^{-1} \)) relaxation for the mode temperatures and the average temperatures of the baths are derived and solved. Time dependencies of these temperatures as well as the heat current show peculiarities at \( t \sim \Delta^{-1} \) relaxation for the mode temperatures. Therefore, it is important to notice that recently a new techniques employing quantum dots as temperature probes for measuring the temperature of a nanoparticle has been developed [57]. The temperature information is inferred from the fluorescent intensity of the quantum dots. As the temperature increases, the maximum intensity of the fluorescent signal shifts toward larger wavelengths and its magnitude decreases. Either of these two changes may be used to find nanoparticle’s temperature. This techniques has the potential to verify predictions of our model.

The validity of Fourier’s law for a chain of the finite-size identical subsystems is discussed. On a short time scale, when \( t \ll \Delta^{-1} \), we return to the case considered in Ref. [47] where Fourier’s law was validated. When \( t \sim \Delta^{-1} \), the temperatures of different baths’ modes deviate from each other preventing thermal equilibrium in each subsystem and the validity of Fourier’s law cannot be established. As is found, when deviations of the initial subsystems’ temperatures \( T_n \) from their average value \( \bar{T} \) are small, the \( t \to \infty \) asymptotic values of the mode temperatures do not depend on the mode number and have the same value \( \bar{T} \) as in the case if Fourier’s law were valid for all times.

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APPENDIX

Taking into account our assumption \[15\], one can drop the index \( \nu \) from the frequencies of the baths’ modes, and the dynamical variables \( x_{\nu i}(t), p_{\nu i}(t) \), and \( \eta(t) \) are determined by the following expressions \[18\]:

\[
x_{\nu i}(t) = \sum_{k=0}^{\infty} \sqrt{\frac{\hbar}{2m_{\nu i} \nu_k}} e_k^i (a_{\nu_k}^+ e^{i \nu_k t} + a_{\nu_k} e^{-i \nu_k t}),
\]

\[
p_{\nu i}(t) = m_{\nu i} \dot{x}_{\nu i}(t),
\]

and

\[
\eta(t) = \sum_{k} \sqrt{\frac{\hbar \gamma_{\nu k} \Delta D^2}{2 \pi (D^2 + \nu_k^2)}} \times [e^{i(\phi_k + \nu_k t)} a_k^+ + e^{-i(\phi_k + \nu_k t)} a_k^c], \quad \phi_k \equiv \mp \gamma_{\nu_k}.
\]

Here \( e_k^i \) are orthonormal eigenvectors corresponding to the \( k \)th mode \[18\], which are determined by

\[
e_k^i = \frac{2 \Delta \omega_i \sin[\phi(\omega_k)]}{\pi (\omega_i^2 - \nu_k^2)} \sqrt{\frac{D^2 + \nu_k^2}{D^2 + \omega_i^2}}.
\]

Using these expressions in the averages \( \langle x_{\nu i}(0) \eta(s) + \eta(s) x_{\nu i}(0) \rangle \) and \( \langle p_{\nu i}(0) \eta(s) + \eta(s) p_{\nu i}(0) \rangle \), the formulas for the Bose occupation numbers

\[
\langle a_{\nu_k}^+ a_{\nu_k^c} + a_{\nu_k} a_{\nu_k^c} \rangle = \coth(\nu_k \hbar \beta_k / 2) \delta_{k k_1},
\]

and for the averages \( \langle a_{\nu_k} a_{\nu_k^c} \rangle = \langle a_{\nu_k^c} a_{\nu_k} \rangle = 0 \), one can find

\[
\langle x_{\nu i}(0) \eta(s) + \eta(s) x_{\nu i}(0) \rangle = \sum_k \sqrt{\frac{\hbar^2 \gamma_{\nu k} \Delta D^2}{4 \pi m_{\nu i} (D^2 + \omega_i^2)}} \times \frac{4 \omega_i \sin(\phi(\omega_k)) \Delta}{\pi (\omega_i^2 - \nu_k^2)} \coth(\beta_k \hbar / 2) \cos(\nu_k t + \phi_k),
\]

and

\[
\langle p_{\nu i}(0) \eta(s) + \eta(s) p_{\nu i}(0) \rangle = \sum_k \sqrt{\frac{\hbar^2 \gamma_{\nu k} \Delta D^2}{4 \pi m_{\nu i} (D^2 + \omega_i^2)}} \times \frac{4 \omega_i \sin(\phi(\omega_k)) \Delta}{\pi (\omega_i^2 - \nu_k^2)} \coth(\beta_k \hbar / 2) \sin(\nu_k t + \phi_k).
\]

Substituting \((A11)\) and \((A12)\) in Eq. 39 and using that

\[
\int_0^t g(t - s) \cos(\nu_k s + \phi_k) ds = G_1(\nu_k, t) \cos(\nu_k t + \phi_k) + G(\nu_k, t) \sin(\nu_k t + \phi_k),
\]

and

\[
\int_0^t g(t - s) \sin(\nu_k s + \phi_k) ds = G_1(\nu_k, t) \sin(\nu_k t + \phi_k) - G(\nu_k, t) \cos(\nu_k t + \phi_k),
\]

where

\[
G_1(\nu_k, t) = \int_0^t g(s) \cos(\nu_k s) ds
\]

and

\[
G(\nu_k, t) = \int_0^t g(s) \sin(\nu_k s) ds,
\]

one finds

\[
\langle P_k \rangle = \hbar \gamma_{\nu k} \Delta D^2 \int k \sin(\phi_k) \coth(\beta_k \hbar \nu_k / 2) \times \left\{ \nu_k [G_1(\nu_k, t) + \phi_k - G(\nu_k, t) \cos(\nu_k t + \phi_k)] S_{1k} - [G(\nu_k, t + \phi_k) + G(\nu_k t + \phi_k)] S_{2k} \right\} + J_{\nu k}'.
\]

In \((A17)\), \( S_{2k} = -\dot{S}_{1k} \) and \( S_{1k} = -\partial_{\nu k}^2 S_k \) with

\[
S_k = \sum_i \frac{\Delta \cos(\omega_i t)}{\omega_i^2 - \nu_k^2 (D^2 + \omega_i^2)} = \frac{A_k - B}{D^2 + \nu_k^2}.
\]

Using \[50\], sums \( A_k \) and \( B \) are determined as

\[
A_k(t) = \sum_i \frac{\Delta \cos(\omega_i t)}{\omega_i^2 - \nu_k^2 (D^2 + \omega_i^2)} = \Delta + \pi \cos(\nu_k t + \phi_k) / 2 k \sin(\phi_k)
\]

and

\[
B(t) = \sum_i \frac{\Delta \cos(\omega_i t)}{D^2 + \omega_i^2} = -\frac{\Delta}{D^2} + \frac{\gamma_{\nu k}(t)}{2 D^2}.
\]

where \( \gamma(t) \) is defined by \[14\]. Thus, \( S_k, S_{1,2k} \) can be found. Taking into account \[13\], \[15\], and relation \( \coth(\nu_k \hbar \beta_k / 2) = 1 + 2 n_{\nu_k} \), \( J_{\nu k}' \) cancels out and \((A17)\) results in

\[
J_{th} = -\frac{\hbar \gamma_{\nu k} D^2}{2 \pi} \sum_k \frac{\Delta \nu_k^2 G(\nu_k, t)}{4 \nu_k^2 (D^2 + \omega_k^2)} (n_{1k} - n_{2k}) + \delta J_{th}.
\]

Here

\[
\delta J_{th} = \frac{\hbar^2 D^3}{2 \pi} [\gamma_+(t) \Gamma_+(t) - \gamma_-(t) \Gamma_-(t)]
\]

with

\[
\Gamma_+(t) = \sum_{k=1}^{N} \frac{n_{1k} \sin(\phi_k)(n_{1k} - n_{2k})}{\nu_k^2 + D^2} \times (G_1(\nu_k, t) \sin(\nu_k t + \phi_k) - G(\nu_k, t) \cos(\nu_k t + \phi_k)),
\]

and

\[
\Gamma_-(t) = D \sum_{k=1}^{N} \frac{n_{1k} \sin(\phi_k)(n_{1k} - n_{2k})}{\nu_k^2 + D^2} \times (G_1(\nu_k, t) \cos(\nu_k t + \phi_k) + G(\nu_k, t) \sin(\nu_k t + \phi_k)),
\]

and \( \gamma_+(t) = \exp(-D t) + \exp(-(T - t) D) \) for \( 0 \leq t \leq T \) and continued periodically with the period \( \tau \) beyond this interval. As is clear, \( \gamma_{\pm}(t) \) are non-zero essentially only within the intervals \( n \tau - \tau \leq t \leq n \tau + \tau \). Also, due to the factor \( n_{1k} - n_{2k} \), the short-scale oscillations from \( \delta J_{th} \) are decaying with time and we neglect \( \delta J_{th} \) which results in \[14\].
