Heat Transport in Mesoscopic Chains

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We present an analytical expression for the heat conductance along a harmonic chain connecting two identical reservoirs at different temperatures. In this model, the end points correspond to Brownian particles with different damping coefficients. Such analytical expression for heat conductance allows for direct comparison with experiments in mesoscopic chains as well as validates the ballistic nature of the heat transport in one-dimensional quantum systems. This implies in the absence of a Fourier law for classical and quantum harmonic chains.

Fourier law in classical macroscopic systems is a well-tested phenomenological statement for both liquids and solids. It states that the heat flux density \( J_E \), which is the amount of heat that flows through a unit area per unit time, can be locally expressed as

\[
J_E = -\kappa \nabla T,
\]

where \( \kappa \) is the thermal conductivity and \( T \) the local temperature. Nevertheless, the emergence of this law from purely microscopic considerations remains elusive \[1\]. The main challenge for obtaining such law lies in its dependence on the temperature gradient. Such dependence implies that if we connect two thermal reservoirs by a bar with thermal conductivity \( \kappa \), the heat flux will decrease with the length of the bar. However, since the work of Rieder et al. \[2\], it has been shown that modeling the solid connecting the reservoirs as a harmonic chain leads to a heat flux which is independent of the length of the bar. This implies that the thermal conductivity is proportional to the number of particles in the harmonic chain, thus diverging in the thermodynamic limit. This behavior is known as anomalous heat conduction. Rieder analysis however takes only classical effects into account and relies on approximations on the coupling mechanism with the reservoirs and Gaussian statistics. It was also found an anomalous temperature profile along the bar. The temperature of the bar is constant until we reach oscillators very near the edge where it starts decreasing (increasing) and then sharply increases (decreases) to reach the temperature of the hot (cold) reservoir \[2\]. As pointed out by \[3\], this result is believed to be a feature of integrable systems.

A large effort was made to take into account quantum effects, different coupling mechanisms, mass disorder, and go beyond the Gaussian approximation \[4,14\]. Of particular importance is the work by Segal et al. \[8\] where numerical studies using Restricted Hartree-Fock methods have hinted an \( 1/N \) dependence on the heat flux. However, the exact solution of a linear chain coupled with two distinct reservoirs taking into account the complete non-Gaussian statistics and coloured noise remains elusive \[10,11\]. For a review on the subject, we refer to \[14\].

Another approach to the problem of heat conduction through mesoscopic devices is based on Landauer theory \[15–24\]. Changing the formalism of Landauer theory to phonons, an expression for the heat conduction through a molecular junction was derived \[25,27\]. Also based on the quantization of the electrical conductance \[28,29\], a quantum thermal conductance was proposed \[25,27\] and measured experimentally soon afterwards \[30\].

In this letter, we study the heat transport in mesoscopic systems for both quantum and classical regimes. For such, we consider a chain of harmonic oscillators whose ends are coupled to thermal reservoirs \( L \) and \( R \), held at different temperatures, as shown in Fig 1. In addition to that, we model each reservoir as an ohmic bath of damped harmonic oscillators. For instants of time much longer than both bath relaxation times, the effective dynamics of the chain degrees of freedom can be expressed through the following quantum Langevin equations \[31–33\].

\[
\begin{align*}
\dot{X}_1 + \eta_L \dot{X}_1 - k(X_2 - X_1) &= F_L(t), \\
\dot{X}_j - k(X_{j+1} - 2X_j + X_{j-1}) &= 0, \quad 2 \leq j < N, \\
\dot{X}_N + \eta_R \dot{X}_N + k(X_N - X_{N-1}) &= F_R(t),
\end{align*}
\]

where \( \eta_{L,R} \) are the damping constants, and \( F_{L,R}(t) \) correspond to fluctuating forces which average to zero, though with non-vanishing correlations, that is,

\[
\langle \{ F_a(t), F_b(t') \} \rangle = \frac{\eta_a \delta_{ab}}{\pi} \int_{-\infty}^{\infty} d\omega \coth \left( \frac{\hbar \omega}{2k_B T_a} \right) e^{i\omega(t'-t)},
\]

for \( a, b = L, R \). In Eq. (5), the angle brackets refer to the thermal average (expectation value over the bath degrees of freedom).

Similar versions of this model were already studied using either white noise instead of the coloured noise \[5\]. Born-
Markov approximation (which fails to capture quantum effects like entanglement \[6\] \[10\] \[11\]), numerical methods \[8\] or treating the coupling perturbatively \[7\]. However, we here provide an analytical solution for the heat flux along a chain connecting two identical reservoirs at different temperatures, in the stationary regime. Such expression allows for direct comparison with experiments as well as provides a quantum mechanical description of the heat transfer along the chain.

The stationary regime of this system is achieved when all the energy transferred from the hotter reservoir to the chain corresponds exactly to the entire energy transferred from the chain to the colder reservoir. In other words, the total energy of the chain must remain constant with time. Since the chain energy is defined through the expectation value of the chain Hamiltonian, that is,

\[
E_{\text{chain}} = \left\langle \sum_{j=1}^{N} \frac{m}{2} \dot{X}_j^2 + \sum_{j=1}^{N-1} \frac{k}{2} (X_{j+1} - X_j)^2 \right\rangle,
\]

it is easy to show, using Eqs. (2-4), that

\[
\frac{d}{dt} E_{\text{chain}} = \frac{1}{2} \left[ \left\langle \dot{X}_1(t), F_L(t) \right\rangle \right] - \eta_L \left\langle \dot{X}_1^2(t) \right\rangle + \frac{1}{2} \left[ \left\langle \dot{X}_N(t), F_R(t) \right\rangle \right] - \eta_R \left\langle \dot{X}_N^2(t) \right\rangle.
\]

Since the coupling to both reservoirs dampens the chain normal modes, these oscillators are expected to reach the stationary regime for sufficiently long time regardless of their initial configuration. In this case, the left hand side of Eq. (7) vanishes and we can relate the heat flux from the left reservoir to the left end of the chain, first line of Eq. (7), with the heat flux from the right end of the chain to the right reservoir, second line of Eq. (7). Thus, the heat flux from the left reservoir to the right one can be defined as

\[
J_E = \lim_{t \to \infty} \left[ \frac{1}{2} \left\langle \dot{X}_1(t), F_L(t) \right\rangle \right] - \eta_L \left\langle \dot{X}_1^2(t) \right\rangle = \lim_{t \to \infty} \left[ \frac{1}{2} \left\langle \dot{X}_N(t), F_R(t) \right\rangle \right] - \eta_R \left\langle \dot{X}_N^2(t) \right\rangle.
\]

Because all the normal modes die out for sufficiently long times, the expectation value coincides with the thermal average.

The scope of this letter is to provide an analytic expression for Eq. (8), hence it is convenient to assume the chain was put in contact to both reservoirs in the far past, i.e., \( t \to -\infty \). Therefore, we can neglect the contribution from the oscillators initial configuration, given that the normal modes decay after some time. This allows us to solve the Eqs. (2-4) via Fourier transform in time, instead of Laplace transform. Let us denote the Fourier transform of the variables by a tilde on top of them.

In order to decouple the set of Eqs. (2-4), let us define the operator valued analytic function

\[
\mathcal{X}(z, \omega) := \sum_{j=1}^{N} \tilde{X}_j(z, \omega) z^j.
\]

This is the finite version of the so-called Z-transform, which is used in signal processing. From this definition, \( \mathcal{X}(z, \omega) \) must vanish at infinity and cannot have any pole of order \( N + 1 \) or higher at \( z = \infty \). The latter imposes that

\[
\oint \mathcal{X}(z, \omega) z^{N+n} dz = 0,
\]

for any non-negative integer \( n \). As a consequence of the Residue Theorem, for any contour \( C \) that encloses \( z = 0 \), we obtain

\[
\tilde{X}_j(\omega) = \frac{1}{2 \pi i} \oint_C \mathcal{X}(z, \omega) z^{j-1} dz, \quad 1 \leq j \leq N.
\]

After some algebra, one can show that \( \mathcal{X}(z, \omega) \) depends only on the endpoint positions, \( \tilde{X}_1 \) and \( \tilde{X}_N \) as well as on the fluctuation forces, \( \tilde{F}_L \) and \( \tilde{F}_R \), i.e.,

\[
\mathcal{X}(z) = \left( \frac{z - 1 - i \eta_L \omega}{k} \right) \tilde{X}_1 + \left( \frac{1}{z} - 1 - i \eta_R \omega \right) \tilde{X}_N z^{N-1} - \frac{\tilde{F}_L + \tilde{F}_R z^{1-N}}{k z^2 - (2 - m \omega^2) z + 1}.
\]

At this point, it is convenient to introduce the parametrization \( \omega = 2 \omega_0 \sin \frac{\theta}{2} \), where \( \omega_0 = \sqrt{k/m} \). This redefinition simplifies the calculation of residues, given that the denominator can be expressed in terms of Chebyshev polynomials of second kind, namely

\[
\frac{1}{z^2 - 2z \cos \theta + 1} = \sum_{n=1}^{\infty} \frac{\sin(n \theta)}{\sin \theta} z^{n-1}.
\]

Taking \( j = N \) in Eq. (12) allows us to express \( \tilde{X}_N \) in terms of \( \tilde{X}_1 \) and \( \tilde{F}_L \), that is,

\[
\tilde{X}_N(\omega) = \frac{\tilde{X}_1(\omega)}{\sin \theta} \left[ \sin(N \theta) - \left( 1 + \frac{i \eta_L \omega}{k} \right) \sin \left( (N - 1) \theta \right) \right] - \frac{\tilde{F}_L(\omega)}{k \sin \theta} \sin \left( (N - 1) \theta \right).
\]

Plugging Eq. (14) into Eq. (13) and imposing Eq. (11), we are able to express \( \tilde{X}_1 \) solely in terms of \( \tilde{F}_L \) and \( \tilde{F}_R \). Thus, the expression for \( \tilde{X}_1 \) can be written as

\[
\tilde{X}_1(\omega) = A(\omega) \tilde{F}_L(\omega) + B(\omega) \tilde{F}_R(\omega),
\]

with

\[
B(\omega) = -\cos \frac{\theta}{2},
\]

\[
A(\omega) = \frac{i \eta_R}{m \omega_0} \sin \left( (N - 1) \theta \right) - \cos \left( (N - \frac{1}{2}) \theta \right),
\]

\[
D(\omega) = m \omega_0 \sin(N \theta) + i(\eta_L + \eta_R) \cos \left( (N - \frac{1}{2}) \theta \right) + \frac{\eta_L \eta_R}{m \omega_0} \sin \left( (N - 1) \theta \right).
\]
Here, $\theta$ must be viewed as an implicit function of $\omega$. Plugging expression (15) into Eq. (8) and using Eq. (5), we end up with

$$J_E = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{h\omega \eta_L}{D(\omega)D(-\omega)} \left\{ \coth \left( \frac{h\omega}{2k_BT_L} \right) \eta_R B(\omega) B(-\omega) \right\}.$$

(19)

For more details, check the Supplementary Material (SM) [35]. Expression (15) is an integral from minus to plus infinity in the variable $\omega$. However, the whole integrand is a function of $\theta$ and, when $|\omega| \geq 2\omega_0$, $\theta$ becomes complex. We can invert the relationship between $\omega$ and $\theta$ by restricting ourselves to the principal branch of the logarithm function (on the upper-half complex plane), that is,

$$\theta = \begin{cases} -2i \ln \left( \frac{\omega}{2\omega_0} + \sqrt{1 - \frac{\omega^2}{4\omega_0^2}} \right), & \text{for } |\omega| \leq 2\omega_0, \\ \pi + 2i \ln \left( \frac{\omega}{2\omega_0} + \sqrt{1 - \frac{\omega^2}{4\omega_0^2}} - 1 \right), & \text{for } \omega > 2\omega_0, \\ -\pi + 2i \ln \left( -\frac{\omega}{2\omega_0} + \sqrt{1 - \frac{\omega^2}{4\omega_0^2}} - 1 \right), & \text{for } \omega < -2\omega_0. \end{cases}$$

(20)

From Eq. (20), one can see that $\theta(-\omega) = -\theta^*(\omega)$. It is not easy to write the integrand explicitly in terms of $\omega$, therefore, to study (19), we express this integral as a contour integral in the complex plane as shown in Fig. 2. Using this contour (C) the final expression for the heat flux is given by

$$J_E = \frac{h\omega_0^2 \eta_L \eta_R}{\pi} \int_C d\theta \frac{\sin \frac{\theta}{2} \cos \frac{\theta}{2}}{m\omega_0 \sin((N-1)\theta) + \frac{\eta_L + \eta_R}{m\omega_0} \sin((N)\theta)} \left[ \coth \left( \frac{h\omega}{k_BT_L} \sin \left( \frac{\theta}{2} \right) \right) - \coth \left( \frac{h\omega}{k_BT_R} \sin \left( \frac{\theta}{2} \right) \right) \right].$$

(21)

The expression (21) can be either expressed as the sum over all the integrand residues “inside” the contour $C$, or broken up into two real integrals. For more details, check the SM [35]. Here it is convenient to introduce the Debye temperature $T_D := \frac{2h\omega_0}{k_B}$. This definition differs slightly from the one in textbooks, since we are neglecting the contribution from transverse phonons.

Notice that the full expression for the heat flux (21) is not proportional to the temperature difference $\Delta T$, but it is instead proportional to the difference between the Bose-Einstein distributions of each reservoir (which can be expressed in terms of hyperbolic cotangents). In the limit of small temperature difference, $\Delta T \ll T, T_D$, we can define the one-dimensional thermal conductance by

$$\mathcal{K} := \frac{h\eta_L \eta_R T_D}{\pi m^2 T^2} \int_C d\theta \frac{\sin \frac{\theta}{2} \cos \frac{\theta}{2} \csch^2 \left( \frac{T_D}{2T} \sin \left( \frac{\theta}{2} \right) \right)}{\sin((N-1)\theta) + \frac{4h^2 \eta_L + \eta_R}{m^2 k_BT_D^2} \sin((N)\theta)} + 4h^2 \left( \frac{\eta_L + \eta_R}{mk_BT_D} \right)^2 \cos^2 \left( (N - \frac{1}{2}) \theta \right).$$

(22)

Although the chain size do not appear explicitly in this formula, one has to remember that, for macroscopic systems, the mass $m$ should be replaced by the linear mass density of the rod multiplied by its length. In order to study the heat conductance without specific considerations about the materials, it is useful to define dimensionless quantities such as $\Theta = T/T_D$, $\alpha_{L,R} = h\eta_{L,R}/mk_BT_D$, as well as the dimensionless heat conductance $\mathcal{K} = \pi \mathcal{K}/k_D^2 T_D$. In terms of these new variables we can express (22) as the sum of two real integrals as

\[
\mathcal{K} := \frac{h\eta_L \eta_R T_D}{\pi m^2 T^2} \int_C d\theta \frac{\sin \frac{\theta}{2} \cos \frac{\theta}{2} \csch^2 \left( \frac{T_D}{2T} \sin \left( \frac{\theta}{2} \right) \right)}{\sin((N-1)\theta) + \frac{4h^2 \eta_L + \eta_R}{m^2 k_BT_D^2} \sin((N)\theta)} + 4h^2 \left( \frac{\eta_L + \eta_R}{mk_BT_D} \right)^2 \cos^2 \left( (N - \frac{1}{2}) \theta \right) \text{.}
\]
Variables $\alpha_{L,R}$ describe the strength of the coupling between the harmonic chain and the left (right) thermal reservoir. Underdamped dynamics is obtained when $\alpha < 1$, whereas the overdamped one refers to $\alpha > 1$. The reduced temperature scale $\Theta$ describes the system in the quantum regime when $\Theta \ll 1$ or classical limit $\Theta \sim 1$.

Hence, we show through the analytic expression (22) that the Fourier law cannot be achieved for a harmonic chain without disorder. This corroborates a well-known result in the literature of 1D systems (see, for example, [3], and references therein) which states that, due to the existence of several conserved quantities, integrable systems always present ballistic heat transport. The so-called normal transport, $J_E \sim N^{-1}$, results from the non-conservation of linear momentum due either to a one-body pinning potential or inelastic (dissipative) effects. Here we should remark that the dissipative motion of the endpoints of our harmonic chain affects at most its boundary effects.

The exact solution given by equations (22) or (23) is the fingerprint of heat transport in harmonic chains and allows for direct comparison with experiments. We suspect that they can be used to test the validity of the harmonic approximation in mesoscopic systems such as gold nanowires.

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FIG. 3. Heat conductance given by equation (23) as a function of $N$ for different temperatures and damping parameters, i.e., a) $\alpha_L = \alpha_R = 0.2$, b) $\alpha_L = 0.2$ and $\alpha_R = 5$ and c) $\alpha_L = \alpha_R = 5$. As one can see from Fig. 3, the thermal conductance of this model saturates for large $N$, which refers to a ballistic transport.

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SUPPLEMENTARY MATERIAL FOR: “HEAT TRANSPORT IN MESOSCOPIC CHAINS”

HEAT FLUX

As shown in Eq. (8), the heat flux can be obtained solely through the asymptotic behavior of $\dot{X}_1(t)$ and $F_L(t)$. From Eq. (15), we can express $\dot{X}_1(t)$ as

$$\dot{X}_1(t) = \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \dot{X}_1(\omega) e^{-i\omega t} = \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} dt' \frac{e^{-i\omega(t-t')}}{iD(\omega)} [A(\omega)F_L(t')+B(\omega)F_R(t')] ,$$

where $B(\omega)$, $A(\omega)$ and $D(\omega)$ are given by Eqs. (16-18) respectively. Plugging Eq. (24) into Eq. (8), we end up with

$$J_E = \lim_{t \to \infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dt'' e^{i\omega(\tau-\tau')} e^{i\omega'/(\tau'-\tau')} \frac{\tau'}{2D(\omega')} \frac{\tau''}{2D(\omega)} [A(\omega) \left( \eta_L A(\omega') - iD(\omega') \right) \left\{ \tilde{F}_L(t''), \tilde{F}_R(t') \right\}]$$

$$+ \eta_L B(\omega) B(\omega') \left\{ \tilde{F}_R(t''), \tilde{F}_R(t') \right\} .$$

Using Eq. (5), one can show that Eq. (25) reduces to Eq. (19), i.e.,

$$J_E = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\hbar \omega \eta_L}{D(\omega) D(-\omega)} \left[ \coth \left( \frac{\hbar \omega}{2k_B T_R} \right) \eta_R B(\omega) B(-\omega) + \coth \left( \frac{\hbar \omega}{2k_B T_L} \right) A(-\omega) \eta_L A(-\omega) - iD(\omega) \right] .$$

Since $A(\omega)$, $B(\omega)$ and $D(\omega)$ are implicit functions of $\omega$, it is convenient to change the integration variable from $\omega$ to $\theta$. For $|\omega| \leq 2\omega_0$, $\theta = 2 \arcsin \left( \frac{\omega}{2\omega_0} \right)$ is real and belongs to the interval $[-\pi, \pi]$. However, for $|\omega| > 2\omega_0$, $\theta = 2 \arcsin \left( \frac{\omega}{2\omega_0} \right)$ cannot be a real number. To see that, we must express $\theta(\omega)$ in terms of the logarithm function

$$\theta = 2 \arcsin \left( \frac{\omega}{2\omega_0} \right) = -2i \ln \left( \frac{i\omega}{2\omega_0} + \sqrt{1 - \frac{\omega^2}{4\omega_0^2}} \right) .$$

If we restrict ourselves to the logarithm principal branch, we can see that there are two possible choices for $\theta$ when $\omega > 2\omega_0$,

$$\theta = \pi + 2i \ln \left( \frac{\omega}{2\omega_0} \pm \sqrt{\frac{\omega^2}{4\omega_0^2} - 1} \right) = \pi + 2i \ln \left( \frac{\omega}{2\omega_0} + \sqrt{\frac{\omega^2}{4\omega_0^2} - 1} \right) ,$$

and other two for $\omega < 2\omega_0$,

$$\theta = -\pi + 2i \ln \left( -\frac{\omega}{2\omega_0} \pm \sqrt{\frac{\omega^2}{4\omega_0^2} - 1} \right) = \pi + 2i \ln \left( -\frac{\omega}{2\omega_0} + \sqrt{\frac{\omega^2}{4\omega_0^2} - 1} \right) ,$$

Therefore, there are 4 possible ways to analytically continue $\arcsin \left( \frac{\omega}{2\omega_0} \right)$ for $|\omega| > 2\omega_0$ and the final result must be independent of this choice. In this work, we choose to analytically continue $\theta$ to the upper-half plane, as shown in Eq. (20), i.e.,

$$\theta = \begin{cases} -2i \ln \left( \frac{i\omega}{2\omega_0} + \sqrt{1 - \frac{\omega^2}{4\omega_0^2}} \right), & \text{for} \ |\omega| < 2\omega_0, \\ \text{sgn}(\omega) \pi, & \text{for} \ |\omega| = 2\omega_0, \\ \text{sgn}(\omega) \pi + 2i \ln \left( \frac{|\omega|}{2\omega_0} + \sqrt{\frac{|\omega|^2}{4\omega_0^2} - 1} \right), & \text{for} \ |\omega| > 2\omega_0. \end{cases}$$

As a contour integral in the complex plane as shown in Fig. 2. Let us denote such contour by $C$, then the heat flux becomes

$$J_E = \frac{\hbar \omega_0 \eta_l}{2\pi} \oint_{C} d\theta \sin \theta \frac{d\theta}{D(\theta) D(-\theta^*)} \left\{ \coth \left[ \frac{\hbar \omega_0 \sin \left( \frac{\theta}{2} \right)}{k_B T_R} \right] \eta_R B(\theta) B(-\theta^*) + \coth \left[ \frac{\hbar \omega_0 \sin \left( \frac{\theta}{2} \right)}{k_B T_L} \right] A(-\theta^*) [\eta_L A(\theta) - iD(\theta)] \right\} .$$

(29)
Let us now write \( \theta = \varphi + i \xi \) and let us break the integral in its 3 parts, as shown in Fig. 2. The second piece (II) is simply the integral over the interval \((-\pi, \pi)\). Therefore, from

\[
B(\varphi)B(-\varphi) = \cos^2(\frac{\varphi}{2}) = B^2(\varphi),
\]

\[
A(-\varphi) [\eta_L A(\varphi) - iD(\varphi)] = -\eta_R \cos^2(\frac{\varphi}{2}) + i \cos ((N - \frac{1}{2})\varphi) \left[ \frac{\eta_R^2}{m\omega_0} \sin ((N - 1)\varphi) - m\omega_0 \sin(N\varphi) \right], \tag{31}
\]

we find that

\[
\text{II} = \frac{\hbar \omega_0^2 \eta_L \eta_R}{2\pi} \int_{-\pi}^{\pi} \frac{d\varphi \sin \varphi}{D(\varphi)D(-\varphi)} B^2(\varphi) \left\{ \coth \left[ \frac{\hbar \omega_0 \sin(\frac{\varphi}{2})}{k_BT_R} \right] - \coth \left[ \frac{\hbar \omega_0 \sin(\frac{\varphi}{2})}{k_BT_L} \right] \right\}, \tag{32}
\]

since the imaginary part of Eq. (31) vanishes when integrated on a symmetric domain. Let us now turn our attention to the first piece (I) of the contour. Using that

\[
B(\pi + i\xi)B(\pi + i\xi) = \sinh^2(\frac{\xi}{2}) = -B^2(\pi + i\xi), \tag{33}
\]

\[
A(\pi + i\xi) [\eta_L A(\pi + i\xi) - iD(\pi + i\xi)] = -\eta_R \sinh^2(\frac{\xi}{2}) + i \sinh ((N - \frac{1}{2})\xi) \left[ \frac{\eta_R^2}{m\omega_0} \sinh ((N - 1)\xi) + m\omega_0 \sinh(N\xi) \right], \tag{34}
\]

together with \( D(\pi + i\xi) = -D(\pi - i\xi) \), we obtain

\[
I = \frac{\hbar \omega_0^2 \eta_L \eta_R}{2\pi} \int_{0}^{\infty} \frac{d\xi \sinh \xi}{D(\pi + i\xi)D(-\pi - i\xi)} B^2(-\pi + i\xi) \left\{ \coth \left[ -\frac{\hbar \omega_0 \cosh(\frac{\xi}{2})}{k_BT_R} \right] - \coth \left[ -\frac{\hbar \omega_0 \cosh(\frac{\xi}{2})}{k_BT_L} \right] \right\} \
- i \frac{\hbar \omega_0^2 \eta_L}{2\pi} \int_{0}^{\infty} \frac{d\xi \sinh \xi \sin((N - \frac{1}{2})\xi)}{D(\pi + i\xi)D(\pi + i\xi)} \left[ \frac{\eta_R^2}{m\omega_0} \sinh ((N - 1)\xi) + m\omega_0 \sinh(N\xi) \right] \coth \left[ -\frac{\hbar \omega_0 \cosh(\frac{\xi}{2})}{k_BT_L} \right]. \tag{35}
\]

Finally, let us focus on the third (III) and last piece. For that, we must consider that

\[
B(\pi + i\xi)B(-\pi + i\xi) = \sinh^2(\frac{\xi}{2}) = -B^2(\pi + i\xi), \tag{36}
\]

\[
A(-\pi + i\xi) [\eta_L A(\pi + i\xi) - iD(\pi + i\xi)] = -\eta_R \sinh^2(\frac{\xi}{2}) + i \sinh ((N - \frac{1}{2})\xi) \left[ \frac{\eta_R^2}{m\omega_0} \sinh ((N - 1)\xi) + m\omega_0 \sinh(N\xi) \right], \tag{37}
\]

and that \( D(\pi + i\xi) = -D(\pi - i\xi) \). Hence, we get

\[
III = \frac{\hbar \omega_0^2 \eta_L \eta_R}{2\pi} \int_{0}^{\infty} \frac{d\xi \sinh \xi}{D(\pi + i\xi)D(-\pi - i\xi)} B^2(\pi + i\xi) \left\{ \coth \left[ \frac{\hbar \omega_0 \cosh(\frac{\xi}{2})}{k_BT_R} \right] - \coth \left[ \frac{\hbar \omega_0 \cosh(\frac{\xi}{2})}{k_BT_L} \right] \right\} \
+ i \frac{\hbar \omega_0^2 \eta_L}{2\pi} \int_{0}^{\infty} \frac{d\xi \sinh \xi \sin((N - \frac{1}{2})\xi)}{D(\pi + i\xi)D(\pi + i\xi)} \left[ \frac{\eta_R^2}{m\omega_0} \sinh ((N - 1)\xi) + m\omega_0 \sinh(N\xi) \right] \coth \left[ \frac{\hbar \omega_0 \cosh(\frac{\xi}{2})}{k_BT_L} \right]. \tag{38}
\]

Adding Eqs. (35), (32) and (38), the heat flux can be written as contour integral of an analytic function of \( \theta \)

\[
J_E = \frac{\hbar \omega_0^2 \eta_L \eta_R}{\pi} \int_{C} d\theta \left[ \coth \left( \frac{\hbar \omega_0}{k_BT_R} \sin(\theta) \right) - \coth \left( \frac{\hbar \omega_0}{k_BT_L} \sin(\theta) \right) \right].
\]

\[
J_E = \frac{\hbar \omega_0^2 \eta_L \eta_R}{\pi} \int_{C} d\theta \left[ \coth \left( \frac{\hbar \omega_0}{k_BT_R} \sin(\theta) \right) - \coth \left( \frac{\hbar \omega_0}{k_BT_L} \sin(\theta) \right) \right] \left[ \frac{\eta_R^2}{m\omega_0} \sin(N\theta) + \frac{\eta_L \eta_R}{m\omega_0} \sin((N - 1)\theta) \right]^2 + \left( \eta_L + \eta_R \right)^2 \cos^2 \left( \frac{(N - \frac{1}{2})\theta}{2} \right). \tag{39}
\]
We can rewrite Eq. (39) explicitly as

\[ J_E = \frac{2\hbar \omega_0 \eta_L \eta_R}{\pi} \int_0^\pi \, d\varphi \, \sin \frac{\varphi}{2} \cos^3 \left( \frac{\varphi}{2} \right) \frac{\coth \left( \frac{T_D}{2T_R} \sin \left( \frac{\varphi}{2} \right) \right) - \coth \left( \frac{T_D}{2T_L} \sin \left( \frac{\varphi}{2} \right) \right)}{m\omega_0 \sin (N\varphi) + \eta_L \eta_R m\omega_0 \sin((N-1)\varphi)} \]

\[- \frac{2\hbar \omega_0^2 \eta_L \eta_R}{\pi} \int_0^\infty \, d\xi \, \sinh^3 \left( \frac{\xi}{2} \right) \cosh \frac{\xi}{2} \frac{\coth \left( \frac{T_D}{2T_R} \cosh \left( \frac{\xi}{2} \right) \right) - \coth \left( \frac{T_D}{2T_L} \cosh \left( \frac{\xi}{2} \right) \right)}{m\omega_0 \sin (N\xi) - \eta_L \eta_R m\omega_0 \sinh((N-1)\xi)} \]

where \( T_D := \frac{2\hbar \omega_0}{k_B} \) is the Debye temperature.