Heat transport in ordered harmonic lattices

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Abstract

We consider heat conduction across an ordered oscillator chain with harmonic interparticle interactions and also onsite harmonic potentials. The onsite spring constant is the same for all sites excepting the boundary sites. The chain is connected to Ohmic heat reservoirs at different temperatures. We use an approach following from a direct solution of the Langevin equations of motion. This works both in the classical and quantum regimes. In the classical case we obtain an exact formula for the heat current in the limit of system size $N \to \infty$. In special cases this reduces to earlier results obtained by Rieder, Lebowitz and Lieb and by Nakazawa. We also obtain results for the quantum mechanical case where we study the temperature dependence of the heat current. We briefly discuss results in higher dimensions.

Key words: Harmonic crystal; Langevin equations; Ohmic baths; Heat Conduction

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1 Introduction

Rieder, Lebowitz and Lieb [1] (RLL) considered the problem of heat conduction across a one-dimensional ordered harmonic chain connected to stochastic heat baths at the two ends. The main results of this paper were: (i) the temperature in the bulk of the system was a constant equal to the mean of the two bath temperatures, (ii) the heat current approaches a constant value for large system sizes and an exact expression for this was obtained. RLL considered the case where only interparticle potentials were present. Nakazawa [2] (N) extended these results to the case with a constant onsite harmonic potential at all sites and also to higher dimensions.

The approach followed in both the RLL and N papers was to obtain the exact nonequilibrium stationary state measure which, for this quadratic problem, is a Gaussian distribution. A complete solution for the correlation matrix was obtained and from this one could obtain both the steady state temperature profile and the heat current.

In this paper we use a different formalism to calculate the heat current in ordered harmonic lattices connected to Ohmic reservoirs (for a classical system this is white noise Langevin dynamics). The formalism has been discussed in detail in [3, 4] and follows from a direct solution, by Fourier transforms, of the Langevin equations of motion. A general formal expression for the heat current can be obtained and this has the form of an integral of the heat transmitted over all frequencies. For the one-dimensional case this expression for current was first obtained by Casher and Lebowitz [5] using different methods. An advantage of the approach used here is that it can be easily generalized to the quantum mechanical regime [4, 6, 7, 8, 9]. As shown in [4] the results obtained are identical to those obtained using the nonequilibrium Green's function method [10, 11]. Here we show how exact expressions for the asymptotic current ($N \to \infty$) can be obtained from this approach. We also briefly discuss the model in the quantum regime and extensions to higher dimensions.

The model we consider here is slightly different from the Nakazawa model. We consider the pinning potentials at the boundary sites to be different from the bulk sites. This allows us to obtain both the RLL and N results as limiting cases. Also it seems that this model more closely mimics the experimental situation. In experiments the boundary sites would be interacting with fixed reservoirs which can be modeled by an effective spring constant that is expected to be different from the interparticle spring constant in the bulk. We also note here that the constant onsite potential present along the wire relates to experimental situations such as that of heat transport in a molecular wire attached to a substrate or, in the two-dimensional case, a monolayer on a substrate. Another example would be the heat current contribution from the optical modes of a polar crystal.

The paper is organized as follows. In Sec.2 we introduce the model and derive the main results of the paper. In Sec.3 we present results for the quantum mechanical case and in Sec.4 generalizations to the higher dimensional case. Finally we conclude with a short discussion in Sec.5.

2 Model and results in the classical case

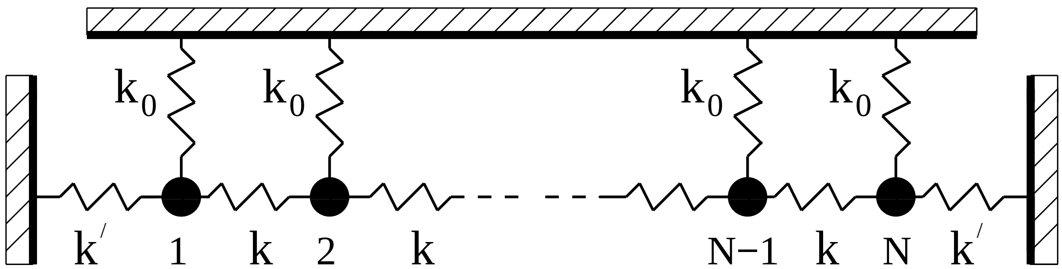

Figure 1: A schematic description of the model.

We consider N particles of equal masses m connected to each other by harmonic springs of equal spring constants k. The particles are also pinned by onsite quadratic potentials with strengths k_o at all sites except the boundary sites where the pinning strengths are $k_o + k'$ [see Fig. (1)]. The Hamiltonian of the harmonic chain is thus:

$$H = \sum_{l=1}^{N} [\frac{1}{2} m \dot{x}_l^2 + \frac{1}{2} k_o x_l^2] + \sum_{l=1}^{N-1} \frac{1}{2} k (x_{l+1} - x_l)^2 + \frac{1}{2} k' (x_1^2 + x_N^2) \ , \tag{2.1}$$

where x_l denotes the displacement of the particle at site l from its equilibrium position. The particles 1 and N at the two ends are immersed in heat baths at temperature T_L and T_R respectively. The heat baths are assumed to be modeled by Langevin equations corresponding to Ohmic baths. In the classical case the steady state heat current from left to right reservoir is given by [3, 5] :

$$\begin{aligned}
J_C &= \frac{k_B (T_L - T_R)}{\pi} \int_{-\infty}^{\infty} d\omega \ \mathcal{T}_N(\omega), \qquad (2.2) \\
\text{where } \mathcal{T}_N(\omega) &= \gamma^2 \omega^2 |G_{1N}|^2 \ , \\
G &= [-m\omega^2 I + \Phi - \Sigma]^{-1} \ , \\
\Phi_{lm} &= (k + k' + k_o) \ \delta_{l,m} - k \ \delta_{l,m-1} \qquad \text{for} \quad l = 1 \ , \\
&= -k \ \delta_{l,m+1} + (2k + k_o) \ \delta_{l,m} - k \ \delta_{l,m-1} \quad \text{for} \quad 2 \le l \le N-1 \ , \\
&= (k + k' + k_o) \ \delta_{l,m} - k \ \delta_{l,m+1} \qquad \text{for} \quad l = N \ , \\
\Sigma_{lm} &= i\gamma\omega \delta_{lm} [\delta_{l1} + \delta_{lN}] \ ,
\end{aligned}$$

and I is a unit matrix. We now write $G = Z^{-1}/k$, where Z is a tri-diagonal matrix with $Z_{11} = Z_{NN} = (k + k_o + k' - m\omega^2 - i\gamma\omega)/k$, all other diagonal elements equal to $2 + k_o/k - m\omega^2/k$ and all off-diagonal elements equal to -1. Then it can be shown easily that $|G_{1N}(\omega)| = 1/(k\ |\Delta_N|)$ where Δ_N is the determinant of the matrix Z. This is straightforward to obtain and after some rearrangements we get:

$$\begin{aligned} \Delta_N &= [a(q)\sin Nq + b(q)\cos Nq]/\sin q \ , \qquad (2.3) \\ \text{where} \ \ a(q) &= [2 - \frac{\gamma^2\omega^2}{k^2} + \frac{k'^2}{k^2} - \frac{2k'}{k}]\cos q + \frac{2k'}{k} - 2 - \frac{2i\gamma\omega}{k}[1 + (\frac{k'}{k} - 1)\cos q] \ , \\ b(q) &= [\frac{\gamma^2\omega^2}{k^2} - \frac{k'^2}{k^2} + \frac{2k'}{k}]\sin q + \frac{2i\gamma\omega}{k}(\frac{k'}{k} - 1)\sin q \ , \end{aligned}$$

and q is given by the relation $2k\cos q = -m\omega^2 + k_o + 2k$. This relation implies that for frequencies outside the phonon band $k_o \leq m\omega^2 \leq k_o + 2k$ the wavevector q becomes imaginary and hence the transmission coefficient $\mathcal{T}(\omega)$ decays exponentially with N. Hence for large N we need only consider the range $0 < q < \pi$ and the current is given by:

$$J_C = \frac{2\gamma^2 k_B(T_L - T_R)}{k^2\pi}\int_0^\pi dq|\frac{d\omega}{dq}|\ \frac{\omega_q^2}{|\Delta_N|^2} \ , \qquad (2.4)$$

with $m\omega_q^2 = k_o + 2k[1 - \cos(q)]$. Now we state the following result:

$$\lim_{N\to\infty}\int_0^\pi dq\frac{g_1(q)}{1 + g_2(q)\sin Nq} = \int_0^\pi dq\frac{g_1(q)}{[1 - g_2^2(q)]^{1/2}} \ , \qquad (2.5)$$

where $g_1(q)$ and $g_2(q)$ are any two well-behaved functions. This result can be proved by making an expansion of the factor $1/[1 + g_2(q)\sin(Nq)]$ (valid for $|g| < 1$ in the integration range), taking the $N \to \infty$ limit and resumming the resulting series. Noting now that Δ_N can be written as $|\Delta_N|^2 = (|a|^2 + |b|^2)[1 + r\sin(2Nq + \phi)]/[2\sin^2(q)]$ where $r\cos\phi = (ab^* + a^*b)/(|a|^2 + |b|^2)$, $r\sin\phi = (|b|^2 - |a|^2)/(|a|^2 + |b|^2)$, we see that Eq. (2.4) has the same structure as the left hand side of Eq. (2.5). Hence using Eq. (2.5) and after some simplification, we finally get:

$$\begin{aligned} J_C &= \frac{\gamma k^2 k_B(T_L - T_R)}{\pi m}\int_0^\pi \frac{\sin^2 q\ dq}{\Lambda - \Omega\cos q} \\ &= \frac{\gamma k^2 k_B(T_L - T_R)}{m\Omega^2}(\Lambda - \sqrt{\Lambda^2 - \Omega^2}) \ , \qquad (2.6) \\ \text{where} \ \ \Lambda &= 2k(k - k') + k'^2 + \frac{(k_o + 2k)\gamma^2}{m} \ \ \text{and} \ \ \Omega = 2k(k - k') + \frac{2k\gamma^2}{m} \ . \end{aligned}$$

Eq. (2.6) is the central result of this paper. We now show that two different special cases lead to the RLL and N results. First in the case of fixed ends and without onsite potentials, *i.e.* $k' = k$ and $k_o = 0$, we recover the RLL result [1]:

$$J_C^{RLL} = \frac{k k_B (T_L - T_R)}{2\gamma} \left[1 + \frac{\nu}{2} - \frac{\nu}{2} \sqrt{1 + \frac{4}{\nu}} \right] \quad \text{where} \quad \nu = \frac{mk}{\gamma^2} \ . \tag{2.7}$$

The case $k' = k, k_o \neq 0$ can also be obtained using the RLL approach [12] and agrees with the result in Eq. (2.6). In the other case of free ends, *i.e.* $k' = 0$, we get the N result [2]:

$$J_C^N = \frac{k \gamma k_B (T_L - T_R)}{2(mk + \gamma^2)} \left[1 + \frac{\lambda}{2} - \frac{\lambda}{2} \sqrt{1 + \frac{4}{\lambda}} \right] \quad \text{where} \quad \lambda = \frac{k_o \gamma^2}{k(mk + \gamma^2)} \ . \tag{2.8}$$

3 Quantum mechanical case

In the quantum case the heat current across a chain described by the Hamiltonian Eq. (2.1) and connected to Ohmic heat baths is given by [4]:

$$J_Q = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \ \hbar \omega \mathcal{T}_N(\omega) [f(\omega, T_L) - f(\omega, T_R)] \ , \tag{3.1}$$

where $f(\omega, T) = 1/[e^{\hbar\omega/(k_B T)} - 1]$ is the phonon distribution function and $\mathcal{T}_N$ is as given in Eq. (2.2). Here we consider the linear response regime where the applied temperature difference $\Delta T = T_L - T_R << T$ with $T = (T_L + T_R)/2$. Expanding the phonon distribution functions $f(\omega, T_{L,R})$ about the mean temperature T we get the following expression for the current:

$$J_Q = \frac{k_B (T_L - T_R)}{\pi} \int_{-\infty}^{\infty} d\omega \ \left(\frac{\hbar \omega}{2 k_B T} \right)^2 \operatorname{cosech}^2 \left(\frac{\hbar \omega}{2 k_B T} \right) \mathcal{T}(\omega) \ . \tag{3.2}$$

We then proceed through the same asymptotic analysis as in the previous section and get, in the limit $N \to \infty$:

$$\begin{aligned} J_Q &= \frac{\gamma k^2 \hbar^2 (T_L - T_R)}{4\pi k_B m T^2} \int_0^{\pi} dq \frac{\sin^2 q}{\Lambda - \Omega \cos q} \ \omega_q^2 \operatorname{cosech}^2 \left(\frac{\hbar \omega_q}{2 k_B T} \right), \qquad (3.3) \\ \text{where} \ \ \omega_q^2 &= [k_o + 2k(1 - \cos q)]/m \ . \end{aligned}$$

We are not able to perform the above integral exactly. Numerically it is easy to obtain the integral for given parameter values and here we examine the temperature dependence of the current (note that in the classical case the current depends only on the temperature difference). In Fig.(2) we plot the current as a function of temperature in three different cases (i) $k' = k, k_o = 0$, (ii) $k' = 0, k_o = 0$ and (iii) $k' = 0, k_o \neq 0$. Particularly interesting is the low temperature ($T << \hbar(k/m)^{1/2}/k_B$) behaviour (shown in inset of Fig.(2)) which is very different for the three cases. The low temperature behaviour can be obtained analytically by examining the integrand at small q. We then find for the three different cases: (i) $J_Q \sim T^3$, (ii) $J_Q \sim T$ and (iii) $J_Q \sim e^{-\hbar\omega_o/(k_B T)}/T^{1/2}$, where $\omega_o = (k_o/m)^{1/2}$.

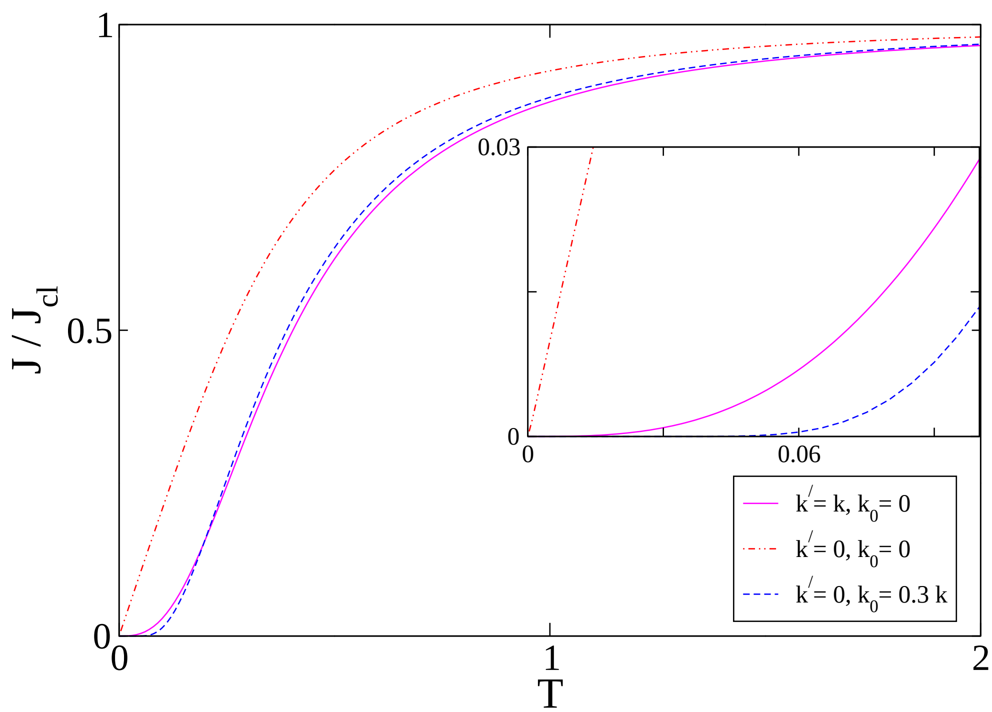

Figure 2: Plot of the scaled heat current with temperature (in units of $\hbar(k/m)^{1/2}/k_B$) for three different parameter regimes (see text). Inset shows the low temperature behaviour.

4 Higher dimensions

Heat conduction in ordered harmonic lattices in more than one dimension was first considered by Nakazawa [2]. The problem can be reduced to an effectively one-dimensional problem. For the sake of completeness we reproduce their arguments here and also give the quantum generalization.

Let us consider a d-dimensional hypercubic lattice with lattice sites labelled by the vector $\mathbf{l} = \{l_\alpha\}, \alpha = 1, 2...d$, where each l_α takes values from 1 to L_α. The total number of lattice sites is thus $N = L_1 L_2 ... L_d$. We assume that heat conduction takes place in the $\alpha = d$ direction. Periodic boundary conditions are imposed in the remaining $d-1$ transverse directions. The Hamiltonian is described by a scalar displacement $X_\mathbf{l}$ and as in the $1D$ case we consider nearest neighbour harmonic interactions with a spring constant k and harmonic onsite pinning at all sites with spring constant k_o. All boundary particles at $l_d = 1$ and $l_d = L_d$ are additionally pinned by harmonic springs with stiffness k' and follow Langevin dynamics corresponding to baths at temperatures T_L and T_R respectively.

Let us write $\mathbf{l} = (\mathbf{l}_t, l_d)$ where $\mathbf{l}_t = (l_1, l_2...l_{d-1})$. Also let $\mathbf{q} = (q_1, q_2...q_{d-1})$ with $q_\alpha = 2\pi n / L_\alpha$ where n goes from 1 to L_α. Then defining variables

$$X_{l_d}(\mathbf{q}) = \frac{1}{L_1^{1/2} L_2^{1/2} ... L_{d-1}^{1/2}} \sum_{\mathbf{l}_t} X_{\mathbf{l}_t, l_d} e^{i\mathbf{q}.\mathbf{l}_t} \ , \tag{4.1}$$

one finds that, for each fixed $\mathbf{q}$, $X_{l_d}(\mathbf{q})$ ($l_d = 1, 2...L_d$) satisfy Langevin equations corresponding to the 1D Hamiltonian in Eq. (2.1) with the onsite spring constant k_o replaced by

$$\lambda(\mathbf{q}) = k_o + 2[d - 1 - \sum_{\alpha=1,d-1} \cos(q_\alpha)] \ . \tag{4.2}$$

For $L_d \to \infty$, the heat current $J(\mathbf{q})$ for each mode with given $\mathbf{q}$ is then simply given by Eq.(2.6) with k_o replaced by $\lambda_\mathbf{q}$. In the quantum mechanical case we use Eq. (3.3). The heat current per bond is then given by:

$$J = \frac{1}{L_1 L_2 .... L_{d-1}} \sum_\mathbf{q} J(\mathbf{q}) \ . \tag{4.3}$$

Note that the result holds for finite lengths in the transverse direction. For infinite transverse lengths we get $J = \int ... \int_0^{2\pi} d\mathbf{q} J(\mathbf{q}) / (2\pi)^{d-1}$.

5 Summary

In this paper we have derived the exact formula for the heat current through an ordered harmonic chain in the limit of infinite system size. Our derivation is different from the methods used by RLL [1] and N [2] and is for a slightly different version of the models studied by them. We have presented the quantum mechanical generalization of the results. In that case one gets, in the linear response regime, a temperature dependent current with interesting low-temperature behaviour. We have also stated the results for the general d-dimensional case.

References

[1] Z. Rieder, J. L. Lebowitz, and E. Lieb, *Properties of a harmonic crystal in a stationary nonequilibrium state*, J. Math. Phys. **8**, 1073 (1967).

[2] H. Nakazawa, *Energy Flow in Harmonic Linear Chain*, Progress of Theoretical Physics **39**, 236 (1968); *On the Lattice Thermal Conduction*, Progress of Theoretical Physics Supplement **45**, 231 (1970).

[3] A. Dhar, *Heat conduction in the disordered harmonic chain revisited*, Phys. Rev. Lett. **86**, 5882 (2001).

[4] A. Dhar and D. Roy, *Heat transport in Harmonic lattices*, J. Stat. Phys. **125**, 801 (2006).

[5] A. Casher and J.L. Lebowitz, *Heat Flow in Regular and Disordered Harmonic Chains*, J. Math. Phys. **12**, 1701 (1971).

[6] U. Zurcher and P. Talkner, *Quantum-mechanical harmonic chain attached to heat baths. II. Nonequilibrium properties*, Phys. Rev. A **42**, 3278 (1990).

[7] K. Saito, S. Takesue, and S. Miyashita, *Energy transport in the integrable system in contact with various types of phonon reservoirs*, Phys. Rev. E **61**, 2397 (2000).

[8] A. Dhar and B. S. Shastry, *Quantum transport using the Ford-Kac-Mazur formalism*, Phys. Rev. B **67**, 195405 (2003).

[9] D. Segal, A. Nitzan and P. Hanggi, *Thermal conductance through molecular wires*, J. Chem. Phys. **119**, 6840 (2003).

[10] T. Yamamoto and K. Watanabe, *Nonequilibrium Green's function approach to phonon transport in defective carbon nanotubes*, Phys. Rev. Lett. **96**, 255503 (2006).

[11] J.-S. Wang, J. Wang and N. Zeng, *Nonequilibrium Green's function approach to mesoscopic thermal transport*, Phys. Rev. B 74, 033408 (2006).

[12] A. Dhar, unpublished notes.