2 Heat conduction in harmonic systems

In the open system description of transport, a system is connected to reservoirs through some system-reservoir couplings. An idealised reservoir acts like a perfect blackbody with zero reflectivity, as used in the Landauer formalism. However in real situations one does not have ideal reservoirs, and it is important to understand the role of reservoirs in transport. Unlike other microscopic approaches such as Boltzmann kinetic theory, or the usual Green-Kubo formalism, where one studies the properties of the system only, the LEGF approach explicitly includes the effect of reservoirs.

In the first three sections of this chapter we introduce and discuss the LEGF approach. In Sec. (2.1) we show the derivation of the generalized quantum Langevin equations for a system coupled to two reservoirs at different temperatures. In Sec. (2.2) we work out the nonequilibrium steady state current expressed in terms of the Green’s function of the system. In Sec. (2.3) we discuss various types of baths that are generally used. Next, in Sec. (2.4) we study heat conduction in d-dimensional harmonic lattices using the LEGF approach. One important new result of the thesis is to develop a recursive Green’s function technique for evaluation of the phonon transmission function. The recursion relation proved here was earlier known for one-dimensional systems. In Sec. (2.4.1) we give the details of the proof of the recursion relation in higher dimensional systems and discuss its numerical implementation to find the transmission function. Applying this technique we evaluate the transmission coefficient and hence the current for harmonic chain in Sec. (2.4.2). Using the results of ordered harmonic chain from previous section we work out current in d-dimensional harmonic system in Sec. (2.4.3).
2.1 Generalized Langevin equations and LEGF approach

Consider a particle of mass $m$ attached to a spring of stiffness $k$ and kept inside a fluid of temperature $T$. Then phenomenologically the simplest way to model the effect of the environment (fluid) is to write the following simple classical equation of motion for the particle:

$$m\ddot{x} = -kx - \gamma \dot{x} + \xi(t).$$  \hspace{1cm} (2.1)

The last two terms correspond to the dissipation and noise respectively. The noise is assumed to be Gaussian and has the following statistical properties

$$\langle \xi(t) \rangle = 0 \text{ and } \langle \xi(t)\xi(t') \rangle = 2\gamma k_B T \delta(t - t').$$ \hspace{1cm} (2.2)

The last equation is called a fluctuation dissipation relation. In the Eq. (2.1) the dissipation is instantaneous and the noise is $\delta$-correlated in time. Often in real systems the situation is somewhat different and a more appropriate description is given in terms of the generalized Langevin equation, which is:

$$m\ddot{x} = -kx - \int_{-\infty}^{\infty} dt' \alpha(t - t') \dot{x}(t') + \xi(t)$$ \hspace{1cm} (2.3)

where the dissipation term involves memory and the noise $\xi(t)$ is Gaussian but correlated in time. The noise properties are now given by

$$\langle \xi(t) \rangle = 0 \text{ and } \langle \xi(t)\xi(t') \rangle = k_B T \alpha(t - t').$$ \hspace{1cm} (2.4)

One can also write Eq. (2.3) in the following form

$$m\ddot{x} = -(k + \alpha(0))x(t) + \int_{-\infty}^{\infty} dt' \frac{d\alpha(t - t')}{dt'} x(t') + \xi(t)$$

$$m\ddot{x} = -(m\omega_0^2)x(t) + \int_{-\infty}^{\infty} dt' \sigma(t - t') x(t') + \xi(t)$$ \hspace{1cm} (2.5)

where we assume that $\lim_{t \to \infty} \alpha(t) = 0$ and have defined $m\omega_0^2 = k + \alpha(0)$, $\sigma(t) = -d\alpha(t)/dt$.

The Eq. (2.5) is the generalized Langevin equation (GLE) for a single harmonic oscillator.
Now we present the details of the LEGF formalism in the context of heat conduction, which will essentially involve solving GLEs for a more general multi-particle harmonic system. The GLEs in this case appear automatically by eliminating the bath degrees of freedom from the Heisenberg equations of motion (or Newton's equations of motion) of the system degrees of freedom. This approach was used by Ford-Kac-Mazur [60] to study Brownian motion in coupled oscillators. Dhar and Shastry [61] extended this approach to study transport in electron and phonon systems. They derived the Landauer formula using this approach. In [62], Dhar and Sen showed how one can get NEGF results for non-interacting electrons modeled by tight binding Hamiltonians, using quantum Langevin equations. There are four basic steps of this approach, which are:

- (i) Write down the equation of motion for both system variables and bath variables.

- (ii) Solve the equations corresponding to bath variables and put these solutions back into the equations for system variables. Thus one gets generalised Langevin equations for system variables. The noises present in GLEs depend of the initial values on bath variables which are chosen from appropriate equilibrium distributions.

- (iii) Solve these generalised Langevin equations by Fourier transform technique and write the solution in such a form so that one can easily identify the phonon green's functions which lead to the identification with NEGF results.

- (iv) To find the steady state value of any quantity take average over noise configurations.

Let us illustrate this approach for a quantum harmonic chain of size $N$ connected to two heat baths at two different temperatures. The baths are also taken to be harmonic oscillators. The first site of the chain is coupled to the left reservoir and the last site ($N^{th}$ site) of the system is coupled to the right reservoir. The left and right reservoirs are at temperatures $T_L$ and $T_R$ respectively. The Hamiltonian of the entire system (system and bath) is ([63]):

$$H = \mathcal{H}_C + \mathcal{H}_L + \mathcal{H}_R + V_L + V_R$$
where $H_C = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m_i} + \frac{k_i x_i^2}{2} \right) + \sum_{i=1}^{N-1} \frac{k(x_{i+1} - x_i)^2}{2}$

$H_L = \sum_{i=1}^{N_L} \frac{p_{IL}^2}{2} + \sum_{i=0}^{N_L} k_0 \frac{(x_{i+1L} - x_{iL})^2}{2}$ with $x_{0L} = x_{N_L+1L} = 0$

$H_R = \sum_{i=1}^{N_R} \frac{p_{IR}^2}{2} + \sum_{i=0}^{N_R} k_0 \frac{(x_{i+1R} - x_{iR})^2}{2}$ with $x_{0R} = x_{N_R+1R} = 0$

$V_L = -k' x_1 x_{1L}$ and $V_R = -k' x_N x_{1R}$ (2.6)

where $H_C$, $H_L$, $H_R$ represent the Hamiltonians of the chain, the left reservoir and the right reservoir of sizes $N$, $N_L$, $N_R$ respectively. The Heisenberg operators $x_i$, $x_{iL}$ and $x_{nR}$ correspond to the particle displacements (assumed to be scalar) about respective equilibrium positions. The conjugate operators corresponding to $x_i$, $x_{iL}$ and $x_{nR}$ are $p_i$, $p_{iL}$ and $p_{nR}$ respectively, which satisfy these commutation relations: $[x_k, p_l] = i\hbar \delta_{kl}$, $[x_{iL}, p_{jl}] = i\hbar \delta_{ij}$ and $[x_{nR}, p_{nR}] = i\hbar \delta_{mn}$. $V_L$ and $V_R$ denote the interaction between the system and the two reservoirs respectively.

Let us consider that, the matrices $U_L$, $U_R$ diagonalize the Hamiltonians $H_L$ and $H_R$ respectively, where $\omega_{\mu L}$ and $\omega_{\mu R}$ are the corresponding eigen frequencies. Then under the variable transformation $x_{iL} = \sum_{\mu=1}^{N_L} U_{i\mu}^L x_{\mu L}$ the Hamiltonian $H_L$ and $V_L$ become

$H_L = \sum_{\mu=1}^{N_L} \left[ \frac{p_{\mu L}^2}{2} + \frac{\omega_{\mu L}^2 x_{\mu L}^2}{2} \right]$ \hfill (2.7)

$V_L = -x_1 \sum_{\mu=1}^{N_L} c_{\mu L} x_{\mu L}$ with $c_{\mu L} = k' U_{1\mu}^L$

and similarly for right reservoir we have

$H_R = \sum_{\mu=1}^{N_R} \left[ \frac{p_{\mu R}^2}{2} + \frac{\omega_{\mu R}^2 x_{\mu R}^2}{2} \right]$ \hfill (2.8)

$V_R = -x_N \sum_{\mu=1}^{N_R} c_{\mu R} x_{\mu R}$ with $c_{\mu R} = k' U_{1\mu}^R$

The full Hamiltonian in Eq. (2.6) now becomes

$H = H_C + H_L + H_R + V_L + V_R$
where \( H_C = \sum_{l=1}^{N} \left( \frac{p_i^2}{2m_i} + \frac{k_i x_i^2}{2} \right) + \sum_{i=1}^{N-1} k(x_{i+1} - x_i)^2 \)

\( H_L = \sum_{\mu=1}^{N_L} \left( \frac{p_{\mu L}^2}{2} + \frac{\omega_{\mu L}^2 x_{\mu L}^2}{2} \right) \)

\( H_R = \sum_{\mu=1}^{N_R} \left( \frac{p_{\mu R}^2}{2} + \frac{\omega_{\mu R}^2 x_{\mu R}^2}{2} \right) \)

\( V_L = -x_1 \sum_{\mu=1}^{N_L} c_{\mu L} x_{\mu L} \)

\( V_R = -x_N \sum_{\mu=1}^{N_R} c_{\mu R} x_{\mu R} \) \quad (2.9)

From the above Hamiltonian we obtain the following Heisenberg equations of motion

\[
\begin{align*}
    m_1 \ddot{x}_1 &= -k_1 x_1 - k(x_1 - x_2) + \sum_{\mu=1}^{N_L} c_{\mu L} x_{\mu L} \\
    m_l \ddot{x}_l &= -k_l x_l - k(2x_l - x_{l-1} - x_{l+1}) \quad 1 < l < N \\
    m_N \ddot{x}_N &= -k_N x_N - k(x_N - x_{N-1}) + \sum_{\mu=1}^{N_R} c_{\mu R} x_{\mu R}, \quad (2.10)
\end{align*}
\]

for the system degrees of freedom, and

\[
\begin{align*}
    \dot{x}_{\mu L} &= -\omega_{\mu L}^2 x_{\mu L} + c_{\mu L} x_1, \quad \mu = 1 \text{ to } N_L \\
    \dot{x}_{\mu R} &= -\omega_{\mu R}^2 x_{\mu R} + c_{\mu R} x_N, \quad \mu = 1 \text{ to } N_R, \quad (2.11)
\end{align*}
\]

for the bath degrees of freedom. We first solve the equations of motion of the bath degrees of freedom by considering them to be linear inhomogeneous equations. We assume that the system reservoir interaction is switched on at time \( t_0 \). The solutions of the equations of motion of the reservoir variables in Eq. (2.11), for \( t > t_0 \), are given by

\[
\begin{align*}
    X_{\mu L}(t) &= \cos \omega_{\mu L}(t - t_0) \ X_{\mu L}(t_0) + \frac{\sin \omega_{\mu L}(t - t_0)}{\omega_{\mu L}} \ X_{\mu L}(t_0) + \int_{t_0}^{t} dt' \frac{\sin \omega_{\mu L}(t - t')}{\omega_{\mu L}} \ c_{\mu L} x_1(t') \\
    X_{\mu R}(t) &= \cos \omega_{\mu R}(t - t_0) \ X_{\mu R}(t_0) + \frac{\sin \omega_{\mu R}(t - t_0)}{\omega_{\mu R}} \ X_{\mu R}(t_0) + \int_{t_0}^{t} dt' \frac{\sin \omega_{\mu R}(t - t')}{\omega_{\mu R}} \ c_{\mu R} x_N(t') \quad (2.12)
\end{align*}
\]
Plugging these solutions into the system’s equations of motion in Eq. (2.10) we get

\[ m_1 \ddot{x}_1 = -k_1 x_1 - k(x_1 - x_2) + \int_{t_0}^{t} dt' \sigma^+_1(t-t')x_1(t') + \eta_1(t) \]

\[ m_i \ddot{x}_i = -k_i x_i - k(2x_i - x_{i-1} - x_{i+1}) \quad 1 < i < N \]

\[ m_N \ddot{x}_N = -k_N x_N - k(x_N - x_{N-1}) + \int_{t_0}^{t} dt' \sigma^+_N(t-t')x_N(t') + \eta_N(t) \]

where \( \sigma^+_i(t) = \sum_{\mu=1}^{N_L} \frac{c_{\mu}^2}{\omega_{\mu}^L} \sin(\omega_{\mu}^L t) \Theta(t) \), \( \sigma^+_N(t) = \sum_{\mu=1}^{N_R} \frac{c_{\mu}^2}{\omega_{\mu}^R} \sin(\omega_{\mu}^R t) \Theta(t) \)

and \( \eta_1(t) = \sum_{\mu=1}^{N_L} c_{\mu} \left[ \cos \omega_{\mu}^L (t - t_0) \ddot{x}_{\mu L}(t_0) + \frac{\sin \omega_{\mu}^L (t - t_0)}{\omega_{\mu}^L} \dot{x}_{\mu L}(t_0) \right] \)

\( \eta_N(t) = \sum_{\mu=1}^{N_R} c_{\mu} \left[ \cos \omega_{\mu}^R (t - t_0) \ddot{x}_{\mu R}(t_0) + \frac{\sin \omega_{\mu}^R (t - t_0)}{\omega_{\mu}^R} \dot{x}_{\mu R}(t_0) \right] \),

and where the function \( \Theta(t) \) is the Heaviside step function. We can easily see that the above equations are in the form of the generalized Langevin equation (Eq. (2.5)). The noises \( \eta_1 \) and \( \eta_N \) involve initial positions and momenta of the reservoir particles. The statistical properties of the noises are determined by the statistical properties of the initial configurations of the reservoirs.

It is assumed that at time \( t_0 \) the left and right reservoirs were in thermal equilibrium at temperatures \( T_L \) and \( T_R \) respectively. The population of the normal modes of the isolated reservoirs is given by the phonon distribution functions \( f_b(\omega, T_{L,R}) = \frac{1}{e^{\hbar \omega/\kappa_b T_{L,R}} - 1} \).

Using these distribution functions it can be easily shown that the equilibrium correlations are given by (for the left reservoir):

\[ \langle \omega_{\mu}^2 \dot{x}_{\mu L}(0) \ddot{x}_{\mu L}(0) \rangle = \langle \ddot{x}_{\mu L}(0) \ddot{x}_{\mu L}(0) \rangle = \frac{\hbar \omega_{\mu L}}{2} \coth(\frac{\hbar \omega_{\mu L}}{2 K_B T_L}) \]

\[ \langle [X_{\mu L}(0) \dot{x}_{\mu L}(0) + \dot{x}_{\mu L}(0) X_{\mu L}(0)] \rangle = 0 \] (2.14)

Using these correlations the noise correlations come out to be

\[ \langle \eta_1(t) \rangle = 0 \quad \text{where} \quad \frac{1}{2} [\langle \eta_1(t) \eta_1(t') \rangle + \langle \eta_1(t') \eta_1(t) \rangle] = K_B T_L k_{\mu L}(t - t') \]

where \( K_L(t) = \sum_{\mu=1}^{N_L} \frac{c_{\mu}^2}{\omega_{\mu}^L} \cos(\omega_{\mu} L t) \frac{\hbar \omega_{\mu L}}{2 k_{\mu} T_L} \coth(\frac{\hbar \omega_{\mu L}}{2 K_B T_L}) \).

(2.15)

Similar relations hold for the right reservoir.
2.2 Stationary solution of the equation of motion and steady state properties

In the limits of infinite reservoir sizes and \( t_0 \to -\infty \), the easiest way to obtain the steady state properties is to solve the equations in (2.13) by Fourier transform. Thus defining the Fourier transforms

\[
\tilde{x}_i(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \ x_i(t) e^{i\omega t}
\]

\[
\tilde{\eta}_{1,N}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \ \eta_{1,N}(t) e^{i\omega t}
\]

\[
\sigma^*_{1,N}(\omega) = \int_{-\infty}^{\infty} dt \ \sigma^*_{1,N}(t) e^{i\omega t}
\]

(2.16)

we get from Eq. (2.13)

\[
-m_1 \omega^2 \tilde{x}_1(\omega) = -k_1 \tilde{x}_1 - k(\tilde{x}_1 - \tilde{x}_2) + \sigma^*_{1}(\omega) \tilde{x}_1(\omega) + \tilde{\eta}_1(\omega)
\]

\[
-m_l \omega^2 \tilde{x}_l(\omega) = -k_l \tilde{x}_l - k(2\tilde{x}_l - \tilde{x}_{l-1} - \tilde{x}_{l+1}) \quad 1 < l < N
\]

\[
-m_N \omega^2 \tilde{x}_N(\omega) = -k_N \tilde{x}_N - k(\tilde{x}_N - \tilde{x}_{N-1}) + \sigma^*_{N}(\omega) \tilde{x}_N(\omega) + \tilde{\eta}_N(\omega).
\]

(2.17)

where the new noise \( \tilde{\eta}_{1,N}(\omega) \) have the following correlations in the Fourier space

\[
\frac{1}{2} [ \langle \tilde{\eta}_{1,N}(\omega) \tilde{\eta}_{1,N}(\omega') \rangle + \tilde{\eta}_{1,N}(\omega') \tilde{\eta}_{1,N}(\omega) ] = \frac{K_B T_{LR}}{2\pi} \tilde{K}_{L,R}(\omega) \delta(\omega + \omega')
\]

where \( \tilde{K}_{L,R}(\omega) = \frac{\hbar}{K_B T_{LR}} \text{Im}[\sigma^*_{1,N}(\omega)] \coth(\frac{\hbar \omega}{2k_B T_{LR}}) \).

(2.18)

One can also show that

\[
\langle \tilde{\eta}_{1,N}(\omega) \tilde{\eta}_{1,N}(\omega') \rangle = \frac{\hbar \text{Im}[\sigma^*_{1,N}(\omega)]}{2\pi} \left[ 1 + f_b(\omega, T_{LR}) \right] \delta(\omega + \omega').
\]

(2.19)

Now we write the equations (2.17) in the following matrix form

\[
[-M \omega^2 + \Phi - \Sigma^*_{L}(\omega) - \Sigma^*_{R}(\omega)] \tilde{X}(\omega) = \tilde{\eta}_L(\omega) + \tilde{\eta}_R(\omega),
\]

(2.20)

where, \( X, \eta \) are column vector with elements \([X]^T = (x_1, x_2, ..., x_N), [\eta]^T = (\eta_L, 0, ..., 0, \eta_R)\) and \( \Sigma^*_{L}(\omega), \Sigma^*_{R}(\omega) \) are \( N \times N \) matrices whose only non-vanishing elements are \([\Sigma^*_{L}]_{11} = \sigma^*_1,\)
\[ [\Sigma^+]_{NN} = \sigma^+_N. \]  
[\Phi]_{N\times N} represents a tridiagonal matrix with elements \([\Phi]_{i,j} = (2k + k_0)\delta_{i,j} - k\delta_{i-1,j} - k\delta_{i+1,j}\) for \(i = 2\) to \(N - 1\) and \([\Phi]_{1,j} = (2k + k_0)\delta_{1,j} - k\delta_{2,j}, [\Phi]_{N,j} = (2k + k_0)\delta_{N,j} - k\delta_{N-1,j}\) for \(j = 1\) to \(N\). From the imaginary part of each element of \(\Sigma^+ L\) and \(\Sigma^+ R\), we construct two more matrices \(\Gamma^+_L\) and \(\Gamma^+_R\) respectively, i.e. \(\Gamma_{L,R}(\omega) = \text{Im}[\Sigma^+_L(\omega)]\).

From Eq. (2.20) we get \(\tilde{X}(\omega) = G^+(\omega)[\tilde{\eta}_L(\omega) + \tilde{\eta}_R(\omega)]\), where

\[
G^+(\omega) = \frac{1}{-M\omega^2 + \Phi - \Sigma^+_L(\omega) - \Sigma^+_R(\omega)}
\]

\[
\langle \tilde{\eta}_L(\omega) \tilde{\eta}_L^T(\omega') \rangle = \frac{\hbar \Gamma_l(\omega)}{2\pi} \left[ 1 + f_\beta(\omega, T_L) \right] \delta(\omega + \omega'),
\]

\[
\langle \tilde{\eta}_R(\omega) \tilde{\eta}_R^T(\omega') \rangle = \frac{\hbar \Gamma_r(\omega)}{2\pi} \left[ 1 + f_\beta(\omega, T_R) \right] \delta(\omega + \omega'),
\]

\[
\langle \tilde{\eta}_L(\omega) \tilde{\eta}_R^T(\omega') \rangle = 0, \quad \Gamma_{L,R}(\omega) = \text{Im}[\Sigma^+_L(\omega)].
\]

(2.21)

Using \(\tilde{X}(\omega)\) we write the solution of the GLEs of the system in steady state as

\[
X(t) = \int_{-\infty}^{\infty} d\omega \tilde{X}(\omega) e^{-i\omega t}.
\]

(2.22)

**Connections to Green’s function:** Now we will show that the function \(G^+(\omega)\) can be identified as Green’s function while \(\Sigma^+_{L,R}\) can be identified as self energy corrections. Since the chain and baths are collections of harmonic oscillators and the interactions among the bath and the chain are quadratic, the Hamiltonian of the entire system in Eq. (2.9) can be expressed as a quadratic Hamiltonian given by:

\[
H = \frac{1}{2} Y^T M Y + \frac{1}{2} Y^T \Phi Y
\]

\[
= \mathcal{H}_C + \mathcal{H}_L + \mathcal{H}_R + \mathcal{V}_L + \mathcal{V}_R
\]

where

\[
\mathcal{H}_C = \frac{1}{2} X^T M C X C + \frac{1}{2} X^T \Phi C X C,
\]

\[
\mathcal{H}_L = \frac{1}{2} X^T M L X L + \frac{1}{2} X^T \Omega^2_L X L,
\]

\[
\mathcal{H}_R = \frac{1}{2} X^T M R X R + \frac{1}{2} X^T \Omega^2_R X R,
\]

\[
\mathcal{V}_L = X^T V L X L, \quad \mathcal{V}_R = X^T V R X R,
\]

(2.23)

where \(M\) denotes the mass matrix of the entire system and \(\Phi\) denotes the force constant.
matrix of the quadratic interactions among the particles of the entire system (chain plus baths). Here, $M_L$ and $M_R$ represent the mass matrices of the left and right reservoirs. Since all particles in both reservoirs have unit masses, $M_L$ and $M_R$ are identity matrices of dimensions $N_L \times N_L$ and $N_R \times N_R$ respectively. The eigenvalues of the two reservoirs are denoted by the matrices $\Omega^2_L$ and $\Omega^2_R$. Here $V_L$ represents a $N \times N_L$ matrix whose only non-vanishing elements are $[V_L]_{1,\mu} = c_{\mu L} = U_{1\mu}^L$, and $V_R$ represents a $N \times N_R$ matrix whose only non-vanishing elements are $[V_R]_{1,\mu} = c_{\mu R} = U_{1\mu}^R$.

The equations of motion for particles of the entire system are:

$$M \ddot{Y} = -\Phi Y. \tag{2.24}$$

If $G^+(t)$ denotes the Green's function of the entire system, then $G^+(t)$ satisfies

$$M \ddot{G}^+(t) + \Phi \dot{G}^+(t) = \delta(t) I. \tag{2.25}$$

It is easy to verify that $G^+(t) = G(t) \Theta(t)$ where $G(t)$ satisfies the equation $M \ddot{G}(t) + \Phi \dot{G}(t) = 0$ with the initial conditions $G(0) = 0$, $\dot{G}(0) = M^{-1}$. The Fourier transform $G^+(\omega) = \int_{-\infty}^{\infty} dt G^+(t) e^{i\omega t}$ of $G^+(t)$ satisfies the equation

$$[-M(\omega + i\epsilon)^2 + \Phi] G^+(\omega) = I. \tag{2.26}$$

The isolated reservoir Green's functions are given by

$$g^+_L(\omega) = \frac{1}{-(\omega + i\epsilon)^2 M_L + \Omega^2_L},$$

$$g^+_R(\omega) = \frac{1}{-(\omega + i\epsilon)^2 M_R + \Omega^2_R}. \tag{2.27}$$

The Green's function element $G^+_{rs}$ is defined between any pair of points $r$ and $s$ on the entire system of chain and baths. We are interested in evaluating $G^+(\omega)$ only between points on the chain. To do that, let us define some notations for various Green's Functions as follows:

- $G^+_C(\omega)$ represents the part of $G^+(\omega)$ whose elements are non-zero only if both the indices represents points on the chain.
• $G_1^L(\omega)$ represents the part of $G_+(\omega)$ whose elements are non-zero only if both the indices represent points on the left reservoir.

• $G_2^R(\omega)$ represents the part of $G_+(\omega)$ whose elements are non-zero only if both the indices represent points on the right reservoir.

• $G_{CL}^+(\omega)$ represents the part of $G_+(\omega)$ whose elements are non-zero only if one index represents a point on the chain while the other one represents point on the left reservoir.

• $G_{CR}^+(\omega)$ represents the part of $G_+(\omega)$ whose elements are non-zero only if one index represents a point on the chain while the other one represents point on the right reservoir.

• $G_{LR}^+(\omega)$ represents the part of $G_+(\omega)$ whose elements are non-zero only if one index represents a point on the left reservoir while the other one represents point on the right reservoir.

Now using the above notations and Eq. (2.27) we can write Eq. (2.26) in the following matrix form:

\[
\begin{pmatrix}
-M_C (\omega + i\epsilon)^2 \hat{I} + \Phi_C & V_L & V_R \\
V_L^T & -M_L (\omega + i\epsilon)^2 \hat{I} + \Omega_L^2 & 0 \\
V_R^T & 0 & -M_R (\omega + i\epsilon)^2 \hat{I} + \Omega_R^2
\end{pmatrix}
\times
\begin{pmatrix}
G_C^+ & G_{CL}^+ & G_{CR}^+ \\
G_{LC}^+ & G_L^+ & G_{CR}^+ \\
G_{RC}^+ & G_{RL}^+ & G_R^+
\end{pmatrix}
= \begin{pmatrix}
\hat{I} & 0 & 0 \\
0 & \hat{I} & 0 \\
0 & 0 & \hat{I}
\end{pmatrix}
\]

This gives the following equations:

\[
[-M_C (\omega + i\epsilon)^2 \hat{I} + \Phi_C]G_C^+ + V_L G_{LC}^+ + V_R G_{RC}^+ = \hat{I}
\]

\[
V_L^T G_C^+ + [-M_L (\omega + i\epsilon)^2 \hat{I} + \Omega_L^2]G_{LC}^+ = 0
\]

\[
V_R^T G_C^+ + [-M_R (\omega + i\epsilon)^2 \hat{I} + \Omega_R^2]G_{RC}^+ = 0.
\]

From the last two equations we get $G_{LC}^+(\omega) = -g_L^+(\omega)V_L^T G_C^+(\omega)$ and $G_{RC}^+(\omega) = \ldots$
Using this in the first equation then gives [24, 62]

\[ [-M_C (\omega + ie)^2 \hat{I} + \Phi_C - V_L g_L^+(\omega)V_L^T - V_R g_R^+(\omega)V_R^T]G_C^+(\omega) = \hat{I} \]

\[ \Rightarrow G_C^+(\omega) = \frac{1}{[-M_C (\omega + ie)^2 \hat{I} + \Phi_C - \Sigma_1^+(\omega) - \Sigma^+(\omega)]} \]

where \( \Sigma_1^+(\omega) = V_L g_L^+(\omega)V_L^T = \sum_{\mu=1}^{N_L} \frac{(U_{1\mu}^L)^2}{-(\omega + ie)^2 M_L + \Omega_L^2} \)

and \( \Sigma^+(\omega) = V_R g_R^+(\omega)V_R^T = \sum_{\mu=1}^{N_R} \frac{(U_{1\mu}^R)^2}{-(\omega + ie)^2 M_R + \Omega_R^2} \). \hspace{1cm} (2.30)

Now comparing the second line of Eq. (2.30) with the third line of Eq. (2.21) we identify that \( G^+(\omega) = G_C^+(\omega) \), and \( \Sigma_{l,R}^+ \) are self energy corrections.

**Steady state properties:** In general, the steady state is represented by the invariant probability distribution of the phase space variables. But it can also be represented by the various cumulants obtained in the steady state. In the case of heat conduction in harmonic systems with correlated noise, it is difficult to obtain the full distribution. However we can calculate a few cumulants which represent various physical quantities. For example, those quantities could be the energy current, local kinetic energy etc. Below we present the calculation of steady state current.

To define the local energy current inside the chain we first define the local energy density associated with the \( l^{th} \) particle (or energy at the lattice site \( l \)) as follows (such that \( H = \sum_{i=1}^{N} \epsilon_i \)) [58].

\[ \epsilon_1 = \frac{p_1^2}{2m_1} + \frac{k_1 x_1^2}{2} + \frac{k}{4}(x_1 - x_2)^2, \]

\[ \epsilon_l = \frac{p_l^2}{2m_l} + \frac{k_l x_l^2}{2} + \frac{k}{4}(x_{l-1} - x_l)^2 + (x_l - x_{l+1})^2 \], \hspace{0.5cm} \text{for} \hspace{0.5cm} l = 2, 3...N - 1

\[ \epsilon_N = \frac{p_N^2}{2m_N} + \frac{k_N x_N^2}{2} + \frac{k}{4}(x_{N-1} - x_N)^2. \hspace{1cm} (2.31) \]

Taking the time derivative of these equations, using Eq. (2.13) and after some straightforward manipulations, we get the continuity equations which are given by:

\[ \dot{\epsilon}_1 = -j_{2,1} + j_{1,L} \]
\[ \dot{e}_l = -j_{l+1,l} + j_{l,l-1} \quad \text{for } l = 2, 3, \ldots, N - 1 \]
\[ \dot{e}_N = j_{N,R} + j_{N,N-1} \]  \hspace{1cm}(2.32)

with \[ j_{l,l-1} = \frac{1}{2} (v_{l-1} + v_l) f_{l,l-1} \] \hspace{1cm}(2.33)

where \[ f_{l,l+1} = -f_{l+1,l} = -k(x_l - x_{l+1}) \]

is the force that the \((l + 1)\)th particle exerts on the \(l\)th particle and \(v_l = \dot{x}_l\). From the above equations one can identify \(j_{l,l-1}\) to be the energy current from site \(l-1\) to \(l\). The terms \(j_{l,L}\) and \(j_{N,R}\) are respectively the rate of energy flow from the left or right reservoir into the boundary particles. It is easy to verify that

\[ j_{1,L}(t) = \dot{x}_1(t) \int_{t_0}^t dt' \sigma^*_1(t-t') x_1(t') + \eta_1(t) \]

and \[ j_{N,R}(t) = \dot{x}_N(t) \int_{t_0}^t dt' \sigma^*_N(t-t') x_N(t') + \eta_N(t) \] \hspace{1cm}(2.34)

Using the fact that in the steady state \(\langle \dot{e}_l \rangle = 0\), we get

\[ \mathcal{J} = \langle j_{1,L} \rangle = \langle j_{2,1} \rangle = \langle j_{3,2} \rangle = \ldots \langle j_{N,N-1} \rangle = -\langle j_{N,R} \rangle \] \hspace{1cm}(2.35)

Now we proceed to calculate \(\mathcal{J} = \langle j_{1,L} \rangle\).

\[ \mathcal{J} = \langle \dot{x}_1(t) \int_{t_0}^t dt' \sigma^*_1(t-t') x_1(t') + \eta_1(t) \rangle \]

\[ = \int_{t_0}^t dt' \langle \dot{X}_1(t) \sigma^*_1(t-t') X(t') \rangle + \langle \dot{X}_1(t) \eta_1(t) \rangle \]

\[ = -i \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \ e^{i(\omega + \omega')t} \ \omega \langle \dot{X}^T(\omega) \Sigma^*_1(\omega') \tilde{X}(\omega') + \tilde{X}^T(\omega) \tilde{\eta}_1(\omega') \rangle \]

\[ = -i \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \ e^{i(\omega + \omega')t} \ \omega \langle Tr \left[ \tilde{X}(\omega') \Sigma^*_1(\omega') \tilde{X}^T(\omega) \right] + Tr \left[ \tilde{\eta}^T_1(\omega') \tilde{X}(\omega) \right] \rangle \].

(2.36)

Using the solution in Eq. (2.21) we get

\[ \mathcal{J} = -i \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \ e^{i(\omega + \omega')t} \ \omega \left( Tr \left[ \Sigma^*_1(\omega') G^*(\omega) \left( \tilde{\eta}_L(\omega') + \tilde{\eta}_R(\omega') \right) \right] \right. \]

\[ \left. \left( \tilde{\eta}^T_1(\omega) + \tilde{\eta}^T_R(\omega) \right) \right) G^{*T}(\omega) \left. \right] + Tr \left[ \left( \tilde{\eta}_L(\omega') \left( \tilde{\eta}^T_L(\omega) + \tilde{\eta}^T_R(\omega) \right) \right) G^{*T}(\omega) \right]. \]
Now consider that part of $\mathcal{J}$, say $\mathcal{J}_R$, which depends only on $T_R$. Clearly this is:

$$
\mathcal{J}_R = -i \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' e^{i(\omega+\omega')t} \omega \, T_R \left[ G^{+T}(\omega) \Sigma^+_L(\omega') G^+(\omega') \left\{ \tilde{h}_R(\omega') \tilde{h}_R^T(\omega) \right\} \right] \\
= -i \int_{-\infty}^{\infty} d\omega \, T_R \left[ G^{+T}(\omega) \Sigma^+_L(-\omega) G^+(-\omega) \Gamma_R(\omega) \right] \frac{\hbar}{\pi} [1 + f_b(\omega, T_R)].
$$

The real part of $\mathcal{J}_R$ is

$$
\mathcal{J}_R = - \int_{-\infty}^{\infty} d\omega \, T_R \left[ G^{+T}(\omega) \Gamma_L(-\omega) G^+(-\omega) \Gamma_R(\omega) \right] \frac{\hbar}{\pi} [1 + f_b(\omega, T_R)].
$$

Including the contribution from the terms involving $T_L$, and noting that the current has to vanish for $T_L = T_R$, it is clear that the net current will then be given by

$$
\mathcal{J} = \int_{-\infty}^{\infty} d\omega \, T_R \left[ G^{+T}(\omega) \Gamma_L(-\omega) G^+(-\omega) \Gamma_R(\omega) \right] \frac{\hbar}{\pi} [f_b(\omega, T_L) - f_b(\omega, T_R)] . \tag{2.37}
$$

Once $G^+(\omega)$ is identified as the system’s Green’s function in the open situation (connected to baths) the above expression is the same expression as one obtains in the NEGF [64] formalism. The above expression for the current is of the Landauer form and has been derived using various other approaches such as scattering theory [65, 66] and the nonequilibrium Green’s function formalism [67, 68].

The classical limit is obtained by taking the high temperature limit so that $\frac{\hbar}{k_B T} \to 0$. In this limit the current in NESS is given by

$$
\mathcal{J} = \frac{K_B(T_L - T_R)}{\pi} \int_{-\infty}^{\infty} d\omega \, T_R \left[ G^{+T}(\omega) \Gamma_L(-\omega) G^+(-\omega) \Gamma_R(\omega) \right] \\
= \frac{K_B(T_L - T_R)}{2\pi} \int_{0}^{\infty} d\omega \, T(\omega) \\
\text{where} \quad T(\omega) = 4 \, T_R \left[ G^{+T}(\omega) \Gamma_L(-\omega) G^+(-\omega) \Gamma_R(\omega) \right]. \tag{2.38}
$$

The quantity $T(\omega)$ is known as transmission coefficient.

Here, we have presented the formalism for a simple one dimensional harmonic chain in such a way that one can easily generalize the formalism for more general systems and higher dimensional systems. (See [24] for general harmonic systems and [62] for tight binding model of electrons.) All of the above derivations will go through for situations more general than a
simple one-dimensional chain, as long as one can write the Hamiltonian for the entire system (the system plus the baths and the interactions of the system with the baths) in a quadratic form as in Eq. (2.23). So far, this approach has mostly been used to study conduction for non-interacting systems; a drawback of this approach is that it is not easy to extend the results to interacting systems.

2.3 Examples of baths

From Eq. (2.13) it is clear that, once the informations about the bath and noise correlations are given one can always start just by writing a set of generalized Langevin equations to obtain the steady state properties. In the equation (2.13), the bath information is given by $\sigma(t) = -\frac{d\alpha(t)}{dt}$. In the Fourier domain this relation reads $\sigma^+ (\omega) = i\omega \alpha^+ (\omega) + \alpha(0)$, which implies that $Im[\sigma^+ (\omega)] = \omega Re[\alpha^+ (\omega)] = \Gamma(\omega)$. Below we present $\sigma^+ (\omega)$, $\Gamma(\omega)$ for some baths commonly used in theoretical studies.

**Ohmic bath:** For ohmic baths one chooses (2.39)

$$\sigma(t) = \frac{\gamma}{l} e^{-|t|/\tau}$$

which in Fourier domain becomes

$$\alpha^+ (\omega) = \frac{\gamma}{1 + \omega^2 \tau^2} + i\frac{\omega \gamma \tau}{1 + \omega^2 \tau^2}$$

and

$$\sigma^+ (\omega) = \alpha(0) + i\omega \alpha^+ (\omega).$$

In the limit $\tau \to 0$ we get the Langevin bath

$$\alpha(t) = 2\gamma \delta(t), \quad \alpha^+ (\omega) = \gamma.$$ (2.41)

In this case, $\alpha(0) \to \infty$. However one can absorb this in the definition of the spring constant.

**Rubin model:** The heat bath in this model is a harmonic chain connected to the system at one end. For simplicity let us consider the system to be a harmonic oscillator of mass $m_s$ and
frequency $\omega_0$. The Hamiltonian of the whole system is written as:

\[
H_s = \frac{p^2}{2m} + \frac{1}{2} m_s \omega_0^2 x^2
\]

\[
H_b = \sum_{i=1}^{N_b} \frac{P_{ib}^2}{2m} + \sum_{i=0}^{N_b+1} k_0 \left( x_{i+1b} + x_{ib} \right)^2 + \sum_{i=1}^{N_b} \frac{1}{2} k_i x_{ib}^2
\]

\[
H_{sb} = -k' x_{1b}.
\]  

(2.42)

We transform to normal mode coordinates using $x_{ib} = \sum_{\alpha} U_{i\alpha} X_{\alpha b}$ and $p_{ib} = \sum_{\alpha} U_{i\alpha} P_{\alpha b}$, where

\[
U_{i\alpha} = \left( \frac{2}{N_b + 1} \right)^{\frac{1}{2}} \sin(q_a) \quad \text{with} \quad q_a = \frac{\pi \alpha}{N_b + 1}, \quad \alpha = 1, 2, \ldots, N_b
\]

and

\[
\omega^2_a = \frac{k_a}{m} \left( 4 \sin^2(q_a/2) + \frac{k_1}{k_0} \right).
\]  

(2.43)

Now, in terms of the new variables $X_{\alpha b}$ and $P_{\alpha b}$ the Hamiltonians $H_b$ and $H_{sb}$ look like

\[
H_b = \sum_{\alpha=1}^{N_b} \frac{P_{\alpha b}^2}{2m} + \frac{1}{2} m \omega^2_a X_{\alpha b}^2
\]

\[
H_{sb} = -\sum_{\alpha=1}^{N_b} c_{\alpha} x X_{\alpha b}
\]

where

\[
c_{\alpha} = k' \left( \frac{2}{N_b + 1} \right)^{\frac{1}{2}} \sin(q_a).
\]  

(2.44)

The equations of motion of the system and bath variables are

\[
m_s \ddot{x} = -m_s \omega_0^2 x + \sum_{\alpha=1}^{N_b} c_{\alpha} X_{\alpha b}
\]

\[
\dot{X}_{\alpha b} = -\omega^2_a X_{\alpha b} + c_{\alpha} x.
\]  

(2.45)

As earlier, solving the equations of motion for bath variables and plugging back those solutions into the equation of motion of the system, we get

\[
m_s \ddot{x} = -m_s \omega_0^2 x + \int_{-t_0}^{t} dt' \sigma(t-t') x(t') + \xi(t)
\]

where

\[
\sigma(t) = \sum_{\alpha=1}^{N_b} \frac{c^2_{\alpha}}{\omega_{\alpha}} \sin(\omega_{\alpha} t),
\]

and

\[
\xi(t) = \sum_{\alpha=1}^{N_b} c_{\alpha} \left[ \cos(\omega_{\alpha} t) X_{\alpha b}(t_0) + \frac{\sin(\omega_{\alpha} t)}{\omega_{\alpha}} \dot{X}_{\alpha b}(t_0) \right].
\]  

(2.46)
We are interested in \( \sigma^+(\omega) = \int_0^\infty dt \sigma(t) e^{i\omega t} \) whose imaginary part is given by

\[
Im[\sigma^+(\omega)] = \Gamma(\omega) = \pi \sum_{\alpha=1}^{N_b} \frac{c_\alpha^2}{2\omega_\alpha} [\delta(\omega - \omega_\alpha) - \delta(\omega + \omega_\alpha)].
\] (2.47)

For \( \omega > 0 \) and \( \sqrt{\frac{k_1}{m}} < \omega < \sqrt{\frac{k_0}{m}} \sqrt{(4 + \frac{k_1}{k_0})}, \)

\[
\Gamma(\omega) = \frac{2k^2}{(N_b + 1)} \sum_q \frac{\sin^2(q)}{\omega_q} \delta(\omega - \omega_q)
\]

\[
= k^2 \int_0^\pi dq \frac{\sin^2(q)}{\omega_q} \delta(\omega - \omega_q)
\]

\[
= \frac{k^2 m}{k_0} \sin(q_0) \quad \text{where,} \quad \sin(q_0/2) = \sqrt{\frac{m}{4k_0}} (\omega^2 - \frac{k_1}{m}),
\] (2.48)

To get the real part of \( \sigma^+(\omega) \) we use the Kramers-Kronig relations and get

\[
Re[\sigma^+(\omega)] = \frac{2}{\pi} \int_0^\infty d\omega' \frac{\omega'}{\omega^2 - \omega'^2} \Gamma(\omega')
\]

\[
= \frac{2}{\pi} \int_{\sqrt{\frac{k_0}{m}} \sqrt{(4 + \frac{k_1}{k_0})}}^{\sqrt{k_1/m}} d\omega' \frac{\omega'}{\omega'^2 - \omega^2} \Gamma(\omega')
\] (2.49)

Now, making the variable transformation \( \cos(\beta) = (1 - \frac{m\omega^2}{2k_0} + \frac{k_1}{2k_0}) \), we get

\[
Re[\sigma^+(\omega)] = \frac{mk^2}{\pi k_0} \int_0^\pi d\beta \frac{\sin^2(\beta)}{x_0 - \cos(\beta)} \quad \text{where,} \quad x_0 = (1 + \frac{k_1}{2k_0} - \frac{m\omega^2}{2k_0})
\]

\[
= \frac{mk^2}{k_0} \cos(q_0) \quad \text{for} \quad \sqrt{\frac{k_1}{m}} < \omega < \sqrt{\frac{k_0}{m}} \sqrt{(4 + \frac{k_1}{k_0})}
\]

\[
= -\frac{mk^2}{k_0} e^{-\nu_1} \quad \text{for} \quad |\omega| > \sqrt{\frac{k_0}{m}} \sqrt{(4 + \frac{k_1}{k_0})}
\]

\[
= \frac{mk^2}{k_0} e^{-\nu_2} \quad \text{for} \quad -\sqrt{\frac{k_1}{m}} < \omega < \sqrt{\frac{k_1}{m}}
\]

where \( \cosh(\nu_1) = (\frac{m\omega^2}{2k_0} - \frac{k_1}{2k_0} - 1) \) and \( \cosh(\nu_2) = (1 + \frac{k_1}{2k_0} - \frac{m\omega^2}{2k_0}) \). (2.50)

Finally collecting the real and imaginary parts we get

\[
\sigma^+(\omega) = \frac{mk^2}{k_0} e^{i\phi_0} \quad \text{for} \quad \sqrt{\frac{k_1}{m}} < \omega < \sqrt{\frac{k_0}{m}} \sqrt{(4 + \frac{k_1}{k_0})}
\]

\[
\text{and} \quad -\sqrt{\frac{k_0}{m}} \sqrt{(4 + \frac{k_1}{k_0})} < \omega < -\sqrt{\frac{k_1}{m}}
\]

33
\[
\begin{align*}
    &= -\frac{m k'^2}{k_0} e^{-\nu_1} \quad \text{for } |\omega| > \sqrt{\frac{k_0}{m} \sqrt{4 + \frac{k_0}{k_0}}} \\
    &= \frac{m k'^2}{k_0} e^{-\nu_2} \quad \text{for } -\sqrt{\frac{k_0}{m} < \omega < \sqrt{\frac{k_0}{m}}.}
\end{align*}
\]

(2.51)

2.4 Current in \(d\)-dimensional disordered harmonic lattice

In this section we consider heat conduction in \(d\)-dimensional classical harmonic lattice. For simplicity we consider only the case where longitudinal and transverse vibration modes are decoupled, allowing us to describe the displacement at each site by a scalar variable. Also we restrict our study to \(d\)-dimensional hypercubic lattices. Let us denote the lattice points by the vector \(n = (n_1, n_2, ..., n_d)\) with \(n_\nu = 1, 2, ..., d\). The displacement of a particle at the lattice site \(n = (n_1, n')\) is given by \(x_n\). In the harmonic approximation the system Hamiltonian is given by

\[
H = \frac{1}{2} \sum_n m_n x_n^2 + \frac{1}{2} \sum_{n_1=1}^{N-1} \sum_{n',\hat{\epsilon}} k_{n_1} (x_n - x_{n+\hat{\epsilon})^2} \\
+ \frac{k_0}{2} \sum_n x_n^2 + \frac{k'}{2} \sum_{n'} \chi^2_{(1,n')} + \frac{k'}{2} \sum_{n'} \chi^2_{(N,n')},
\]

(2.52)

where \(\hat{\epsilon}\) refers to the \(2d\) nearest neighbors of any site and we impose different boundary conditions which will be specified later. The parameter \(k_0\) represents the spring constant of the external pinning potential whereas \(k'\) is the spring constant of the external potential at the boundary \(n_1 = 1\) and \(n_1 = N\). The mass of the particle at site \(n\) is denoted by \(m_n\).

We couple all the particles at \(n_1 = 1\) and \(n_1 = N\) to heat reservoirs, at temperatures \(T_L\) and \(T_R\) respectively, and use periodic boundary conditions in the other \((d-1)\) directions. The heat conduction takes place along the \(\nu = 1\) direction. Each layer with constant \(n_1\) consists of \(N' = N^{d-1}\) particles. The heat baths are modeled by white noise Langevin equations of motion for the particles coupled to the baths. The equations of motion are given by:

\[
m_n \ddot{x}_n = - \sum_{\hat{\epsilon}} k (x_n - x_{n+\hat{\epsilon})} - k_0 x_n + \delta_{n_1,1} (-\gamma \dot{x}_n)
\]

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where the dissipative and noise terms are related by the usual fluctuation dissipation relations

\[
\langle \eta_{n}^{L}(t)\eta_{n}^{L}(t') \rangle = 2\gamma k_{B}T_{L}\delta(t-t')\delta_{n,n'},
\]

\[
\langle \eta_{n}^{R}(t)\eta_{n}^{R}(t') \rangle = 2\gamma k_{B}T_{R}\delta(t-t')\delta_{n,n'}. \tag{2.54}
\]

The particles at the surfaces \( n_1 = 1, N \) experience additional harmonic pinning potentials with spring constants \( k' \) arising from coupling to the heat reservoirs. We consider two kinds of boundary conditions at the surfaces connected to reservoirs: (i) fixed BCs \( k' > 0 \) and (ii) free BCs \( k' = 0 \). A schematic of the models and the different boundary conditions is given in Fig. (2.1).

![Figure 2.1](image)

(a) Free boundaries (b) Fixed boundaries (c) Pinned lattice

Figure 2.1: A schematic diagram of a two-dimensional mass-disordered lattice of particles connected by harmonic springs and connected to heat baths at temperatures \( T_L \) and \( T_R \). Red and green colours indicate particles of different masses. Pinning refers to the presence of a spring attaching a particle to the substrate. In (a) there is no pinning, in (b) boundary particles are pinned and in (c) all sites are pinned.

The two different BCs emerge naturally if we model the heat reservoirs themselves by infinite ordered harmonic crystals. One then obtains Langevin type equations on eliminating the bath degrees of freedom. Fixed BCs correspond to reservoirs with properties different from the system (e.g. different spring constants) and in this case one finds that effectively the particles at the boundaries (those coupled to reservoirs) experience an additional harmonic
pining potential. Free BCs correspond to the case where the reservoir is simply an extension of the system (without disorder) and in this case the end particles are unpinned.

Driven by the reservoirs at two different temperatures $T_L$ and $T_R$, the system reaches a nonequilibrium steady state. We are mainly interested in the steady state heat current. Given the Langevin equations of motion Eq (2.53), one can find a formal general expression for the current. Let us denote by $X$ a column vector with $N^d$ elements consisting of the displacements at all lattice sites. Similarly let $\dot{X}$ represent the vector for velocities at all sites. Then we can write the Hamiltonian in Eq. (2.52) in the compact form as in Eq. (2.23),

$$H = \frac{1}{2} X^T M \dot{X} + \frac{1}{2} X^T \mathcal{V} X,$$

which defines the diagonal mass matrix $M$ and the force constant matrix $\mathcal{V}$. Now following the four steps of LEGF formalism one gets an expression for the current $J$ in terms of the transmission coefficient $\mathcal{T}(\omega)$.

It is convenient to express all the results in terms of dimensionless variables. These variables are as follows: force-constants are measured in units of $k$, masses in units of the average mass $\bar{m}$, time in units of the inverse frequency $\Omega_0^{-1} = (\bar{m}/k)^{1/2}$, displacements are in units of the lattice spacing $a$, friction constant $\gamma$ in units of $\bar{m}\Omega$, and finally, temperature is measured in units of $\bar{m}a^2\Omega_0^2/k_B$. With this notation, we write the steady state current per bond from the left to the right reservoir from Eq. (2.38) [24, 17]:

$$J = \frac{\Delta T}{4\pi N'} \int_{-\infty}^{\infty} d\omega \mathcal{T}(\omega), \quad (2.55)$$

where $\mathcal{T}(\omega) = 4 \text{Tr}[\mathcal{I}_L(\omega)\mathcal{G}^+(\omega)\mathcal{I}_R(\omega)\mathcal{G}^-(\omega)]$, $\mathcal{G}^+(\omega) = [-\omega^2 M + \mathcal{V} - S_L^+ - S_R^+]^{-1}$, $\mathcal{G}^- = [\mathcal{G}^+]^\dagger$, $I_L = \text{Im}[S_L^+]$, and $I_R = \text{Im}[S_R^+]$.

$$I_L = \text{Im}[S_L^+] \quad \text{and} \quad I_R = \text{Im}[S_R^+] \quad (2.57)$$

and $\Delta T = T_L - T_R$. The matrices $S_L^+$ and $S_R^+$ represent the coupling of the system to the left and right reservoirs respectively, and can be written as $N \times N$ block matrices where each block is a $N' \times N'$ matrix. The block structures are as follows:

$$S_L^+ = \begin{pmatrix} \Sigma_L^+ & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \end{pmatrix}, \quad S_R^+ = \begin{pmatrix} 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & \Sigma_R^+ \end{pmatrix}. \quad (2.58)$$
where

\[ \Sigma_L^+ = \Sigma_R^+ = i \gamma \omega I , \]  

(2.59)

\( I \) is a \( N' \times N' \) unit matrix, and \( 0 \) is a \( N' \times N' \) matrix with all elements equal to zero. Similarly the matrices \( M \) and \( \mathcal{V} \) have the following block structure:

\[
M = \begin{pmatrix}
M_1 & 0 & \ldots & 0 \\
0 & M_2 & \ldots & 0 \\
0 & 0 & \ldots & 0 \\
0 & 0 & \ldots & M_N
\end{pmatrix}, \quad \mathcal{V} = \begin{pmatrix}
\Phi & -I & \ldots & 0 \\
-\Phi & \Phi & \ldots & 0 \\
0 & 0 & \ldots & 0 \\
0 & 0 & \ldots & -I \Phi
\end{pmatrix},
\]  

(2.60)

where \( M_n \) denotes the diagonal mass-matrix for the \( n_1 = n \) layer and \( \Phi \) is a force-constant matrix whose off-diagonal terms correspond to coupling to sites within a layer. Hence the matrix \( \mathcal{G}^{-1} = [-M \omega^2 + \mathcal{V} - S_L^+ - S_R^+] \) has the following structure:

\[
[\mathcal{G}]^{-1} = \begin{pmatrix}
a_1 & -I & 0 & \ldots & 0 \\
-\Phi & a_2 & -I & \ldots & 0 \\
\ldots & \ldots & \ldots & \ldots & \ldots \\
0 & \ldots & 0 & -I & a_{N-1} \\
0 & \ldots & 0 & -I & a_N
\end{pmatrix},
\]  

(2.61)

where \( a_i = -M_i \omega^2 + \Phi - \delta_{i,1} \Sigma_L^+ - \delta_{i,N} \Sigma_R^+ \). With the form of \( S_{LR}^+ \) given in Eqs. (2.58)and (2.59), we find that the expression for the transmission coefficient reduces to the following form:

\[
\mathcal{T}(\omega) = 4 \text{Tr}[\Gamma_L(\omega)G_N^+(\omega)\Gamma_R(\omega)G_N^-],
\]

where \( \Gamma_{LR} = \text{Im}[\Sigma_{LR}^+] \) 

(2.62)

and \( G_N^+ \) is the \((1,N)\)th block element of \( \mathcal{G} \) and \( G_N^- = [G_N^+]^\dagger \). We now show that \( G_N^+ \) satisfies some simple recursion relations and using those recursion relations the transmission coefficient \( \mathcal{T}(\omega) \) can be expressed as a product of random matrices.
2.4.1 Transfer matrix approach and recursion relations for Green’s functions

Here we will see that because of the block tridiagonal nature of the force constant matrix one can find simple recursion relations among the elements of Green’s function. Before doing that we first introduce some notations. Let $\mathcal{Y}^{(l,l+n-1)}$ with $1 \leq n \leq N - l + 1$ denote a $n \times n$ tridiagonal block matrix whose diagonal entries are $a_l, a_{l+1}, \ldots a_{l+n-1}$, where each $a_l$ is a $N' \times N'$ matrix. The off-diagonal entries are given by $-I$. For an arbitrary block matrix $\mathcal{A}^{(l,m)}$, $\mathcal{A}^{(l,m)}_{(i,j)}$ will denote the block sub-matrix of $\mathcal{A}^{(l,m)}$ beginning with $i$th block row and column and ending with the $j$th block row and column, while $A^{(l,m)}_{i,j}$ will denote the $(i, j)^{th}$ block element of $\mathcal{A}^{(l,m)}$. Also $I_n$ will denote a $n \times n$ block-diagonal matrix with diagonal elements $I$.

The inverse of $\mathcal{Y}^{(1,N)}$ is denoted by $[\mathcal{Y}^{(1,N)}]^{-1} = \mathcal{G}^{(1,N)}$ and satisfies the equation:

$$\mathcal{Y}^{(1,N)} \mathcal{G}^{(1,N)} = I_N .$$

According to our notation, we have $\mathcal{G}^{(1,N)} = \mathcal{G}^*$ and $\mathcal{G}^{(1,N)}_{1,N} = \mathcal{G}^*_N$. The matrix $\mathcal{Y}^{(1,N)}$ has the following structure:

$$\mathcal{Y}^{(1,N)} = \begin{pmatrix} \mathcal{Y}^{(1,N-1)} & W_N \\ W_N^T & a_N \end{pmatrix},$$

(2.63)

where $W_N = (0, 0, \ldots, -I)$ is a $1 \times N - 1$ block vector. We then write Eq. (2.63) in the form

$$\begin{pmatrix} \mathcal{Y}^{(1,N-1)} & W_N \\ W_N^T & a_N \end{pmatrix} \begin{pmatrix} \mathcal{G}^{(1,N)}_{1,N-1} & \mathcal{U}_N \\ \mathcal{U}_N^T & \mathcal{G}^{(1,N)}_{N,N} \end{pmatrix} = \begin{pmatrix} I_{N-1} & 0 \\ 0 & I \end{pmatrix},$$

(2.64)

where $\mathcal{U}_N = [\mathcal{G}^{(1,N)}_{1,N}, \mathcal{G}^{(1,N)}_{2,N}, \ldots, \mathcal{G}^{(1,N)}_{N-1,N}]$ is a $1 \times N - 1$ block vector. From Eq (2.64) we get the four following equations:

$$\mathcal{Y}^{(1,N-1)} \mathcal{G}^{(1,N)}_{1,N-1} + W_N \mathcal{U}_N^T = I_{N-1},$$

$$W_N^T \mathcal{G}^{(1,N)}_{1,N-1} + a_N \mathcal{U}_N^T = 0,$$

$$\mathcal{Y}^{(1,N-1)} \mathcal{U}_N + W_N \mathcal{G}^{(1,N)}_{N,N} = 0,$$

$$W_N^T \mathcal{U}_N + a_N \mathcal{G}^{(1,N)}_{N,N} = I .$$

(2.65)
Noting that \( \mathcal{Y}^{(N-1)}_N = \mathcal{G}^{(N-1)}_N \) and using the third equation above and the form of \( \mathcal{W}_N \), we get:

\[
\mathcal{U}_N = -\mathcal{G}^{(N-1)}_N \mathcal{W}_N \mathcal{G}^{(N)}_{N,N},
\]
or
\[
\mathcal{G}^{(N)}_{i,N} = \mathcal{G}^{(N-1)}_{i,N-1} \mathcal{G}^{(N)}_{N,N}, \text{ for } i = 1, 2, ..., N - 1.
\] (2.66)

From the fourth equation in Eq. (2.65) we get:

\[
\mathcal{G}^{(1,N)}_{N-1,N} = a_N \mathcal{G}^{(1,N)}_{N,N} - I.
\] (2.67)

We will now use Eqs. (2.66),(2.67) to obtain a recursion relation for \( \mathcal{G}^{(1,N)}_{1,N} = \mathcal{G}^{*_1}_N \) in Eq. (2.62), which is the main object of interest. Let us define \( \mathcal{P}^{(l_n)} = [\mathcal{G}^{(l_n)}_{1,n-1}]^{-1} \) where \( \mathcal{G}^{(l_m)} = [\mathcal{Y}^{(l_m)}]^{-1} \). Then setting \( i = 1 \) in Eq. (2.66) and taking an inverse on both sides we get:

\[
\mathcal{P}^{(1,N)} = [\mathcal{G}^{(1,N)}_{N,N}]^{-1} \mathcal{P}^{(1,N-1)}.
\] (2.68)

Setting \( i = N - 1 \) in Eq. (2.66) we get \( \mathcal{G}^{(1,N)}_{N-1,N} = \mathcal{G}^{(1,N-1)}_{N-1,N-1} \mathcal{G}^{(1,N)}_{N,N} \) and using this in Eq. (2.67) we get \( [\mathcal{G}^{(1,N)}_{N,N}]^{-1} = [a_N - \mathcal{G}^{(1,N-1)}_{N-1,N-1}] \). Inserting this in the above equation we finally get our required recursion relation:

\[
\mathcal{P}^{(1,N)} = a_N \mathcal{P}^{(1,N-1)} - \mathcal{P}^{(1,N-2)}.
\] (2.69)

The initial conditions for this recursion are: \( \mathcal{P}^{(1,0)} = I_M \) and \( \mathcal{P}^{(1,1)} = a_1 \). By proceeding similarly as before we can also obtain the following recursion relation:

\[
\mathcal{P}^{(n,N)} = \mathcal{P}^{(n-1,N)} a_1 - \mathcal{P}^{(n-2,N)}, \quad n = 1, 2, ..., N - 1,
\] (2.70)

and \( \mathcal{P}^{(1,N)} \) can be recursively obtained using the initial conditions \( \mathcal{P}^{(N+1,N)} = I_M \) and \( \mathcal{P}^{(N,N)} = a_N \). Given the set \( \{a_i\} \), by iterating either of the above equations one can numerically find \( \mathcal{P}^{(1,N)} \) and then invert it to find \( \mathcal{G}^{(1,N)}_{1,N} \).

However this scheme runs into accuracy problems since the numerical values of the matrix elements of the iterates grow rapidly. We describe now a different way of performing the
recursion which turns out to be numerically more efficient. We first define
\[ r_N = p^{(1,N)}[p^{(1,N-1)}]^{-1}. \]
(2.71)

From Eq. (2.69) we immediately get:
\[ r_N = a_N - \frac{1}{r_{N-1}}, \]
(2.72)
with the initial condition \( r_1 = a_1 \). Then \( G^{(1,N)}_{1,N} \) is given by:
\[
G^{(1,N)}_{1,N} = [p^{(1,N)}]^{-1} = [r_N r_{N-1} \ldots r_1]^{-1} = r_1^{-1} r_2^{-1} \ldots r_N^{-1}.
\]
(2.73)

This form where at each stage \( r_i^{-1} \) is evaluated turns out to be numerically more accurate.

Finally, we show that one can express \( G^{(1,N)}_{1,N} \) in the form of a product of matrices. The product form is such that the system and reservoir contributions are separated. First, we note that the form of the matrices \( a_i \) for our specific problem is: \( a_i = c_i - \delta_{i1} \Sigma_1 - \delta_{iN} \Sigma_N \) where \( c_i = -M_i \omega^2 + \Phi \). We define system-dependent matrices \( Q^{(1,n)} \), \( Q^{(n,N)} \) by replacing \( a_1, a_N \) by \( c_1, c_N \) in the recursions for \( P \)’s. Thus \( Q^{(1,n)} = p^{(1,n)}(a_1 \rightarrow c_1, a_N \rightarrow c_N) \) and \( Q^{(n,N)} = p^{(n,N)}(a_1 \rightarrow c_1, a_N \rightarrow c_N) \). Clearly \( Q \)’s satisfy the same recursion as the \( P \)’s with \( a_i \) replaced by \( c_i \). Then using Eqs. (2.69),(2.70), and similar equations for the \( Q \)’s’ we get:
\[
p^{(1,N)} = Q^{(1,N)} - Q^{(2,N)} \Sigma_1 - \Sigma_N Q^{(1,N-1)} + \Sigma_N Q^{(2,N-1)} \Sigma_1
\]
= \[ (1 - \Sigma_N) \begin{pmatrix} Q^{(1,N)}_{1,N-1} & -Q^{(2,N)}_{1,N-1} \\ Q^{(1,N-1)} & -Q^{(2,N-1)} \end{pmatrix} \begin{pmatrix} 1 \\ \Sigma_1 \end{pmatrix}, \]
(2.74)

From the recursion relations for the \( Q \)’s’, it is easy to see that
\[
\begin{pmatrix} Q^{(1,N)}_{1,N-1} & -Q^{(2,N)}_{1,N-1} \\ Q^{(1,N-1)} & -Q^{(2,N-1)} \end{pmatrix}
= \begin{pmatrix} a_N & -I \\ I & 0 \end{pmatrix} \begin{pmatrix} Q^{(1,N-1)}_{1,N-2} & -Q^{(2,N-1)}_{1,N-2} \\ Q^{(1,N-2)} & -Q^{(2,N-2)} \end{pmatrix}
= \tilde{T}_N \tilde{T}_{N-1} \ldots \tilde{T}_1,
\]
(2.75)
where
\[
\hat{T}_I = \begin{pmatrix} a_I & -I \\ I & 0 \end{pmatrix}.
\] (2.76)

From Eq. (2.74) we then obtain \( P^{(1,N)} \) and from which we get \( G_N^+ = [P^{(1,N)}]^{-1} \). Using this and noting that the baths are white noise Langevin baths we get
\[
\mathcal{J} = \frac{K_B(T_L - T_R)}{\pi N} \int_{-\infty}^{\infty} d\omega \omega^2 \gamma^2 Tr \left[ [P_{1,N}^+(\omega)P_{1,N}^{+T}(-\omega)]^{-1} \right].
\] (2.77)

Comparing the above equation with Eq. (2.55), we get
\[
\mathcal{T}(\omega) = 4\omega^2 \gamma^2 Tr \left[ [P_{1,N}^+(\omega)P_{1,N}^{+T}(-\omega)]^{-1} \right].
\] (2.78)

### 2.4.2 Current in one dimensional harmonic system:

For 1D chain the Hamiltonian in Eq. (2.52) looks like
\[
H = \sum_{i=1}^{N} \left[ \frac{1}{2} m_i \dot{x}_i^2 + \frac{1}{2} k_0 x_i^2 \right] + \sum_{i=1}^{N-1} \frac{1}{2} k(x_{i+1} - x_i)^2 + \frac{1}{2} k'(x_i^2 + x_{i+1}^2),
\] (2.79)

and the corresponding langevin equations look like
\[
m_1 \ddot{x}_1 = -(k' + k_0) x_1 - k(x_1 - x_2) + \gamma \dot{x}_1 + \eta_1(t)
m_l \ddot{x}_l = -k_0 \dot{x}_l - k(2x_l - x_{l-1} - x_{l+1}), \quad 1 < l < N
m_N \ddot{x}_N = -(k' + k_0) x_N - k(x_N - x_{N-1}) + \gamma \dot{x}_N + \eta_N(t)
\] (2.80)

In the classical case, the steady state heat current from left to right reservoir is obtained from Eq. (2.77) \[17, 13\]
\[
\mathcal{J}_N(\omega) = \gamma^2 \omega^2 |G_N|^2,
\]
\[
G_N(\omega) = [P^{(1,N)}]^{-1}(\omega),
\]
\[
\mathcal{V}_{lm} = (1 + k' + k_0) \delta_{l,m} - \delta_{l,m-1} \quad \text{for} \quad l = 1.
\]
\[
\sum_{lm} = i\gamma\omega\delta_{ln}[\delta_{11} + \delta_{1N}],
\]

All the variables and parameters in the above expressions are now dimensionless quantities and \([P^{(1,N)}]^{-1}\) is now just a complex number. It is easy to identify that

\[
P^{(1,N)} = \Delta_N
\]  

(2.81)

where \(\Delta_N\) is the determinant of the matrix \(Z = [-\omega^2 M + V - \Sigma]\).

**Disordered case:** This has been extensively studied and is well understood [14, 15, 17, 19, 22, 69]. The matrix formulation explained in the last section leads to a clear analytic understanding of the main results. From the products of \(N\) random matrices of size \((2 \times 2)\) one calculates \(P^{(1,N)}\) numerically and hence \(T(\omega)\). Clearly \(T(\omega)\) and \(J\) will be different for different disorder realisations. Since we will mostly be interested in disorder averages of these quantities we need to introduce some notation for the disorder average. We consider \([x]\) to be the disorder average of the quantity \(x\). We denote disordered averaged \(T_N(\omega)\) and \(J\) by \(T(\omega) = [T]\) and \(J = [J]\) respectively.

There are three observations that enable one to determine the asymptotic system size dependence of the current. These are:

(i) \(P^{(1,N)} = [G_N^+]^{-1}\) given by Eqs. (2.74), (2.76) is a complex number which can be expressed in terms of the product of \(N\) random \(2 \times 2\) matrices. Using Furstenberg’s theorem it can be shown that for almost all disorder realizations, the large \(N\) behaviour of \(P^{(1,N)}\) for fixed \(\omega > 0\) is \(|P^{(1,N)}| \sim e^{bN\omega^2}\), where \(b > 0\) is a constant. This is to be understood in the sense that \(\lim_{N \to \infty} (1/N) \log |P^{(1,N)}| \sim b\omega^2\) for \(\omega \to 0\). Since \(T(\omega) \sim |P^{(1,N)}|^{-2} \sim e^{-2bN\omega^2}\), this implies that transmission is significant only for low frequencies \(\omega \lesssim \omega_c(N) \sim 1/N^{1/2}\). The current is therefore dominated by the small \(\omega\) behaviour of \(T(\omega)\).

(ii) The second observation made in [19] is that the transmission for \(\omega < \omega_c(N)\) is ballistic in the sense that \(T(\omega)\) is insensitive to the disorder. This can be seen in fig. (2.2) where the
Figure 2.2: Frequency dependence of $|Q^{(1,N)}|$ at small $\omega$ for $\Delta = 0.2$ and $N = 1024$ with fixed BC is compared with the same for an ordered chain. In disordered case $|Q^{(1,N)}|^2$ is averaged over $10^4$ different realisation of masses.

disorder average of $|Q^{(1,N)}|^2$ for a chain of length $N = 1024$ is plotted along with the same for an ordered chain.

(iii) The final important observation is that the form of the prefactors of $e^{-bN\omega^2}$ in $T(\omega)$ for $\omega < \omega_c(N)$ depends strongly on boundary conditions and bath properties [19, 22]. For the white noise Langevin baths, one finds $T(\omega) \sim \omega^2 e^{-bN\omega^2}$ for fixed BC and $T(\omega) \sim \omega^0 e^{-bN\omega^2}$ for free BC [22]. This difference arises because of the scattering of long wavelength modes by the boundary pinning potentials. Now, the asymptotic $N$ dependence of the disorder averaged current in the NESS will be

$$J \sim \int_0^{\omega_c(N)} T(\omega)$$

$$\sim N^{-\frac{1}{2}} \text{ for free BC}$$

$$\sim N^{-\frac{3}{2}} \text{ for fixed BC.}$$

(2.82)

In Fig. (2.3), we plot numerical results showing $T(\omega)$ for the 1D mass-disordered lattice with both fixed and free boundary conditions. We consider a binary mass disordered crystal
in which we set the masses of exactly half the particles at randomly chosen sites to be $\bar{m} - \Delta$ and the rest to be $\bar{m} + \Delta$. Thus $\Delta$ gives a measure of the disorder. One can clearly see the two features discussed above, namely (i) dependence of frequency cut-off on system size and (ii) dependence of the form of $T(\omega)$ on boundary conditions. Using the three observations made above it is easy to arrive at the conclusion that $J \sim N^{-3/2}$ for fixed BC and $J \sim N^{-1/2}$ for free BC. In the presence of a pinning potential the low-frequency modes are suppressed and one obtains a heat insulator with $J \sim e^{-cN}$, with $c$ a constant [69] (see also [21] and references therein).

**Ordered case:** In this case, masses of all the particles are the same (say, $m$). Hence one can write a closed form expression for $\Delta_N$. After some straightforward calculations and rearrangements one can show that [11]:

$$\Delta_N = \frac{[a(q) \sin Nq + b(q) \cos Nq]}{\sin q}, \quad (2.83)$$
where \( a(q) = [2 - \gamma^2 \omega^2 + k'^2 - 2k'] \cos q + 2k' - 2 - 2i \gamma \omega [1 + (k' - 1) \cos q] \),
\[ b(q) = [\gamma^2 \omega^2 - k'^2 + 2k'] \sin q + 2i \gamma \omega (k' - 1) \sin q, \]
\[ 2 \cos q = -m \omega^2 + k_o + 2. \] (2.84)

From the relation in Eq. (2.84), it is clear that for frequencies outside the phonon band \( k_o \leq m \omega^2 \leq k_o + 2 \) the wave vector \( q \) becomes imaginary and hence, from Eq. (2.83), we note that the transmission coefficient \( T(\omega) \) decays exponentially with \( N \). Hence, for large \( N \) we need to consider only the range \( 0 < q < \pi \) and the current is given by:
\[ J_C = \frac{2 \gamma^2 (T_L - T_R)}{\pi} \int_0^\pi dq \frac{d \omega}{dq} \left| \frac{\omega_q^2}{|\Delta_N|^2} \right|, \] (2.85)
with \( m \omega_q^2 = k_o + 2[1 - \cos(q)] \). We now state the following result. For any two well-behaved functions \( g_1(q) \) and \( g_2(q) \)
\[ \lim_{N \to \infty} \int_0^\pi dq \frac{g_1(q)}{1 + g_2(q) \sin Nq} \frac{g_1(q)}{[1 - g_2(q)]^{1/2}} = \int_0^\pi dq \frac{g_1(q)}{[1 - g_2(q)]^{1/2}}. \] (2.86)

There are three steps required to prove this result: (i) expand the factor \( 1/[1 + g_2(q) \sin(Nq)] \) (valid for \( |g| < 1 \) in the integration range), (ii) take the \( N \to \infty \) limit, (iii) resum the resulting series. It is easy to see that the Eq. (2.85) has the same structure as the left hand side of Eq. (2.86) once we note that \( \Delta_N \) can be written as
\[ |\Delta_N|^2 = (|a|^2 + |b|^2)(1 + r \sin(2Nq + \phi))/(2 \sin^2(q)) \]
where \( r \cos \phi = (ab^* + a^*b)/(|a|^2 + |b|^2) \)
and \( r \sin \phi = (|b|^2 - |a|^2)/(|a|^2 + |b|^2) \). (2.87)

Hence using Eq. (2.86) and simplifying, we get [22]:
\[ J_C = \frac{\gamma k^2 k_B (T_L - T_R)}{\pi m} \int_0^\pi \frac{\sin^2 q dq}{\Lambda - \Omega \cos q} = \frac{\gamma k^2 k_B (T_L - T_R)}{m \Omega^2} (\Lambda - \sqrt{\Lambda^2 - \Omega^2}), \] (2.88)
where \( \Lambda = 2k(k - k') + k'^2 + \frac{(k_o + 2k)\gamma^2}{m} \) and \( \Omega = 2k(k - k') + \frac{2k\gamma^2}{m} \).
2.4.3 Current in d-dimensional ordered harmonic system

The current in a d-dimensional ordered lattice can be calculated by using the observation that the problem of heat conduction in a d-dimensional ordered harmonic lattice can be related to heat conduction across $N^{d-1}$ independent ordered harmonic chains with different onsite potentials. Hence the transmission coefficient $T(\omega)$ for the d-dimensional lattice can be expressed as a sum of the transmission coefficients of the 1D chains. Now we will see how one can relate the d-dimensional problem to a one dimensional problem. The Hamiltonian of the d-dimensional system is given in sec. (2.4). We recall that $x_n$ is the displacement of a particle at the lattice site $n = (n_1, n')$. Let us consider that for each $n$ there exists a $q = (q_1, q_2, ..., q_{d-1}, q_d) = (q_1, q')$ with $q_\alpha = \frac{2\pi l}{N}$ where $l$ goes from 1 to $N$ such that

$$\frac{1}{N^{d-1}} \sum_{q'} e^{iq' \cdot \Delta n} e^{-iq' \cdot \Delta n'} = \delta_{\Delta n', \Delta n}$$

(2.89)

Now, if we define

$$x_{n_1}(q') = \frac{1}{N^{d-1}} \sum_{n'} x_{(n_1, n')} e^{iq' \cdot \Delta n'},$$

(2.90)

then one can show that, for each $q'$, $x_{n_1}(q')$ satisfies a Langevin equation corresponding to a one-dimensional Hamiltonian with the onsite spring constant replaced by

$$\lambda(q') = k_o + 2k(d - 1 - \sum_{\alpha=2,...,d} \cos q_\alpha).$$

(2.91)

Hence in the ordered case the d-dimensional harmonic system can be decomposed into $N^{d-1}$ harmonic chains. For $N \rightarrow \infty$, the heat current $J(q')$ for each mode with given $q'$ is then simply given by Eq.(2.88) with $k_o$ replaced by $\lambda(q')$. The heat current per bond is then given by:

$$J = \frac{1}{N^{d-1}} \sum_{q'} J(q').$$

(2.92)

The above result also holds for finite lengths in the transverse direction. For infinite trans-
verse lengths, we get $J = \int ... \int_0^{2\pi} dq J(q)/(2\pi)^{d-1}$. Heat conduction in higher dimensional disordered harmonic systems is studied in the next chapter.