4 Green-Kubo formula for open systems

The Green-Kubo formula [84, 85] is a cornerstone of the study of transport phenomena. In sec. (1.1.3) we saw that for a system governed by Hamiltonian dynamics, the currents that flow in response to small applied fields can be related to the equilibrium correlation functions of the currents. For the case of heat transport the Green-Kubo formula (in the classical limit) gives:

\[
\kappa = \frac{1}{K_B T^2} \lim_{\varepsilon \to 0} \int_0^\infty dt e^{-\varepsilon t} \lim_{L \to \infty} \frac{1}{L} \langle \hat{J}_E(t) \hat{J}_E(0) \rangle,
\]

where \( \kappa \) is the thermal conductivity of a system of linear dimension \( L \) at temperature \( T \). For a d-dimensional system this formula can be written as:

\[
\kappa = \frac{1}{K_B T^2} \lim_{\varepsilon \to 0} \int_0^\infty dt e^{-\varepsilon t} \lim_{L \to \infty} \frac{1}{L^d} \langle \hat{J}_E(t) \hat{J}_E(0) \rangle.
\]

The autocorrelation function on the right hand side is evaluated in equilibrium, without a temperature gradient. Since in this chapter we will be talking about heat current \( J_E \) only, for the rest of the chapter we denote it by \( J \). The total heat current in the system is \( J(t) = \int j(x, t) dx \), where \( j(x, t) \) is the heat flux density. The order of the limits in Eq. (4.2) is important. With the correct order of limits, one can calculate the correlation functions with arbitrary boundary conditions and apply Eq. (4.2) to obtain the response of an open system with reservoirs at the ends. There have been a number of derivations of Eq. (4.2) by various authors [84, 85, 86]. In the introduction of this thesis we have presented one such derivation.

There are several situations where the Green-Kubo formula in Eq. (4.2) is not applicable. For example, for the small structures that are studied in mesoscopic physics, the thermo-
dynamic limit is meaningless, and one is interested in the conductance of a specific finite system. Secondly, in many low dimensional systems, heat transport is anomalous and the thermal conductivity diverges [59]. In such cases it is impossible to take the limits as in Eq. (4.2); one is then interested in the thermal conductance as a function of $L$ instead of an $L$-independent thermal conductivity. The usual procedure that has been followed in the heat conduction literature is to put a cut-off at $t_c \sim L$, in the upper limit in the Green-Kubo integral [59]. There is no rigorous justification of this assumption. A related case is that of integrable systems, where the infinite time limit of the correlation function in Eq. (4.2) is non-zero. Another way of using the Green-Kubo formula for finite systems is to include the infinite reservoirs also while applying the formula and this was done, for example, by Allen and Ford [87] for heat transport and by Fisher and Lee [88] for electron transport. Both these cases are for non-interacting systems and the final expression for conductance is what one also obtains from the nonequilibrium Green's function approach, a formalism of transport commonly used in the mesoscopic literature. More recently, it has been shown that Green-Kubo like expressions for finite open systems can be derived rigorously by using the steady state fluctuation theorem (SSFT) [89, 90, 91, 92].

There are mainly two parts of this chapter. In this first part of this chapter, we derive a Green-Kubo like formula for open systems, without invoking the SSFT. Our proof applies to all classical systems, of arbitrary size and dimensionality, with a variety of commonly used implementations of heat baths. The proof consists in first solving the equation of motion for the phase space probability distribution to find the $O(\Delta T)$ correction to the equilibrium distribution function. The average current at this order can then be expressed in terms of the equilibrium correlation $\langle J(t)J_{fp}(0) \rangle$, where $J_{fp}$ is a specified current operator. Secondly we use the energy continuity equations to relate two different current-current correlation functions, namely $\langle J(0)J(t) \rangle$ and $\langle J(0)J_b(t) \rangle$ where $J_b$ is an instantaneous current operator involving heat flux from the baths. Finally one relates $\langle J(0)J_b(t) \rangle$ to $\langle J(0)J_{fp}(t) \rangle$ and then, using time-reversal invariance, to $\langle J(t)J_{fp}(0) \rangle$. For baths with stochastic dynamics, time-reversal invariance follows from the detailed balance principle, which is an essential requirement of
our proof.

In the second part we obtain an exact expression for the time auto-correlation function for heat current in the NESS for a mass disordered harmonic chain of arbitrary length, expressed in terms of the non-equilibrium Green’s functions. We show that it satisfies the GK formula derived in the first section. Using this correlation function we also calculate the asymptotic system size scaling of fluctuations in current in NESS.

The entire chapter is organised as follows. In Sec. (4.1) we present our proof of the formula for 1D lattice model in detail and outline the proof for other baths in Sec. (4.2). In Sec. (4.3) we extend our proof for higher dimensional lattice models. We also prove this formula for fluid system coupled to Maxwell baths in Sec. (4.4). Finally in Sec. (4.5) we present the calculation of time autocorrelation function and prove that it also satisfies a similar open system formula.

4.1 Proof of the formula for 1D lattice model

We first give a proof of our linear response result for a 1D lattice model with white noise Langevin baths. We consider the following general Hamiltonian:

\[ H = \sum_{i=1}^{N} \left[ \frac{m_i v_i^2}{2} + V(x_i) \right] + \sum_{i=1}^{N-1} U(x_i - x_{i+1}), \tag{4.3} \]

where \( x = \{x_i\} \), \( v = \{v_i\} \) with \( i = 1, 2...N \) denotes displacements of the particles about their equilibrium positions and their velocities, and \( \{m_i\} \) denotes their masses. The particles at the ends are connected to two white noise heat baths of temperatures \( T_L \) and \( T_R \) respectively. The equations of motion of the system are given by:

\[ m_i \ddot{x}_i = f_i - \delta_{i,1} [\gamma^L v_1 - \eta^L] - \delta_{i,N} [\gamma^R v_N - \eta^R], \tag{4.4} \]

where \( f_i = -\partial H/\partial x_i \), and \( \eta^{R,L}(t) \) are Gaussian noise terms with zero mean and satisfying the fluctuation dissipation relations: \( \langle \eta^{L,R}(t) \eta^{L,R}(t') \rangle = 2\gamma^{L,R} k_B T_{L,R} \delta(t - t') \). There are three stages toward proving the open system GK formula.

First stage: In the first part of the proof we obtain an expression for the nonequilibrium
steady state average $\langle J \rangle_{\Delta T}$, at linear order in $\Delta T$, and then we relate this to the equilibrium correlation function $\langle J(t)J(0) \rangle$. The $\langle \ldots \rangle$ denotes a thermal equilibrium average. Time-dependent equilibrium correlation functions require an averaging both over initial conditions as well as over paths. In the Fokker-Planck representation this can be obtained using the time-evolution operator, while in the Langevin representation thermal noise occurs explicitly and has to be averaged over. Corresponding to the stochastic Langevin equations in Eq. (4.4), one has a Fokker-Planck (FP) equation for the phase space distribution $P(x, v, t)$.

Setting $T_L = T + \Delta T/2$ and $T_R = T - \Delta T/2$ we write the FP equation in the following form:

$$\frac{\partial P(x, v, t)}{\partial t} = \hat{L}P(x, v, t) + \hat{L}^{\Delta T} P(x, v, t) , \quad (4.5)$$

where $\hat{L}(x, v) = \hat{L}^H + \sum_{i=1}^{N} \frac{\gamma_l}{m_i} \frac{\partial}{\partial v_l} \left( \frac{1}{2} \frac{k_BT}{m_i} \frac{\partial}{\partial v_l} \right)$

$$\hat{L}^{\Delta T}(v) = \frac{k_BT \Delta T}{2} \left( \frac{\gamma^L}{m_1^2} \frac{\partial^2}{\partial v_1^2} - \frac{\gamma^R}{m_N^2} \frac{\partial^2}{\partial v_N^2} \right) , \quad (4.6)$$

where $\hat{L}^H = -\sum_i \left[ \frac{\partial}{\partial x_1} (f_l/m_i) \frac{\partial}{\partial v_l} \right]$ is the Hamiltonian Liouville operator and $\gamma_l = \gamma^L, \gamma^N = \gamma^R$. For $\Delta T = 0$ the steady state solution of the FP equation is known and is just the usual equilibrium Boltzmann distribution $P_0 = e^{-\beta H}/Z$, where $Z = \int dx dv e^{-\beta H}$ is the canonical partition function $[\beta = (k_BT)^{-1}]$. It is easily verified that $\hat{L}P_0 = 0$. For $\Delta T \neq 0$, we solve Eq. (4.5) by perturbation theory, starting from the equilibrium solution at time $t = -\infty$.

Writing $P(x, v, t) = P_0 + p(x, v, t)$, we obtain the following solution at $O(\Delta T)$:

$$p(x, v, t) = \int_{-\infty}^{t} dt' \, e^{\hat{L}^{\Delta T} (t-t')} \hat{T}^{\Delta T} P_0(x, v) = \Delta \beta \int_{-\infty}^{t} dt' \, e^{\hat{L}^{\Delta T} (t-t')} J_{fp}(v) P_0(x, v) ,$$

with $J_{fp}(v) = (\Delta \beta P_0)^{-1} \hat{L}^{\Delta T} P_0 = -\frac{\gamma_l}{2} \left[ \frac{v_l^2 - k_BT}{m_l} \right] + \frac{\gamma_R}{2} \left[ \frac{v_N^2 - k_BT}{m_N} \right] . \quad (4.7)$

To define the current operator, one first defines the local energy density at the $l$th site:

$$\epsilon_l = m_l v_l^2 / 2 + V(x_l) + \frac{1}{2} [U(x_{l-1} - x_l) + U(x_l - x_{l+1})] .$$

Taking a time derivative gives the energy continuity equation

$$d\epsilon_l/dt + j_{l+1} - j_{l-1} = j_{l,L} \delta_{l,1} + j_{N,R} \delta_{l,N} , \quad (4.8)$$
where \( j_{i+1,l} = \frac{1}{2} (v_l + v_{l+1}) f_{l+1,l} \)
gives the current from the \( l \)th to the \( l + 1 \)th site (\( f_{l+1,l} \) is the force on \( l + 1 \)th particle due to \( l \)th particle). We define the total current flowing through the system as \( J = \sum_{l=1}^{N-1} j_{i+1,l} \). The expectation value of the total current is then given by:

\[
\langle J \rangle_{\Delta T} = \int dx dv J \rho(x, v) = \Delta \beta \int_0^\infty dt \int dx dv J e^{Lt} J f_p P_0 = \Delta \beta \int_0^\infty dt \langle J(t) J f_p(0) \rangle.
\] (4.9)

**Second stage**: In this part we prove

\[
\langle J(t) J f_p(0) \rangle = -\langle J(0) J f_p(t) \rangle.
\] (4.10)

Eq. (4.10) is a statement of time-reversal symmetry. To prove this we write \( \langle J f_p(t) J(0) \rangle = \int dq \int dq' J f_p(q) J(q') P_0(q') W(q, tlq', 0) \) where \( W(q, tlq', 0) \) denotes the transition probability from \( q' = (x', v') \) to \( q = (x, v) \) in time \( t \). Then, using the detailed balance principle,

\[
W(x, v, tlx', v', 0) P_0(x', v') = W(x', -v', tlx, -v, 0) P_0(x, -v)
\] (see [93, 94, 95]) and the fact that \( J \) is odd in the velocities while \( J f_p \) is even, one gets \( \langle J f_p(t) J(0) \rangle = -\langle J f_p(0) J(t) \rangle \) as follows.

\[
\langle J f_p(t) J(0) \rangle_T = \int dq \int dq' J f_p(q) J(q') P_0(q') W(q, tlq', 0)
= \int dq \int dq' J f_p(q') J(q) P_0(q) W(q', tlq, 0)
= \int dq \int dq' J f_p(q') J(q) P_0(x', -v') W(x, -v, tlx', -v', 0)
= \int dq \int dq' J f_p(x', -v') J(x, -v) P_0(q') W(q, tlq', 0)
= -\langle J(t) J f_p(0) \rangle_T,
\] (4.11)

where we have interchanged \( q \) and \( q' \) in the second line and used detailed balance in the third line. Finally in the fourth line we have reversed all the velocity variables and used the fact that \( J(x, v) \) is odd under velocity reversal while \( J f_p \) is not. The Eq. (4.10) can be
proved in a direct but equivalent way which is as follows: An integration by parts followed
by the transformation \( v \to -v \) yields: \( \langle J(t)J_{fp}(0) \rangle = \int dx dv J e^{Lt} J_{fp} P_0 = \int dx dv J_{fp} P_0 e^{Lt} J = -\int dx dv J_{fp} P_0 e^{Lt} J \) where \( \hat{T} \hat{T}^\dagger = \hat{L}^\dagger = \hat{L}^H - \sum_{i=1,N} [v_i - (\beta m_i)^{-1}\partial_{v_i}](\gamma_i' / m_i)\partial_{v_i} \) and \( \hat{T} \) denotes time reversal. We now note the operator identities \( \hat{L} P_0 = P_0 \hat{L}^\dagger \) and consequently \( e^{Lt} P_0 = P_0 e^{Lt} \) which can be proved using the form of \( P_0 \). Using this in the above equation immediately gives: \( \langle J(t)J_{fp}(0) \rangle = -\int dx dv J_{fp} e^{Lt} J P_0 = -\langle J(0)J_{fp}(t) \rangle \). Using this relation in Eq. (4.9) we get

\[
\langle J \rangle_{\Delta T} = \frac{\Delta T}{K_B T^2} \int_0^{\infty} dt \, \langle J_{fp}(t)J(0) \rangle .
\] (4.12)

Third stage: Here we prove the following relations

\[
\int_0^\infty dt \langle J(t)J(0) \rangle = (N-1) \int_0^\infty dt \langle J(0)J_b(t) \rangle .
\] (4.13)

and \( \langle J(0)J_b(t) \rangle = \langle J(0)J_{fp}(t) \rangle \) (4.14)

which together complete the proof. For this let us define the current variable \( J_b \) as the mean of the instantaneous heat currents flowing into the system from the left reservoir and flowing out of the system to the right reservoir. Thus we have

\[
J_b(t) = \frac{1}{2} (J_{1,h} - J_{N,R})
\] (4.15)

where \( J_{1,h}(t) = -\gamma^L v_1^2(t) + \eta^L(t)v_1(t) \), \( J_{N,R}(t) = -\gamma^R v_N^2(t) + \eta^R(t)v_N(t) \). (4.16)

It is easy to note that \( \langle J(0) \rangle = 0 \). Now we prove

\[
\langle J(0)\eta^L(t)v_1(t) \rangle = \langle J(0)\eta^R(t)v_N(t) \rangle = 0 .
\] (4.17)

To prove this we use Novikov’s theorem [96] which says: if \( \{\eta_i\} \) be a set of arbitrary Gaussian noise variables with \( \langle \eta_i(t)\eta_j(t') \rangle = K_{ij}(t,t') \) and \( H[\eta] \) be a functional of the noise variables, then

\[
< \eta(t)H[\eta] > = \sum_i \int \langle \eta_i(t)\eta_j(t') \rangle \left( \frac{\delta H[\eta]}{\delta \eta_j(t')} \right) dt' ,
\]
where \( \delta H[\eta]/\delta \eta(t') \) represents a functional derivative of \( H[\eta] \) with respect to \( \eta \). Using the fact \( \langle J(0) \rangle = 0 \) and Eq. (4.17) we get Eq. (4.14).

To prove Eq. (4.13) let us define \( D_i(t) = \sum_{k=1}^{l} \epsilon_k - \sum_{l=i+1}^{N} \epsilon_k \) for \( l = 1, 2, \ldots, N - 1 \). Then from the continuity equation Eq. (4.8) one can show that

\[
\frac{dD_i}{dt} = -2j_{i+1,i}(t) + 2J_b(t) . \tag{4.18}
\]

We multiply this equation by \( J(0) \), take a steady state average, and integrate over time from \( t = 0 \) to \( \infty \). Since \( D_iJ \) has an odd power of velocity, we get \( \langle D_i(0)J(0) \rangle = 0 \). Also \( \langle D_i(\infty)J(0) \rangle = \langle D_i(\infty) \rangle \langle J(0) \rangle = 0 \), and using these we immediately get \( \int_0^{\infty} dt \langle j_{i+1,i}(t)J(0) \rangle = \int_0^{\infty} dt \langle J_b(t)J(0) \rangle \). Summing over all bonds thus proves Eq. (4.13). Now using Eq. (4.14) first and then Eq. (4.13) we write Eq. (4.12) as:

\[
\langle J \rangle_{\Delta T} = \frac{\Delta T}{k_B T^2} \frac{1}{N-1} \int_0^{\infty} dt \langle J(t)J(0) \rangle . \tag{4.19}
\]

Dividing both sides of the above equation by \( (N-1) \) and defining the steady state current per bond between the reservoir and the system as \( \bar{j} = J/(N-1) \) we write Eq.(4.19) as

\[
\langle \bar{j} \rangle_{\Delta T} = \frac{\Delta T}{k_B T^2} \int_0^{\infty} dt \langle \bar{j}(t)\bar{j}(0) \rangle . \tag{4.20}
\]

Finally the conductance is given by

\[
G = \lim_{\Delta T \to 0} \frac{\langle \bar{j} \rangle_{\Delta T}}{\Delta T} = \frac{1}{k_B T^2} \int_0^{\infty} dt \langle \bar{j}(t)\bar{j}(0) \rangle . \tag{4.21}
\]

Except the proofs of Eq. (4.10) and Eq. (4.14), other parts of the proof are quite general and independent of the heat baths used. Proofs of Eq. (4.10) and Eq. (4.14) depend on the specific bath chosen. In the next section we extend the proof to the cases where the noises from the baths are exponentially correlated in time and noises are obtained by coupling the lattice Hamiltonian to a deterministic bath model. Later we also give the proof of this formula for fluid systems.
4.2 One dimensional lattice with other baths

We outline the proof for two other models of baths coupled to the lattice Hamiltonian. These are (i) the Nose-Hoover bath and (ii) a Langevin bath with exponentially correlated noise.

**Nose-Hoover bath:** In this case the equations of motion are:

\[ m_1 \dot{v}_1 = f_1 - \delta_{L1} \xi_L v_1 - \delta_{L, N} \xi_R v_N, \]  
(4.22)

where \( \xi_L, \xi_R \) are themselves dynamical variables satisfying the equations of motion:

\[ \dot{\xi}_L = \frac{1}{\theta_L} \left( \frac{m_1 v_1^2}{k_B T_L} - 1 \right), \]
\[ \dot{\xi}_R = \frac{1}{\theta_R} \left( \frac{m_N v_N^2}{k_B T_R} - 1 \right). \]

For small \( \Delta T \), we then write an equation of motion for the extended distribution function \( P(x, v, \xi_L, \xi_R, t) \). This has the same form as Eq. (4.5) but now with:

\[ \hat{\mathcal{L}}^T = \hat{\mathcal{L}}^H + \frac{\xi_L}{m_1} \frac{\partial}{\partial v_1} v_1 - \frac{1}{\theta_L} \frac{\partial}{\partial \xi_L} \left( \frac{m_1 v_1^2}{k_B T_L} - 1 \right) \]
\[ + \frac{\xi_R}{m_N} \frac{\partial}{\partial v_N} v_N - \frac{1}{\theta_R} \frac{\partial}{\partial \xi_R} \left( \frac{m_N v_N^2}{k_B T_R} - 1 \right) \]
\[ \hat{\mathcal{L}}^{\Delta T} = \frac{\Delta T}{2k_B T^2} \left( \frac{m_1 v_1^2}{\theta_L} \frac{\partial}{\partial \xi_L} - \frac{m_N v_N^2}{\theta_R} \frac{\partial}{\partial \xi_R} \right). \]  
(4.23)

If \( T_L = T_R = T \), it is easy to verify that the equilibrium phase space density is given by:

\[ \hat{P}_0 = P_0(x, v) \exp \left[ -\frac{1}{2} \left( \frac{\theta_L \xi_L^2}{m_1} + \frac{\theta_R \xi_R^2}{m_N} \right) \right], \]
(4.24)

and we assume that there is convergence to this distribution. Acting with \( \hat{\mathcal{L}}^{\Delta T} \) on this, we then obtain:

\[ J_{fp} = -\frac{1}{2} (v_1^2 \xi_L - v_N^2 \xi_R). \]  
(4.25)

On the other hand, since \( -\xi_L v_1 \) is the force from the left reservoir on the first particle, hence \( j_{1,L} = -\xi_L v_1^2 \) and similarly, \( j_{N,R} = -\xi_R v_N^2 \). Hence from the definition of \( J_b \) in Eq. (4.15), we obtain \( J_{fp} = -J_b \). This gives Eq. (4.14) with a minus sign on the right hand side i.e. \( \langle J(0)J_b(t) \rangle = -\langle J(0)J_{fp}(t) \rangle \). Now proceeding as in the second stage of the proof we get
\[ \langle J(t)J_{fp}(0) \rangle = \langle J(0)J_{fp}(t) \rangle \text{ without the minus sign (as there in Eq. (4.10))}. \] This can be seen from Eqs.(4.22) and (4.23). Under time reversal \((x, v, \zeta) \rightarrow (x, -v, -\zeta)\), and since \(J, J_{fp}\) both are odd under time reversal, there is no minus sign in Eq.(4.11). Rest of the proof is similar to the previous case.

**Exponentially correlated bath:** A simple way of realizing exponentially correlated heat baths is to consider the following set of equations of motion:

\[ m_1 \dot{v}_1 = f + \delta_{1,1} y_L + \delta_{1,N} y_R, \quad (4.26) \]

where \(y_L, y_R\) satisfy the following equations of motion:

\[ \begin{align*}
\dot{y}_L &= -\frac{y_L}{\gamma_L} - \gamma_L v_1 + \eta^L \\
\dot{y}_R &= -\frac{y_R}{\gamma_R} - \gamma_R v_N + \eta^R,
\end{align*} \]

where \(\eta^L, \eta^R\) are Gaussian white noise satisfying \(\langle \eta^L(t) \eta^R(t') \rangle = 2k_B T_{LR} / v^{LR} \delta(t - t')\). Assuming that the baths are coupled to the system at time \(t = -\infty\), the solution of the above equations is:

\[ \begin{align*}
y_L &= -\gamma_L \int_{-\infty}^{t} dt' e^{-\gamma_L (t-t')/v^L} v_1(t') + \xi^L(t) \\
y_R &= -\gamma_R \int_{-\infty}^{t} dt' e^{-\gamma_R (t-t')/v^R} v_N(t') + \xi^R(t),
\end{align*} \]

where \(\xi^L = \int_{-\infty}^{t} dt' e^{-\gamma_L (t-t')/v^L} \eta^L(t')\) and \(\xi^R = \int_{-\infty}^{t} dt' e^{-\gamma_R (t-t')/v^R} \eta^R(t')\).

The noise variables \(\xi^{LR}\) satisfy \(\langle \xi^{LR}(t) \xi^{LR}(t') \rangle = k_B T_{LR} v^{LR} e^{-|t-t'|/v^{LR-LR}}, \) and so we verify that \(y_{LR}\) are of the required form of exponentially correlated baths.

In this case we write a Fokker-Planck equation for the probability distribution for \(P(x, v, y_L, y_R)\) and the forms of \(\hat{L}^T\) and \(\hat{L}^{AT}\) are given by:

\[ \hat{L}^T = \hat{L}^H - \frac{y_L}{m_1} \frac{\partial}{\partial v_1} + \frac{\gamma_L v_1}{m_1} \frac{\partial}{\partial y_L} \left( \frac{y_L}{v^L} \frac{\partial}{\partial y_L} + \frac{k_B T}{v^L} \frac{\partial}{\partial y_L} \right) - \frac{y_R}{m_N} \frac{\partial}{\partial v_N} + \frac{\gamma_R v_N}{m_N} \frac{\partial}{\partial y_R} \left( \frac{y_R}{v^R} \frac{\partial}{\partial y_R} + \frac{k_B T}{v^R} \frac{\partial}{\partial y_R} \right), \]
One can verify that the equilibrium distribution is, in this case, given by:

$$\hat{P}_0 = P_0(x, v) \exp \left[ -\frac{1}{2} \left( \frac{y_L^2}{\gamma_L^2} + \frac{y_R^2}{\gamma_R^2} \right) \right],$$

while $J_{fp}$ is given by:

$$J_{fp} = \frac{1}{2\gamma_L} \left( \frac{y_L^2}{(\gamma_L)^2} - \frac{k_B T}{\gamma_L} \right) - \frac{1}{2\gamma_R} \left( \frac{y_R^2}{(\gamma_R)^2} - \frac{k_B T}{\gamma_R} \right).$$

Now using the equation

$$\frac{d}{dt} \left( \frac{y_L^2}{2\gamma_L^2} \right) = -\frac{y_L^2}{\gamma_L} \frac{v_L}{(\gamma_L)^2} - y_L v_1 + \frac{y_L \eta^L}{\gamma_L},$$

and the fact that $\langle J(0)y_L(t)\eta^L(t) \rangle_T = 0$, it follows that:

$$\int_0^\infty dt \left( \frac{y_L^2(t)}{\gamma_L(t)^2} \right)_T = -\int_0^\infty dt \langle J(0)y_L(t)v_1(t) \rangle_T,$$

and a similar result for the right reservoir. From the equations of motion Eq. (4.26), we get $j_{1L} = y_L v_1$, $j_{N,R} = y_R v_N$. Hence from the above equation and from the definitions of $J_b$ in Eq. (4.15), and of $J_{fp}$ in Eq. (4.29), we again get $\langle J(0)J_{fp}(t) \rangle_T = \langle J(0)J_b(t) \rangle_T$. The other steps of the proof are the same as for the white-noise case.

### 4.3 Lattice models in higher dimensions

In this section we give a generalization of the derivation to arbitrary dimensions, for the case of white noise reservoirs. The extension to the baths in sec. (4.2) is straightforward. We consider a system of particles with mean positions on a $d$-dimensional hypercubic lattice with points represented by $l = (l_1, l_2, ..., l_d)$ where $l_\alpha = 1, 2, ..., N$ with $\alpha = 1, 2, ..., d$. The Hamiltonian of the system is given by:

$$H = \sum_1^N \left[ \frac{m_1 v_1^2}{2} + V(x_1) \right] + \sum_{<1,k>} U(x_1 - x_k),$$

(4.31)
where $x_i$ and $v_i$ are the $d$-dimensional displacement about lattice positions and velocity vectors respectively, of the particle at $I$ and $<I,k>$ denotes nearest neighbors. Heat conduction takes place in the $\alpha = v$ direction because of heat baths at temperature $T_L$ and $T_R$ that are attached to all lattice points on the two hypersurfaces $l_v = 1$ and $l_v = L$. The corresponding Langevin equations of motion are:

$$m_i \ddot{x}_i = f_i + \delta_{i,1} [\eta^L_v - \gamma^L_v v_i] + \delta_{l_v,L} [\eta^R_v - \gamma^R_v v_i],$$

(4.32)

where $I = (l_v, Y)$, so that $I'$ denotes points on a constant $l_v$ hypersurface. The noise terms at different lattice points and in different directions are assumed to be uncorrelated, and satisfy the usual fluctuation-dissipation relations. We define the local energy as:

$$\epsilon_l(t) = \frac{1}{2} m_i \dot{v}_i^2 + V(x_i) + \frac{1}{2} \sum_{\tilde{e}} U(x_i - x_{i+\tilde{e}}),$$

(4.33)

where the sum is over all the $2d$ unit vectors $\tilde{e}$ which specify the nearest neighbours of the site $I$. The corresponding continuity equations are easily found to be:

$$\dot{\tilde{e}}_{l,v} = \sum_{\tilde{e}'} \tilde{j}_{l,v}(l,v), \quad \dot{\tilde{e}}_i = \sum_{\tilde{e}} \tilde{j}_{i+\tilde{e},v}, \quad \text{for } l_v = 2, 3 \ldots N - 1$$

$$\dot{\tilde{e}}_{N,v} = \sum_{\tilde{e}'} \tilde{j}_{N,v}(N,v),$$

(4.34)

where $\tilde{j}_{l,v}$ denotes the force on particle at $l$ by particle at $k$, and $\sum_{\tilde{e}}$ is a sum over neighbors but excluding points on $l_v = 0, N + 1$. Further, if we define $\epsilon_{l,v} = \sum_{Y} \epsilon_{l(v,Y)}$, then these satisfy equations of the 1D form:

$$\dot{\epsilon}_l = -\dot{j}_{2,1}^{l_v}(t) + \dot{j}_{1,l(1)}^{l_v}(t)$$

$$\dot{\epsilon}_{l,v} = \dot{j}_{l,v,l(1)}^{l_v,v}(t) - \dot{j}_{l,v,l(1)}^{l_v,v}(t), \quad \text{for } l_v = 2, 3 \ldots N - 1$$
\[ \epsilon_N = \mathcal{J}_{N,N-1}^\nu(t) + \mathcal{J}_{N,R}^\nu(t) \]

where

\[ \mathcal{J}_{L,v-1}^\nu = \sum_{\nu} j^{(\nu),v,(v-1),v} \]

\[ \mathcal{J}^\nu_{IL} = \sum_{\nu} j^{(1),v}_{(1),v} \], \[ \mathcal{J}^\nu_{IR} = \sum_{\nu} j^{R}_{(N),v} \]. \tag{4.35}

Defining now the total current operator as \( \mathcal{J}^\nu = \sum_{v=1}^{N-1} \mathcal{J}^\nu_{v,v+1} \) where \( \mathcal{J}^\nu_{v,v+1} \) is the heat current flowing in the \( \nu \) direction between the \( v \)th and \( v+1 \)th hypersurfaces, and the boundary current operator

\[ \mathcal{J}^\nu_b = -\frac{(\mathcal{J}_{IL}^\nu - \mathcal{J}_{NR}^\nu)}{2} = \frac{1}{2} \sum_{\nu} \left[ \left[ \gamma^L_{v^{(1)},v} v^{2}_{v^{(1)},v} - \eta^L_{v^{(1)},v} \right] - \left[ \gamma^R_{v^{(N)},v} v^{2}_{v^{(N)},v} - \eta^R_{v^{(N)},v} \right] \right]. \tag{4.36} \]

and by following the same steps as in the 1D case, we can again prove the analogue of Eq. (4.13). In this case this is \( \int_0^\infty dt \langle J'(t) J'(0) \rangle = (N - 1) \int_0^\infty dt \langle J'(0) J'_b(t) \rangle \).

The Fokker-Planck equation corresponding to the Langevin equations in Eq. (4.32) have the same form as Eq. (4.5) with:

\[ L^{\Delta T} = \frac{k_B T}{2} \sum_{\nu} \left[ \gamma^L_{v^{(1)},v} v^{2}_{v^{(1)},v} - \gamma^R_{v^{(N)},v} v^{2}_{v^{(N)},v} \right]. \tag{4.37} \]

As in the 1D case, the deviation of the expectation value of any observable \( A(x, v) \) from its stationary value is given by \( \Delta T / (k_B T^2) \int_0^\infty dt \langle A(t) J_{fp}^\nu(0) \rangle \), where now:

\[ J_{fp}^\nu = \frac{1}{2} \sum_{\nu} \left\{ \gamma^L_{v^{(1)},v} \left[ \frac{d k_B T}{m^{(1),v}} \right] - \gamma^R_{v^{(N)},v} \left[ \frac{d k_B T}{m^{(N),v}} \right] \right\}. \tag{4.38} \]

With \( J_b^\nu \) and \( J_{fp}^\nu \) given by Eqs. (4.36,4.38), it is clear that we can repeat the arguments for the 1D case. We then get \( \langle J'(0) J'_b(t) \rangle = \langle J'(0) J'_{fp}(t) \rangle = -\langle J'(t) J'_{fp}(0) \rangle \), where the last step requires use of the detailed balance principle. Thus we finally have the required results corresponding to Eqs. (4.9,4.10,4.13,4.14), from which we get the required formula, which is of the same form as Eq. (4.21) with \( i \) replaced by \( \nu = J'/\langle N - 1 \rangle \).

### 4.4 Fluid system coupled to Maxwell baths

We first consider a 1D system of particles in a box of length \( L \). The end particles (1 and \( N \)) interact with baths at temperatures \( T_L \) and \( T_R \) respectively. Whenever the first particle
hits the left wall it is reflected back with a random velocity chosen from the distribution:
\[ \Pi(v) = m_1 \beta_L \theta(v) v \exp[-\beta_L m_1 v^2/2] , \]
with a similar rule at the right end. Otherwise the dynamics is Hamiltonian.

We find the FP current by noting that \( J_{fp} = (\Delta \beta)^{-1} [\partial_t P/P]_{P=P_0} \). There are two parts to the evolution of the phase space density: the Hamiltonian dynamics inside the system, and the effect of the heat baths. After a small time interval \( \epsilon \), the phase space density \( P(x; v; t + \epsilon) \) is

\[
J_1 = \frac{\partial m_1 e^{-\frac{1}{2} \beta_L m_1 v^2} \int_0^\infty P(0, x' - v' \epsilon; -v_0, v' - a' \epsilon; t)v_0 dv_0}{\epsilon}, \quad \text{for } x_1 < v_1 \epsilon
\]
\[
J_N = \frac{\beta R m_N e^{-\frac{1}{2} \beta R m_N v^2} \int_0^\infty P(x' - v' \epsilon, L; v' - a' \epsilon, v_0; t)v_0 dv_0}{\epsilon}, \quad \text{for } x_N > L + v_N \epsilon
\]
\[
= P(x - v \epsilon, v - a \epsilon, t) \quad \text{otherwise} \quad (4.39)
\]

where the primed variables in the first and second lines leave out particles 1 and \( N \) respectively. (Note that since \( 0 < x_1 \) and \( x_N < L \), the conditions in the second and third lines imply \( v_1 > 0 \) and \( v_N < 0 \).)

If \( T_L = T_R = T \), and \( P(x, v, t) = P_0 \), the equilibrium phase space density for the temperature \( T \), then the phase space density at time \( t + \epsilon \) is the same. Now if \( T_{LR} = T \pm \Delta T/2 \), with \( P(x, v, t) \) still equal to \( P_0 \), then

\[
P(x; v; t + \epsilon) = P_0 + \frac{\Delta T}{2T} \left[ \frac{1}{2} \beta m_1 v_1^2 - k_B T \right] \theta(v_1 - x_1) - \frac{1}{2} \beta m_N v_N^2 - 1) \theta(x_N - L - v_N \epsilon) P_0.
\]

Dividing by \( \epsilon \) throughout and taking \( \epsilon \to 0 \), we see that

\[
J_{fp} = \frac{1}{2} \left[ \frac{1}{2} \beta m_1 v_1^2 - k_B T \right] v_1^2 \delta(x_1) \theta(v_1) - \frac{1}{2} \left[ \frac{1}{2} \beta m_N v_N^2 - k_B T \right] v_N^2 \delta(x_N - L) \theta(-v_N) \quad (4.40)
\]

We have to use continuum energy density \( \epsilon(x, t) \) and current \( j(x, t) \), and the total heat current is now \( J = \int j(x) dx \) instead of \( \sum_{i=1} J_i \). The continuity equation is still valid, and defining \( D(x, t) = \int_0^x d x' \epsilon(x', t) - \int_x^L \epsilon(x', t) \) and \( A(t) = \int_0^L dx D(x) \), we get the analogue of Eq. (4.13):

\[
\int_0^\infty \langle J(t)J(0) \rangle dt = L \int_0^\infty \langle J_b(t)J(0) \rangle dt.
\]

(4.41)
Here \( J_b = \frac{1}{2}[j_{1,L} - j_{N,R}] \) as before, and

\[
\begin{align*}
    j_{1,L} &= \frac{1}{2}m_1 v_1 (v_{1,L}^2 - v_1^2) \delta(x_1) \theta(-v_1) \\
    j_{N,R} &= \frac{1}{2}m_N v_N (v_{N,L}^2 - v_N^2) \delta(x_N - L) \theta(v_N).
\end{align*}
\]

The \( \delta \)-functions enforce the condition that the particle is colliding with the bath, and \( v_{1,L} \) and \( v_{N,R} \) are the random velocities with which they emerge from the collision. Invoking detailed balance, using the explicit forms of \( J_{fp} \) and \( J_b \), and the fact that \( J(0) \) is uncorrelated with \( v_{1,L}, v_{N,R} \) we can show that \( \langle J(0)J_b(t) \rangle = -\langle J(t)J_{fp}(0) \rangle \). Using this relation and Eq. (4.41) in Eq. (4.9), we obtain Eq. (4.21) with \( (N - 1) \) replaced with \( L \).

The generalization to a \( d \)-dimensional system is straightforward. First, any particle can interact with the baths at the ends if it reaches \( x = 0 \) or \( x = L \). Including the effect of the components of the velocity transverse to the heat-flow direction the derivation of Eq. (4.40) gets modified and gives

\[
\begin{align*}
    J_{fp} &= \sum_l \left[ -\frac{1}{2}(\frac{1}{2}m_l v_l^2 - \frac{1}{2}(d + 1)k_BT)v_l^r \delta(x_l^r) \theta(v_l^r) \\
    &\quad - \frac{1}{2}(\frac{1}{2}m_l v_l^2 - \frac{1}{2}(d + 1)k_BT)v_l^r \delta(x_l^r - L) \theta(-v_l^r) \right].
\end{align*}
\]

The expression for \( J_b \) changes similarly, so that the final result of the previous paragraph is still valid.

All the above derivations of open system GK formula for different systems uses Fokker-Planck description of stochastic systems and hence is only applicable for those currents which can be expressed solely in terms of phase space variables (e.g. currents inside the bulk of the system). Since boundary currents naturally involve noises explicitly, derivation given in this section is not applicable to them. The general expectation is that, even for boundary currents, one can prove an open finite system GK formula as given in Eq.(4.21). In the next section we explicitly calculate boundary current-current auto correlation function in the context of heat transport for a finite mass disordered harmonic chain in NESS and show that integration of the equilibrium correlation function gives the NESS current.

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4.5 Proof of the formula for boundary currents

Time correlation functions are useful quantities in the study of transport processes. They are related to various transport coefficients. For example, the diffusion constant of a Brownian particle is given by the integral of the equilibrium velocity-velocity time auto-correlation function. Similarly the friction coefficient of an over-damped particle is also related to the time correlation function of the instantaneous force experienced by the particle. There are few examples where exact time auto-correlation functions in equilibrium state have been obtained for many-particle systems. For Hamiltonian systems some examples of exact calculations are velocity auto-correlation function for ordered harmonic lattices [97] and for a one dimensional gas of elastically colliding hard rods [98]. Recently authors of [99] have shown explicitly that integration of the heat current auto-correlation function gives the current in non-equilibrium steady state for a two particle harmonic system. In this section we obtain an exact expression for the time auto-correlation function for heat current in the NESS for a disordered harmonic chain of arbitrary length, expressed in terms of the non-equilibrium Green’s functions. We show that it satisfies the GK formula derived in previous section. Using this correlation function we also calculate the asymptotic system size scaling of fluctuations in current in NESS.

4.5.1 Definition of the model

We consider a chain of oscillators of N particles described by the Hamiltonian $H$:

$$H = \sum_{l=1}^{N} \left[ \frac{1}{2} m_l x_l^2 + \frac{1}{2} k_o x_l^2 \right] + \sum_{l=1}^{N-1} \frac{1}{2} k (x_{l+1} - x_l)^2 + \frac{1}{2} k' (x_1^2 + x_N^2), \quad (4.42)$$

where $x_l$ are displacements of the particles about their equilibrium positions, $k$, $k_o$ are the inter-particle and on-site spring constants respectively, and $m_l$ is mass of the $l^{th}$ particle. $k'$ is the spring constant of the potentials at the boundaries. For different values of $k'$ and $k_0$ we get different boundary-conditions (BCs). If $k'$ and $k_0$ both are zero we get free BC, otherwise we get fixed BC ($k' \neq 0$ and $k_0 = 0$) and pinned case ($k_0 \neq 0$). The particles 1 and $N$
are connected to two white noise heat baths of temperatures $T_L$ and $T_R$ respectively. The equation of motion of the $l^{th}$ particle is given by [19]

$$m_i \ddot{x}_l = -k(2x_l - x_{l-1} - x_{l+1}) - k_v x_l - \delta_{l1}[(k' - k)x_l + \gamma_L x_l - \eta_L]$$

$$-\delta_{lN}[(k' - k)x_l + \gamma_R x_N - \eta_R]$$

where $l = 1, 2...N$ and $x_0 = x_{N+1} = 0$ (4.43)

where $\eta_{L,R}(t)$ are Gaussian noise terms with zero mean and satisfy the following fluctuation dissipation relations

$$\langle \eta_{L,R}(t) \eta_{L,R}(t') \rangle = 2\gamma_{L,R} k_B T_{L,R} \delta(t - t')$$

$$\langle \eta_L(t) \eta_R(t') \rangle = 0, \quad \langle \eta_{L,R}(t) \rangle = 0$$ (4.44)

We first define the local energy density associated with the $l^{th}$ particle (or energy at the lattice site $l$) as earlier:

$$\epsilon_1 = \frac{p_1^2}{2m_1} + \frac{k_v x_1^2}{2} + \frac{k'}{4} (x_1 - x_2)^2,$$

$$\epsilon_l = \frac{p_l^2}{2m_l} + \frac{k_v x_l^2}{2} + \frac{k}{4} \left[ (x_{l-1} - x_l)^2 + (x_l - x_{l+1})^2 \right],$$

for $l = 2, 3...N - 1$

$$\epsilon_N = \frac{p_N^2}{2m_N} + \frac{k_v x_N^2}{2} + \frac{k'}{4} (x_{N-1} - x_N)^2.$$ (4.45)

Taking time derivative of these energy densities we write continuity equations, from which we get two instantaneous currents $j_{1,L}$ and $j_{N,R}$ which are flowing from the left and right reservoirs into the system respectively. These currents are given by [59, 58]

$$j_{1,L}(t) = -\gamma_L \dot{x}_1^2(t) + \eta_L(t) \dot{x}_1(t),$$

and

$$j_{N,R}(t) = -\gamma_R \dot{x}_N^2(t) + \eta_R(t) \dot{x}_N(t).$$ (4.46)
4.5.2 Steady state properties and current calculation

In order to obtain the steady state properties we have to find out the steady state solution of the Eq. (4.43). For that we write Eq. (4.43) in Matrix form as:

\[ M\ddot{X} + \Gamma \dot{X} + \Phi X = \eta(t), \]

(4.47)

where, \( X, \eta \) are column vectors with elements \( [X]^T = (x_1, x_2, \ldots, x_N) \), \( [\eta]^T = (\eta_L, 0, \ldots, 0, \eta_R) \) and \( \Gamma \) is a \( N \times N \) matrix with only non-vanishing elements \( [\Gamma]_{11} = \gamma_L \), \( [\Gamma]_{NN} = \gamma_R \). \( [\Phi]_{N \times N} \) represents a tridiagonal matrix with elements [13]

\[
\Phi_{lm} = \begin{cases} (k + k' + k_o)\delta_{l,m} - k\delta_{l,m-1} & \text{for } l = 1 \\ -k\delta_{l,m-1} + (2k + k_o)\delta_{l,m} - k\delta_{l,m+1} & \text{for } 2 \leq l \leq N - 1 \\ (k + k' + k_o)\delta_{l,1} - k\delta_{l,m+1} & \text{for } l = N , \end{cases}
\]

(4.48)

and \( M_{lm} = m_l\delta_{lm} \) where \( m_l \) is chosen uniformly from the range \([1 - \Delta, 1 + \Delta]\). If \( G^+(t) \) denotes the Green’s function of the entire system then \( G^+(t) \) satisfies

\[
M\ddot{G}^+(t) + \Gamma \dot{G}^+(t) + \Phi G^+(t) = \delta(t)I , \]

(4.49)

It is easy to verify that \( G^+(t) = G(t)\Theta(t) \) where \( G(t) \) satisfies the homogeneous equation

\[
M\ddot{G} + \Gamma \dot{G} + \Phi G = 0 , \]

(4.50)

with the initial conditions \( G(0) = 0 \), \( \dot{G}(0) = M^{-1} \). Here \( \Theta(t) \) is the Heaviside function. Assuming that the heat baths have been switched on at \( t = -\infty \) we write the steady state solution of Eq. (4.47) as

\[
X(t) = \int_{-\infty}^{t} dt' G(t-t')\eta(t').
\]

(4.51)

For equilibration we require that \( G(t) \to 0 \) as \( t \to \infty \). From Eq. (4.51), we get

\[
\dot{x}_1(t) = \int_{-\infty}^{t} dt_1 \left[ \dot{G}_{11}(t-t_1)\eta_L(t_1) + \dot{G}_{1N}(t-t_1)\eta_R(t_1) \right].
\]

(4.52)
Next we calculate $J = \langle j_{1,L} \rangle$ in the NESS. Here $\langle ... \rangle$ denotes the average over the noise variables $\eta_L(t)$ and $\eta_R(t)$. Putting $\dot{x}_1(t)$ from Eq. (4.52) in the expression of $j_{1,L}(t)$ in Eq. (4.46) and using the noise correlation in Eq. (4.44) we get:

\[
J = -\gamma_L \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 \left[ \dot{G}_{11}(t-t_1)\dot{G}_{11}(t-t_2) \times \langle \eta_L(t_1)\eta_L(t_2) \rangle \right]
+ \dot{G}_{1N}(t-t_1)\dot{G}_{1N}(t-t_2) \times \langle \eta_R(t_1)\eta_R(t_2) \rangle \right] + \int_{-\infty}^{t} dt_1 \dot{G}_{11}(t-t_1) \langle \eta_L(t)\eta_L(t_1) \rangle
\]
\[
= 2\gamma_L K_B \left[ \frac{T_L}{2} \dot{G}_{11}(0) - (\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)) \right], \tag{4.53}
\]

where we have used the definition

\[
A_i(t) = \int_{0}^{\infty} dt' \dot{G}_{11}(t + t')\dot{G}_{11}(t') \quad \forall \ t. \tag{4.54}
\]

We now note the following identity (for proof see appendix)

\[
\gamma_L A_1(t) + \gamma_R A_N(t) = \frac{\dot{G}_{11}(t)}{2}, \tag{4.55}
\]

which can be obtained from Eqs. (4.54, 4.50). Using this in Eq. (4.53) we get

\[
J = 2\gamma_L \gamma_R K_B (T_L - T_R) A_N(0). \tag{4.56}
\]

If we go to the frequency ($\omega$) space using the following definition

\[
G^*(\omega) = \int_{0}^{\infty} dt G(t)e^{i\omega t}, \tag{4.57}
\]

we can identify that

\[
A_i(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \omega^2 |G_{1i}^*(\omega)|^2 e^{i\omega t}, \tag{4.58}
\]

and

\[
G^*(\omega) = \left[ -M\omega^2 + i\omega \Gamma + \Phi \right]^{-1}. \tag{4.59}
\]

With this identification we see that the expression given in Eq. (4.56) reduces to the form

\[
J = \frac{K_B(T_L - T_R)}{2\pi} \int_{0}^{\infty} d\omega T(\omega), \tag{4.60}
\]

\[\text{105}\]
\[ T(\omega) = 4\gamma L\gamma R \omega^2 |G_{1N}^+(\omega)|^2, \tag{4.61} \]

is the transmission coefficient for frequency \( \omega \). The above expression for the current \( J \) is seen to be identical to the well-known expression for the current given in [17, 24].

In the next section we proceed to obtain the time auto-correlation function \( C_{\Delta T}(t, t') \) defined as:

\[ C_{\Delta T}(t, t') = \langle j_{1,L}(t) j_{1,L}(t') \rangle - \langle j_{1,L} \rangle^2, \tag{4.62} \]

in the NESS. The subscript \( \Delta T \) represents the difference between the temperature at the two ends i.e. \( \Delta T = T_L - T_R \). In the stationary state \( \langle j_L(t) j_L(t') \rangle \) will be a function of \( |t - t'| \) only.

Hence we set \( t' = 0 \). If we take \( \Delta T = 0 \) in the expression of \( C_{\Delta T}(t) \) we get the equilibrium auto-correlation which is denoted by \( C_0(t) \) and we show that integral of \( C_0(t) \) is related to the average current \( \langle j_L \rangle \), whereas integral of \( C_{\Delta T}(t) \) is related to its fluctuations in the NESS.

### 4.5.3 Calculation of auto-correlation function

Using the forms of \( j_{1,L} \) from Eq. (4.46) we write current current auto-correlation \( \langle j_{1,L}(t) j_{1,L}(0) \rangle \) for \( t > 0 \) as:

\[ \langle j_{1,L}(t) j_{1,L}(0) \rangle = J_{L1} + J_{L2} + J_{L3} + J_{L4}, \]

where

\[ J_{L1} = \gamma L \langle \dot{x}_1^2(t) \dot{x}_1^2(0) \rangle, \quad J_{L2} = -\gamma L \langle \eta_L(t) \dot{x}_1(t) \dot{x}_1^2(0) \rangle, \]
\[ J_{L3} = -\gamma L \langle \eta_L(0) \dot{x}_1^2(0) \dot{x}_1(t) \rangle, \quad J_{L4} = \langle \eta_L(t) \dot{x}_1(t) \eta_L(0) \dot{x}_1(0) \rangle. \tag{4.63} \]

Now we will calculate all these \( J \)'s using Eq. (4.52) and Eq. (4.44). We will present the calculation of \( J_{L1} \) explicitly and state the results for other \( J \)'s. Putting the form of \( x_1(t) \) in the expression of \( J_{L1} \) in Eq. (4.63) we get

\[ J_{L1} = \gamma L \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 \int_{-\infty}^{t} dt_3 \int_{-\infty}^{t} dt_4 \times K_1(t_1, t_2, t_3, t_4, t), \tag{4.64} \]
where

\[ K_1(t_1, t_2, t_3, t_4, t) = \]

\[ \left\langle \left[ \hat{G}_{11}(t - t_1)\eta_L(t_1) + \hat{G}_{12}(t - t_1)\eta_R(t_1) \right] \times \left[ \hat{G}_{11}(t - t_2)\eta_L(t_2) + \hat{G}_{12}(t - t_2)\eta_R(t_2) \right] \times \left[ \hat{G}_{11}(-t_3)\eta_L(t_3) + \hat{G}_{12}(-t_3)\eta_R(t_3) \right] \times \left[ \hat{G}_{11}(-t_4)\eta_L(t_4) + \hat{G}_{12}(-t_4)\eta_R(t_4) \right] \right\rangle . (4.65) \]

After taking the average over noises and using their Gaussian property, we get

\[ K_1(t_1, t_2, t_3, t_4, t) = 4 \left( K_1^{(1)}(t_1, t_2, t_3, t_4, t)\delta(t_1 - t_2)\delta(t_3 - t_4) + \right. \]

\[ K_1^{(2)}(t_1, t_2, t_3, t_4, t)\delta(t_1 - t_3)\delta(t_2 - t_4) + K_1^{(3)}(t_1, t_2, t_3, t_4, t)\delta(t_1 - t_4)\delta(t_2 - t_3) \right) \]  

(4.66)

where expressions for these \( K_1 \)s are given in appendix. Putting the expression of \( K_1(t_1, t_2, t_3, t_4, t) \) in Eq. (4.64) and arranging the terms we get

\[ J_{L1} = 4\gamma_L^2 K_B^2 [\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)]^2 + 2[\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)]^2, \quad (4.67) \]

where we have used the definitions of \( A_1(t) \) in Eq. (4.54). Similarly we calculate other \( J_1 \)'s and their expressions are

\[ J_{L2} = -4\gamma_L^2 T_L K_B^2 \left[ \frac{1}{2} \hat{G}_{11}(0)(\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)), \right. \]

\[ J_{L3} = -4\gamma_L^2 T_L K_B^2 \left[ \frac{1}{2} \hat{G}_{11}(0)(\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)) \right. \]

\[ + \left. 2\hat{G}_{11}(t)(\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)) \right] \],

\[ J_{L4} = 4\gamma_L T_L K_B^2 [\delta(t)(\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)) + \gamma_L T_L \left( \frac{1}{4} \hat{G}_{11}^2(0) \right) \right]. \quad (4.68) \]

Collecting all the expressions for \( J_1 \)’s from Eqs. (4.67) and (4.68) in Eq. (4.63) and subtracting \( \langle j_{1L} \rangle^2 \) we finally obtain

\[ C_{AT}(t) = 4\gamma_L T_L K_B^2 [\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)]\delta(t) \]

\[ - 8\gamma_L^2 K_B^2 [\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)] \times \left[ T_L \gamma_L A_1(t) + (2T_L - T_R)\gamma_R A_N(t) \right] \right], \quad (4.69) \]

\[ g_{AT}(t) = 8\gamma_L^2 K_B^2 [\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)] \]

\[ \times \left[ T_L \gamma_L A_1(t) + (2T_L - T_R)\gamma_R A_N(t) \right] , \quad (4.70) \]
Figure 4.1: Plots of \([g_0(t)]\) vs. \(t\) for \(N = 4\) and \(N = 8\). The parameters for the figure are \(T_L = 2.0, T_R = 2.0, k = 1.0, k_0 = 0.0, k' = 0.0, \gamma_L = \gamma_R = 2.5\) and \(\Delta = 0.4\). Here \([g_0(t)]\) denotes disorder averaged \(g_0(t)\). The average is done over 100 disorder realisations. Inset shows the plots of \(A_1(t)\) and \(A_N(t)\) for \(N = 8\) for a single disorder configuration.

and we have used the identity in Eq. (4.55). From the above expression of \(g_{\Delta T}(t)\) we note that \(g_0(t)\) is always positive. Thus we have obtained a closed form expression for the non-equilibrium current-current auto-correlation function expressed in terms of the Green’s function for a disordered harmonic chain of length \(N\). The delta function appearing in the above equation is purely due to the white nature of the noises. More generally one can define the current operator on any bond on the harmonic chain. However the detailed form of the bond-correlation function is quite different from that of the boundary-correlation function. The notable difference that we find is the absence of the \(\delta\)-function peak. We have verified that the integral of bond-correlation agrees with the value for the boundary-correlation.

4.5.4 Numerical results

In this section we plot the function \(g_{\Delta T}(t) = 4\gamma_L T_L K^2_R(\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0))\delta(t) - C_{\Delta T}\). To find the functional form of \(g_{\Delta T}(t)\) we need to know the functional forms of the functions \(A_i(t)\). These functions can be obtained by Fourier transforming \(\omega^2[G_{ii}(\omega)]^2\) as shown in Eq. (4.58).
Figure 4.2: Plots of $|A_N(t)|$ vs. $t$ for different system sizes. The parameters for the figure are same as those for Fig. 4.1. $\Delta = 0.4$.

For a general N-particle mass disordered chain it is difficult to find analytical expressions for the functions $|G_{i j}^+(\omega)|^2$. For the ordered case $G_{i j}^+(\omega)$ can be obtained analytically using the tridiagonal nature of the force matrix $\Phi$ (see for example Refn. [13]). However in case of disordered chain, $G_{1N}^+(\omega)$ and $G_{11}^+(\omega)$ can be obtained through transfer matrix approach in which $G_{1N}^+(\omega)$ and $G_{11}^+(\omega)$ are expressed in terms of a product of $N$ random matrices [19]. We numerically evaluate $G_{1N}^+(\omega)$ and $G_{11}^+(\omega)$ using this transfer matrix approach. We observe that at large $\omega > \omega_d = \sqrt{\frac{km}{N\sigma^2}}$, $|G_{1N}^+(\omega)|^2$ decays as $e^{-an\omega^2}$ ($a$ is a positive constant) where $m = [m_t]$ and $\sigma^2 = [(m_t - m)^2]$. Here [...] denotes disorder average. This behaviour was proved analytically by Matsuda and Ishi [14] and was first observed numerically by Dhar [19]. A further observation made by Dhar was that for $\omega < \omega_d$ disordered average of $|G_{1N}^+(\omega)|^2$ is almost identical to that of an ordered chain for both the BCs (discussed in detail in chapter (2)). Another observation which we made is that for $\omega > \omega_m$ the function $|G_{11}^+(\omega)|^2$ decays as $1/\omega^4$, where $\omega_m$ is the maximum normal mode frequency. This $1/\omega^4$ behaviour can be easily obtained through the transfer matrix approach. For small frequencies disorder average of $|G_{11}^+(\omega)|^2$ oscillates with $\omega$ and is again identical to that of ordered chain. Here we make use of these observations.
After integrating Eq. (4.58) numerically, we obtain $A_i(t)$ and $G_{ij}(t)$ and hence $g_0(t)$ for different system sizes with different disorder configurations. In Fig. 4.1 we plot $[g_{\Delta T}(t)]$ versus $t$ for system sizes $N = 4, 8$ and $16$ with free BC. We observe that the correlation functions for two system sizes remain almost identical at short times and start being different significantly after some time scale. These observations can be made by looking at the dominant contributions of $\omega^2|G_{11}^+(\omega)|^2$ in the integrand of Eq. (4.58) for fixed $t$. At large $\omega$ the function $|G_{1N}^+(\omega)|^2$ decays as $e^{-aN\omega^2}$ ($a$ is a positive constant)$^{[14, 19]}$ whereas $|G_{11}^+(\omega)|^2$ decays as $1/\omega^4$. At small frequencies both $G_{1N}^+(\omega)$ and $G_{11}^+(\omega)$ are oscillating functions of $\omega$ and the frequency of oscillation increases with system size $N$. As a result $A_1(t)$ is independent of system size $N$ at small times and starts depending on $N$ after some time scale, where contribution from small $\omega$ becomes important. Whereas, in case of $A_N(t)$, only a small range of $\omega$ contributes to the Fourier transform of $\omega^2|G_{1N}^+(\omega)|^2$(Eq. (4.58)). For large $N$, at small times $A_1(t)$ is much larger that $A_N(t)$ and contributes most in $g_0(t)$, which makes $g_0(t)$ to be independent of $N$ at small times. Inset in Fig. 4.1 compares $A_1(t)$ and $A_N(t)$ for $N = 8$. In the next paragraph we will see that physically interesting quantities like current, fluctuations in current in NESS are related to the time integral of $C_{\Delta T}(t)$ and this integral depends only on $A_N(t)$, though $A_1(t)$ has dominant contribution in the correlation function itself. Hence it is more relevant to see the behaviour of $A_N(t)$ with system size $N$. In Fig. 4.2 we plot $[A_N(t)]$ for different system sizes. Here we prefer to give plots of disorder-averaged quantities.

Let $Q(\tau) = \int_0^\tau dt j_{1,L}(t)$ be the heat transfer in duration $\tau$ from left reservoir to the system. Using stationarity property of the correlation function it is easy to show that the $2^{nd}$ order cumulant of $Q(\tau)$ is related to $C_{\Delta T}(t)$ as

$$\lim_{\tau \to \infty} \frac{\langle Q^2(\tau) \rangle_c}{\tau} = \int_0^\infty dt C_{\Delta T}(t). \quad (4.71)$$

Now integrating the expression of $C_{\Delta T}(t)$ given in Eq. (4.69) from 0 to $\infty$ and again using the identity in Eq.(4.55) we get

$$\int_0^\infty dt C_{\Delta T}(t) = 2\gamma_L\gamma_RT_LT_RT_B^2A_N(0) + 8\gamma_L^2\gamma_R^2K_B^2(T_L - T_R)^2\int_0^\infty dt A_N^2(t). \quad (4.72)$$

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In the frequency space the Eq. (4.72) can be written as an integration over $\omega$ of the transmission coefficient $T(\omega)$ defined in Eq. (4.61) and we obtain

$$\int_0^\infty dt C_\Delta(t) = \frac{K_B^2 T_L T_R}{2\pi} \int_0^\infty d\omega T(\omega) + \frac{K_B^2 T_L - T_R}{4\pi} \int_0^\infty d\omega T^2(\omega). \quad (4.73)$$

This expression matches with the expression given in [100] for quantum mechanical systems in the high temperature limit. Now if we put $T_L = T_R = T$ in the expression in Eq. (4.72) and use Eq.(4.56) we get a relation between the current in the non-equilibrium steady state and the equilibrium correlation function similar to the GK relation given in Eq. (4.20) of the previous section

$$\int_0^\infty dt C_0(t) = \frac{K_B^2 T^2}{2\pi} \int_0^\infty d\omega T(\omega) = K_B T^2 \frac{\mathcal{J}}{(T_L - T_R)}, \quad (4.74)$$

where $C_0(t)$ is the equilibrium auto-correlation function for the open system. The inset of Fig. 4.3 shows the system size dependence of the disorder average of current.

In general for large system sizes $[\mathcal{J}]$ and $[\langle Q^2(r) \rangle]$ scale with $N$ as $N^{-\beta}$ and $N^{-\alpha}$ respectively. Using the frequency dependence of $T(\omega) = [T(\omega)]$ and $[T^2(\omega)]$ one can predict the values of $\alpha$ and $\beta$ for different BC's. By computing $[\mathcal{J}]$ in NESS, several authors have already studied asymptotic size dependence of $[\mathcal{J}]$. Rubin and Greer [101] obtained $\beta = 1/2$ for free BC, which was later proved rigorously by Verheggen[102]. Casher and Lebowitz [17] studied the same model and obtained a lower bound for $[\mathcal{J}] \geq N^{-3/2}$ and simulations by Rich and Vischer [103] confirmed the exponent to be $\beta = 3/2$. Later Dhar[19] obtained $\mathcal{J}$ for both the boundary conditions using Langevin Equation and Green Function approach and obtained $\beta = 1/2$ for free BC and $\beta = 3/2$ for fixed BC. Here we follow the same procedure described in [19] to find the asymptotic size dependence of $[\langle Q^2(r) \rangle]$ from the expression given in Eq. (4.73).

We numerically observe that for both the BCs $[T^2(\omega)]$ is much smaller than $T(\omega)$ for each $N$. Hence, in determining the asymptotic $N$ dependence, dominant contribution comes from the integration of $T(\omega)$ over $\omega$. To determine $\alpha$, we use the fact (discussed in the first paragraph of this section) that for $\omega$ greater than $\omega_d \sim N^{-1/2}$, $T(\omega)$ decays exponentially
Figure 4.3: This figure shows the dependence of non-equilibrium current fluctuation on system size for free BC. The parameters for the figure are same as those for Fig. 4.1 except $T_L = 3.0$ and $T_R = 2.0$. Inset shows the dependence of non-equilibrium current on system size for free BC. Disorder average is taken over 100 different disorder realizations. Standard deviation corresponding to each point is smaller that the size of the point symbol.

as $e^{-aN\omega^2}$, whereas for $\omega < \omega_d$, $T(\omega)$ is almost identical to $T_o(\omega)$ of an ordered chain. It is shown in chapter (3) shown that transmission coefficient of an ordered chain, denoted by $T_o(\omega)$, is independent of $\omega$ for free BC and goes as $\omega^2$ for fixed BC. Now putting these forms of $T_o(\omega)$ and integrating up to $\omega_d \sim N^{-1/2}$ we get $\alpha = 1/2$ for free BC and 3/2 for fixed BC. We see that the asymptotic size dependence of current fluctuation is same as that of NESS current. We numerically evaluate the RHS of Eq. (4.72) for free BC and obtain $\frac{(\langle Q^2(\tau) \rangle_{\tau}}{\tau}$ for $\tau \rightarrow \infty$ for different system sizes. In Fig. 4.3 we plot $[\frac{(\langle Q^2(\tau) \rangle_{\tau}}{\tau}$ versus system size $N$, which shows that the fluctuation in current scales with system size as $N^{-1/2}$, when both ends of the chain are free. In the pinned case, since there are no low frequency modes, $T(\omega)$ decays exponentially and hence fluctuations in current decay exponentially with $N$. 

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4.6 Conclusions

In this chapter we have derived an exact expression for the linear response conductance in a system connected to heat baths. Our results are valid in arbitrary dimensions and have been derived both for a solid where particles execute small displacements about fixed lattice positions as well as for a fluid system where the motion of particles is unrestricted, and various heat bath models have been considered. We also have given an expression for the boundary current-current correlation for a one dimensional mass-disordered harmonic system in NESS. The correlation function has been expressed in terms of the phonon Green's functions which are easy to evaluate numerically. We show that the integration of equilibrium correlation function gives current satisfying the finite size open system Green-Kubo formula whereas the integration of non-equilibrium correlation function gives information about current fluctuation in the NESS.

The important differences with the usual Green-Kubo formula are worth noting. In the present formula, one does not need to first take the limit of infinite system size; the result is valid for finite systems. The fact that a sensible answer is obtained even for a finite system (unlike the case for the usual Green-Kubo formula) is because here we are dealing with an open system. Secondly the correlation function here has to be evaluated not with Hamiltonian dynamics, but for an open system evolving with heat bath dynamics. Finally we note that unlike the usual derivation of the Green-Kubo formula where the assumption of local thermal equilibrium is crucial, the present derivation requires no such assumption. The results are thus valid even for integrable Hamiltonian models, the only requirement being that they should attain thermal equilibrium when coupled to one or more heat reservoirs all at the same temperature.

Our derivation here is based on using both the microscopic equations of motion and also the equation for the phase space distribution. The broad class of systems and heat baths for which we have obtained our results strongly suggests that they are valid whenever detailed balance is satisfied.
4.7 appendix

4.7.1 Proof of Eq. [4.55]

Let us first define few quantities:

\[ \tilde{G} = M^{-\frac{1}{2}}GM^{\frac{1}{2}}, \tilde{\Gamma} = M^{-\frac{1}{2}}\Gamma M^{\frac{1}{2}} \text{ and } \tilde{\Phi} = M^{-\frac{1}{2}}\Phi M^{\frac{1}{2}} \]

Using this above definitions Eq. (4.50) can be written as

\[ \ddot{\tilde{G}}(t) + \tilde{\Gamma}\dot{\tilde{G}}(t) + \tilde{\Phi}\tilde{G}(t) = 0. \tag{4.75} \]

We use the above equation to evaluate \( \frac{d}{dt}[\tilde{G}^T(t')\dot{\tilde{G}}(t' + t)] \) and get

\[ \frac{d}{dt}[\tilde{G}^T(t')\dot{\tilde{G}}(t' + t)] = -2\tilde{G}^T(t')\tilde{\Gamma}\dot{\tilde{G}}(t' + t) + \frac{d}{dt}[\tilde{G}^T(t')\tilde{\Phi}\tilde{G}(t' + t)]. \]

Now integrating both side of the above equation over \( t' = 0 \) to \( t' = \infty \) we get

\[ \dot{\tilde{G}}(t) = 2 \int_0^{\infty} dt' \tilde{G}^T(t')\tilde{\Gamma}\dot{\tilde{G}}(t' + t). \tag{4.76} \]

To the above equation we have used the following: \( \tilde{G}(0) = M^{-1}, G(0) = 0, G(t) \to 0 \) as \( t \to \infty \). Now we know that \( \Gamma_{ij} = (\frac{2\alpha}{m_1} \delta_{i1} + \frac{2\alpha}{m_2} \delta_{iN})\delta_{ij} \). Taking \((11)^{th}\) element on the both side of the matrix equation (4.76) we get

\[ \frac{\tilde{G}_{11}(t)}{2} = \int_0^{\infty} dt' [\gamma_L \tilde{G}_{11}(t')\dot{\tilde{G}}_{11}(t' + t) + \gamma_R \tilde{G}_{1N}(t')\dot{\tilde{G}}_{1N}(t' + t)] \]

\[ = \gamma_L A_1(t) + \gamma_R A_N(t). \tag{4.77} \]

4.7.2 Expressions of \( K_1s \)

\[ K_1^{(1)}(t_1, t_2, t_3, t_4, t) = [\gamma_L^2 T_L^2 \tilde{G}_{11}(t - t_1)\tilde{G}_{11}(t - t_2)\tilde{G}_{11}(-t_3)\tilde{G}_{11}(-t_4) \]

\[ + \gamma_R^2 T_R^2 \tilde{G}_{1N}(t - t_1)\tilde{G}_{1N}(t - t_2)\tilde{G}_{1N}(-t_3)\tilde{G}_{1N}(-t_4) \]

\[ + \gamma_L T_L \gamma_R T_R [\tilde{G}_{1N}(t - t_1)\tilde{G}_{1N}(t - t_2)\tilde{G}_{11}(-t_3)\tilde{G}_{11}(-t_4) \]

\[ + \tilde{G}_{11}(t - t_1)\tilde{G}_{11}(t - t_2)\tilde{G}_{1N}(-t_3)\tilde{G}_{1N}(-t_4)]]. \]
\[ K_1^{(2)}(t_1, t_2, t_3, t_4, t) = \left[ \gamma_L^2 T_L^2 \dot{G}_{11}(t - t_1) \dot{G}_{11}(t - t_2) \dot{G}_{11}(-t_3) \dot{G}_{11}(-t_4) \\
+ \gamma_R^2 T_R^2 \dot{G}_{1N}(t - t_1) \dot{G}_{1N}(t - t_2) \dot{G}_{1N}(-t_3) \dot{G}_{1N}(-t_4) \\
+ \gamma_L T_L T_R (\dot{G}_{1N}(t - t_1) \dot{G}_{11}(t - t_2) \dot{G}_{1N}(-t_3) \dot{G}_{11}(-t_4)) \\
+ \dot{G}_{11}(t - t_1) \dot{G}_{1N}(t - t_2) \dot{G}_{11}(-t_3) \dot{G}_{1N}(-t_4) \right] \]

and

\[ K_1^{(3)}(t_1, t_2, t_3, t_4, t) = \left[ \gamma_L^2 T_L^2 \dot{G}_{11}(t - t_1) \dot{G}_{11}(t - t_2) \dot{G}_{11}(-t_3) \dot{G}_{11}(-t_4) \\
+ \gamma_R^2 T_R^2 \dot{G}_{1N}(t - t_1) \dot{G}_{1N}(t - t_2) \dot{G}_{1N}(-t_3) \dot{G}_{1N}(-t_4) \\
+ \gamma_L T_L T_R (\dot{G}_{11}(t - t_1) \dot{G}_{1N}(t - t_2) \dot{G}_{1N}(-t_3) \dot{G}_{11}(-t_4)) \\
+ \dot{G}_{1N}(t - t_1) \dot{G}_{11}(t - t_2) \dot{G}_{11}(-t_3) \dot{G}_{1N}(-t_4) \right].\]