Heat transport in harmonic lattices

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Abstract

We work out the non-equilibrium steady state properties of a harmonic lattice which is connected to heat reservoirs at different temperatures. The heat reservoirs are themselves modeled as harmonic systems. Our approach is to write quantum Langevin equations for the system and solve these to obtain steady state properties such as currents and other second moments involving the position and momentum operators. The resulting expressions will be seen to be similar in form to results obtained for electronic transport using the non-equilibrium Green's function formalism. As an application of the formalism we discuss heat conduction in a harmonic chain connected to self-consistent reservoirs. We obtain a temperature dependent thermal conductivity which, in the high-temperature classical limit, reproduces the exact result on this model obtained recently by Bonetto, Lebowitz and Lukkarinen.

Key words: Harmonic crystal; Quantum Langevin equations; Non-equilibrium Green's Function; Fourier's Law

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1 Introduction

The harmonic crystal is one of the the simplest model that one learns in solid state physics and it is known to reproduce, for example, some of the correct experimental features for the specific heat of an insulating solid. The harmonic approximation basically involves expanding the full atomic potential of the solid about its minimum (which one assumes is a crystal) and keeping terms up to second order. If one transforms to normal mode coordinates then the harmonic crystal can be viewed as a collection of noninteracting phonons. While many equilibrium properties can be understood satisfactorily within the harmonic approximation, transport properties (heat conduction) of the harmonic lattice are anomalous because of absence of interactions between the phonons.

In discussions of transport properties (see for example Ref. [1]) of an insulating solid it is usual to first think of the pure harmonic crystal. One can then introduce various mechanisms for scattering of the phonons, two important ones being impurity scattering and phonon-phonon scattering. Impurity scattering can arise because of randomness in the masses of the particles or in the spring constants. In this case the phonons still do not interact with each other. One can think of the phonons of the original pure crystal getting elastically scattered by impurities. Alternatively, since the system is still harmonic, one can think of heat transmission by the new normal modes of the disordered system. The second mechanism for scattering is through phonon-phonon interactions and this occurs if we include the higher order nonlinear terms (*i.e* beyond quadratic order) of the interparticle potential. Phonon-phonon interactions are usually classified into those which conserve momentum and those which do not (Umklapp processes).

One important question that has attracted a lot of attention is: what are the necessary and sufficient conditions for the validity of Fourier's law of heat conduction [2, 3] ? We recall that Fourier's law states that for a solid with a spatially varying temperature field $T(\mathbf{x})$ inside it, the local heat current density $\mathbf{J}$ at a point $\mathbf{x}$ is given by:

$$\mathbf{J}(\mathbf{x}) = -\kappa \nabla T(\mathbf{x}) \tag{1.1}$$

where κ defines the thermal conductivity of the solid and is expected to be an intrinsic property of the material. Fourier's law is a phenomenological law which is expected to be true in the hydrodynamic linear response regime. However till now there does not exist any purely mechanical model (without external potentials) in which a first principle demonstration of the validity of Fourier's law, either numerically or analytically, has been achieved.

Infact it is now pretty much clear that in one dimensional momentum conserving systems Fourier's law is not valid and one cannot define a system-size independent thermal conductivity for these systems [4, 5, 6] (Note that the momentum one is referring to here is the total real momentum, and not the crystal momentum. This is conserved

if there are no external potentials). Apart from a large number of numerical studies various theoretical approaches have been used for different classes of systems to arrive at this conclusion regarding non-validity of Fourier's law in one dimensions. In the case of interacting systems (nonlinear) the anomalous behaviour of thermal conductivity has been understood within the Green-Kubo formalism and has been related to long-time tails in the current-current auto-correlation functions [5, 6]. For non-interacting (harmonic) disordered systems heat transport occurs through independent phonon modes and the main contribution comes from low frequency extended modes [7]. One finds a situation similar to that of electronic transport in mesoscopic systems [8, 9] where it is important to include the reservoirs in discussing transport. In this case it is more natural to talk of heat conductance of a system and one finds that this depends on the details of the reservoirs.

For a three dimensional solid, based on kinetic theory and Boltzmann equation approaches, the expectation is that the thermal conductivity should be finite (and Fourier's law valid) at high temperatures where Umklapp processes dominate. At low temperatures Umklapp processes are rare and non-Umklapp ones cannot lead to a finite thermal conductivity. However it is expected that, if in addition to these non-Umklapp processes, one also includes impurity scattering , then one should get a finite conductivity [1]. Unfortunately there is no clear proof of any of these physically motivated expectations. One possible approach to this problem is through a rigorous study of the phonon Boltzmann equation (see for example [10]).

In this paper we discuss a formalism for transport in harmonic lattices based on the Langevin equation approach. This approach was first used to study heat conduction in a one-dimensional ordered harmonic lattice [11]. Subsequently this approach was used to study heat conduction in disordered harmonic lattices in one [12, 13, 7] and two dimensions [14]. The quantum mechanical case has also been studied by several authors [15, 16, 17, 18, 19, 20, 21] using an open system description either through quantum Langevin equations or through density matrices. The open system description for harmonic systems closely resembles the Landauer formalism used for electron transport and Ref. [20] gives a derivation of the basic Landauer results using the Langevin equation approach, both for electrons and phonons. Another rigorous approach to studying electron transport in mesoscopic systems is the non-equilibrium Green's function formalism (NEGF)[8] and Ref. [22] shows how this can be derived, for non-interacting electrons modeled by tight-binding Hamiltonians, using a quantum Langevin equation approach. We note that the Landauer formalism has also been discussed in the context of wave propagation in disordered media [23, 24]. The problems of heat conduction in disordered harmonic lattices and wave propagation in disordered media are closely related. It is expected that some of the work in the latter area, for example on localization, will be useful in the heat conduction context.

In the present paper we show how the quantum Langevin equations method for harmonic lattices leads to NEGF-like expressions for phonon transport. For simplicity we restrict ourselves to harmonic Hamiltonians with scalar displacement variables at each lattice site. It is straightforward to extend the calculations to the case of vector displacements. The basic steps in the calculation are: (i) one thinks of the full system as consisting of the sample we are interested in (henceforth called wire) as well as the reservoirs at different temperatures which are connected to the wire, (ii) the wire and the reservoir Hamiltonians are taken to be harmonic, (iii) we eliminate the reservoir degrees of freedom and this leads to Langevin equations of motion for the wire variables, (iv) the linear Langevin equations are solved and steady state properties such as expectation values of the current are found. Finally (v) the solution is written in a form where one can identify the usual phonon Green's functions commonly used in solid state physics. This leads to the identification with results from the NEGF formalism. We note that Landauer-like results for phonons have been proposed earlier [25, 26] and a recent paper [27] derives NEGF results for phonon transport using the Keldysh approach.

The paper is organized as follows. In Sec. 2 we present the basic model and derive the quantum Langevin equations describing the wire. In Sec. 3 we solve the equations of motion to obtain the stationary long-time solution which is used in Sec. 4 to obtain formal expressions for various steady state quantities such as the heat current. In Sec. 5 we discuss an application of the present approach to studying heat conduction in a harmonic wire with self-consistent reservoirs at all lattice points. Finally we conclude with a discussion in Sec. 6.

2 Quantum Langevin equations

We consider a harmonic system which consists of a wire (denoted by W) coupled to reservoirs which are also described by harmonic interactions. In most of our discussions we consider the case of two reservoirs, labeled as L (for left) and R (right) , which are at two different temperatures. It is easy to generalize the case where there are more than

two reservoirs. The Hamiltonian of the entire system of wire and reservoirs is taken to be

$$\begin{aligned} \mathcal{H} &= \frac{1}{2}\dot{X}^T M \dot{X} + \frac{1}{2} X^T \Phi X \qquad (2.1) \\ &= \mathcal{H}_W + \mathcal{H}_L + \mathcal{H}_R + \mathcal{V}_L + \mathcal{V}_R \\ \text{where} \quad \mathcal{H}_W &= \frac{1}{2}\dot{X}_W^T M_W \dot{X}_W + \frac{1}{2} X_W^T \Phi_W X_W \ , \\ \mathcal{H}_L &= \frac{1}{2}\dot{X}_L^T M_L \dot{X}_L + \frac{1}{2} X_L^T \Phi_L X_L \ , \\ \mathcal{H}_R &= \frac{1}{2}\dot{X}_R^T M_R \dot{X}_R + \frac{1}{2} X_R^T \Phi_R X_R \ , \\ \mathcal{V}_L &= X_W^T V_L X_L, \qquad \mathcal{V}_R = X_W^T V_R X_R \ , \end{aligned}$$

where $M,\ M_W,\ M_L,\ M_R$ are real diagonal matrices representing masses of the particles in the entire system, wire, left, and right reservoirs respectively. The quadratic potential energies are given by the real symmetric matrices $\Phi,\ \Phi_W,\ \Phi_L,\ \Phi_R$ while V_L and V_R denote the interaction between the wire and the two reservoirs. The column vectors $X,\ X_W,\ X_L,\ X_R$ are Heisenberg operators which correspond to particle displacements, assumed to be scalars, about some equilibrium configuration. Thus $X = \{X_1, X_2, ...X_{N_s}\}^T$ where X_r denotes the position operator of the r^{th} particle and N_s denotes the number of points in the entire system. Also $\dot{X} = M^{-1}\ P$ where P_r denotes the momentum operator, with $\{X_r,\ P_r\}$ satisfying the usual commutation relations $[X_r, P_s] = i\hbar\delta_{rs}$.

The Heisenberg equations of motion for the system are:

$$M_W \ddot{X}_W = -\Phi_W X_W - V_L X_L - V_R X_R \ , \qquad (2.2)$$

and the equations of motion for the two reservoirs are

$$\begin{aligned} M_L \ddot{X}_L &= -\Phi_L X_L - V_L^T X_W \ , \qquad (2.3) \\ M_R \ddot{X}_R &= -\Phi_R X_R - V_R^T X_W \ . \qquad (2.4) \end{aligned}$$

We solve these equations by considering them as linear inhomogeneous equations. Thus for the left reservoir the general solution to Eq. (2.3) is (for $t > t_0$):

$$\begin{aligned} X_L(t) &= f_L^+(t-t_0) M_L X_L(t_0) + g_L^+(t-t_0) M_L \dot{X}_L(t_0) \\ &\quad - \int_{t_0}^{t} dt'\ g_L^+(t-t') V_L^T X_W(t') \ , \qquad (2.5) \\ \text{with} \quad f_L^+(t) &= U_L \cos(\Omega_L t) U_L^T\ \theta(t), \quad g_L^+(t) = U_L \frac{\sin(\Omega_L t)}{\Omega_L} U_L^T\ \theta(t) \ , \end{aligned}$$

where $\theta(t)$ is the Heaviside function and $U_L,\ \Omega_L$ are the normal mode eigenvector and eigenvalue matrices respectively and which satisfy the equations:

$$U_L^T \Phi_L U_L = \Omega_L^2 \ , \quad U_L^T M_L U_L = I \ .$$

Similarly, for the right reservoir we obtain

$$\begin{aligned} X_R(t) &= f_R^+(t-t_0) M_R X_R(t_0) + g_R^+(t-t_0) M_R \dot{X}_R(t_0) \\ &\quad - \int_{t_0}^{t} dt' \ g_R^+(t-t') V_R^T X_W(t') \ . \end{aligned} \tag{2.6}$$

We plug these solutions back into the equation of motion for the system to get

$$\begin{aligned} M_W \ddot{X}_W &= -\Phi_W X_W \ + \ \eta_L \ + \ \int_{t_0}^{t} dt' \ V_L \ g_L^+(t-t') \ V_L^T \ X_W(t') \\ &\quad + \ \eta_R \ + \ \int_{t_0}^{t} dt' \ V_R \ g_R^+(t-t') \ V_R^T \ X_W(t') \ , \end{aligned} \tag{2.7}$$

where

$$\begin{aligned} \eta_L &= -V_L \ [f_L^+(t-t_0) M_L X_L(t_0) \ + \ g_L^+(t-t_0) M_L \dot{X}_L(t_0)] \\ \eta_R &= -V_R \ [f_R^+(t-t_0) M_R X_R(t_0) \ + \ g_R^+(t-t_0) M_R \dot{X}_R(t_0)] \ . \end{aligned} \tag{2.8}$$

This equation has the form of a quantum Langevin equation. The properties of the noise terms η_L and η_R are determined using the condition that, at time t_0, the two isolated reservoirs are described by equilibrium phonon distribution functions. At time t_0 the left reservoir is in equilibrium at temperature T_L and the population of the normal modes (of the isolated left reservoir) is given by the distribution function $f_b(\omega, T_L) = 1/[e^{\hbar\omega/k_B T_L} - 1]$. The equilibrium correlations are then given by:

$$\begin{aligned} \langle X_L(t_0) X_L^T(t_0) \rangle &= U_L \frac{\hbar}{2\Omega_L} \coth\left(\frac{\hbar\Omega_L}{2k_B T_L}\right) U_L^T \ , \\ \langle \dot{X}_L(t_0) \dot{X}_L^T(t_0) \rangle &= U_L \frac{\hbar\Omega_L}{2} \coth\left(\frac{\hbar\Omega_L}{2k_B T_L}\right) U_L^T \\ \langle X_L(t_0) \dot{X}_L^T(t_0) \rangle &= U_L \left(\frac{i\hbar}{2}\right) U_L^T \\ \langle \dot{X}_L^T(t_0) X_L(t_0) \rangle &= U_L \left(\frac{-i\hbar}{2}\right) U_L^T \ . \end{aligned}$$

Using these we can determine the correlations of the noise terms in Eq. (2.8). Thus we get for the left reservoir noise correlations:

$$\begin{aligned}\langle \eta_L(t)\eta_L^T(t')\rangle &= V_L U_L \left[\cos\Omega_L(t-t')\frac{\hbar}{2\Omega_L}\coth\left(\frac{\hbar\Omega_L}{2k_BT_L}\right)\right. \\ &\left. -i\sin\Omega_L(t-t')\frac{\hbar}{2\Omega_L}\right] U_L^T V_L^T \ , \end{aligned} \tag{2.9}$$

and a similar expression for the right reservoir.

3 Stationary solution of the equations of motion

Now let us take the limits of infinite reservoir sizes and let $t_0 \to -\infty$. We can then solve Eq. (2.7) by taking Fourier transforms. Thus defining the Fourier transforms

$$\begin{aligned}\tilde{X}_W(\omega) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\ X_W(t)e^{i\omega t} \ , \\ \tilde{\eta}_{L,R}(\omega) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\ \eta_{L,R}(t)e^{i\omega t} \ , \\ g^+_{L,R}(\omega) &= \int_{-\infty}^{\infty} dt\ g^+_{L,R}(t)e^{i\omega t} \ , \end{aligned} \tag{3.1}$$

we get from Eq. (2.7)

$$\begin{aligned}(-\omega^2\ M_W + \Phi_W)\tilde{X}_W(\omega) &= [\ \Sigma_L^+(\omega) + \Sigma_R^+(\omega)\ ]\ \tilde{X}_W(\omega) + \tilde{\eta}_L(\omega) + \tilde{\eta}_R(\omega) \\ \text{where}\quad \Sigma_L^+(\omega) &= V_L g_L^+(\omega) V_L^T, \quad \Sigma_R^+(\omega) = V_R g_R^+(\omega) V_R^T \ . \end{aligned} \tag{3.2}$$

The noise correlations can be obtained from Eq. (2.9) and we get (for the left reservoir):

$$\begin{aligned}\langle \tilde{\eta}_L(\omega)\tilde{\eta}_L^T(\omega')\rangle &= \delta(\omega+\omega')\ V_L\ Im[g_L^+(\omega)]\ V_L^T\ \frac{\hbar}{\pi}[1+f_b(\omega,T_L)] \\ &= \delta(\omega+\omega')\ \Gamma_L(\omega)\ \frac{\hbar}{\pi}[1+f_b(\omega,T_L)] \qquad (3.3) \\ &\text{where}\quad \Gamma_L(\omega) = Im[\Sigma_L^+(\omega)] \qquad (3.4) \end{aligned}$$

which is a fluctuation-dissipation relation. This also leads to the more commonly used correlation:

$$\frac{1}{2}\langle\ \tilde{\eta}_L(\omega)\tilde{\eta}_L^T(\omega') + \tilde{\eta}_L(\omega')\tilde{\eta}_L^T(\omega)\ \rangle = \delta(\omega+\omega')\ \Gamma_L(\omega)\ \frac{\hbar}{2\pi}\ \coth(\frac{\hbar\omega}{2k_BT_L}). \tag{3.5}$$

Similar relations hold for the noise from the right reservoir. We then get the following stationary solution to the equations of motion:

$$\begin{aligned} X_W(t) &= \int_{-\infty}^{\infty} d\omega \tilde{X}_W(\omega) e^{-i\omega t} \ , \\ \text{with} \quad \tilde{X}_W(\omega) &= G_W^+(\omega) \ [\tilde{\eta}_L(\omega) + \tilde{\eta}_R(\omega)] \ , \qquad (3.6) \\ \text{where} \quad G_W^+ &= \frac{1}{[-\omega^2 M_W + \Phi_W - \Sigma_L^+(\omega) - \Sigma_R^+(\omega)]} \ . \qquad (3.7) \end{aligned}$$

The identification of $G_W^+(\omega)$ as a phonon Green function, with $\Sigma_{L,R}^+(\omega)$ as effective self energy terms, is the main step that enables a comparison of results derived by the quantum Langevin approach with those obtained from the NEGF method. In App. A we show explicitly how this identification is made.

For the reservoirs we get, from Eqs. (2.5-2.6),

$$\begin{aligned} -V_L \tilde{X}_L(\omega) &= \tilde{\eta}_L(\omega) + \Sigma_L^+ \tilde{X}_W(\omega) \ , \\ -V_R \tilde{X}_R(\omega) &= \tilde{\eta}_R(\omega) + \Sigma_R^+ \tilde{X}_W(\omega) \ . \qquad (3.8) \end{aligned}$$

4 Steady state properties

Current: The simplest way to evaluate the steady state current is to evaluate the following expectation value for left-to-right current:

$$J = -\langle \ \dot{X}_W^T V_L X_L \ \rangle = \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \ e^{-i(\omega+\omega')t} i\omega \ \langle \tilde{X}_W^T(\omega) V_L \tilde{X}_L(\omega') \rangle \ ,$$

which is just the rate at which the left reservoir does work on the wire. Using the solution in Eq. (3.6-3.8) we get

$$\begin{aligned} J &= -\int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \ e^{-i(\omega+\omega')t} i\omega \ \langle \ (\ \tilde{\eta}_L^T(\omega) + \tilde{\eta}_R^T(\omega) \ ) \ {G_W^+}^T(\omega) \\ &\quad \times [\ \tilde{\eta}_L(\omega') + \Sigma_L^+(\omega') \ G_W^+(\omega') \ (\ \tilde{\eta}_L(\omega') + \tilde{\eta}_R(\omega') \ ) \ ] \ \rangle \ . \qquad (4.1) \end{aligned}$$

Now consider that part of J, say J^R, which depends only on T_R. Clearly this is:

$$\begin{aligned} J^R &= -\int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \ e^{-i(\omega+\omega')t} \ i \ \omega \\ &\quad \times Tr \ [\ {G_W^+}^T(\omega) \ \Sigma_L^+(\omega') \ G_W^+(\omega') \ \langle \ \tilde{\eta}_R(\omega') \tilde{\eta}_R^T(\omega) \ \rangle \ ] \\ &= -i \int_{-\infty}^{\infty} d\omega \ Tr[\ {G_W^+}^T(\omega) \ \Sigma_L^+(-\omega) G_W^+(-\omega) \Gamma_R(\omega)] \ \frac{\hbar\omega}{\pi} \ [1 + f_b(\omega, T_R)] \ . \end{aligned}$$

Using the identities ${G_W^+}^T = G_W^+$, $G_W^+(-\omega) = G_W^-(\omega)$ and taking the real part of above equation we obtain, after some simplifications,

$$J^R = -\int_{-\infty}^{\infty} d\omega \; Tr[\; G_W^+(\omega)\; \Gamma_L(\omega)\; G_W^-(\omega)\; \Gamma_R(\omega)\;]\; \frac{\hbar\omega}{\pi}\; [1 + f_b(\omega, T_R)]\; .$$

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 be given by

$$J = \int_{-\infty}^{\infty} d\omega \; Tr[\; G_W^+(\omega)\; \Gamma_L(\omega) G_W^-(\omega)\; \Gamma_R(\omega)]\; \frac{\hbar\omega}{\pi}\; [f(\omega, T_L) - f(\omega, T_R)]\; . \tag{4.2}$$

This expression for current can be seen to be of identical form as the NEGF expression for electron current (see for example [8, 28, 29]).

Two point correlation functions: We can also easily compute expectation values of various correlations. Thus the velocity-velocity correlations are given by

$$\begin{aligned}
K &= \langle \dot{X}_W \dot{X}_W^T \rangle \\
&= \int_{-\infty}^{\infty} d\omega\; \frac{\omega}{\pi}\; [\; G_W^+(\omega)\Gamma_L(\omega)G_W^-(\omega)\hbar\omega(1 + f_b(\omega, T_L)) \\
&\qquad + G_W^+(\omega)\Gamma_R(\omega)G_W^-(\omega)\hbar\omega(1 + f_b(\omega, T_R))\;] \\
&= \int_{-\infty}^{\infty} d\omega \frac{\omega}{\pi}\; [\; G_W^+(\omega)\Gamma_L(\omega)G_W^-(\omega)\frac{\hbar\omega}{2}\coth(\frac{\hbar\omega}{2k_BT_L}) \\
&\qquad + G_W^+(\omega)\Gamma_R(\omega)G_W^-(\omega)\frac{\hbar\omega}{2}\coth(\frac{\hbar\omega}{2k_BT_R})\;]\; ,
\end{aligned} \tag{4.3}$$

where the last line is easily obtained after writing $K = (K + K^*)/2$. We see that for $T_L = T_R$ this reduces to the equilibrium result of Eq. (B.3) *provided that there are no bound states*.

Similarly the position-position and position-velocity correlations are given by:

$$\begin{aligned}
P &= \langle X_W X_W^T \rangle \\
&= \int_{-\infty}^{\infty} d\omega \frac{\hbar}{2\pi}\; [\; G_W^+(\omega)\Gamma_L(\omega)G_W^-(\omega)\coth(\frac{\hbar\omega}{2k_BT_L}) \\
&\qquad + G_W^+(\omega)\Gamma_R(\omega)G_W^-(\omega)\coth(\frac{\hbar\omega}{2k_BT_R})\;]\; , \\
C &= \langle X_W \dot{X}_W^T \rangle \\
&= \int_{-\infty}^{\infty} d\omega \frac{i}{\pi}\; [\; G_W^+(\omega)\Gamma_L(\omega)G_W^-(\omega)\frac{\hbar\omega}{2}\coth(\frac{\hbar\omega}{2k_BT_L}) \\
&\qquad + G_W^+(\omega)\Gamma_R(\omega)G_W^-(\omega)\frac{\hbar\omega}{2}\coth(\frac{\hbar\omega}{2k_BT_R})\;]\; .
\end{aligned} \tag{4.4}$$

The correlation functions K and P can be used to define the local energy density which can in turn be used to define the temperature profile in the non-equilibrium steady state of the wire. Also we note that the correlations C give the local heat current density. In the next section we will find that it is sometimes more convenient to evaluate the total steady state current from this expression rather than the one in Eq. (4.2).

Classical limits: The classical limit is obtained by taking the high temperature limit so that $\hbar\omega/k_BT \to 0$. Then we obtain the following expressions for the various steady state properties computed in the last section. The current is given by

$$J = \frac{k_B\ (T_L - T_R)}{\pi}\ \int_{-\infty}^{\infty} d\omega\ Tr[\ G_W^+(\omega)\ \Gamma_L(\omega) G_W^-(\omega)\ \Gamma_R(\omega)]\ , \tag{4.5}$$

while other correlation functions are given by:

$$\begin{aligned}
K &= \frac{k_BT_L}{\pi}\int_{-\infty}^{\infty} d\omega\ \omega\ G_W^+(\omega)\Gamma_L(\omega)G_W^-(\omega) \\
&\quad + \frac{k_BT_R}{\pi}\int_{-\infty}^{\infty} d\omega\ \omega\ G_W^+(\omega)\Gamma_R(\omega)G_W^-(\omega)\ , \\
P &= \frac{k_BT_L}{\pi}\int_{-\infty}^{\infty} d\omega\ \frac{1}{\omega}\ G_W^+(\omega)\Gamma_L(\omega)G_W^-(\omega) \\
&\quad + \frac{k_BT_R}{\pi}\int_{-\infty}^{\infty} d\omega\ \frac{1}{\omega}\ G_W^+(\omega)\Gamma_R(\omega)G_W^-(\omega)\ , \\
C &= \frac{ik_BT_L}{\pi}\int_{-\infty}^{\infty} d\omega\ G_W^+(\omega)\Gamma_L(\omega)G_W^-(\omega) \\
&\quad + \frac{ik_BT_R}{\pi}\int_{-\infty}^{\infty} d\omega\ G_W^+(\omega)\Gamma_R(\omega)G_W^-(\omega)\ .
\end{aligned} \tag{4.6}$$

For one dimensional wires these lead to [20] expressions for current and temperature used in earlier studies of heat conduction in disordered harmonic chains [12, 13, 7].

5 An application: one-dimensional harmonic crystal with self-consistent reservoirs

As an application of the Langevin equation-Green functions formalism we consider the problem of heat transport in a harmonic chain with each site connected to self-consistent heat reservoirs. The classical version of this model was first studied by [30, 31] who introduced the self-consistent reservoirs as a simple scattering mechanism which might ensure local equilibration and the validity of Fourier's law. This model was recently solved

exactly by Bonetto et al [33] who proved local equilibration and validity of Fourier's law and obtained an expression for the thermal conductivity of the wire. They also showed that the temperature profile in the wire was linear. The quantum version of the problem was also studied by Visscher and Rich [32] who analyzed the limiting case of weak coupling to the self-consistent reservoirs. We will show here how the present formalism can be used to obtain results in the quantum-mechanical case. The classical results of Bonetto et al are obtained as the high temperature limit while the quantum mechanical results of Vischer and Rich are obtained in the weak coupling limit.

In this model one considers a one-dimensional harmonic wire described by the Hamiltonian

$$\begin{aligned} H_W &= \sum_{l=1}^{N} \frac{m}{2}[\dot{x}_l^2 + \omega_0^2 x_l^2] + \sum_{l=1}^{N+1} \frac{m\omega_c^2}{2}(x_l - x_{l-1})^2 \ , \\ &= \frac{1}{2}\dot{X}_W^T M_W \dot{X}_W + \frac{1}{2} X_W^T \Phi_W X_W \end{aligned} \tag{5.1}$$

where the wire particles are denoted as $X^T = \{x_1, x_2, ...x_N\}$ and we have chosen the boundary conditions $x_0 = x_{N+1} = 0$. All the particles are connected to heat reservoirs which are taken to be Ohmic. The coupling strength to the reservoirs is controlled by the dissipation constant γ. The temperatures of the first and last reservoirs are fixed and taken to be $T_1 = T_L$ and $T_N = T_R$. For other particles, *i.e* $l = 2, 3...(N-1)$, the temperature of the attached reservoir T_l is fixed self-consistently in such a way that the net current flowing into any of the reservoirs $l = 2, 3...(N-1)$ vanishes. The Langevin equations of motion for the particles on the wire are:

$$m\ddot{x}_l = -m\omega_c^2(2x_l - x_{l-1} - x_{l+1}) - m\omega_0^2 x_l - \gamma\dot{x}_l + \eta_l \quad l = 1, 2...N \ , \tag{5.2}$$

where the noise-noise correlation is easier to express in frequency domain and given by

$$\frac{1}{2}\langle\ \eta_l(\omega)\eta_m(\omega') + \eta_l(\omega')\eta_m(\omega)\ \rangle = \frac{\gamma\hbar\omega}{2\pi}\coth(\frac{\hbar\omega}{2k_B T_l})\ \delta(\omega+\omega')\ \delta_{lm} \ . \tag{5.3}$$

From the equations of motion it is clear that the l^{th} particle is connected to a bath with a self energy matrix $\Sigma_l^+(\omega)$ whose only non vanishing element is $[\Sigma_l^+]_{ll} = i\gamma\omega$. Generalizing Eq. (4.2) to the case of multiple baths we find that the heat current from the l^{th} reservoir into the wire is given by:

$$\begin{aligned} J_l &= \sum_{m=1}^{N} \int_{-\infty}^{\infty} d\omega\ Tr[\ G_W^+(\omega)\ \Gamma_l(\omega) G_W^-(\omega)\ \Gamma_m(\omega)]\frac{\hbar\omega}{\pi}\ [f(\omega, T_l) - f(\omega, T_m)] \ , \\ &\text{where} \quad G_W^+ = [\ -\omega^2\ M_W + \Phi_W - \sum_l \Sigma_l^+(\omega)\ ]^{-1} \ , \quad \Gamma_l = Im[\Sigma_l^+] \ . \end{aligned} \tag{5.4}$$

Using the form of Γ_l we then get:

$$J_l = \sum_{m=1}^{N} \gamma^2 \int_{-\infty}^{\infty} d\omega\ \omega^2 \mid [G_W^+(\omega)]_{lm} \mid^2 \ \frac{\hbar\omega}{\pi}\ [f(\omega, T_l) - f(\omega, T_m)] \ .$$

To find the temperature profile we need to solve the $N-2$ nonlinear equations $J_l = 0$ for $l = 2, 3...N-1$ with $T_1 = T_L$ and $T_N = T_R$. To proceed we consider the linear response regime with the applied temperature difference $\Delta T = T_L - T_R << T$ where $T = (T_L + T_R)/2$. In that case we expand the phonon distribution functions $f(\omega, T_l)$ about the mean temperature T and get the following simpler expressions for the currents

$$J_l = \gamma^2 \int_{-\infty}^{\infty} d\omega\ \frac{\hbar\omega^3}{\pi} \frac{\partial f(\omega, T)}{\partial T}\ \sum_{m=1}^{N}\ \mid [G_W^+(\omega)]_{lm} \mid^2\ (T_l - T_m) \ . \tag{5.5}$$

We write $G^+ = Z^{-1}/(m\omega_c^2)$ where Z is a tridiagonal matrix with offdiagonal elements equal to -1 and diagonal elements are all equal to $z = 2 + \omega_0^2/\omega_c^2 - \omega^2/\omega_c^2 - i\gamma\omega/(m\omega_c^2)$. It is then easy to find its inverse using the formula $Z_{lm}^{-1} = D_{1,l-1}\ D_{m+1,N}/D_{1,N}$, where D_{ij} is the determinant of the sub-matrix of Z beginning with the ith row and column and ending with the jth row and column. The determinant is given by $D_{ij} = \sinh\left[(j-i+2)\ \alpha\right]/\sinh(\alpha)$, where $e^\alpha = z/2 \pm [(z/2)^2 - 1]^{1/2}$ (any of the two roots can be taken). For points far from the boundaries of the wire ($l = yN$ where $y = O(1)$, $1 - y = O(1)$) we then find that

$$G_{lm}^+ = \frac{e^{-\alpha|l-m|}}{2m\omega_c^2 \sinh\alpha} \ , \tag{5.6}$$

where we choose the root α such that $\alpha_R = Re[\alpha] > 0$. In Ref. [33], where the classical version of the present model was studied, it was shown that in the limit $N \to \infty$ the temperature profile obtained by solving the self-consistent equations has the linear form

$$T_l = T_L + \frac{l-1}{N-1}(T_R - T_L) \ . \tag{5.7}$$

From the form of G_{lm}^+ in Eq. (5.6) we see at once that, for any point l in the bulk of the wire, the zero-current condition $J_l = 0$ is satisfied since $\sum_{m=-\infty}^{\infty}(l-m)|e^{-\alpha|l-m|}|^2 = 0$. For points which are within distance $O(1)$ from the boundaries the temperature profile deviates from the linear form.

To find the net left-right current in the wire we could use the formula for $J_1 = -J_N$ given in Eq. (5.4). However we notice that use of this formula requires us to know the accurate form of T_m for points m close to the boundaries since these terms contribute

significantly to the sum in Eq. (5.4). We instead use a different expression for the current. We evaluate the left-right current $J_{l,l+1}$ on the bond connecting sites l and $(l+1)$. Using Eq. (4.4) and in the linear response limit, making expansions about T, we get

$$\begin{aligned} J_{l,\ l+1} &= m\omega_c^2\ \langle x_l \dot{x}_{l+1}\rangle = -\frac{m\omega_c^2\gamma}{\pi}\int_{-\infty}^{\infty} d\omega\ \omega\ \left(\frac{\hbar\omega}{2k_BT}\right)^2 \mathrm{cosech}^2(\frac{\hbar\omega}{2k_BT}) \\ &\times \sum_{m=-\infty}^{\infty} k_BT_m\ Im\{[G_W^+(\omega)]_{lm}[G_W^+(\omega)]^*_{l+1\ m}\}\ . \end{aligned}$$

The current value is independent of l and we choose to evaluate it at a value of l in the bulk of the wire. In that case terms in the sum above which contain T_m with m close to the boundaries are exponentially small ($\sim e^{-\alpha N}$) and so do not contribute. Hence we can use the linear temperature profile for T_m and the form of G_W^+ in Eq. (5.6) to evaluate the heat current. We get:

$$\begin{aligned} J &= -\frac{\gamma}{8m\omega_c^2\pi i}\int_{-\infty}^{\infty} d\omega\ \frac{\omega}{|\sinh\alpha|^2}\ \left(\frac{\hbar\omega}{2k_BT}\right)^2 \mathrm{cosech}^2(\frac{\hbar\omega}{2k_BT}) \\ &\times \sum_{m=-\infty}^{\infty} k_BT_m\ [e^{-\alpha|l-m|}e^{-\alpha^*|l+1-m|} - e^{-\alpha^*|l-m|}e^{-\alpha|l+1-m|}]\ , \end{aligned}$$

where the additional terms in the summation over m are exponentially small contributions. Also as before we choose the root $\alpha(\omega)$ such that $Re[\alpha] > 0$. Using the notation $\alpha_R(\omega) = Re[\alpha],\ \alpha_I(\omega) = Im[\alpha]$ we get, after some algebra, the following expression for the thermal conductivity $\kappa = JN/\Delta T$ (obtained in the large N limit):

$$\kappa = \frac{\gamma k_B}{16m\omega_c^2\pi i}\int_{-\infty}^{\infty} d\omega\ \frac{\omega}{\sinh^2\alpha_R}\left(\frac{\hbar\omega}{2k_BT}\right)^2 \mathrm{cosech}^2(\frac{\hbar\omega}{2k_BT})\ \left(\frac{1}{\sinh\alpha} - \frac{1}{\sinh\alpha^*}\right)\ . \quad (5.8)$$

In the high temperature limit we get $(\hbar\omega/2k_BT)^2\mathrm{cosech}^2(\hbar\omega/2k_BT)\ \rightarrow\ 1$. This gives the classical result for the thermal conductivity. In this limit a change of variables from ω to α_I leads to the following result for the thermal conductivity:

$$\begin{aligned} \kappa_{cl} &= \frac{2k_Bm\omega_c^2(2+\nu^2)}{\gamma\pi}\int_0^{\pi/2} d\alpha_I\ \frac{\sin^2(\alpha_I)}{(2+\nu^2)^2 - 4\cos^2(\alpha_I)} \\ &= \frac{k_Bm\omega_c^2}{\gamma\ (2+\nu^2+[\nu^2(4+\nu^2)]^{1/2})}\ , \end{aligned} \quad (5.9)$$

where $\nu = \omega_0/\omega_c$. This agrees with the result obtained in Ref. [33].

An interesting limiting case is the case of weak coupling to the reservoirs ($\gamma \to 0$). In this case Eq. (5.8) gives:

$$\begin{aligned} \kappa_{wc} &= \left(\frac{\hbar\omega_c^2}{k_B T}\right)^2 \frac{m k_B}{4\gamma\pi} \int_0^\pi d\alpha_I \ \sin^2\alpha_I \ \mathrm{cosech}^2(\frac{\hbar\omega_\alpha}{2k_B T}) \ , \qquad (5.10) \\ \text{where} \quad \omega_\alpha^2 &= \omega_0^2 + 2\omega_c^2[1-\cos(\alpha_I)] \ . \end{aligned}$$

This agrees with the result obtained in [32]. The temperature profile obtained by them differs from the linear form obtained by us and also by [33] and is incorrect. They nevertheless obtain the correct thermal conductivity, presumably because their derivation only uses the temperature profile close to the centre of the chain where it is again linear. In the low temperature limit, Eq. (5.10) gives $\kappa_{wc} \sim e^{-\hbar\omega_0/k_B T}/T^{1/2}$ for $\omega_0 \neq 0$ and $\kappa_{wc} \sim T$ for $\omega_0 = 0$. As noted in [32] the expression for thermal conductivity (in the weak scattering limit) is consistent with a simple relaxation-time form for the thermal conductivity. The temperature dependence of κ_{wc} then simply follows the temperature dependence of the specific heat of the 1-dimensional chain.

Finally we examine the general case where the coupling constant has a finite value. In Figs. (1,2) we plot the thermal conductivity as a function of temperature for two sets of parameter: (i) $\gamma/(m\omega_c) = 0.2, \nu = 0.5$ and (ii) $\gamma/(m\omega_c) = 0.2, \nu = 0.0$. The insets in the two figures show the low-temperature behaviour. As before, the low-temperature behaviour depends on whether or not there is an onsite potential. However we see that the form of the low-temperature behaviour is very different from the case of weak coupling. For small T it is easy to pull out the temperature dependence of the integral in Eq. (5.8) and we find that $\kappa \sim T^3$ for $\nu \neq 0$ and $\kappa \sim T^{1/2}$ for $\nu = 0$, in agreement with the numerical result shown in Figs. (1,2).

6 Discussion

In this paper, using the quantum Langevin equation approach, we have derived NEGF-like expressions for the heat current in a harmonic lattice connected to external reservoirs at different temperatures. We note that unlike other approaches such as the Green-Kubo formalism and Boltzmann equation approach, the Langevin equation approach explicitly includes the reservoirs. The Langevin equation is also physically appealing since it gives a nice picture of the reservoirs as sources of noise and dissipation. Also just as the Landauer formalism and NEGF have been extremely useful in understanding electron transport in mesoscopic systems it is likely that a similar description will be useful for the case of heat transport in insulating nanotubes, nanowires, etc. We note here that the single-channel Landauer results follow from NEGF if one considers one-dimensional reservoirs [20] and have been useful in interpreting experimental results [34].

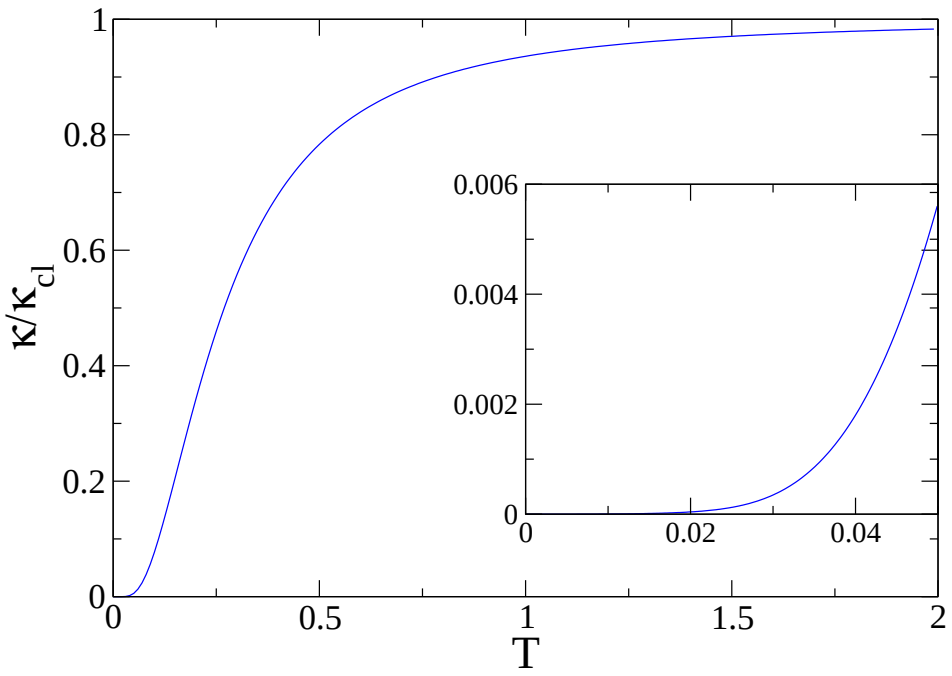

Figure 1: Plot of the scaled thermal conductivity as a function of temperature (in units of $\hbar\omega_c/k_B$) for $\nu = 0.5$. Inset shows the low temperature behaviour.

We think that the similarity, between heat conduction studies in harmonic systems and electron transport in noninteracting wires, is an interesting and useful point to note. The two areas have developed quite independently using different theoretical tools. In the former case most of the earlier studies were done on classical systems using either a Langevin or a Fokker Planck description. More recent studies on quantum systems have used either a quantum Langevin or a density matrix approach. On the other hand, for the electron case, which is inherently quantum-mechanical, the most popular and useful approach has been the Landauer and the NEGF formalism. As we have demonstrated, in this paper for the phonon case, and in Ref [22] for the electron case, the NEGF results can be easily derived using the Langevin approach at least in the noninteracting case.

As an application of the NEGF results we have studied the problem of heat conduction in a one dimensional harmonic chain connected to self-consistent reservoirs. The classical version of this problem was solved exactly by Bonetto et al [33], using different methods. The quantum mechanical case was studied earlier by Vischer and Rich [32] and they obtained the thermal conductivity in the limit of weak coupling. The advantage of the

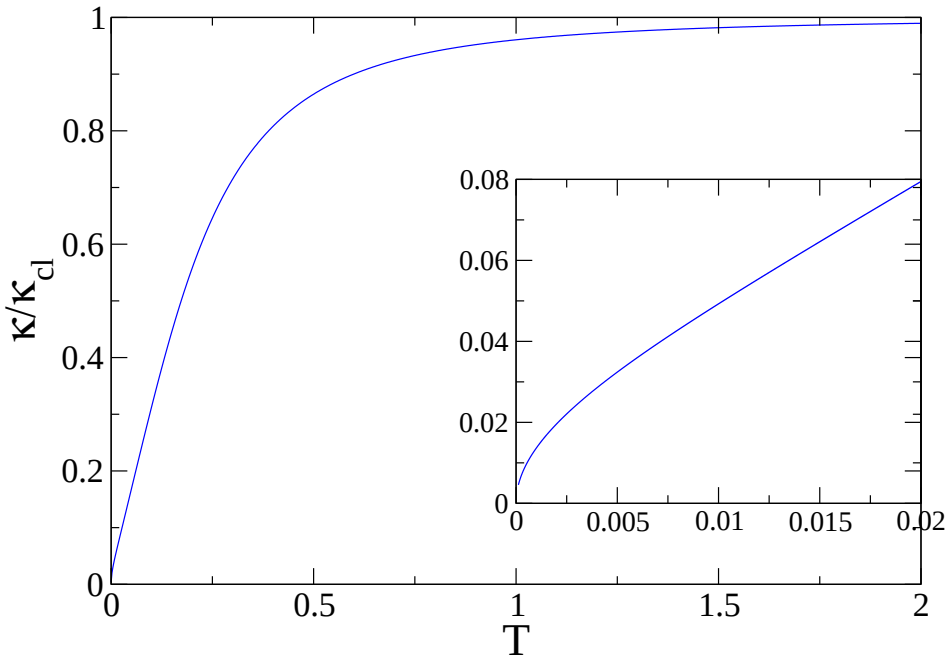

Figure 2: Plot of the scaled thermal conductivity as a function of temperature (in units of $\hbar\omega_c/k_B$) for $\nu = 0.0$. Inset shows the low temperature behaviour.

present approach is that it's implementation is simple and straightforward. We obtain a general expression for the thermal conductivity, which in limiting cases gives both the classical result in [33] and the weak-coupling result in [32]. We also find that, at low temperatures, the temperature dependence of thermal conductivity in the case of finite coupling is completely different from the weak coupling case. In the classical case it was shown in [33] that the thermal conductivity of the harmonic chain with self-consistent reservoirs can also be obtained from the Kubo formula. An interesting problem would be to demonstrate this in the quantum-mechanical case. It is interesting to note that the self-consistent reservoirs are very similar to the Buttiker probes [35, 36] which have been used to model inelastic scatterering in electron transport. In the electron case they lead to Ohm's law being satisfied just as in the harmonic chain the introduction of self-consistent reservoirs leads to Fourier's law being satisfied. In fact we have recently shown how one can obtain Ohm's law using self-consistent reservoirs modeled microscopically by noninteracting electron baths [37].

The Langevin equation approach has some advantages. For example, in the classical heat conduction case, it is easy to write Langevin equations for nonlinear systems and study them numerically. Also they might be useful in studying time dependent phenom-

ena. Examples of this are the treatment of quantum pumping in [38] and the treatment of the question of approach to the non-equilibrium steady state in [22]. We feel that it is worthwhile to explore the possibility of using the quantum Langevin equation approach to the harder and more interesting problems involving interactions and time-dependent potentials in both the electron and phonon case.

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A Green's function properties

We will consider some properties of the Phonon Green's functions. We denote by $\mathcal{G}^+(t)$ the full Green's function of the coupled system of wire and reservoirs. Let U and Ω^2 respectively denote the normal mode eigenvector and eigenvalue matrices satisfying the equations:

$$U^T \Phi U = \Omega^2, \quad U^T M U = \hat{I} \ . \tag{A.1}$$

We define the Green's function $\mathcal{G}^+(t)$ as

$$\mathcal{G}^+(t) = U \ \frac{\sin(\Omega t)}{\Omega} \ U^T \ \theta(t) \ . \tag{A.2}$$

It satisfies the equation

$$M\ddot{\mathcal{G}}^+(t) + \Phi \ \mathcal{G}^+(t) = \delta(t) \ \hat{I} \ . \tag{A.3}$$

The Fourier transform $\mathcal{G}^+(\omega) = \int_{-\infty}^{\infty} dt \ \mathcal{G}^+(t) e^{i\omega t}$ is thus given by

$$\mathcal{G}^+(\omega) = \frac{1}{-(\omega + i\epsilon)^2 M + \Phi} \ . \tag{A.4}$$

The isolated reservoir Green's functions are given by:

$$\begin{aligned} g_L^+(\omega) &= \frac{1}{-(\omega + i\epsilon)^2 M_L + \Phi_L} \\ g_R^+(\omega) &= \frac{1}{-(\omega + i\epsilon)^2 M_R + \Phi_R} \ . \end{aligned}$$

We can also represent $\mathcal{G}^+(\omega)$ as follows:

$$\begin{aligned}\mathcal{G}^+_{rs}(\omega) &= -\sum_Q \frac{U_{rQ}U_{sQ}}{(\omega+\omega_Q+i\epsilon)(\omega-\omega_Q+i\epsilon)} \\ &= -\sum_Q \frac{U_{rQ}U_{sQ}}{\omega^2-\omega_Q^2} + \frac{i\pi}{2\omega}\sum_Q U_{rQ}U_{sQ}[\delta(\omega-\omega_Q)+\delta(\omega+\omega_Q)] \ . \end{aligned} \tag{A.5}$$

We will now express the wire-part of the full Green's function in terms of the uncoupled reservoir Green's functions. We write the equation for $\mathcal{G}^+(\omega)$ in the following form:

$$\begin{pmatrix} -M_W\ (\omega+i\epsilon)^2\hat{I}+\Phi_W & V_L & V_R \\ V_L^T & -M_L\ (\omega+i\epsilon)^2\hat{I}+\Phi_L & 0 \\ V_R^T & 0 & -M_R\ (\omega+i\epsilon)^2\hat{I}+\Phi_R \end{pmatrix} \times \begin{pmatrix} G^+_W & G^+_{WL} & G^+_{WR} \\ G^+_{LW} & G^+_L & G^+_{LR} \\ G^+_{RW} & G^+_{RL} & G^+_R \end{pmatrix} = \begin{pmatrix} \hat{I} & 0 & 0 \\ 0 & \hat{I} & 0 \\ 0 & 0 & \hat{I} \end{pmatrix} . \tag{A.6}$$

From these equations we obtain the following expression for $G^+_W(\omega)$:

$$\begin{aligned} G^+_W(\omega) &= \frac{1}{-(\omega+i\epsilon)^2\ M_W+\Phi_W-\Sigma^+_L-\Sigma^+_R} \ , \\ \text{where}\quad \Sigma^+_L(\omega) &= V_L\ g^+_L(\omega)\ \ V_L^T \ , \\ \Sigma^+_R(\omega) &= V_R\ g^+_R(\omega)\ V_R^T \ . \end{aligned} \tag{A.7}$$

B Equilibrium properties

In this section we will calculate the canonical ensemble expectation value of $K = \langle\ \dot{X}_W \dot{X}_W^T\ \rangle$ where the average is taken over the equilibrium density matrix of the entire coupled system of wire and reservoirs. Denoting by Z_Q the normal mode coordinates of the entire

system we get, for points i, j on the wire:

$$\begin{aligned}
K_{ij}^{eq} &= \langle \dot{X}_i \dot{X}_j \rangle_{eq} \\
&= \sum_Q U_{iQ} U_{jQ} \langle \dot{Z}_Q^2 \rangle_{eq} \\
&= \sum_Q U_{iQ} U_{jQ} [\frac{\hbar\omega_Q}{2} + \hbar\omega_Q f(\omega_Q, T)] \\
&= \int_{-\infty}^{\infty} d\omega \frac{\omega}{\pi} \sum_Q U_{iQ} U_{jQ} \frac{\pi}{2\omega} [\delta(\omega - \omega_Q) + \delta(\omega + \omega_Q)] \frac{\hbar\omega}{2} \coth(\frac{\hbar\omega}{2k_B T}) \\
&= \int_{-\infty}^{\infty} d\omega \frac{\omega}{2\pi i} [(G_W^+ - G_W^-)]_{ij} \frac{\hbar\omega}{2} \coth(\frac{\hbar\omega}{2k_B T}) \ . \qquad \text{(B.1)}
\end{aligned}$$

Now from Eq. (A.7) we have:

$$\begin{aligned}
(G_W^-)^{-1} - (G_W^+)^{-1} &= (\Sigma_L^+ - \Sigma_L^-) + (\Sigma_R^+ - \Sigma_R^-) + 4i\epsilon\omega M_W \\
&= 2\ i\ (\Gamma_L + \Gamma_R) + 4i\epsilon\omega M_W \\
\Rightarrow G_W^+ - G_W^- &= 2\ i\ G_W^+\ (\Gamma_L + \Gamma_R)\ G_W^- + 4i\epsilon\omega\ G_W^+ M_W G_W^- \ . \qquad \text{(B.2)}
\end{aligned}$$

Hence we finally get:

$$\begin{aligned}
K_{ij}^{eq} &= \int_{-\infty}^{\infty} d\omega\ \frac{\omega}{\pi}\ [\ G_W^+\ (\Gamma_L + \Gamma_R)\ G_W^-\ ]_{ij}\ \frac{\hbar\omega}{2}\ \coth(\frac{\hbar\omega}{2k_B T}) \\
&\quad + \int_{-\infty}^{\infty} d\omega\ \frac{2\epsilon\omega}{\pi}\ [\ G_W^+\ M_W\ G_W^-\ ]_{ij}\ \frac{\hbar\omega}{2}\ \coth(\frac{\hbar\omega}{2k_B T}) \ . \qquad \text{(B.3)}
\end{aligned}$$

Since we eventually take the limit $\epsilon \to 0$, the second term is non-vanishing only when the equation

$$Det[-\omega^2 M_W + \Phi_W - \Sigma_L^+(\omega) - \Sigma_R^+(\omega)] = 0 \qquad \text{(B.4)}$$

has solutions for real ω. These solutions correspond to the *bound states*[1] of the coupled system of wire and reservoirs [22].

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