Time autocorrelation function and Green-Kubo formula: Study on a disordered harmonic chain

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We have considered heat conduction in a one-dimensional mass-disordered harmonic chain of N particles connected to two Langevin type reservoirs at different temperatures. An exact expression for the boundary heat current-current autocorrelation function in the nonequilibrium steady state (NESS) is obtained in terms of nonequilibrium phonon Green's functions. The time integral of the correlation function gives expected result, both in nonequilibrium as well as equilibrium cases. Using the form of this correlation function we show that asymptotic system size dependence of current fluctuation in NESS for a mass-disordered harmonic chain is $N^{-\alpha}$ for different boundary conditions. For free and fixed boundary conditions we get $\alpha=1/2$ and 3/2, respectively, while for pinned case the fluctuation decays exponentially with system size.

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I. INTRODUCTION

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 autocorrelation function. Similarly the friction coefficient of an overdamped particle is also related to the time correlation function of the instantaneous force experienced by the particle. Let us consider a stochastic process described by the vector $\mathbf{x}(t)$. Then the time correlation function of any quantity $A(t)=A(\mathbf{x}(t))$ is defined as: $\langle A(t)A(t')\rangle$ where $\langle\ \rangle$ represents the average over initial conditions and trajectories. In terms of phase space variables, $\langle A(t)A(t')\rangle$ is given by

$$\langle A(t)A(t')\rangle = \int d\mathbf{x} \int d\mathbf{y} A(\mathbf{x})A(\mathbf{y})W(\mathbf{x},t;\mathbf{y},t')P(\mathbf{y},t'), \tag{1}$$

where, $P(\mathbf{y},t')$ is the probability of $\mathbf{y}$ at time t' and W is the transition probability from $\mathbf{y}$ to $\mathbf{x}$ in time $t-t'$. In general the equilibrium time correlation function of some quantity is related to the response of a system to small perturbations. These relations are called Green-Kubo formula (GK) [1,2].

For the case of heat transport the GK formula relates the response of a system to a small temperature gradient to the equilibrium heat current autocorrelation function. The response to temperature gradient defines the thermal conductivity κ and the GK formula gives

$$\kappa = \lim_{\tau\to\infty}\lim_{L\to\infty} \frac{1}{k_B T^2 L^d}\int_0^\tau dt\langle J(t)J(0)\rangle, \tag{2}$$

where $J(t)$ is the heat current through the system at time t and L is the linear dimension of a d-dimensional system. In Eq. (2) the order of the limits is very important. Although this is a very useful formula, there are some difficulties associated with this formula. The formula in Eq. (2) is not applicable to small mesoscopic structures. Also in case of anomalous transport, which occurs in many low dimensional systems, the thermal conductivity diverges [3,4]. In such cases it is not possible to take the limits as in Eq. (2). There are various derivations of this formula [5,6]. Recently, we have derived a formula similar to Eq. (2) for open systems, which is applicable to systems of arbitrary size in any dimensions [7]. This derivation uses Fokker-planck description of stochastic systems and hence is only applicable for those currents, which can be expressed 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 [7] is not applicable for them. General expectation is, for boundary currents also one can proof a open finite system GK formula as given in [7]. In this paper, we explicitly calculate boundary current-current autocorrelation 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.

There are few examples where exact time autocorrelation functions in equilibrium state have been obtained for many-particle systems. For Hamiltonian systems some examples of exact calculations are velocity autocorrelation function for ordered harmonic lattices [8] and for a one-dimensional gas of elastically colliding hard rods [9]. Recently authors of [10] have shown explicitly that integration of the heat current autocorrelation function gives the current in nonequilibrium steady state for a two particle harmonic system. In this paper, we obtain an exact expression for the time autocorrelation function for boundary heat current in the NESS for mass-disordered harmonic chains of arbitrary length, expressed in terms of the nonequilibrium Green's functions. We show that it satisfies the GK formula derived in [7]. Using this correlation function we also calculate the asymptotic system size scaling of fluctuations in current in NESS.

The paper is organized as follows. In Sec. II, we give the description of the model, define some relevant quantities and notations and calculate the current in the NESS. In Sec. III, we present the calculation of the time correlation function. In Sec. IV, we discuss our results and finally in Sec. V we conclude.

II. DEFINITION OF MODEL

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

$$H = \sum_{l=1}^{N} \left[\frac{1}{2} m_l \dot{x}_l^2 + \frac{1}{2} k_o x_l^2 \right] + \sum_{l=1}^{N-1} \frac{1}{2} k (x_{l+1} - x_l)^2 + \frac{1}{2} k' (x_1^2 + x_N^2), \tag{3}$$

where x_l are displacements of the particles about their equilibrium positions, k, k_0 are the interparticle and on-site spring constants, respectively, and m_l is mass of the lth 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 lth particle is given by [11]

$$\begin{aligned} m_l \ddot{x}_l = & -k(2x_l - x_{l-1} - x_{l+1}) - k_o x_l \\ & - \delta_{l,1}[(k' - k)x_l + \gamma_L \dot{x}_1 - \eta_L] \\ & - \delta_{l,N}[(k' - k)x_l + \gamma_R \dot{x}_N - \eta_R] \\ & \text{where} \quad l = 1, 2 \ldots N \quad \text{and} \quad x_0 = x_{N+1} = 0 \end{aligned} \tag{4}$$

where $\eta_{L,R}(t)$ are Gaussian noise terms with zero mean and related to the dissipative terms with these relations

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

$$\langle \eta_L(t)\, \eta_R(t') \rangle = 0, \quad \langle \eta_{L,R}(t) \rangle = 0. \tag{5}$$

(In this paper we have set $K_B = 1$.) To define the local energy current inside the chain we first define the local energy density associated with the lth particle (or energy at the lattice site l) as follows:

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

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

$$\text{for} \quad l = 2, 3 \ldots N - 1,$$

$$\epsilon_N = \frac{p_N^2}{2m_N} + \frac{k_o x_N^2}{2} + \frac{k' x_N^2}{2} + \frac{k}{4}(x_{N-1} - x_N)^2. \tag{6}$$

Using this energy density we write a continuity equation, from which we get two instantaneous currents j_L and j_R which are flowing from the left and right reservoirs into the system respectively. These currents are given by [3,4]

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

$$\text{and} \quad j_R(t) = -\gamma_R \dot{x}_N^2(t) + \eta_R(t) \dot{x}_N(t). \tag{7}$$

In order to obtain the steady state properties we have to find out the steady state solution of the Eq. (4). For that we write Eq. (4) in Matrix form as

$$M\ddot{X} + \Gamma \dot{X} + \Phi X = \eta(t), \tag{8}$$

where, X, η are column vectors with elements $[X]^T = (x_1, x_2, \ldots x_N)$, $[\eta]^T = (\eta_L, 0, \ldots .0, \eta_R)$ and Γ is a $N \times N$ matrix with only nonvanishing elements $[\Gamma]_{11} = \gamma_L$, $[\Gamma]_{NN} = \gamma_R$. $[\Phi]_{N \times N}$ represents a tridiagonal matrix with elements [12]

$$\begin{aligned} \Phi_{lm} &= (k + k' + k_o)\delta_{l,m} - k\delta_{l,m-1}, \quad \text{for} \quad l = 1 \\ &= -k\delta_{l,m-1} + (2k + k_o)\delta_{l,m} - k\delta_{l,m+1}, \quad \text{for} \quad 2 \leq l \leq N - 1 \\ &= (k + k' + k_o)\delta_{l,j} - k\delta_{l,m+1}, \quad \text{for} \quad l = N, \end{aligned} \tag{9}$$

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

$$M\ddot{\mathcal{G}}^+(t) + \Gamma \dot{\mathcal{G}}^+(t) + \Phi \mathcal{G}^+(t) = \delta(t) I, \tag{10}$$

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

$$M\ddot{G} + \Gamma \dot{G} + \Phi G = 0, \tag{11}$$

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. (8) as

$$X(t) = \int_{-\infty}^{t} dt' G(t - t')\, \eta(t'). \tag{12}$$

For equilibration we require that $G(t) \to 0$ as $t \to \infty$. From Eq. (12), we get

$$\dot{x}_1(t) = \int_{-\infty}^{t} dt_1 [\dot{G}_{11}(t - t_1)\, \eta_L(t_1) + \dot{G}_{1N}(t - t_1)\, \eta_R(t_1)]. \tag{13}$$

Next we calculate $\langle j_L \rangle$ in the NESS. Here $\langle \ldots \rangle$ denotes the average over the noise variables $\eta_L(t)$ and $\eta_R(t)$. From now we denote $\langle j_L \rangle$ by j. Putting $\dot{x}_1(t)$ from Eq. (13) in the expression of $j_L(t)$ in Eq. (7) and using the noise correlation in Eq. (5) we get

$$\begin{aligned} j = & -\gamma_L \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 [\dot{G}_{11}(t - t_1)\dot{G}_{11}(t - t_2) \times \langle \eta_L(t_1)\, \eta_L(t_2) \rangle \\ & + \dot{G}_{1N}(t - t_1)\dot{G}_{1N}(t - t_2) \times \langle \eta_R(t_1)\, \eta_R(t_2) \rangle] \\ & + \int_{-\infty}^{t} dt_1 \dot{G}_{11}(t - t_1) \langle \eta_L(t)\, \eta_L(t_1) \rangle \\ = & \, 2\gamma_L \left[\frac{T_L}{2} \dot{G}_{11}(0) - (\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)) \right], \end{aligned} \tag{14}$$

where we have used the definition

$$A_i(t) = \int_0^{\infty} dt' \dot{G}_{1i}(t + t') \dot{G}_{1i}(t') \quad \forall\, t. \tag{15}$$

We now note the following identity (for proof see Appendix A)

$$\gamma_L A_1(t) + \gamma_R A_N(t) = \frac{\dot{G}_{11}(t)}{2}, \tag{16}$$

which can be obtained from Eqs. (15) and (11). Using this in Eq. (14) we get

$$j = 2\gamma_L \gamma_R (T_L - T_R) A_N(0). \tag{17}$$

If we go to the frequency ω space using the following definition:

$$G^+(\omega) = \int_0^\infty dt G(t) e^{i\omega t}, \tag{18}$$

we can identify that

$$A_i(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \omega^2 |G_{1i}^+(\omega)|^2 e^{i\omega t}, \tag{19}$$

and

$$G^+(\omega) = [-M\omega^2 + i\omega\Gamma + \Phi]^{-1}. \tag{20}$$

With this identification we see that the expression given in Eq. (17) reduces to the form

$$j = \frac{(T_L - T_R)}{2\pi} \int_0^\infty d\omega \mathcal{T}(\omega), \tag{21}$$

where

$$\mathcal{T}(\omega) = 4\gamma_L \gamma_R \omega^2 |G_{1N}^+(\omega)|^2, \tag{22}$$

is the transmission coefficient for frequency ω. The above expression for the current j is seen to be identical to the well-known expression for the current given in [13,14].

In the next section we proceed to obtain the time autocorrelation function $C_{\Delta T}(t,t')$ defined as

$$C_{\Delta T}(t,t') = \langle j_L(t) j_L(t') \rangle - \langle j_L \rangle^2, \tag{23}$$

in the NESS. The subscript ΔT 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 autocorrelation 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.

III. CALCULATION OF AUTOCORRELATION FUNCTION

Using the forms of j_L from Eq. (7) we write current-current autocorrelation $\langle j_L(t) j_L(0) \rangle$ as

$$\langle j_L(t) j_L(0) \rangle = J_{L1} + J_{L2} + J_{L2} + J_{L4},$$

where

$$J_{L1} = \gamma_L^2 \langle \dot{x}_1^2(t) \dot{x}_1^2(0) \rangle,$$

$$J_{L2} = -\gamma_L \langle \eta_L(t) \dot{x}_1(t) \dot{x}_1^2(0) \rangle,$$

$$J_{L3} = -\gamma_L \langle \eta_L(0) \dot{x}_1^2(0) \dot{x}_1(t) \rangle,$$

$$J_{L4} = \langle \eta_L(t) \dot{x}_1(t) \eta_L(0) \dot{x}_1(0) \rangle, \tag{24}$$

where $t > 0$.

Now we will calculate all these J's using Eqs. (13) and (5). 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. (24) we get

$$J_{L1} = \gamma_L^2 \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 \int_{-\infty}^{0} dt_3 \int_{-\infty}^{0} dt_4 \times K_1(t_1,t_2,t_3,t_4,t), \tag{25}$$

Where $K_1(t_1,t_2,t_3,t_4,t)$ is given by

$$\begin{aligned} K_1(t_1,t_2,t_3,t_4,t) = \langle & [\dot{G}_{11}(t-t_1)\eta_L(t_1) + \dot{G}_{1N}(t-t_1)\eta_R(t_1)] \\ & \times [\dot{G}_{11}(t-t_2)\eta_L(t_2) + \dot{G}_{1N}(t-t_2)\eta_R(t_2)] \\ & \times [\dot{G}_{11}(-t_3)\eta_L(t_3) + \dot{G}_{1N}(-t_3)\eta_R(t_3)] \\ & \times [\dot{G}_{11}(-t_4)\eta_L(t_4) + \dot{G}_{1N}(-t_4)\eta_R(t_4)] \rangle. \end{aligned} \tag{26}$$

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

$$\begin{aligned} K_1(t_1,t_2,t_3,t_4,t) = & 4(K_1^{(1)}(t_1,t_2,t_3,t_4,t)\delta(t_1-t_2)\delta(t_3-t_4) \\ & + K_1^{(2)}(t_1,t_2,t_3,t_4,t)\delta(t_1-t_3)\delta(t_2-t_4) \\ & + K_1^{(3)}(t_1,t_2,t_3,t_4,t)\delta(t_1-t_4)\delta(t_2-t_3)) \end{aligned} \tag{27}$$

where expressions for these $K_1^{\prime s}$ are given in Appendix B.

Putting the expression of $K_1(t_1,t_2,t_3,t_4,t)$ in Eq. (25) and arranging the terms we finally get

$$\begin{aligned} J_{L1} = & 4\gamma_L^2 [\{\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)\}^2 \\ & + 2\{\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)\}^2], \end{aligned} \tag{28}$$

where we have used the definitions of $A_i(t)$ in Eq. (15). Similarly we calculate other J's and their expressions are

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

$$J_{L3} = -4\gamma_L^2 T_L \left[\frac{1}{2} \dot{G}_{11}(0) \{\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)\} + 2\dot{G}_{11}(t) \times \{\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)\}, \right]$$

$$\begin{aligned} J_{L4} = 4\gamma_L T_L \Bigg[& \delta(t) \{\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)\} \\ & + \gamma_L T_L \left\{ \frac{1}{4} \dot{G}_{11}^2(0) \right\} \Bigg]. \end{aligned} \tag{29}$$

Collecting all the expressions for J's from Eqs. (28) and (29) in Eq. (24) and subtracting $\langle j_L \rangle^2$ we finally obtain

$$C_{\Delta T}(t) = 4\gamma_L T_L\{\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)\}\delta(t) - 8\gamma_L^2[\{\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)\} \times \{T_L \gamma_L A_1(t) + (2T_L - T_R)\gamma_R A_N(t)\}],$$

$$= 4\gamma_L T_L\{\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)\}\delta(t) - g_{\Delta T}(t), \quad (30)$$

where

$$g_{\Delta T}(t) = 8\gamma_L^2[\{\gamma_L T_L A_1(t) + \gamma_R T_R A_N(t)\} \times \{T_L \gamma_L A_1(t) + (2T_L - T_R)\gamma_R A_N(t)\}], \quad (31)$$

and we have used the identity in Eq. (16). 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 nonequilibrium current-current autocorrelation 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 δ-function peak. We have verified that the integral of bond correlation agrees with the value for the boundary correlation.

IV. DISCUSSIONS

In this section we plot the function $g_{\Delta T}(t) = 4\gamma_L T_L\{\gamma_L T_L A_1(0) + \gamma_R T_R A_N(0)\}\delta(t) - C_{\Delta T}$. 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 $\omega^2|G_{1i}(\omega)|^2$ as shown in Eq. (19). For a general N-particle mass-disordered chain it is difficult to find analytical expressions for the functions $|G_{ij}^+(\omega)|^2$. For the ordered case, $G_{ij}^+(\omega)$ can be obtained analytically using the tridiagonal nature of the force matrix Φ (see for example Ref. [12]). 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 [11]. We numerically evaluate $G_{1N}^+(\omega)$ and $G_{11}^+(\omega)$ using this transfer matrix approach. We observe that at large $\omega > \omega_d = \frac{km}{N\sigma^2}$, $[\![|G_{1N}^+(\omega)|^2]\!]$ decays as $e^{-aN\omega^2}$ (a is a positive constant) where $m = [\![m_l]\!]$ and $\sigma^2 = [\![(m_l - m)^2]\!]$. Here $[\![\ldots]\!]$ denotes disorder average. This behavior was proved analytically by Matsuda and Ishii [15] and was observed numerically by Dhar [11]. Another 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. We make use of this observation in this paper. Another observation which we made is that for $\omega > \omega_m$ the function $|G_{11}^+(\omega)|^2$ decays as $1/\omega^4$, where ω_m is the maximum normal mode frequency. This $1/\omega^4$ behavior can be easily obtained through the transfer matrix approach. For small frequencies disorder average of $|G_{11}^+(\omega)|^2$ oscillates with ω and is again identical to that of ordered chain.

After integrating Eq. (19) 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. 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 remains almost identical at short times and starts being different significantly after some time scale. These observations can be made by looking at the dominant contributions of $\omega^2|G_{1i}^+(\omega)|^2$ in the integrand of Eq. (19) for fixed t. At large ω the functions $|G_{1N}^+(\omega)|^2$ decays as $e^{-aN\omega^2}$ (a is a positive constant) [11,15] whereas $|G_{11}^+(\omega)|^2$ decays as $1/\omega^4$. At small frequencies both $G_{1N}^+(\omega)$ and $G_{11}^+(\omega)$ are oscillating function of ω 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 ω becomes important. Whereas, in case of $A_N(t)$, only a small range of ω contribute in the Fourier transform of $\omega^2|G_{1N}^+(\omega)|^2$ [Eq. (19)]. For large N, at small times $A_1(t)$ is much larger than $A_N(t)$ and contributes most in $g_0(t)$, which makes $g_0(t)$ to be independent of N at small times. Inset in Fig. 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 behavior of $A_N(t)$ with system size N. In Fig. 2, we plot $[\![A_N(t)]\!]$ for different system sizes. Here we prefer to give plots of disordered averaged quantities, since very often we are interested in disorder averaged quantities.

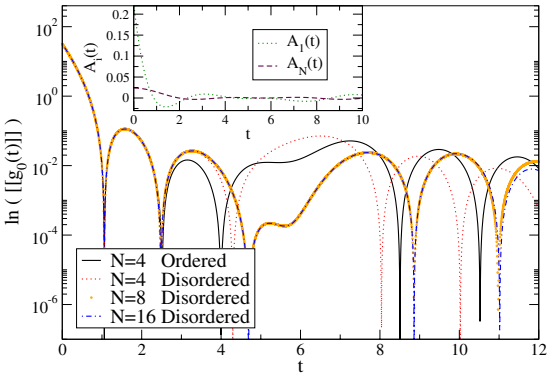

FIG. 1. (Color online) Plots of $[\![g_0(t)]\!]$ vs t for $N=4$ and $N=8$. The parameters for the figure are $T_L=2.0$, $T_R=2.0$, $k=1.0$, $k_0=0.0$, $k'=0.0$, $\gamma_L=\gamma_R=2.5$, and $\Delta=0.4$. Here $[\![g_0(t)]\!]$ denotes disorder averaged $g_0(t)$. The average is done over 100 disorder realizations. Inset shows the plots of $A_1(t)$ and $A_N(t)$ for $N=8$ for a single disorder configuration.

Let $Q(\tau) = \int_o^\tau dt j_L(t)$ be the heat transfer in duration τ from left reservoir to the system. Using stationarity property of the correlation function it is easy to show that the second order cumulant of $Q(\tau)$ is related to $C_{\Delta T}(t)$ as

$$\lim_{\tau\to\infty} \frac{\langle Q^2(\tau)\rangle_c}{\tau} = \int_0^\infty dt C_{\Delta T}(t). \quad (32)$$

Now integrating the expression of $C_{\Delta T}(t)$ given in Eq. (30) from 0 to ∞ and again using the identity in Eq. (16) we get

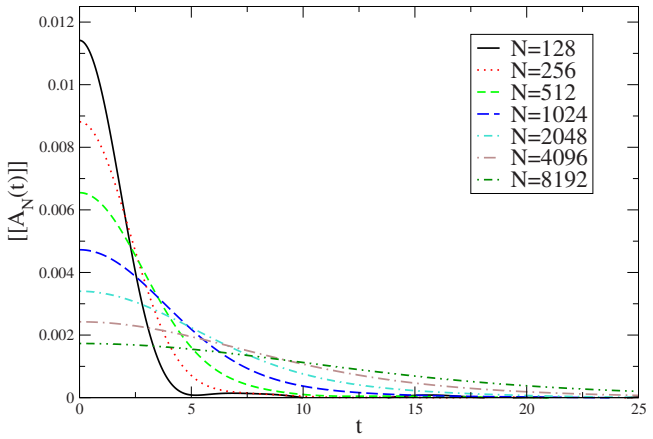

FIG. 2. (Color online) Plots of $[\![A_N(t)]\!]$ vs t for different system sizes. The parameters for the figure are same as those for Fig. 1. $\Delta=0.4$.

$$\int_0^\infty dt C_{\Delta T}(t) = 2\gamma_L\gamma_R T_L T_R A_N(0) + 8\gamma_L^2\gamma_R^2(T_L - T_R)^2 \int_0^\infty dt A_N^2(t). \quad (33)$$

In the frequency space the Eq. (33) can be written as an integration over ω of the transmission coefficient $\mathcal{T}(\omega)$ defined in Eq. (22) and we obtain

$$\int_0^\infty dt C_{\Delta T}(t) = \frac{(T_L - T_R)^2}{4\pi}\int_0^\infty d\omega \mathcal{T}^2(\omega) + \frac{T_L T_R}{2\pi}\int_0^\infty d\omega \mathcal{T}(\omega). \quad (34)$$

This expression matches with the expression given in [16] for quantum mechanical systems, in the high temperature limit. Now if we put $T_L=T_R=T$ in the expression in Eq. (33) and use Eq. (17) we get a relation between the current in the nonequilibrium steady state and the equilibrium correlation function similar to the GK relation derived in [7]

$$\int_0^\infty dt C_0(t) = \frac{T^2}{2\pi}\int_0^\infty d\omega \mathcal{T}(\omega) = T^2\frac{j}{(T_L - T_R)}, \quad (35)$$

where $C_0(t)$ is the equilibrium autocorrelation function for the open system. The inset of Fig. 3 shows the system size dependence of the disorder average of current.

In general for large system sizes $[\![j]\!]$ and $[\![\frac{\langle Q^2(\tau)\rangle_c}{\tau}]\!]$ scales with N as $N^{-\beta}$ and $N^{-\alpha}$, respectively. Using the frequency dependence of $T(\omega)=[\![\mathcal{T}(\omega)]\!]$ and $[\![\mathcal{T}^2(\omega)]\!]$ one can predict the value of α and β for different BC's. By computing $[\![j]\!]$ in NESS, several authors have already studied asymptotic size dependence of $[\![j]\!]$. Rubin and Greer [17] obtained $\beta=1/2$ for free BC, which was latter proved rigorously by Verheggen [18]. Casher and Lebowitz [13] studied the same model and obtained a lower bound for $[\![j]\!]\geq N^{-3/2}$ and simulations by Rich and vischer [19] confirmed the exponent to be $\beta=3/2$. Later Dhar [11] obtained j for both the boundary conditions using Langevin equation and Green's function approach and obtained $\beta=1/2$ for free BC and $\beta=3/2$ for fixed BC. Here

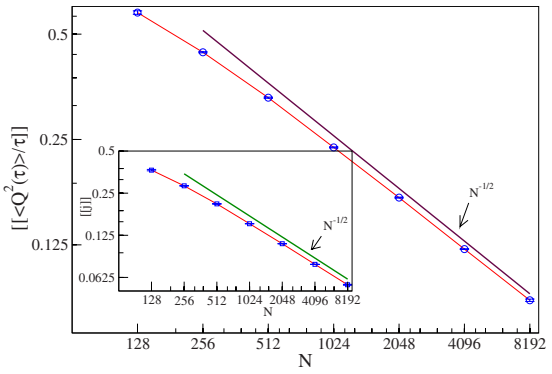

FIG. 3. (Color online) This figure shows the dependence of nonequilibrium current fluctuation on system size for free BC. The parameters for the figure are same as those for Fig. 1 except $T_L=3.0$ and $T_R=2.0$. Inset shows the dependence of nonequilibrium current on system size for free BC. Disorder average is taken over 100 different disorder realizations. Standard deviation corresponding to each point is smaller that the size of the point symbol.

we follow the same procedure described in [11] to find the asymptotic size dependence of $[\![\frac{\langle Q^2(\tau)\rangle_c}{\tau}]\!]$ from the expression given in Eq. (34).

We numerically observe that for both the BCs $[\![\mathcal{T}^2(\omega)]\!]$ 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 ω. To determine α, we use the fact (discussed in the first paragraph of this section) that for ω greater than $\omega_d \sim N^{-1/2}$, $T(\omega)$ decays exponentially as $e^{-aN\omega^2}$ whereas, for $\omega < \omega_d$, $T(\omega)$ is almost identical to $\mathcal{T}_o(\omega)$ of an ordered chain. It can be shown that transmission coefficient of an ordered chain, denoted by $\mathcal{T}_o(\omega)$, is independent of ω for free BC and goes as ω^2 for fixed BC. Now putting these forms of $\mathcal{T}_o(\omega)$ 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. (33) for free BC and obtain $\frac{\langle Q^2(\tau)\rangle_c}{\tau}$ for $\tau\to\infty$ for different system sizes. In Fig. 3 we plot $[\![\frac{\langle Q^2(\tau)\rangle_c}{\tau}]\!]$ 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 decays exponentially with N.

V. CONCLUSION

In conclusion, we have given an expression for the 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 nonequilibrium correlation function gives information about current fluctuation in the NESS. Using the nonequilibrium correlation function we ob-

tain asymptotic system size scaling of the fluctuation in the steady state current. A possible application of our results is that they can serve to test numerical codes for simulations studying correlations in nonequilibrium systems. In this paper, we have considered a classical one dimensional system with white noise Langevin dynamics. It will be straightforward to get an expression for correlation function in quantum systems and higher dimensional systems.

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APPENDIX A: PROOF OF EQ. (16)

Let us first define few quantities

$$\tilde{G} = M^{1/2} G M^{1/2}$$

$$\tilde{\Gamma} = M^{-1/2} \Gamma M^{-1/2}$$

$$\tilde{\Phi} = M^{-1/2} \Phi M^{-1/2}$$

Using this above definitions Eq. (11) can be written as

$$\ddot{\tilde{G}}(t) + \tilde{\Gamma}\dot{\tilde{G}}(t) + \tilde{\Phi}\tilde{G}(t) = 0. \tag{A1}$$

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

$$\frac{d}{dt'}[\dot{\tilde{G}}^T(t')\dot{\tilde{G}}(t'+t)]$$

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

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

$$\dot{\tilde{G}}(t) = 2\int_0^\infty dt' \dot{\tilde{G}}^T(t')\tilde{\Gamma}\dot{\tilde{G}}(t'+t). \tag{A2}$$

To the above equation we have used the following: $\dot{G}(0) = M^{-1}$, $G(0)=0$, $G(t)\to 0$ as $t\to\infty$. Now we know that $\Gamma_{ij} = (\frac{\gamma_L}{m_1}\delta_{i1} + \frac{\gamma_R}{m_N}\delta_{iN})\delta_{ij}$. Taking (11)th element on the both side of the matrix Eq. (A2) we get

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

$$= \gamma_L A_1(t) + \gamma_R A_N(t). \tag{A3}$$

APPENDIX B: EXPRESSIONS OF K_1's

$$K_1^{(1)}(t_1,t_2,t_3,t_4,t)$$

$$= [\gamma_L^2 T_L^2 \dot{G}_{11}(t-t_1)\dot{G}_{11}(t-t_2)\dot{G}_{11}(-t_3)\dot{G}_{11}(-t_4)$$

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

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

$$+ \dot{G}_{11}(t-t_1)\dot{G}_{11}(t-t_2)\dot{G}_{1N}(-t_3)\dot{G}_{1N}(-t_4)\}],$$

$$K_1^{(2)}(t_1,t_2,t_3,t_4,t)$$

$$= [\gamma_L^2 T_L^2 \dot{G}_{11}(t-t_1)\dot{G}_{11}(t-t_2)\dot{G}_{11}(-t_3)\dot{G}_{11}(-t_4)$$

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

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

$$+ \dot{G}_{11}(t-t_1)\dot{G}_{1N}(t-t_2)\dot{G}_{11}(-t_3)\dot{G}_{1N}(-t_4)\}],$$

and

$$K_1^{(3)}(t_1,t_2,t_3,t_4,t)$$

$$= [\gamma_L^2 T_L^2 \dot{G}_{11}(t-t_1)\dot{G}_{11}(t-t_2)\dot{G}_{11}(-t_3)\dot{G}_{11}(-t_4)$$

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

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

$$+ \dot{G}_{1N}(t-t_1)\dot{G}_{11}(t-t_2)\dot{G}_{11}(-t_3)\dot{G}_{1N}(-t_4)\}].$$

[1] M. S. Green, J. Chem. Phys. **22**, 398 (1954).
[2] R. Kubo, M. Yokota, and S. Nakajima, J. Phys. Soc. Jpn. **12**, 1203 (1957).
[3] S. Lepri, R. Livi, and A. Politi, Phys. Rep. **377**, 1 (2003).
[4] A. Dhar, Adv. Phys. **57**, 457 (2008).
[5] H. Mori, Phys. Rev. **112**, 1829 (1958); M. S. Green, *ibid.* **119**, 829 (1960); L. P. Kadanoff and P. C. Martin, Ann. Phys. **24**, 419 (1963); W. M. Visscher, Phys. Rev. A **10**, 2461 (1974).
[6] J. M. Luttinger, Phys. Rev. **135**, A1505 (1964).
[7] A. Kundu, A. Dhar, and O. Narayan, J. Stat. Mech.: Theory Exp. (2009) L03001.
[8] P. Mazur and E. Montroll, J. Math. Phys. **1**, 70 (1960).
[9] D. W. Jepsen, J. Math. Phys. **6**, 405 (1965).
[10] W. A. M. Morgado and D. O. Soares-Pinto, Phys. Rev. E **79**, 051116 (2009).
[11] A. Dhar, Phys. Rev. Lett. **86**, 5882 (2001).
[12] D. Roy and A. Dhar, J. Stat. Phys. **131**, 535 (2008).
[13] A. Casher and J. L. Lebowitz, J. Math. Phys. **12**, 1701 (1971).
[14] D. Roy and A. Dhar, J. Stat. Phys. **125**, 4 (2006).
[15] H. Matsuda and K. Ishii, Prog. Theor. Phys. **45**, 56 (1970).
[16] K. Saito and A. Dhar, Phys. Rev. Lett. **99**, 180601 (2007).
[17] R. Rubin and W. Greer, J. Math. Phys. **12**, 1686 (1971).
[18] T. Verheggen, Commun. Math. Phys. **68**, 69 (1979).
[19] M. Rich and W. M. Visscher, Phys. Rev. B **11**, 2164 (1975).