

Comment on “Can Disorder Induce a Finite Thermal Conductivity in 1D Lattices?”

In a recent Letter, Li *et al.* [1] have reported that the steady state of the disordered harmonic chain is not unique and depends on initial conditions. Their claim is based on a molecular dynamics simulation using Nosé-Hoover thermostats to model the heat baths. We point out that the uniqueness of the nonequilibrium steady state of the disordered harmonic chain for a large class of heat baths has been proven exactly [2,3]. In this Comment we consider a particular case where it is easy to explicitly demonstrate the uniqueness of the steady state. This is the case where the heat bath is modeled by Langevin dynamics. The results of Li *et al.* appear to be due to either insufficient equilibration times or an artifact of using Nosé-Hoover thermostats.

Consider heat conduction through a one-dimensional mass-disordered harmonic chain. The Hamiltonian of the system is

$$H = \sum_{l=1}^N \frac{p_l^2}{2m_l} + \sum_{l=0}^N \frac{(x_l - x_{l+1})^2}{2}, \quad (1)$$

where $\{x_l\}$ are the displacements of the particles about their equilibrium positions, $\{p_l\}$ are their momenta, and $\{m_l\}$ are the random masses. We put the boundary conditions $x_0 = x_{N+1} = 0$. The particles in the bulk evolve through the classical equations of motion while the boundary particles, namely particles 1 and N , are coupled to Langevin heat baths as in Ref. [2].

The equations of motion for the particles are:

$$\begin{aligned} m_1 \ddot{x}_1 &= -2x_1 + x_2 - \dot{x}_1 + \eta_L(t); \\ m_l \ddot{x}_l &= -(2x_l - x_{l-1} - x_{l+1}), \\ l &= 2, 3, \dots, (N-1); \\ m_N \ddot{x}_N &= -(2x_N + x_{N-1}) - \dot{x}_N + \eta_R(t), \end{aligned} \quad (2)$$

where η_L and η_R are Gaussian white noises with the correlations $\langle \eta_{L,R}(t) \eta_{L,R}(t') \rangle = 2T_{L,R} \delta(t - t')$. Denoting the coordinates and momenta collectively by the variables q_l so that $\{q_1, q_2, \dots, q_{2N}\} = \{x_1, x_2, \dots, x_N, p_1, p_2, \dots, p_N\}$ Eqs. (2) can be written in the form

$$\dot{q}_l = - \sum_{k=1}^{2N} a_{lk} q_k + \eta_l, \quad (3)$$

where the vector η has all elements zero except $\eta_{N+1} = \eta_L$ and $\eta_{2N} = \eta_R$ and the $2N \times 2N$ matrix a is given by

$$a = \begin{pmatrix} 0 & J \\ \Phi & \gamma \end{pmatrix} \quad \text{with}$$

$$\begin{aligned} J_{kl} &= -\delta_{k,l}/m_k; & \Phi_{kl} &= 2\delta_{k,l} - \delta_{k,l-1} - \delta_{k,l+1}; \\ \gamma_{kl} &= \delta_{k,l}(\delta_{k,1}/m_1 + \delta_{k,N}/m_N). \end{aligned} \quad (4)$$

In the steady state $\langle d(q_k q_l)/dt \rangle = 0$. From this and using Eq. (3) we get the matrix equation

$$a \cdot b + b \cdot a^T = d, \quad (5)$$

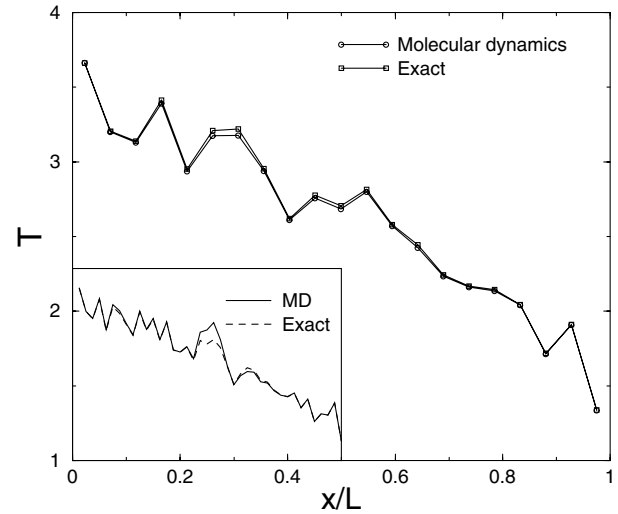


FIG. 1. The exact temperature profiles as obtained from inverting Eq. (5) are compared with those from molecular dynamics simulations for two lattice sizes $N = 20$ and $N = 40$ (inset).

where b is the correlation matrix with elements $b_{kl} = \langle q_k q_l \rangle$ and $d_{kl} = \delta_{k,l}(2T_L \delta_{k,N+1} + 2T_R \delta_{k,2N})$. We can invert this equation to obtain b and thus all the moments including the local temperatures $T_l = \langle p_l^2/m_l \rangle$. The uniqueness of the steady state then depends on whether or not Eq. (5) has a unique inverse. For chains of finite length and for given disorder realizations it is easy to verify numerically that Eq. (5) does have a unique inverse. We also find that a molecular dynamics simulation (using a simple Euler discretization), with Langevin heat baths, reproduces the exact temperature profile and is independent of initial conditions. This is shown in Fig. 1. For the $N = 20$ lattice, averaging over 10^7 time units is sufficient to achieve steady-state values. The $N = 40$ data are averaged over 10^8 time units. We find that equilibration times increase rapidly with system size.

Finally, we note that for Langevin heat bath dynamics, the unique steady-state distribution is, in fact, known exactly [2] and is a Gaussian given by

$$P(\{q_l\}) = (2\pi)^{-N} \text{Det}[b]^{-1/2} e^{-1/2 \sum b_{lm}^{-1} q_l q_m}. \quad (6)$$

Abhishek Dhar
Raman Research Institute
Bangalore 560080
India

Received 15 March 2001; published 24 July 2001
DOI: 10.1103/PhysRevLett.87.069401
PACS numbers: 44.10.+i, 05.45.-a, 05.70.Ln, 66.70.+f

- [1] B. Li, H. Zhao, and B. Hu, Phys. Rev. Lett. **86**, 63 (2001).
- [2] A. J. O'Connor and J. L. Lebowitz, J. Math. Phys. (N.Y.) **15**, 692 (1974); A. Casher and J. L. Lebowitz, J. Math. Phys. (N.Y.) **12**, 1701 (1971).
- [3] H. Spohn and J. L. Lebowitz, Commun. Math. Phys. **54**, 97 (1977).