Heat Conduction in a Two-Dimensional Harmonic Crystal with Disorder

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We study the problem of heat conduction in a mass-disordered two-dimensional harmonic crystal. Using two different stochastic heat baths, we perform simulations to determine the system size (L) dependence of the heat current (J). For white noise heat baths we find that $J \sim 1/L^{\alpha}$ with $\alpha \approx 0.59$, while correlated noise heat baths give $\alpha \approx 0.51$. A special case with correlated disorder is studied analytically and gives $\alpha = 3/2$, which agrees also with results from exact numerics.

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Introduction.—The problem of proving or verifying Fourier's law, $J = -\kappa \nabla T$, where κ is the thermal conductivity, in any system evolving through Newtonian dynamics has been a challenge for theorists [1,2]. So far most studies have been restricted to one-dimensional systems for the simple reason that they are easier to study through simulations and through whatever analytic methods that are available. Also the hope is that such studies on one-dimensional systems provide insights which will be useful when one confronts the more difficult (and experimentally more relevant) problem of higher dimensional systems. For one-dimensional systems, some of the most interesting results that have been obtained are as follows: (i) For momentum conserving nonlinear systems, the heat current J decreases with system size L as $J \sim 1/L^{\alpha}$, where $\alpha < 1$ [3]. Thus Fourier's law (which predicts $\alpha = 1$) is not valid. The exponent α is expected to be universal, but its exact value is still not known. A renormalization group analysis of the hydrodynamic equations [4] predicts $\alpha = 2/3$, while mode-coupling theory [5] gives $\alpha = 3/5$. The results from simulations are not able to convincingly decide between either of these. (ii) For disordered harmonic systems, we get $J \sim 1/L^{\alpha}$ again, but the exponent α depends on the properties of the heat baths [6–9].

In dimensions higher than one, there are few detailed studies and it is fair to say that it is totally unclear as to whether Fourier's law will hold, and if not, then what the value of the exponent α is. For nonlinear systems which are expected to show local thermal equilibrium, both the hydrodynamic approach and mode-coupling theories predict a logarithmic divergence of the conductivity in two dimensions. There have been simulations by Lippi and Livi [10] who find a logarithmic divergence, but simulations on larger-size systems by Grassberger and Yang [11] seem to obtain a power law divergence. A disordered harmonic model in two dimensions was studied in simulations by Yang [12], who claimed that beyond some critical disorder one gets Fourier's law, i.e., $\alpha = 1$. It is doubtful that this claim is correct. The data in the paper seems to indicate $J \sim 1/L^2$, which is *not* Fourier's law. Besides, these simulations were done with Nose-Hoover heat baths and it is known that these can be problematic when applied to harmonic systems [13]. Simulations by Hu *et al.* [14] on the same model but with stochastic heat baths do not find a Fourier behavior. Finally, an older study by Poetzsch and Bottger [15] looked at heat conduction in a 2D system with both disorder and nonlinearity and they give some evidence for Fourier behavior.

In this Letter, we consider heat conduction in a 2D disordered harmonic system. Let us first try to see what one should expect theoretically. We expect localization phenomena (for phonons) to play an important role. A renormalization group calculation [16] predicts the following: in one dimension, all modes with $\omega > 1/L^{1/2}$ are localized; in two dimensions, all modes with $\omega > [\log(L)]^{-1/2}$ are localized; in three dimensions, there is a finite band of frequencies of extended states. This is similar to results for electron localization with the important difference that here the $\omega \to 0$ modes are extended even in one and two dimensions. Also for the case of electrons, only electrons near the Fermi-level contribute significantly to transport, while in heat transport, all phonons contribute. From the localization results we expect that in three dimensions the current in a disordered harmonic system should be independent of system size ($\alpha = 0$). In one and two dimensions it is the small number of low-frequency phonons ($\omega < \omega_c$) which dominate transport properties. The fact that $\omega_c \to 0$ with increasing L immediately implies that $\alpha > 0$. In one dimension it has been shown [6] that the exact value of α depends on the low-frequency spectral properties of the bath. A similar calculation is not available in the 2D case, and we address this specific question.

Here we present results from a detailed simulational study to determine the exponent α for a mass-disordered harmonic system. Two different kinds of stochastic baths are considered, one with white noise and the other with correlated noise. We also study a special case where the disorder is correlated.

Definition of model.—We consider heat conduction in a two-dimensional mass-disordered harmonic crystal described by the Hamiltonian

$$H = \sum_{\substack{i=1,L_x \\ j=1,L_y}} \frac{p_{ij}^2}{2m_{ij}} + \sum_{\substack{i=1,L_x \\ j=1,L_y}} \frac{1}{2}[(x_{ij} - x_{i-1j})^2 + (x_{ij} - x_{i+1j})^2 + (x_{ij} - x_{ij-1})^2 + (x_{ij} - x_{ij+1})^2],$$

where $\{x_{ij}, p_{ij}, m_{ij}\}$ denote the position (particle displacements about equilibrium positions), momentum, and mass of a particle at the site (i, j). We set the masses of exactly half the particles to one and the remaining to two and make all configurations equally probable. Heat conduction takes place in the x direction, and we assume that the ends of the system are fixed by the boundary conditions $x_{0j} = 0 = x_{L_x+1j}$. We will assume periodic boundary conditions along the y direction so that $x_{ij+L_y} = x_{ij}$. The heat baths are modeled through Langevin equations and thus we get the following equations of motion:

$$\begin{aligned} m_{1j}\ddot{x}_{1j} &= -4x_{1j} + x_{2j} + x_{1j-1} + x_{1j+1} + h_j^L, \\ m_{L_xj}\ddot{x}_{L_xj} &= -4x_{L_xj} + x_{L_x-1j} + x_{L_xj-1} + x_{L_xj+1} + h_j^R, \\ m_{ij}\ddot{x}_{ij} &= -4x_{ij} + x_{i-1j} + x_{i+1j} + x_{ij-1} + x_{ij+1} \end{aligned} \quad (1)$$

(for $1 < i < L_x$ and $1 \le j \le L_y$), where h_j^L and h_j^R denote the forces from the heat baths. We will consider two different models for the heat baths: the Gaussian white noise source and the Gaussian exponentially correlated source.

Gaussian white noise source.—Thus $h_j^L = -\gamma\dot{x}_{1j} + \eta_j^L$; $h_j^R = -\gamma\dot{x}_{L_xj} + \eta_j^R$, where the noise terms have the properties $\langle\eta_j^L\rangle = \langle\eta_j^R\rangle = 0$, $\langle\eta_j^L(t)\eta_{j'}^L(t')\rangle = 2T_L\gamma\delta(t - t')\delta_{jj'}$, and $\langle\eta_j^R(t)\eta_{j'}^R(t')\rangle = 2T_R\gamma\delta(t - t')\delta_{jj'}$.

Gaussian exponentially correlated source.—In this case, the bath forces have the forms

$$\begin{aligned} h_j^L &= -\int_{-\infty}^t dt'\tilde{\gamma}(t - t')\dot{x}_{1j}(t') + \eta_j^L, \\ h_j^R &= -\int_{-\infty}^t dt'\tilde{\gamma}(t - t')\dot{x}_{L_xj}(t') + \eta_j^R, \end{aligned} \quad (2)$$

with $\langle\eta_j^L(t)\eta_{j'}^L(t')\rangle = T_L\tilde{\gamma}(t - t')\delta_{jj'}$, $\langle\eta_j^R(t)\eta_{j'}^R(t')\rangle = T_R\tilde{\gamma}(t - t')\delta_{jj'}$, and $\tilde{\gamma}(t) = e^{-\gamma t}$. A simple way of implementing correlated baths in the simulations is by introducing new dynamical variables y_j^L, y_j^R for the bath and setting $h_j^L = y_j^L$, $h_j^R = y_j^R$. These satisfy the equations of motion $\dot{y}_j^L = -\gamma y_j^L - \dot{x}_{1j} + \eta_j^L$, etc. In the long time limit it can be easily seen that the solutions $y_j^L(t)$ and $y_j^R(t)$ have the required properties of correlated baths. We now discuss the results from simulations of the two different bath models.

Simulations with white noise.—Equilibration times in simulations of disordered harmonic lattices can be very long and this can sometimes lead to wrong conclusions (see for, e.g., [17]). To avoid such problems we first compare our simulation results with exact numerical results on steady state properties of small systems. We now briefly describe the numerical technique.

With $N = L_xL_y$ let us define the new variables $\{q_1, q_2, \ldots, q_{2N}\} = \{x_{11}, x_{12}\ldots, x_{L_xL_y}, p_{11}, p_{12}\ldots, p_{L_xL_y}\}$. Then Eq. (1) can be rewritten in the form

$$\dot{q}_l = -\sum_{m=1}^{2N} \mathbf{a}_{lm}q_m + \xi_l, \quad (3)$$

where the vector ξ has all elements zero except $\xi_{N+j} = \eta_j^L$; $\xi_{2N-L_y+j} = \eta_j^R$ (for $1 \le j \le L_y$) and the $2N \times 2N$ matrix $\mathbf{a}$ is given by

$$\mathbf{a} = \begin{pmatrix} 0 & -M^{-1} \\ \Phi & \Gamma \end{pmatrix},$$

where the $N \times N$ matrices M, Φ, and Γ can be labeled by the double indices (i, j) and are given by

$$\begin{aligned} M_{(ij),(i'j')} &= \delta_{ii'}\delta_{jj'}m_{ij}, \\ \Phi_{(ij)(i'j')} &= 4\delta_{ii'}\delta_{jj'} - \delta_{ii'}(\delta_{jj'-1} + \delta_{jj'+1}) \\ &\quad - \delta_{jj'}(\delta_{ii'-1} + \delta_{ii'+1}), \\ \Gamma_{(ij)(i'j')} &= \gamma\delta_{ii'}\delta_{jj'}(\delta_{i1}/m_{1j} + \delta_{iL_x}/m_{L_xj}). \end{aligned} \quad (4)$$

In the steady state, $\langle d(q_nq_l)/dt\rangle = 0$. From this and using Eq. (3) we get the matrix equation [18]

$$\mathbf{a}\,\mathbf{b} + \mathbf{b}\mathbf{a}^T = \mathbf{d} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{e} \end{pmatrix}, \quad (5)$$

where $\mathbf{b}$ is the correlation matrix with elements $\mathbf{b}_{nl} = \langle q_nq_l\rangle$ and $\mathbf{e}_{(ij)(i'j')} = \gamma\delta_{ii'}\delta_{jj'}(2T_L\delta_{i1} + 2T_R\delta_{iL_x})$. Inverting this equation one obtains $\mathbf{b}$ and thus all the moments which include the local temperatures $T_{ij} = \langle p_{ij}^2/m_{ij}\rangle$ and currents $J_{ij}^x = \langle x_{i-1j}p_{ij}/m_{ij}\rangle$. The dimension of the matrix which has to be inverted is $N(2N + 1) \times N(2N + 1)$, and by using the fact that it is a sparse matrix we have been able to numerically [19] obtain $\mathbf{b}$ for system sizes up to $L_x = L_y = L = 8$.

The molecular dynamics simulations were performed using a velocity-verlet scheme [20]. We chose a step size of $\Delta t = 0.005$ and averaging over 10^8 time steps (for $L = 256$ we took $\Delta t = 0.02$ and $10^7 - 5 \times 10^7$ time steps). The temperatures at the two ends were set to $T_L = 0.5$ and $T_R = 2.0$. In Fig. 1, we plot T_{ij} at every site, as obtained from the simulations and from the exact solution, for a particular realization of disorder. The agreement is clearly very good. We also find that current fluctuations decay faster than fluctuations of the local temperature. This is because, in the harmonic model, *decay of fluctuations takes place only through coupling to the reservoirs* and this is weak for localized modes that contribute to the temperature. This means that equilibrated values for the current can be obtained in smaller simulation runs.

Simulations were performed for sizes $L_x = L_y = L = 4, 8, 16, \ldots, 256$, and in Fig. 2 we plot the system size dependence of the current, averaged over 100 samples (9 samples for $L = 256$). Error bars shown are those calcu-

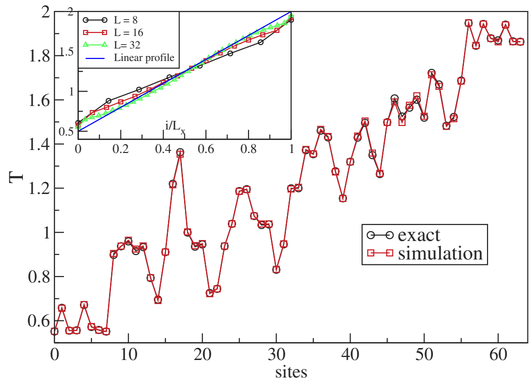

FIG. 1 (color online). Temperature at all the sites of a 8×8 fully disordered lattice, from simulations and from the exact solution. The inset shows the disorder-averaged temperature profiles for different system sizes and seems to approach a linear form.

lated from the disorder averaging, the thermal ones being much smaller. For larger system sizes we find that we need to average over a smaller number of realizations since the rms spread in the current decreases rapidly. From our data, we estimate $\alpha = 0.59 \pm 0.01$.

We briefly note that Eq. (5) can be solved exactly for the ordered case, using methods similar to those in [18]. The current is independent of system size and is given by

$$J = \frac{(T_L - T_R)}{4\pi\gamma} \int_0^{2\pi} dq \phi_1(q),$$

where $\phi_1(q) = 1 + \frac{1}{2}(\gamma^{-2} + \lambda_q) - \frac{1}{2}[4(\gamma^{-2} + \lambda_q) + (\gamma^{-2} + \lambda_q)^2]^{1/2}$ and $\lambda = 2[1 - \cos(q)]$. The temperature in the bulk of the system takes the constant value $T = (T_L + T_R)/2$.

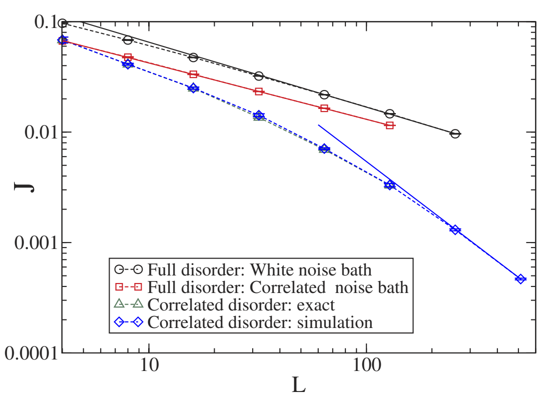

FIG. 2 (color online). Plot of disorder-averaged-current versus system size for the two different heat baths and for the case of correlated disorder with white noise. For the full disorder cases, the solid lines are fits to the last three points and have slopes 0.59 and 0.51. For the case of correlated disorder, the slope from exact numerics (and also simulations) is compared to 1.5, which is what one expects analytically.

Simulations with correlated noise.—In this case the simulations were done by using a slightly modified version of the velocity-verlet algorithm with a step size $\Delta t = 0.001$ and averaging over 10^8 time steps. The accuracy of the algorithm was tested in one dimension, where exact numerical results are available [6]. Simulations were performed for sizes $L = 4, 8, 16, \ldots, 128$ with disorder averages over 100 samples (22 for $L = 128$). The results are plotted in Fig. 2 and we estimate the exponent $\alpha = 0.51 \pm 0.01$ in this case, which is somewhat different from the slope of $\alpha \approx 0.59$ for the case of uncorrelated noise. It is possible that the small difference is a finite-size effect, and for larger system sizes we might see the same exponent. The error bars given are statistical errors, while those from finite-size effects are more difficult to estimate. The next example throws some light on this aspect.

Correlated disorder.—Finally, we consider a special case of correlated disorder (with white noise baths) which was discussed in [7]. This case is analytically tractable and gives us some insights on possible finite-size effects. In this model, in a given column, say, the ith, all particles have the same mass m_i. This case can be reduced to an effective 1D problem [7]. Using the fact that there is order in the transverse direction, we transform to new variables using an orthogonal basis $\psi_j(q)$, which satisfies the equation $2\psi_j(q) - \psi_{j-1}(q) - \psi_{j+1}(q) = \lambda_q \psi_j(q)$. We choose the $\psi_j(q)$ to be real and find that $\lambda_q = 2[1 - \cos(q)]$, with $q = 2s\pi/L_y$ where $s = 1, 2, \ldots, L_y$. The new variables $x_i(q) = \sum_j x_{i,j}\psi_j(q)$ satisfy the following equations of motion:

$$\begin{aligned} m_1 \ddot{x}_1(q) &= -\mu(q)x_1 + x_2 - \gamma\dot{x}_1 + \eta^L(q), \\ m_{L_x}\ddot{x}_{L_x}(q) &= -\mu(q)x_{L_x} + x_{L_x-1} - \gamma\dot{x}_{L_x} + \eta^R(q), \\ m_i \ddot{x}_i(q) &= -\mu(q)x_i + x_{i-1} + x_{i+1} \end{aligned} \quad (6)$$

(for $1 < i < L_x$), where $\mu(q) = 2 + \lambda_q$. The transformed noise variables $\eta^L(q, t) = \sum_j \eta_j^L(t)\psi_j(q)$ satisfy $\langle \eta^L(q, t)\eta^L(q', t')\rangle = 2T_L\gamma\delta(t - t')\delta_{qq'}$ and similarly for $\eta^R(q, t)$. Thus for every q we have an equation identical to that of a 1D disordered chain with an additional on-site potential $V = \lambda_q x^2/2$. The heat current in terms of the transformed variables is

$$J = \frac{1}{L_y}\sum_q \langle [-\gamma\dot{x}_1(q) + \eta^L(q)]\dot{x}_1(q)\rangle. \quad (7)$$

Fourier transforming Eq. (6) using $\tilde{x}_i(q, \omega) = \int dt x_i(q, t)e^{-i\omega t}$, $\tilde{\eta}^{L,R}(q, \omega) = \int dt \eta^{L,R}(q, t)e^{-i\omega t}$, we get the following set of equations:

$$\begin{aligned} [\mu(q) - m_1\omega^2 + i\gamma\omega]\tilde{x}_1 - \tilde{x}_2 &= \tilde{\eta}^L, \\ -\tilde{x}_{i-1} + [\mu(q) - m_i\omega^2]\tilde{x}_i - \tilde{x}_{i+1} &= 0, \\ -\tilde{x}_{L_x-1} + [\mu(q) - m_{L_x}\omega^2 + i\gamma\omega]\tilde{x}_{L_x} &= \tilde{\eta}^R, \end{aligned}$$

which in matrix notation can be written as $\mathcal{Y}(q, \omega)\tilde{x}(q, \omega) = \tilde{\eta}(q, \omega)$, where $\tilde{x}$ and $\tilde{\eta}$ are the vectors

$(\tilde{x}_1(q,\omega),\ldots,\tilde{x}_{L_x}(q,\omega))^T$ and $(\tilde{\eta}^L(q,\omega),0,0,\ldots,\tilde{\eta}^R(q,\omega))^T$. The matrix $\mathcal{Y}=k\Phi-\omega^2M+i\omega\Gamma$ where $M_{nl}=\delta_{nl}m_n$; $\Phi_{nl}=\mu(q)\delta_{nl}-\delta_{nl-1}-\delta_{nl+1}$ and $\Gamma_{nl}=\gamma\delta_{nl}(\delta_{n1}/m_1+\delta_{nL_x}/m_{L_x})$. After some manipulations the current in Eq. (7) simplifies to give

$$J=\frac{\gamma^2(T_L-T_R)}{\pi L_y}\sum_q\int_{-\infty}^{\infty}d\omega\,\omega^2|\mathcal{Y}^{-1}_{1L_x}(\omega,q)|^2. \qquad (8)$$

The inverse element is given by [6] $|\mathcal{Y}^{-1}_{1L_x}(\omega,q)|^2=|\mathrm{Det}[\mathcal{Y}]|^{-2}$, where $\mathrm{Det}[\mathcal{Y}]=D_{1,L_x}+i\gamma\omega(D_{2,L_x}+D_{1,L_x-1})-\gamma^2\omega^2D_{2,L_x-1}$ and $D_{i,i'}$ is defined to be the determinant of the submatrix of $k\hat{\Phi}-\omega^2M$ beginning with the ith row and column and ending with the i'th row and column. These matrix elements can be expressed in terms of products of random matrices [6]. Using these results one can very efficiently compute the integral in Eq. (8) and obtain J accurately for quite large system sizes ($L=512$). In Fig. 2 we show the system size dependence of the current as obtained from the exact numerical method and also from simulations. They agree very well and give $\alpha\approx1.5$. This value can be understood analytically by noting that the leading contribution to the current in Eq. (8) comes from the $q\to0$ term (finite q modes decay exponentially with system size) and this is identical to a pure 1D chain for which $\alpha=3/2$.

The fact that the simulation results agree extremely well with the exact numerical results (for sizes up to $L=128$) proves the accuracy of our simulations. Further, we see that for the correlated disorder case the asymptotic result for the exponent can already be seen at around $L=512$. This gives us confidence that for the case of the fully disordered lattice we might already be close to the asymptotic value. This is also supported by the fact that the change in slope of the J-versus-L curves in Fig. 2 over the system sizes studied is very small.

Conclusions.—We have performed extensive simulations of heat conduction in a mass-disordered harmonic solid in two dimensions, which give exponents $\alpha\approx0.59$ for white noise heat baths and $\alpha\approx0.51$ for correlated noise baths. A system with correlated disorder gives, somewhat surprisingly, a larger exponent $\alpha=3/2$. The combination of simulations and exact numerics gives us confidence on the accuracy of our results and also additional insight. Some interesting open problems are the exact determination of the exponent α in two dimensions, for any heat bath model, and an analytical understanding of dependence of α on bath properties.

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