Heat conduction in the disordered Fermi-Pasta-Ulam chain

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We address the question of the effect of disorder on heat conduction in an anharmonic chain with interactions given by the Fermi-Pasta-Ulam (FPU) potential. In contrast to the conclusions of an earlier paper [Phys. Rev. Lett. **86**, 63 (2001)], which found that disorder could induce a finite thermal conductivity at low temperatures, we find no evidence of a finite-temperature transition in conducting properties. Instead, we find that at low temperatures, small system-size transport properties are dominated by disorder but the asymptotic system size dependence of current is given by the usual FPU result $J \sim 1/N^{2/3}$. We also present interesting results on the binary-mass ordered FPU chain.

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It is now generally believed that heat conduction in one-dimensional (1D) linear momentum-conserving systems is anomalous [1,2]. In the absence of an external pinning potential, as is the case in most realistic situations, one finds that Fourier's law is not satisfied [3]. One of the predictions from Fourier's law is the scaling form of heat current J with system size N for a system with a fixed applied temperature difference. From Fourier's law one gets $J \sim 1/N$. The conclusion, from a large number of studies of 1D momentum-conserving systems, seems to be

$$J \sim \frac{1}{N^{1-\alpha}}, \quad \alpha \neq 0. \tag{1}$$

The main results on the exponent α can be summarized as follows: (i) for a pure harmonic chain $J \sim N^0$ [4], (ii) for a disordered harmonic chain α depends on the spectral properties of the bath and on boundary conditions [5–7], and (iii) for a nonlinear system without disorder α seems to be independent of properties of heat baths and the results from the most recent simulations indicate a universal value of $\alpha = \frac{1}{3}$ [2,8].

Transport in systems with both disorder and interactions has recently attracted a lot of interest both theoretically [9–13] and experimentally [14]. The main interest is to understand the transition from an insulating state governed by the physics of Anderson localization to a conducting state as one increases interactions. In the context of oscillator chains, we note that the physics of the disordered harmonic chain is dominated by localization physics, which has its strongest effect in 1D systems. The question of the effect of anharmonicity on localization was recently addressed for a system in which the harmonic part of the Hamiltonian included an external pinning potential and the anharmonicity was a quartic on-site potential [12]. In this case, in the absence of the anharmonic term, $J \sim e^{-cN}$. Surprisingly it was found that adding a small amount of anharmonicity leads to a conducting (Fourier-like) behavior with a power-law decay $J \sim 1/N$ and no transition to the insulating state was found on decreasing the anharmonicity. An important feature seen was that with decreasing anharmonicity one had to go to larger system sizes to see the true asymptotic behavior of the current.

In the present paper, we investigate the same question, namely that of the effect of interactions (phonon-phonon) on localization, but in the absence of any external pinning potential. We study the mass disordered Fermi-Pasta-Ulam (FPU) model with interactions put in through a quartic interparticle potential. In the absence of pinning, for the harmonic case, low-frequency modes with $\omega \lesssim 1/N^{1/2}$ remain extended and this gives rise to a power-law dependence of J on N [5–7]. On the other hand, for the pure FPU chain also, low-frequency modes are believed to play an important role in transport and give rise to anomalous transport. An earlier study by Li *et al.* [9] on this model concluded that this model showed a transition, from a Fourier-like scaling $J \sim 1/N$ at low temperatures to a pure FPU-like behavior with $J \sim 1/N^{0.57}$ at high temperatures. Our study suggests that this conclusion may not be correct. We do not find any evidence of a finite-temperature transition. Instead we find that a small amount of anharmonicity leads to the same system-size dependence as seen in the pure system. We discuss possible sources of error in the conclusions of Li *et al.* We also present results on the ordered binary mass FPU chain, including nontrivial scaling properties of the system-size dependence of current.

I. MODEL

We consider the following FPU Hamiltonian:

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m_l} + \sum_{l=1}^{N+1} \left(\frac{(x_l - x_{l-1})^2}{2} + \nu \frac{(x_l - x_{l-1})^4}{4} \right), \tag{2}$$

where $\{x_l, p_l\}$ denotes the position and momenta of particles and we use fixed boundary conditions $x_0 = x_{N+1} = 0$. The interparticle harmonic spring constant has been set to 1 and ν denotes the strength of the quartic interaction. We consider a binary random alloy and set the masses of half of the particles, at randomly chosen sites, to m_1 and the rest to m_2. The

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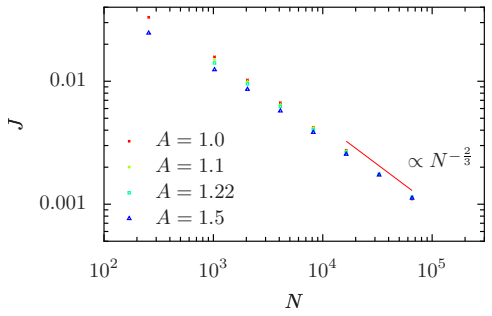

FIG. 1. (Color online) Plot of the heat current J versus system size in the binary mass ordered chain for different values of the mass ratio $A=1.0$, 1.1, 1.22, and 1.5.

particles at the two ends of the chain are connected to stochastic white noise heat baths at different temperatures. The equations of motion of the chain are then given by

$$m_l\ddot{x}_l = -(2x_l - x_{l-1} - x_{l+1}) - \nu[(x_l - x_{l-1})^3 + (x_l - x_{l+1})^3] - \gamma_l\dot{x}_l + \eta_l, \tag{3}$$

with $\eta_l = \eta_L\delta_{l,1} + \eta_R\delta_{l,N}$, $\gamma_l = \gamma(\delta_{l,1} + \delta_{l,N})$, and where the noise terms satisfy the fluctuation dissipation relations $\langle \eta_L(t)\eta_L(t')\rangle = 2\gamma k_B T_L \delta(t-t')$, $\langle \eta_R(t)\eta_R(t')\rangle = 2\gamma k_B T_R \delta(t-t')$, k_B being Boltzmann's constant. The heat current is given by $J = \Sigma_l \langle f_{l,l-1}\dot{x}_l\rangle/(N-1)$, where $f_{l,l-1}$ is the force exerted by the $(l-1)$th particle on the lth particle and $\langle\cdots\rangle$ denotes a steady-state average. We will denote by $[J]$ an average over disorder. As noted in [12], Eqs. (3) are invariant under the transformation $T_{L,R} \to sT_{L,R}$, $\{x_l\} \to \{s^{1/2}x_l\}$, and $\nu \to \nu/s$. This implies the scaling relation $J(sT_L, sT_R, \nu) = sJ(T_L, T_R, s\nu)$ and thus the effect of changing ν can be equivalently studied by changing T_L, T_R. In the present study, we will fix temperatures and consider the effect of changing ν.

Let us consider first the harmonic case $\nu=0$. In this case, it is known from detailed numerical work and analytic arguments that the exponent α depends on the properties of the bath and on boundary conditions. For white noise baths one finds $\alpha = -\frac{1}{2}$ for fixed boundaries and $\alpha = \frac{1}{2}$ for free boundaries. In the presence of anharmonicity it is expected, and indeed we have verified in simulations, that α does not depend on boundary conditions. Here we use fixed boundary conditions only.

Before presenting the results of simulations for the binary-mass disordered anharmonic chain, it is important to know the value of α for the binary ordered chain. Let us thus discuss this first. This case was studied earlier in [8], where it was found that the temperature profile showed oscillations with an amplitude that decreased as $N^{-1/2}$. Let us denote the mass ratio $m_1/m_2 = A$. For $A=1$, the simulations in [8] gave strong evidence for an exponent $\alpha = \frac{1}{3}$. However, for the value $A=2.62$ a clear convergence could not be obtained. Here we will argue that the exponent remains unchanged from the $A=1$ value. In Fig. 1, we present simulation results for the N dependence of the current J in the binary-mass ordered chain for different values of the parameter A, all corresponding to the same average mass $(m_1+m_2)/2=1$. Remarkably we find that at large enough system sizes the actual

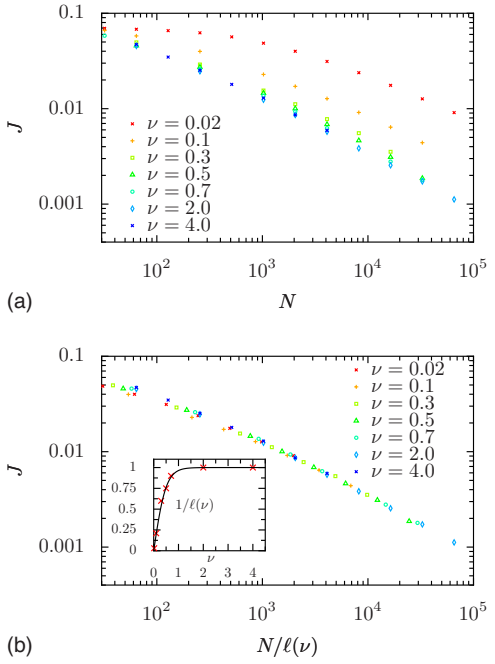

FIG. 2. (Color online) Plot of the heat current J versus system size for the binary mass ordered chain, for different values of ν and with the mass ratio $A=1.5$ (a). (b) shows the same data plotted with a scaled x axis.

values of the currents for different A tend to converge to the same value as the $A=1$ value. Thus clearly the exponent α remains unchanged for any value of A. However, for a large mass ratio one has to go to large system sizes to see the true exponent. A similar effect was seen in Ref. [2] for the binary hard-particle gas. In our simulations, we used the velocity-Verlet algorithm with time steps $dt=0.005$ [15]. For small system sizes we used $O(10^7)-O(10^8)$ steps for relaxation and the same number of steps for averaging, while for larger systems, up to $O(10^9)$ steps were used. In all our simulations, we used $T_L=1.25$, $T_R=0.75$, and $\gamma=1.0$.

For the disordered anharmonic case, we wish to study the cases with weak and strong anharmonicity and see if there is a transition in the value of α. For small ν we expect the system's behavior to be close to a harmonic one, and so one would have to go to very large system sizes to see the effect of anharmonicity and the correct exponent. It then becomes necessary to try and understand the data using some sort of a scaling analysis. Let us first do this for the ordered case. We fix the value of $A=1.5$ and look at the N dependence of the current for different values of ν. The results are shown in Fig. 2(a). For small system sizes, we find a flat region, which is expected since for system sizes smaller than the phonon-phonon scattering length scale we expect the system to behave as a harmonic chain. The scattering length should be larger for smaller ν, and this can be seen in the plot. At large enough system sizes all curves tend to show the same decay coefficient $\alpha = \frac{2}{3}$. To see this clearly, we scale the system size by a length factor $\ell(\nu)$. Figure 2(b) shows a nice collapse of the data and the value of the exponent is confirmed. We find empirically that the ν dependence of the length parameter is given by $\ell(\nu) = 1/\tanh(2\nu)$. We note the interesting and

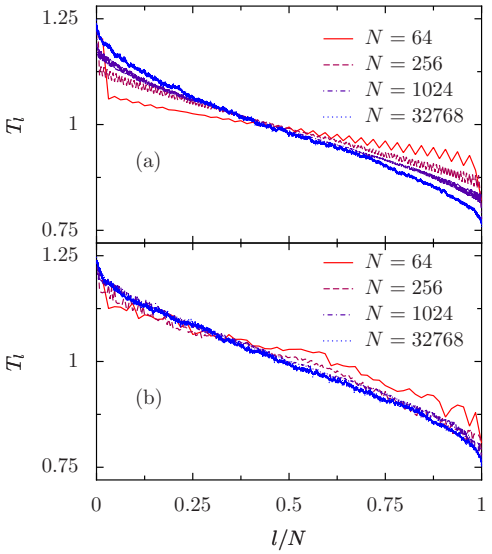

FIG. 3. (Color online) Plot of the temperature profiles in the (a) ordered and (b) disordered lattices for ν=0.1 and for different system sizes.

somewhat surprising point that for any given system size, the value of the current saturates as we keep increasing ν. In Fig. 3(a), we show the temperature profiles for different system size for ν=0.1. As noted earlier in [8], we see the large oscillations in temperature. An interesting general feature of temperature profiles in FPU chains is the following. A coarse-grained temperature profile obtained by averaging over many particles would be smooth and monotonic. However, the temperature gradient is nonmonotonic and this appears to be true even for small temperature differences. This implies that it may not even be possible to write a phenomenological relation such as $J=-\kappa_N(T)\nabla T$.

Finally, we now give the results for the disordered anharmonic case. We take averages over 50–100 samples $N<1024$, 10 samples for N=1024–16 384, and 2 samples for N=32 768 and 65 536. In Fig. 4, we plot the results of simulations for $[J]$ for ν=0.004 and 0.02. Also we show the result for ν=0.0. For small values of ν we see that, at small system

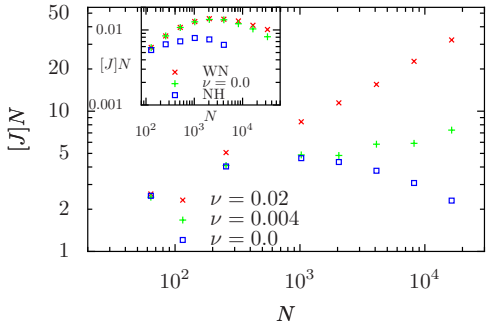

FIG. 4. (Color online) Plot of heat current versus system size, for the disordered anharmonic chain, for different values of ν and with m_1=1.2, m_2=0.8. The data in the inset correspond to parameters (T_L,T_R)=(0.001,0.0005) with Gaussian white noise bath for ν=1 (WN) and ν=0, and Nose-Hoover bath (NH) for ν=1. The error bars corresponding to numerical errors and disorder averaging are smaller than the size of the points.

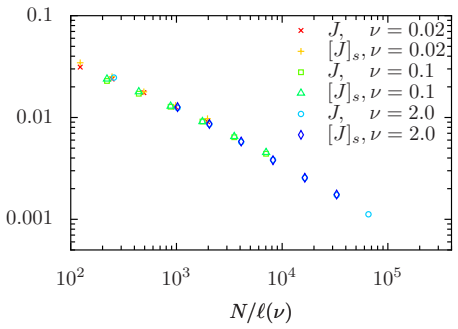

FIG. 5. (Color online) Plot of scaled heat current versus scaled system size, for the binary-mass ordered (J) and disordered ($[J]_s$) anharmonic chains, for different values of ν and with m_1=1.2, m_2=0.8. The error bars corresponding to numerical errors and disorder averaging are smaller than the size of the points.

sizes the current value is close to the ν=0 value. As expected, one has to go to large system sizes to see the effect of the weak anharmonicity. At sufficiently large N, we find the same system-size dependence of $[J]$ as obtained for the ordered FPU chain, namely that given by $\alpha=\frac{1}{3}$. In fact, by scaling the current by appropriate factors we find that the data for the disordered case can be made to collapse on to the binary-mass ordered case. This is shown in Fig. 5 (for ν =0.02,0.1,2.0). Thus our results show that the asymptotic power-law dependence of the current is always dominated by anharmonicity while disorder only decreases the overall conductance of a sample. In Fig. 3(b), we plot the temperature profile for ν=0.1 and find that the asymptotic profile is similar to the ordered case. We now shed some light on the reasons that led to the erroneous conclusions in [9], of a transition in conducting properties at low temperatures (or equivalently small anharmonicity). Consider the data for $[J]N$ plotted in Fig. 4 for ν=0.004. We see that at around $N\sim$1000–2000 the data seem to flatten, and if one had just looked at data in this range, as was done by [9], one would conclude that Fourier's law is valid. However, the behavior changes drastically when one looks at larger system sizes and one again gets the usual FPU behavior. To verify that this is indeed what happens for the particular case studied by Li *et al.*, we have repeated simulations with their set of parameters but for much larger system sizes, and the results are shown in the inset of Fig. 4. This case corresponds to a much smaller value of ν and so it is expected that it will follow the ν=0 curve up to very long length scales, and this is clearly seen. However, at around N=16 384 we see a tendency for the curve to turn up and we expect that the same asymptotic behavior will eventually show up. While a transition cannot be ruled out at even lower temperatures, this seems unlikely. Also, if there is such a transition, one would expect that at low temperatures the effect of anharmonicity would be negligible and so one would see only the effect of disorder. In that case, one should see the corresponding exponent for the disordered harmonic chain, which gives $[J]\sim 1/N^{3/2}$.

II. TEMPERATURE DEPENDENCE OF CONDUCTIVITY

The scaling property of the current, mentioned earlier [after Eq. (3)], implies that the thermal conductivity has the

form $\kappa=\kappa(\nu T)$. For small anharmonicity ($\nu \ll 1$), our earlier results imply that at large system sizes $\kappa \sim N^{1/3}\nu^{-2/3}$ and from the scaling property this immediately gives $\kappa \sim T^{-2/3}$ at low temperatures. However, at small system sizes $[N \ll \ell(\nu)]$, we expect the system to behave like a harmonic system with $\kappa \sim T^0$. At high temperatures, the conductivity will saturate to a constant value.

III. DISCUSSION

Our main conclusion is that there is no change in the asymptotic power-law dependence of the current on system size on decreasing the temperature in the disordered FPU problem. At low temperatures, one has to go to much larger system sizes to see the true exponent, whose value ($\alpha=\frac{1}{3}$) is the same as that for the ordered FPU chain. While we have mostly presented results from simulations with Langevin baths, we have also done some simulations with Nose-Hoover baths, and the conclusions are similar. We also find several interesting results for the binary-mass ordered FPU chain: (i) the exponent α is independent of the mass ratio A and is the same as the $A=1$ value, (ii) the data for different values of ν can be collapsed by scaling the system size by a ν-dependent length scale. Also we make the interesting and somewhat surprising observation that for a finite FPU chain, $J \to \text{const} \neq 0$ as $\nu \to \infty$.

Experiments measuring heat conduction in quasi-1D systems such as individual nanowires, nanotubes [16], are now being done. The predictions of anomalous thermal conduction and diverging conductivity have most recently been verified in an experiment on individual nanotubes [17]. In this experiment, on samples of carbon and boron nitride nanotubes, it was found that even at length scales much larger than phonon mean free paths, the conductivity kept increasing with length. One expects that a detailed verification of the predicted exponent will also soon be possible. Interestingly, the boron nitride sample is isotopically disordered, and so the two systems studied correspond precisely to the ordered and disordered FPU chains studied here. Our prediction, namely that disorder will lower the current in a wire while the system-size dependence of $[J]$ is unaffected, is consistent with current experimental results [17,18]. Experimentally, the temperature dependence of the thermal conductivity may be easier to measure and one can verify if this is unaffected by disorder.

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