Equilibration and Universal Heat Conduction in Fermi-Pasta-Ulam Chains

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It is shown numerically that for Fermi-Pasta-Ulam (FPU) chains with alternating masses and heat baths at slightly different temperatures at the ends, the local temperature (LT) on small scales behaves paradoxically in steady state. This expands the long established problem of equilibration of FPU chains. A well-behaved LT appears to be achieved for equal mass chains; the thermal conductivity is shown to diverge with chain length N as $N^{1/3}$, relevant for the much debated question of the universality of one-dimensional heat conduction. The reason why earlier simulations have obtained systematically higher exponents is explained.

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It has long been established [1] that Fermi-Pasta-Ulam (FPU) chains (one-dimensional chains of particles with anharmonic forces between them) may not be able to achieve thermal equilibrium with seemingly reasonable initial conditions. This has interesting implications for the ergodic hypothesis at the foundation of statistical mechanics. The results of Ref. [1] led to the discovery of solitons in continuum versions [2], and eventually an understanding of chaotic dynamics. With regard to the initial results, a vast body of work has established [3,4] that quasiperiodic solutions exist below an energy threshold, above which the system does equilibrate.

Although all this work has been with closed boundary conditions, the study of FPU chains has expanded to include heat bath boundary conditions: with slightly different temperatures imposed at the two ends, the thermal conductivity can be measured and shows anomalous properties [5,6]. Since the baths at the ends are at different temperatures, the concept of equilibrium has to be extended: a local temperature (LT) that varies smoothly along the chain has to be defined. Surprisingly, this has not been fully investigated, even though the discussion of heat conductivity is in terms of Fourier's law [5], which is meaningless if the local temperature is ill behaved. When the heat baths at the two ends have *equal* temperatures, one can prove analytically that the only possible steady state is the one in thermal equilibrium [7].

In this Letter, we demonstrate for the first time that, for FPU chains with heat bath boundary conditions, the LT behaves paradoxically on small scales. In particular, we show through numerical simulations that for FPU-β chains with alternating light and heavy masses, connected to heat baths at temperatures T_L and T_R at the left and right end, respectively, (with $\Delta T = T_L - T_R$ sufficiently small that the system is in the linear response regime), the kinetic temperature of the particles oscillates as one moves along the chain. The ratio of amplitude of these oscillations to $\Delta T/N$ is constant as ΔT is reduced, and increases with the chain length N: in the vicinity of the $2i$th particle, the temperature difference between heavy and light particles scales approximately as $\delta T \sim [\Delta T/\sqrt{N}]f(i/N)$. Thus if one were to coarse grain over a region of the order of the mean free path, the intracell temperature uncertainty $O(\Delta T/\sqrt{N})$ would dominate the $O(\Delta T/N)$ change in temperature between adjacent cells. [Similar results are obtained when the heavy and light particles are randomly ordered, so that *no* $O(1)$ coarse-graining length would work.] Nor is this a boundary effect with a characteristic decay length, since the dependence on i is through i/N. We also show that there are no problems when the FPU chain has equal masses. For one-dimensional gases, lack of energy equipartition between heavy and light particles has been observed for hard particle systems [8], but we have verified that $T(x)$ as a function of position x (instead of particle number i) is smooth. For the FPU system, where the lattice constant can be taken to be arbitrarily large, this resolution of the problem is not applicable.

For equal mass FPU chains, having verified the existence of a well-behaved LT, we measure the heat conductivity $\kappa(N)$ and demonstrate that

$$\kappa(N) \sim N^{\alpha} \tag{1}$$

with $\alpha = 1/3$, in agreement with the earlier renormalization group (RG) analytical result [9] for a fluid model. We do this by simulating very long FPU chains with up to $N = 65\,536$ particles, showing that $\alpha = 1/3$ is attained in this regime. This result is insensitive to system parameters, in contrast to the apparent exponents for smaller N. We also explain why the apparent α for smaller N is systematically higher than $1/3$, as seen in various earlier numerical simulations [6,10–13]. This supports the assertion that there is only one universality class for heat conduction in one-dimensional momentum conserving systems (that have a well-behaved LT), contrary to earlier suggestions [10–13].

The generalized FPU chain consists of a sequence of particles connected by springs between nearest neighbors. The Hamiltonian is $\sum_i m_i \dot{x}_i^2/2 + V(x_i - x_{i+1})$, where the

potential energy of the interparticle springs is $V(z) = k_2 z^2/2 + k_3 z^3/3 + k_4 z^4/4 + \ldots$. For all figures shown in this Letter, we use the FPU-β model where $k_2 = k_4 = 1$ and other k_i's are zero. As noted in the original FPU paper [1], the incidental even symmetry of this potential may cause nonmixing of even and odd modes, but this is not the case with the heat bath boundary conditions used here. After fixing ΔT, we allow the system to reach steady state and then measure the kinetic temperature $T_i = m_i \langle v_i^2 \rangle$ of each particle. Unless otherwise noted, the end particles $i = 1$ and $i = N$ are connected to Langevin baths at temperatures $T_L = 2.0$ and $T_R = 0.5$, respectively, by adding damping and noise terms to their equations of motion, which are integrated with an accurate Verlet-like algorithm [14].

Figure 1 shows T_i as a function of particle number i for a dimer chain with $N = 128$ and mass ratio 2.62. An unusual oscillating temperature profile is seen; the lighter particles are hotter than the heavier ones on the left and colder on the right. Since the sign, not just the magnitude, of $T_{i+1} - T_i$ oscillates, it is not because of a thermal conductivity κ that oscillates on the microscopic scale. The behavior shown here is robust to changes in the mass ratio, although the oscillation amplitude changes, or the interparticle potential (e.g., if an exponential potential is used, i.e., a Toda lattice with alternating masses). Oscillations in T_i as a function of

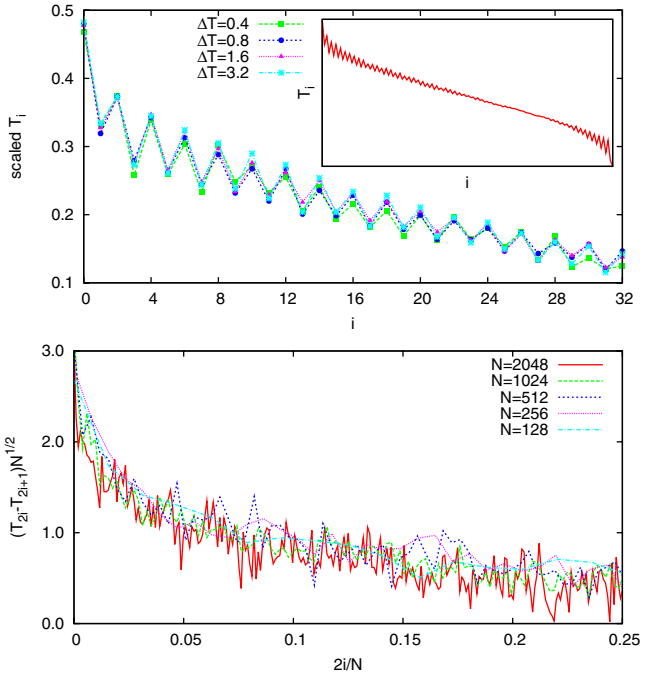

FIG. 1 (color online). Oscillations of the kinetic temperature profile for FPU-β dimer chains with mass ratio 2.62, $\gamma = 2$. (Top inset) Full profile for a system with $N = 128$ and $T_L = 2.0$, $T_R = 0.5$. (Top) $N = 128$ particles, $T_{L,R} = 2 \pm \Delta T/2$. The scaled temperature is $(T - 2)/\Delta T$; the different plots line up. (Bottom) $(T_{2i} - T_{2i+1})N^{1/2}$ versus $2i/N$ for different N. $T_{L,R} = 2.0, 0.5$. The $N^{1/2}$ and $2i/N$ are chosen to approximately match the vertical and horizontal scales of the plots. Together, the figures imply $\delta T \approx [\Delta T/\sqrt{N}] f(i/N)$.

i are also seen when the Langevin baths are replaced with Nose-Hoover baths [15].

Figure 1 also shows that if ΔT is reduced or N is increased, the temperature difference between the $2i$th and $(2i + 1)$th particles scales approximately as $\delta T \sim [\Delta T/\sqrt{N}] f(i/N)$. Thus coarse graining over a region of size $O(1)$, comparable to the mean free path, creates an unusual LT: the uncertainty in temperature in a coarse-grained region is greater than the variation between adjacent regions. Moreover, the "decay length" over which the oscillations penetrate into the interior of the chain is a fixed fraction of N, showing that this is not negligible for large N. Nonmonotonic temperature profiles are also seen when the heavy and light particles are ordered randomly, in which case the heavy and light kinetic temperatures track two separate smooth curves.

Our results show that anharmonicity and disorder are not sufficient for a well-behaved LT even with heat bath boundaries imposing a $O(1/N)$ temperature gradient. When a well-behaved LT *is* achieved, e.g. (as we will show) for equal mass FPU chains, it should be viewed as being fragile. The question remains: what are the necessary and sufficient conditions for a local temperature?

We also simulate FPU-β chains of equal mass particles (of unit mass) as described in the previous paragraphs. When steady state is reached, we observe an approximately linear temperature profile as shown by Fig. 2. There is a slight curvature near the boundaries, which decreases with N. Figure 2 also shows that the velocity distributions are Gaussian (at least for large N) which is necessary for a LT. This indicates that the equal mass FPU chain with heat baths at the boundaries has a well-behaved LT.

With this reassurance, we proceed to measure the heat conductivity as a function of N for the equal mass case. With a small temperature difference applied across the system, Fourier's law predicts that the heat current j should be equal to $-\kappa \nabla T$, with a κ that depends on microscopic

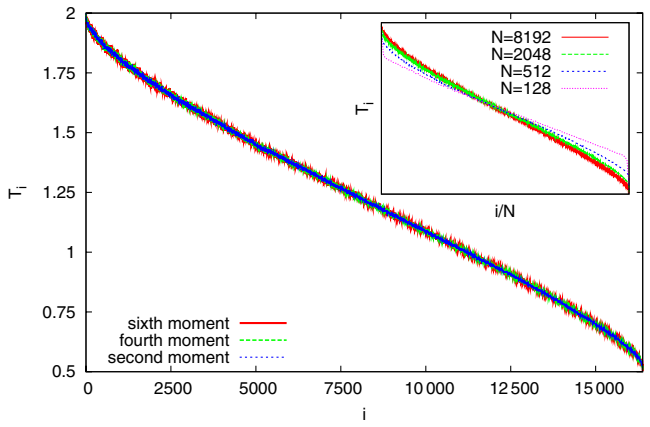

FIG. 2 (color online). Kinetic temperature profile for a FPU-β chain with $N = 16\,384$, $T_L = 2.0$, $T_R = 0.5$, and $\gamma = 2.0$. The first three even moments of the velocity are shown; their agreement indicates a Gaussian velocity distribution. (Inset) Normalized temperature profiles for different N.

properties. Equivalently, $j = -\kappa(\Delta T/N)$, where we have defined ∇T as $\Delta T/N$. By measuring $j(N)$, deviations from $j \sim 1/N$ are interpreted as a N-dependent conductivity $\kappa(N)$ and a consequent breakdown of Fourier's law.

For one-dimensional momentum conserving systems where a well-behaved LT exists, a RG study of the hydrodynamic equations of a normal fluid [9] showed that Eq. (1) is satisfied with $\alpha = 1/3$. This has been confirmed by simulations of hard particle gases [16–18], although very large systems are required [19] and the issue is not completely settled [20]. On the other hand, numerical simulations of oscillator chains, including FPU chains, give various exponents [6,10–13] for different systems, often slightly higher than $1/3$. This seems consistent with early results from mode-coupling theory (MCT), which predict a heat conductivity exponent of $\alpha = 2/5$ [10–12], although recent MCT analyses predict exponents that depend on the leading nonlinearity [13,21] and the extent of transverse motion [12]. The apparent agreement between the numerical and MCT results has led to speculation that there may be two (or more) universality classes with different exponents [12,13]. The most recent MCT analysis [13,21] predicts that $\alpha \neq 1/3$ is restricted to even potentials $V(z)$, which is why we have studied the FPU-β model here.

Recently, two of us have extended the earlier RG treatment to systems with broken symmetry [22], which can occur on intermediate length scales in one dimension (as in nanotubes). The resulting crystalline hydrodynamic equations also yielded $\alpha = 1/3$, like the earlier fluid result [23]. From numerical results, it was argued that the apparent $\alpha > 1/3$ found for FPU chains is probably a crossover effect from hard particle systems. However, the possibility that the crossover could be pushed out to $N \to \infty$ could not be ruled out. Thus the numerical and analytical evidence so far allow for FPU chains to be a singular limit for the RG with a special value of the conductivity exponent α, motivating our numerical simulations.

The heat current flowing in steady state is measured as a function of N for equal mass FPU chains. The time averaged current j is defined by $j = -[\sum_i \dot{x}_i V'(x_{i+1} - x_i)/N]$, where x_i is the displacement from equilibrium of the ith particle. As shown in Fig. 3, $\kappa(N) = -jN/\Delta T$ satisfies Eq. (1) for large N with $\alpha = 0.333 \pm 0.004$, in strong agreement with the RG prediction.

To test the sensitivity of this result to different baths, we run simulations with Langevin baths with different damping constants $\gamma = 0.4$, 2, and 10. We also replace the stochastic Langevin baths with deterministic Nose-Hoover [15] thermostats, for which we use the fourth order Runge-Kutta integrator. Figure 3 compares the RG prediction and the MCT prediction for systems with these different baths and bath parameters. As can be seen in the figure, an asymptotic exponent of $1/3$ is attained for *all* these systems, whereas the apparent exponents for smaller N depend on system parameters. Moreover, it is possible to understand the deviation of the apparent exponent from

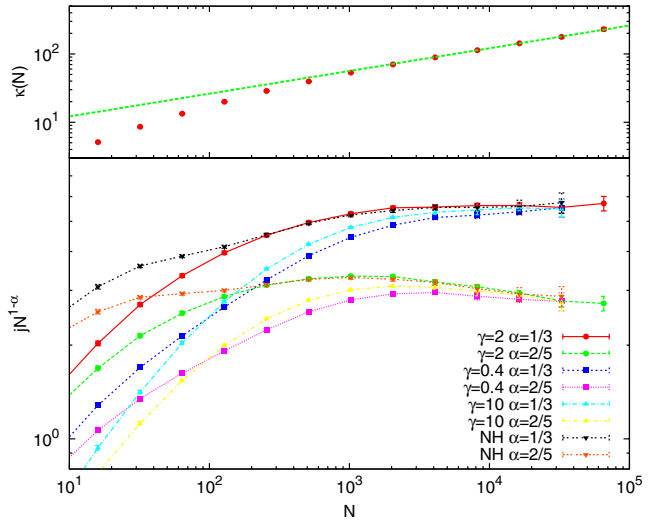

FIG. 3 (color online). Heat current as a function of N. Root mean square errors from $O(10^5 - 10^6)$ measurements are shown except when they are smaller than the points. (Top) Conductivity versus N. The last five points fit to a slope of $\alpha = 0.333 \pm 0.004$. The baths are described in Fig. 2. (Bottom) $jN^{1-\alpha}$ versus N for $\alpha = 1/3$ and $\alpha = 2/5$. In the large N regime, α is definitely less than $2/5$ and appears to agree quite well with the $1/3$ prediction for all data sets. Langevin baths with $\gamma = 0.4$, 2, and 10, and one data set with Nose-Hoover baths, are shown.

$1/3$ for small system sizes. As shown in Ref. [6], if the damping constant for the Langevin baths is very large or small, there is a large "contact resistance" at the boundaries of the chain. The current only depends weakly on N, resulting in an apparent $\alpha > 1/3$. (Similar considerations apply to Nose-Hoover baths [24].) This is confirmed by our results: the plot for $\gamma = 2$ reaches the asymptotic limit fastest, whereas $\gamma = 0.4$, 10 have apparent exponents closer to 0.4 for small N. Taken together, the large-N exponent of $1/3$, the universality with respect to bath parameters, and the explanation for how the apparent exponent behaves as a function of N and γ for small N convincingly supports the RG prediction.

Since Fourier's law is only applicable in the linear response regime, we halve the temperature difference between the ends and simulate the same spring system with Langevin baths with $\gamma = 2$, $T_L = 1.625$, and $T_R = 0.875$. Though the error bars are larger, α still agrees with $1/3$, verifying that the system is in the linear response regime.

The exponent α measured in our simulations of FPU chains clearly differs from the measurements from other simulations [10–13]. This disagreement is mainly because very large system sizes are needed. Moreover, we use a step size $h = 0.0025$–0.005 that is an order of magnitude smaller than the step size used for the dynamics in [11]; by comparing numerical and exact results for harmonic springs, we have found that a small h is necessary for proper convergence. Finally, we have shown the results as a function of the coupling to the bath, which has not been done before, and explained why the baths increase the

apparent α, especially if the coupling is not optimal. We note that only equilibrium correlations for a periodic FPU-β chain are shown in Ref. [13]. As discussed in the second paper in Ref. [18], this is problematic.

However, in Ref. [11], where purely quartic springs ($k_2 = 0$) and system sizes similar to our simulations were used, $\alpha \sim 0.44$ was extrapolated from an indirect measurement and $\alpha \gtrsim 0.4$ was measured directly from nonequilibrium simulations. We have found $\alpha = 0.38$–0.39 for this system. Because the analytical results all obtain the same asymptotic α for the FPU-β and quartic models, and we have shown that the apparent α decreases with N for the FPU-β model, we believe that α for the quartic system will also asymptotically change to $1/3$. The alternative, that α for the FPU-β chain will reverse its change with N and revert to ≈ 0.4, seems unlikely. Indeed, the latest MCT results [21] obtain $\alpha = 0.5$ for even potentials (including the quartic model and the FPU-β model) which is quite far from earlier work [13] and our numerical results. Nevertheless, it is unclear why the pure quartic system should need exceptionally large N. A final resolution of the issue requires an analytical demonstration of an error in one of the competing methods.

The existence of a paradoxical LT on small scales for slight alterations to the equal mass FPU chain could be partly responsible for the unusually large N needed to reach the asymptotic limit (most notably for purely quartic potentials). Conversely, slight changes can improve the convergence to $\alpha = 1/3$ as seen by adding a cubic term [13,21], transverse motion [12], or collisions [11,22]. Recent simulations of nanotubes obtain $\alpha = 1/3$ [25].

In summary, we have shown that the local temperature behaves paradoxically when an $O(1/N)$ temperature gradient is applied to FPU chains with unequal masses; coarse graining with any $O(1)$ averaging length does not cure this. This renders existing analytical models for heat conductivity inapplicable. However, a well-behaved LT is established for equal mass chains, or when the baths are at the same temperature [7]. For equal mass chains, large scale simulations support the much debated heat conductivity exponent being $1/3$ as predicted [9].

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