Universality of One-Dimensional Heat Conductivity

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We show analytically that the heat conductivity of oscillator chains diverges with system size $N$ as $N^{1/3}$, which is the same as for one-dimensional fluids. For long cylinders, we use the hydrodynamic equations for a crystal in one dimension. This is appropriate for stiff systems such as nanotubes, where the eventual crossover to a fluid only sets in at unrealistically large $N$. Despite the extra equation compared to a fluid, the scaling of the heat conductivity is unchanged. For strictly one-dimensional chains, we show that the dynamic equations are those of a fluid at all length scales even if the static order extends to very large $N$. The discrepancy between our results and numerical simulations on Fermi-Pasta-Ulam chains is discussed.

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I. INTRODUCTION

When a small temperature gradient is applied across a system, the heat current that flows through it is expected to follow Fourier’s law, $j = -\kappa \nabla T$. However, for one-dimensional systems there are numerous examples of systems where numerical simulations or exact analytical results have shown that Fourier’s law breaks down. The thermal conductivity $\kappa$ is observed to be anomalous, i.e., dependent on the system size and divergent in the thermodynamic limit. Despite the existence of an analytical renormalization group (RG) prediction for the behavior of $\kappa$, there is still considerable controversy about whether the theory applies to chains of stiff oscillators, where the particles form a lattice to an excellent approximation. Since this is the appropriate description for nanotubes, this class of systems is of great topical interest. An understanding of $\kappa$ also has broader implications, since other transport coefficients can also be anomalous in low dimensional systems.

Numerical and analytical studies show $\kappa \propto N^\alpha$ for various one-dimensional systems, where $N$ is the size of the system and $\alpha > 0$. A renormalization group (RG) analysis has shown that for one-dimensional non-integrable systems with momentum conservation, $\alpha$ has the universal value of $1/3$, and that without momentum conservation the conductivity is normal (i.e., $\alpha = 0$). This result was derived using the hydrodynamic equations of a normal fluid. Simulations on one-dimensional hard particle gases have yielded a wide range of values for $\alpha$ even for small $N$. This is because very large system sizes are needed before the large $N$ behavior is reached, presumably because of the limited phase space accessed in one-dimensional elastic collisions. This problem has been circumvented by using a random collision (RC) model, where convergence to the asymptotic regime is seen for small $N$. Recent simulations measuring energy diffusion in hard particle systems have confirmed that $\alpha = 1/3$.

In marked contrast to these results, chains of nonlinear oscillators such as Fermi-Pasta-Ulam (FPU) chains and their variants consistently show numerical results that disagree with the RG prediction. Varying parameters within a given model gives different values for $\alpha$, but they generally lie between 0.37 and 0.44 with occasional exceptions. This is contrary to the RG prediction, but is compatible with the result from a mode-coupling analysis that yields $\alpha = 2/5$. These numerical results have led to suggestions that there are (at least) two universality classes for heat conduction in one-dimensional momentum conserving systems, and that the “fluid-like” RG analysis is not appropriate for oscillator chains, which are better described as a crystal with small fluctuations in particle positions.

Although any one-dimensional system will eventually renormalize to fluid like behavior at sufficiently long length scales, for stiff oscillator chains the crystalline order persists to very large $N$. Since the hydrodynamic equations for a crystal are different from those for a fluid, the large $N$ behavior for such chains could be different from the fluid prediction.

In this paper, we show that this is not the case: $\alpha$ should be $1/3$ even for stiff oscillator chains. In this light, the numerical results on FPU chains are probably due to the well-known difficulties with equilibrating them, necessitating extremely large $N$ before the asymptotic behavior is seen.

In Section II, we first argue that the earlier RG analysis applies to chains as well as gases. This result is surprising in view of the fact that the standard hydrodynamic description of crystals introduces extra degrees of freedom for broken symmetries, and is peculiar to one-dimensional chains with single-well interparticle interaction potentials. We then derive the hydrodynamic equations for chains with multiple-well interaction potentials and for quasi one-dimensional systems such as tubes. There are four equations instead of three for a fluid, because of the extra degree of freedom corresponding to the broken symmetry. We show that these modified hydrodynamic equations also yield $\alpha = 1/3$. In Section III, we elucidate the discrepancy between numerical results on FPU chains and the analytical predic-
tion by performing simulations on FPU chains with collisions, which interpolate continuously between the RC model and pure (collisionless) FPU chains. As we tune parameters to move towards pure FPU chains, a new intermediate length scale regime emerges and increases in range, while leaving the large $N$ scaling of $\kappa$ unchanged. This corroborates the analytical prediction that $\alpha = 1/3$ asymptotically, but shows that this will be seen at unusually large $N$ for pure FPU chains. Finally, in Section IV, we discuss the applicability of these predictions to physical systems.

II. 1-D HYDRODYNAMICS

The RG analysis discussed earlier \cite{17} uses the hydrodynamic equations for a one-dimensional fluid \cite{22, 25},

\[ \partial_t \rho + \partial_x g = 0, \]
\[ \partial_t g + \partial_x (gv) = -\partial_x p + \eta \partial_x^2 v, \]
\[ \partial_t \epsilon + \partial_x [(\epsilon + p)v] = \kappa \partial_x^2 T + \eta [(\partial_x v)^2 + v \partial_x^2 v] \]

(1)

where $\rho$, $g$ and $\epsilon$ are the local mass, momentum and energy densities respectively. The thermodynamic fields, temperature, pressure, and velocity are represented by $T$, $p$, and $v$ respectively. There are two transport coefficients, the viscosity $\eta$ and the thermal conductivity $\kappa$.

The RG analysis adds noise terms to the second and third of Eqs. (1) (the first is an exact identity and therefore has no noise term). Using the Green-Kubo relations \cite{26, 27}, the critical exponents are derived from the equilibrium fluctuations of a system at constant temperature. This can be done without approximations by invoking Galilean invariance and the condition that equal time correlations must obey equilibrium statistical mechanics.

For a crystal, broken symmetries introduce additional long-lived hydrodynamic modes \cite{22, 24, 25}. For a $d$ dimensional crystal, the extra $d$ broken symmetry degrees of freedom are associated with \cite{24} the $d - 1$ transverse sound modes, which become propagating instead of diffusing, and an extra vacancy diffusion mode \cite{24}. This vacancy diffusion mode is the only one that survives for $d = 1$. The number of hydrodynamic equations is increased from three to four. We are thus led to enquire whether the results of Ref. \cite{17} are altered for a stiff chain, which can be viewed as a one-dimensional crystal.

Before doing this, we show that for one-dimensional monoatomic systems, if the interparticle interaction has only one minimum, vacancies do not exist. The fluid description of Ref. \cite{17} is therefore valid even if the interactions are sufficiently stiff that the particles are almost on a perfect lattice. This is true for FPU chains.

This result can be shown on physical grounds: if we remove a single particle from an otherwise perfect $d$ dimensional crystal, there is a slight distortion in its vicinity, but a vacancy remains. This vacancy only moves when a neighboring particle hops into the empty site, resulting in very slow diffusive motion of vacancies (and interstitials) through the system. In contrast, if a particle is removed from a FPU-like one-dimensional chain, its neighbors move immediately, on microscopic — i.e. non-hydrodynamic — time scales to close the gap. Although the reduction in mass density caused by removing the particle is not eliminated, but only smeared out, this is what one would expect, since mass density is conserved in Eqs. (1). The extra degree of freedom introduced in the standard hydrodynamic treatment of crystals \cite{22, 24, 25, 26}, distortions of the broken symmetry, is thus indistinguishable from density fluctuations, and the fluid description of Eqs. (1) remains valid.

There are two ways in which the argument of the previous paragraph can break down. First, if the interparticle potential has multiple minima, it is possible to create a situation where the separation between adjacent particles is $x_{i+1} - x_i = a + \delta_{i,n} b$ for some $n$, and the force on all the particles is zero. Here $a$ is the lattice constant and $b$ is the separation between minima of the interparticle potential, in the simplest case equal to $a$. The resulting vacancy at site $n$ will diffuse slowly through the system and is therefore a hydrodynamic mode, distinct from lattice distortions and momentum which combine to produce longitudinal sound. Second, if the system is only quasi one-dimensional, for example a cylinder, vacancies can be introduced as for $d > 1$. Neither of these exceptions applies to FPU chains.

The second exception is, however, applicable to nanotubes. In view of their importance, we derive the hydrodynamic equations for a one-dimensional crystal, modifying Eqs. (1), and show that the heat conductivity exponent $\alpha$ is still not changed. This is because the assumptions that allowed $\alpha$ to be calculated exactly for a fluid are still valid for the crystal. (Nanotubes have additional transverse and torsional degrees of freedom, but we will argue later that these do not affect $\alpha$ either.)

A hydrodynamic theory is formed from the continuity equation of the conserved quantities and the time derivative of all the broken symmetries. In the case of the 1-d crystal, the equations are

\[ \partial_t \rho + \partial_x g = 0, \]
\[ \partial_t g + \partial_x \pi = 0, \]
\[ \partial_t \epsilon + \partial_x j^\epsilon = 0, \]
\[ \partial_t u = v + j^u, \]

(2)

where $u$ is the displacement and the currents, $\pi$, $j^\epsilon$, and $j^u$, are still to be determined. Galilean invariance demands the inclusion of the $v$ in the last equation.

Following the methods from \cite{27} and \cite{28}, constitutive equations can be derived from entropy arguments. The first law of thermodynamics for this system can be rewritten in terms of densities,

\[ T ds = d\epsilon - \mu d\rho - vd\eta - h d(\partial_x u), \]

(3)

where $s$ is the entropy density and $\mu$ is the chemical potential per unit mass. A uniform translation cannot alter
the energy, therefore energy can only depend on gradients of \( u \). The conjugate field to \( \partial_x u \) is \( h = \partial E/\partial (\partial_x u) \) at constant \( s, \rho, \) and \( g \). The displacement variable also changes the pressure to

\[
p = -\epsilon + Ts + \mu \rho + vg + h \partial_x u.
\]  

Using these two relations and the continuity equations, we can derive an entropy “continuity” equation with source terms,

\[
T[\partial_t s + \partial_x (vs + Q)] = -\frac{Q}{T} \partial_x T - (g - \rho v) \partial_x \mu + (j^u + \nu \partial_x u) \partial_x h - (\pi + h - p - gv) \partial_x v,
\]

\[Q = j^\pi - \mu (g - \rho v) - \pi v + h j^u - \epsilon v + gv^2 + h v \partial_x u.\]  

By integrating both sides of Eq. (5) over a large volume where the entropy “current” \( vs + Q/T \) is negligible at the surface, we have an expression for the time derivative of the total entropy,

\[
T \frac{dS}{dt} = \int dx [-\frac{Q}{T} \partial_x T + (\rho v - g) \partial_x \mu + (j^u + \nu \partial_x u) \partial_x h - (\pi + h - p - gv) \partial_x v].
\]

The constitutive equations for the currents can now be derived by using the condition of entropy creation, \( dS/dt \geq 0 \) \[22\]. The equality holds only when there is no dissipation. Without dissipation, each term of Eq. (7) must independently be zero, giving the reactive terms of the currents:

\[
g = \rho v,
\]

\[j^g_R = -\nu \partial_x u,
\]

\[\pi_R = p - h + gv,
\]

\[Q_R = 0,
\]

\[j^\pi_R = (\epsilon + p - h)v.
\]

The \(-\nu \partial_x u\) term in the displacement current does not appear in the derivation of crystal hydrodynamics from \[22\] but appears to us to be correct. With dissipation, entropy is produced and the currents have dissipative components:

\[j^g_D = \Gamma \partial_x h - \lambda \partial_x T,
\]

\[\pi_D = -\eta \partial_x v,
\]

\[Q_D = -\kappa \partial_x T - \lambda T \partial_x h,
\]

\[j^\pi_D = -(\kappa - \lambda h) \partial_x T - (\lambda T + \Gamma h) \partial_x h - \eta v \partial_x v.
\]

The transport coefficients \( \kappa, \eta, \lambda, \) and \( \Gamma \) are all positive. In general, there are higher order terms in the gradient expansion, but we will only retain these order terms (which is valid for small gradients). The mass current \( g \), does not have a dissipative term because it is a conserved density itself.

The displacement field introduces two new transport coefficients: one associated to the relaxation of its conjugate field \( h \) and the second due to the possibility of cross coupling between the heat current and the displacement field (and the displacement current and temperature field). This cross coupling is possible because the field and the current have opposite signs under time-reversal, a necessary condition for dissipative currents \[22\]. For this reason, there are no cross couplings with \( \pi \). Using these expressions for the currents in the continuity equations closes our set of equations,

\[
\partial_t \rho + \partial_x g = 0,
\]

\[\partial_t g + \partial_x (gv) = -\partial_x p + \partial_x h + \eta \partial_x^2 v + \zeta_g,
\]

\[\partial_t \epsilon + \partial_x [(\epsilon + p - h)v] = \kappa \partial_x^2 T + \eta [(\partial_x v)^2 + \nu \partial_x^2 v] + \Gamma [(\partial_x h)^2 + h \partial_x^2 h] + \lambda [T \partial_x^2 h - h \partial_x^2 T] + \zeta_e,
\]

\[\partial_t u + (\partial_x u - 1)v = \Gamma \partial_x h - \lambda \partial_x T + \zeta_u.
\]

Eqs. (10) are the full nonlinear hydrodynamic equations of the 1-d crystal. Noise, represented by the \( \zeta \)'s, is introduced to the last three equations for the RG analysis.

The hydrodynamic modes and their dispersion relations can be solved for the linearized theory. The three variable normal fluid has three modes, a heat diffusion mode and two propagating sound modes \[22\]. The additional displacement variable now introduces another diffusive mode representing vacancy diffusion. A vacancy diffusion mode is seen in the longitudinal hydrodynamics of the three dimensional crystal as well \[23\]. In these linearized theories, quantities such as the susceptibilities and correlations can be calculated and Green-Kubo relations can be derived \[22\]. Although the details of such calculations are different with four hydrodynamic modes instead of three, Eqs. (10) are clearly still Galilean invariant, and — when no temperature gradient is imposed externally — have equal time fluctuations that are drawn from the canonical ensemble. As in Ref. \[17\], the various critical exponents are therefore determined and, in particular, \( \alpha = 1/3 \).

In summary, for one-dimensional momentum-conserving crystals (that reach local thermal equilibrium), Eqs. (10) describe the hydrodynamics when vacancies are not possible, as is the case for FPU chains. When vacancies are possible, Eqs. (10) apply, but the symmetry arguments that determine \( \alpha = 1/3 \) for Eqs. (10) are still valid. In the next section, we numerically show the possible source of the discrepancy between prior numerical results on FPU-like lattices \[4\], \[10\], \[11\] and \[12\] and this exact result.

III. NON-EQUILIBRIUM SIMULATIONS

Results of past numerical simulations \[4\], \[10\], \[11\], \[12\], \[13\] consistently measure an exponent larger than 1/3 for FPU-like chains. Due to the exact derivation of the analytical prediction, the good agreement between this prediction and gas simulations \[4\], \[5\], \[6\] and the well-known problems of convergence in one-dimensional systems \[22\], we conjecture that the FPU simulations have not reached the asymptotic large \( N \) regime. Going to
larger and larger system sizes to confirm this would be prohibitive. Instead, we use a tunable model which smoothly interpolates between the RC gas and the FPU chain, where this is easier to see.

We introduce FPU-like springs to the random collision model. As the springs become stiffer, the system continuously evolves from the pure RC gas with $\alpha = 1/3$ to the collisionless FPU chain: from a fluid to a “crystal”. As the spring constants are increased, we observe that an intermediate length scale regime emerges, whereas the large $N$ scaling of $\kappa$ remains $\sim N^{1/3}$.

For the simulations, we numerically integrate a system of $N$ particles with nearest neighbor interactions. The interaction potential between every pair of particles is of the generalized FPU form

$$V(z) = \frac{k_2}{2} z^2 + \frac{k_3}{3} z^3 + \frac{k_4}{4} z^4 + \ldots,$$  \hspace{1cm} (11)

where $z = x_{i+1} - x_i$ is the compression (or elongation) of the spring and $x_i$ is the deviation from the equilibrium position of the $i^{th}$ particle. Collisions can be neglected in the limit when the lattice constant $a$ is large, but for finite $a$ and finite temperature, the probability of two particles colliding is nonzero. When two particles come into contact, $z = -a$, they undergo a random collision as in Ref. \cite{20}.

For the simulations, we only use terms up to fourth order in Eq. (11). In their original work, Fermi, Pasta, and Ulam \cite{20} noticed that the odd frequency normal modes do not mix with the even frequency normal modes when the interparticle potential is even. To avoid this problem and any others that may arise from this accidental symmetry of an FPU-\beta chain, we use a finite $k_3$ in all of our chain simulations.

Heat baths are connected to the end particles to maintain a temperature gradient across the system. The scaling of the conductivity is determined by measuring the size dependence of the current maintaining a (small) temperature difference between the baths. For our numerics, the leftmost ($i = 1$) and rightmost ($i = N$) particles are connected to Nose-Hoover heat baths \cite{30} \cite{31}. The auxiliary degree of freedom introduced in the RC model, the transverse momentum, does not couple to the baths or enter the dynamics except in collisions, and so is not seen in the pure FPU (collisionless) limit.

We adopt a convention in which the energy contained in each spring is symmetrically shared by the two particles attached to it. The first and last springs are only in each spring is symmetrically shared by the two particles attached to it. Thus the total current flowing through the system is

$$jN = \sum_{i=1}^{N} e_i v_i - \frac{1}{2} \sum_{i=1}^{N} (x_{i+1} - x_i) (v_{i+1} + v_i) V'(x_{i+1} - x_i).$$  \hspace{1cm} (12)

It is possible to show that the time average $\langle jN \rangle$ is equal to $-(a/2) \sum_i (v_{i+1} + v_i) V'(x_{i+1} - x_i)$. However, with collisions it is more useful to keep Eq. (12) in its entirety, since $x_{i+1} - x_i + a = 0$ at collisions, where $V'$ is singular. In fact, for hard sphere particles, $jN = \sum_{i=1}^{N} e_i v_i$.

Numerical integration of this system is complicated by the combination of collisions and springs. Without springs, the particles travel freely and a fast event driven simulation can be implemented \cite{4}. For a collisionless system, the equations of motion can simply be integrated numerically by standard algorithms. For our simulations, the fourth order Runge-Kutta algorithm is used. Because of the occurrence of collisions, our algorithm checks for collisions after every trial timestep. If a collision is seen to have occurred, the trial step is discarded, and the integrator evolves the system by a smaller stepsize to the (extrapolated) point at which the two particles collide. Because of the need for trial steps, integrating systems with collisions and springs requires substantial amounts of computational time.

We use a stepsize of $dt = 0.01$ for all simulations and check that the results do not change for smaller stepizes. We allow the system to equilibrate for $\sim 10^8$ steps before measurements are taken. Each measurement consists of the particle and time averaged current, where a block of $10^8$ timesteps is used for the time average and $10^5$ steps separate each block. Each data point in figure 4 is the mean of many such measurements and the error bars shown are the root mean square errors of the block measurements.

The parameters in the model are the masses of the particles $m_i$, the lattice constant $a$, the temperatures of the baths $T_L$ and $T_R$, and the spring constants $k_i$ in Eq. (11). Alternating masses are used due to the fast convergence seen in the pure RC model for such systems \cite{5}. In particular, we use a mass ratio of 2.62 and $m_i = 1$ for all odd $i$. The bath temperatures are 1.2 and 1.0 for the left and right baths, respectively. For these temperatures, we have checked that the system is in the linear response regime. With the temperatures of the baths and the masses of the particles fixed at these values, the collision rate can be altered by changing the lattice constant and/or spring constants. We have chosen to fix the lattice constant to $a = 1/2$.

Figure 4 shows the kinetic temperature profile after steady state is reached for systems of size $N = 256$, showing increasing curvature as collisions decrease. For the pure FPU system, the masses of all the particles are chosen to be the same. This is because with alternating masses, the kinetic temperature for particles in the pure FPU chain also shows an odd-even oscillation, indicating that equilibrating the system with Nose-Hoover baths is problematic. All other systems simulated have alternat-
is reached for relatively small systems ($N \geq 128$). As the springs are turned on, an intermediate length scale regime emerges and the asymptotic large $N$ regime moves out, but the slope in the large $N$ regime is still $1/3$. For the strongest springs shown in Figure 2, the asymptotic regime has moved out of the range simulated. Figure 2 also shows the results for a pure FPU chain, which agrees with earlier results [10, 11, 12, 13]. The slope of $> 0.4$ for this system is comparable to the strong spring system with collisions, supporting the assertion that this is an intermediate length scale phenomenon. As discussed in the previous paragraph, the masses of all the particles in the pure FPU chain are chosen to be equal. This is the cause for the different behavior for very small $N$, where the slope increases with $N$ instead of decreasing.

IV. DISCUSSION

In the light of the experience with hard particle gases and the random collision model, it is natural to expect that introducing extra degrees of freedom would cause FPU chains to show their large $N$ behavior more rapidly. In this context, Wang and Li [14] have shown that when one transverse degree of freedom is added to the FPU chain, the conductivity exponent is numerically seen to be $1/3$. It would be interesting to see whether other extensions of the FPU model can achieve the same result. More ambitiously, it would be very useful if a criterion could be obtained that would easily determine numerically whether a system reaches local thermal equilibrium, allowing one to decide whether the hydrodynamic theory is applicable.

The study of low dimensional transport is not merely of theoretical interest; the vast potential applications of real quasi one-dimensional systems, namely nanotubes, demand an understanding of their physical properties. Specifically, research and production of electronic devices at the micrometer and nanometer scale have shown that carbon nanotubes may be used in very efficient cooling systems [32]. Experimentally, the thermal conductivity of nanotubes has been found to be extremely high [33] which makes nanotubes obvious candidates for cooling devices in microelectronics. This potential for applications motivates a theoretical investigation of the heat transport properties of low dimensional systems. Experimental [33, 34] and numerical [35, 36] studies of nanotubes have shown that the phonon contribution to heat transport is much larger than the electronic contribution, so that the fact that we have only considered lattice motion in this paper is not a problem.

The two dimensional nature of the tube allows for the existence of vacancies. The tubular shape also introduces other transverse hydrodynamic modes (a broken symmetry and conserved momentum for torsional and the two transverse motions), but as mentioned earlier, these modes do not affect the symmetry arguments, and the heat conductivity exponent is expected to still
be $1/3$. The longitudinal hydrodynamics for this quasi one-dimensional system is the four component theory, Eqs. (10).

There are a few concerns in applying the prediction of $\alpha = 1/3$. First, on short length scales, the phonon motion is ballistic. The phonon mean free path in carbon nanotubes is $\sim 1\mu m$ [31], and our discussion in this paper would apply to systems that are larger than this scale. Recent thermal conductivity measurements have only been made on systems with lengths in this order of magnitude [34]. The unusually high conductivity in such systems is correctly attributed to the ballistic transport nature at these scales [31]. There have yet to be extensive experiments on the length dependence of $\kappa$ to our knowledge. To test our prediction and measure the actual heat conductivity exponent, length dependent experiments of long ($> 1\mu m$) nanotubes must be done. Second, even beyond this length scale it is possible (based on what we have seen for FPU chains) that equilibration is imperfect. However, this is less likely to be a problem with the extra transverse modes [14] which are present in a nanotube, and in any case would only change $\alpha$ slightly. Third, under renormalization, the system flows to its fixed point only for large $N$. It is not clear what limitation this imposes, but the nonlinearity in the hydrodynamic equations that causes anomalous scaling behavior is the advective term, whose strength is unity and whose effect should therefore be seen even for small system sizes [38, 39].

In this paper, we have shown analytically that one-dimensional chains of particles connected with nonlinear springs have a heat conductivity that diverges as a function of the chain length $N$ as $\sim N^{1/3}$, which is the same as the earlier result for hard sphere particles and other fluid systems. For quasi one-dimensional systems, this result is obtained from the crystalline hydrodynamic equations. It does not rely on the eventual crossover from a crystal to a fluid which must happen for any one-dimensional system. For Fermi-Pasta-Ulam chains and other examples where the interparticle potential has a single minimum, we have obtained the stronger result that the fluid hydrodynamic theory [17] is applicable on all length scales for the dynamics, even when there is excellent static ordering. In the light of these analytical results, the numerical results on FPU chains that show a heat conductivity exponent of $\sim 0.4$ is probably due to imperfect equilibration.

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[38] The dimensionless coupling constant in a renormalization group calculation is not unity, but at high temperatures this should not create problems. We thank Sriram Ramaswamy for bringing this to our attention.
[39] Advection takes place in a stiff system even though the particles do not move far from their lattice positions. The collective motion of the particles in a large region can transport energy forward, transmitting the energy to neighboring regions through interactions, just as in a fluid.