Violations of local equilibrium and stochastic thermostats

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We quantitatively investigate the violations of local equilibrium in the $\phi^4$ theory under thermal gradients, using stochastic thermostats. We find that the deviations from local equilibrium can be quite well described by a behavior $\sim (\nabla T)^2$. The dependence of the quantities on the thermostat type is analyzed and its physical implications are discussed.

The physics of non-equilibrium is ubiquitous and is an essential ingredient in a wide spectrum of issues in physics, from the early universe, transport in solid state physics to heavy ion collisions. Because of this importance, the field has been studied for a long time, yet some basic problems remain. A deep and interesting issue is what the microscopic properties of the systems in non-equilibrium are. In particular, a crucial question is whether local equilibrium is broken when global equilibrium is broken, and if it is, how the breaking occurs. Non-equilibrium situations occur in various situations and there is no general theory on how systems should behave away from equilibrium. In steady state systems, the validity of local equilibrium has been addressed from various approaches, though few have studied the deviations from it quantitatively. The violations of local equilibrium were studied quantitatively in the FPU (Fermi–Pasta–Ulam) model and the $\phi^4$ theory under thermal gradients through the behavior of momentum cumulants, making use of numerical simulations. There, the violations of local equilibrium were seen and their dependence on the non-equilibrium nature of the system could be well described by $(\nabla T)^2$, where $T$ is the local temperature. Furthermore, it was found that the linear response theory also breaks down by about the same amount, relatively. These non-equilibrium states were numerically constructed using deterministic thermostats in a standard manner. However, it has not yet been established whether these deviations also occur if completely different type of thermostats are used, such as stochastic ones. Since the non-equilibrium situation itself is created by the action of the thermostats, whether the non-equilibrium effects are artifacts of using a particular type of thermostat needs to be clarified.

The possible dependence of physics properties on thermostats is not a purely theoretical concept; the physical quantities can depend on the thermostats in a non-trivial way, in real physical systems. A thermostat thermalizes the degrees of freedom attached to it at a prescribed temperature. However, what happens away from the thermostatted regions is not unique and is a dynamical property of the system. For instance, it has been known for some time that the internal gradient (be it shear or heat flow), depends on the boundary conditions in a non-trivial way through the boundary jumps or slips. For thermostats, these slips depend not only on the temperature but also on the type of thermostat used, which is quite understandable if one considers real systems. The issue involves a deeper question — which physical quantities are universal or intrinsic to the system, independently of the boundary conditions. In particular, for systems with bulk behavior, physical quantities that are universal in this sense should be independent of the size of the system and the thermostat used. The boundary conditions determine the flow and gradients inside the system, away from the boundaries, but whether their influence on physical quantities is solely through these quantities is unclear. Determining which quantities are universal in the sense that they are independent of the thermostats and the boundary conditions is crucial if one wants to develop general theories regarding the behavior of systems in non-equilibrium, such as in the approach of so-called non-equilibrium thermodynamics.

In this work, we quantitatively investigate the steady state non-equilibrium behavior of the $\phi^4$ theory in one spatial dimension using stochastic thermostats. (For a review of one dimensional systems see, for instance, [10].) We find that the behavior is similar to that of systems using deterministic thermostats, but differs in a subtle way. The Hamiltonian of the massless $\phi^4$ theory in one dimension, which we study, is

$$H = \sum_{j=1}^{L} \left[ \frac{\pi_j^2}{2} + \frac{(\nabla \phi_j)^2}{2} + \frac{\phi_j^4}{4} \right]$$

(1)

with $L$ being the size of the system and the discrete spatial gradient defined as $\nabla \phi_j \equiv \phi_{j+1} - \phi_j$. $\phi^4$ theory is a typical model in which bulk behavior can be seen in the $(1 + 1)$ dimensional model. The model is a prototypical one in field theory so that it allows us to understand the problem in a broader context and it is applicable to various problems.

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in solid state and particle physics. We adopt the so called “ideal gas temperature”, \( \langle \pi_j^2 \rangle = T_j \) as the definition of temperature. This widely used definition is convenient for systems we study, since it is simple and local. We note that it is quite sensible to consider local quantities in the system as we are considering physical quantities averaged over a large number of ensembles.

In this study, we analyze the \( \phi^4 \) theory under thermal gradients, where thermostats are applied to one site each at both ends of the system, with their temperatures \( T_{1,2}^0 \). Inside the system, the equations of motion are solely those derived from the Hamiltonian \( \mathcal{H} \). We integrate the equations of motion numerically computing the values of relevant observables at every step and averaging them over time at the end in the standard manner. We used time steps of \( 0.005 \sim 0.05 \) over \( 10^9 \sim 10^{10} \) steps and have checked that the results do not depend on the time step size.

We apply the stochastic thermostats following the ideas in [11]. Concretely, at every \( t_{kick} \) time interval, we replace the momenta at the boundaries, \( \pi_1, \pi_L \), with values selected randomly from the Maxwell distribution for the thermostat temperatures, \( T_{1,2}^0 \). Physically, these thermostats can be thought of as particles at the boundaries of the chain striking the walls at given temperatures, though the situation is more general since \( \phi_j \) needs not have any relation to a spatial direction. For instance, in the lattice \( \phi^4 \) field theory, \( \phi_j \) is an internal degree of freedom, not a spatial one. \( t_{kick} \) affects how well the thermostats work and has to be controlled so that thermalization is achieved at the boundaries. Given the boundary temperatures, one still needs to specify the type of thermostat to apply and this is not just a theoretical choice; given the boundary temperatures, the choice of the type of thermostat used affect the physical quantities in real systems also. If the system displays bulk behavior, quantities such as thermal conductivity should have no thermostat dependence.

![Figure 1](image-url)

**FIG. 1:** Temperature profile (top) and \( \langle \langle \pi_j^4 \rangle \rangle/T^2 \) cumulant profile (bottom) for boundary temperatures \( (T_{1,2}^0) = (0.5, 1.5) \). Thermostats used were stochastic with \( t_{kick} = 0.5 \) (solid), \( t_{kick} = 1 \) (dashes) and deterministic (small dashes).

In Fig. 1, we show some spatial profiles of the temperature and \( \pi^4 \) cumulants, \( \langle \langle \pi_j^4 \rangle \rangle = \langle \pi_j^4 \rangle - 3(\langle \pi_j^2 \rangle)^2 \), with the boundary temperatures controlled by the stochastic thermostats. The profiles include temperature jumps at the boundaries and thermal profiles inside which can be curved. These features are quite generic. Given a Maxwellian
distribution, all the cumulants vanish, except for $\langle \langle \pi^2 \rangle \rangle$. When the distribution is not Maxwellian, there is no unique definition of $T$ and in this sense, local equilibrium does not hold. The cumulant profiles show that the boundaries are indeed thermalized but local equilibrium is broken inside the system. The behavior of the cumulants are quite different but the corresponding temperature profiles are also quite different. We analyze these properties in more detail below. Considering cumulants of $\pi$ in non-equilibrium is reminiscent of Grad’s moment expansion in kinetic theory of some time ago. In that approach, one tries to obtain the distribution function $f(\pi_j, \phi_k)$ in non-equilibrium by constraining the coefficients the expansion in $\pi$ and $\phi$ using macroscopic observables.

To study the dynamics of the system, let us first measure the thermal conductivity, $\kappa$, directly. We perform this task by choosing temperature boundary conditions $(T - \delta T, T + \delta T)$ with varying $\delta T$ around the same central temperature. In this manner, we can verify directly that Fourier’s law, $J = -\kappa \nabla T$ holds in the non–equilibrium steady state system and obtain the thermal conductivity. Here, $J = -\pi \nabla \phi_i$ is the heat flow in the system, which is constant inside, since the flow is one dimensional.

![Graph](image)

**FIG. 2:** $J$ vs. $\nabla T$. The relation is linear when the system is not too far from equilibrium, showing that Fourier’s law holds. Thermostats used were stochastic with $t_{kick} = 1$ (□), $t_{kick} = 0.5$ (○) and deterministic (△). Straight line represents bulk conductivity and we see that the the data all agree, independently of the thermostat type in the linear regime, as expected. The curved lines represent (2) (see text).

In Fig. 2, the relation between $J$ and $\nabla T$ is shown for $L = 42$ systems with central temperature $T = 1$. We have plotted the cases using stochastic thermostats with $t_{kick} = 0.5, 1$ and for comparison, deterministic thermostats which generalize the Nosé–Hoover thermostats, as detailed in [14]. We see that Fourier’s law is obeyed for systems not too far from equilibrium. The straight line is Fourier’s law in the bulk behavior regime with $\kappa = 2.75$ obtained previously using deterministic thermostats. It can be seen that the agreement with the results using both types of stochastic thermostats is excellent, as we expect. At this temperature, bulk behavior in thermal conductivity holds quite well at $L = 42$. The thermal conductivity is independent of both system size and of thermostat type and is universal.

For systems far from equilibrium, we see that the linear response theory starts to break down. The manner in which it breaks down is similar to the case with deterministic thermostats and can be reasonably well depicted by the relation,

$$\delta_{LR} = \frac{J - J_{LR}}{J_{LR}} = C_{LR} \left( \frac{\nabla T}{T} \right)^2$$

(2)

This is shown in Fig. 2 with $C_{LR} = -414$ (dashes), $-215$ (dot–dashes) for $t_{kick} = 0.5, 1$ cases respectively. It should be emphasized that to analyze the deviations from linear response theory, we also need to consider the possible breaking of local equilibrium. Unless local equilibrium is preserved, the meaning of temperature is not unique so that the significance of linear response breaking implicitly depends on the definition of the temperature.

To this end, we quantitatively investigate the deviations from local equilibrium and we do so through the momentum cumulants, $\langle \langle \pi^4 \rangle \rangle/T^2$. In the $\phi^4$ theory and the FPU model thermostatted by deterministic thermostats, it was found that the local equilibrium breaking can be described by a simple behavior,

$$\delta_{LE} = \frac{\langle \langle \pi^4 \rangle \rangle}{3T^2} = C_{LE} \left( \frac{\nabla T}{T} \right)^2$$

(3)
In Fig. 3, we plot the behavior of $\langle \langle \pi^4 \rangle \rangle / T^2$ at $T = 1$ against $\nabla T / T$, for $L = 42$. To do so, we averaged the cumulants for small number of lattice sites having local temperature close to $T = 1$ inside the system. By “inside” here, we refer to lattice sites away by more than the mean free path from the boundaries. The mean free path and other properties of this system can be found in [14]. In the plot, systems using stochastic boundary thermostats with $t_{kick} = 0.5, 1$ are included. Fits to the behavior of (3), using coefficients $C_{LE} = 146, 87$, respectively, are also shown. For comparison, we also included the behavior of the case with deterministic thermostats similar in type to those in [14]. In the plot, each point represents an averaged cumulant from a configuration with a particular set of temperature boundary conditions. We see that the behavior is quite well described by the formula (3) in all cases. For both $C_{LE}, C_{LR}, t_{kick} = 0.5$ case is larger than $t_{kick} = 0.5$ case by a factor of roughly two, but its precise reason is unclear.

So we see that the breaking of local equilibrium also occurs when using stochastic thermostats, which are quite different from deterministic ones, and that the behavior of the breaking is semi–quantitatively the same. However, we also see that the behavior is non–universal in that the coefficient $C_{LE}$ depends on the thermostat type. While the behavior of local equilibrium breaking itself is generic and simple, the coefficient, though of the same order, is not universal. When using deterministic thermostats, the coefficient $C_{LE}$ is dependent on $L$ even though the theory has bulk behavior [8], so that dependence on thermostat type is perhaps not surprising. On the technical side, we have found it significantly more demanding to obtain reliable numerical simulation data from stochastic simulations than from deterministic ones.

Let us discuss the significance of the non–universality in the coefficient $C_{LE}$. For contrast, let us first consider the thermal conductivity, which is universal or intrinsic to the theory. Thermal conductivity can be obtained from the temperature profile and the current $J$. But both these quantities are strongly boundary condition dependent; they depend on the system size and the boundary temperatures. Furthermore, they depend also on the thermostat type since the boundary temperature jumps depend on it and hence the temperature profile. Thermal conductivity is boundary condition independent only in the sense that when we inspect the relation between $J$ and $T$, Fourier’s Law $J = -\kappa \nabla T$ holds and $\kappa$ is independent of $L$, boundary temperatures and thermostat type. Had we not tried to use $\nabla T$ or looked at the appropriate relation, we could have concluded that the thermal transport properties are non–universal.

Now consider the cumulant: This is a property of the local distribution function. Let us define the full distribution function, $f(\pi_1, \pi_2, \ldots \pi_L; \phi_1, \phi_2, \ldots \phi_L)$ which is a function of all physical degrees of freedom. The local distribution function for $\pi$ is obtained by integrating out all other degrees of freedom.

$$f_j(\pi_j) = \int \prod_{k \neq j} d\pi_k \prod_k d\phi_k f(\pi_1, \pi_2, \ldots \pi_L; \phi_1, \phi_2, \ldots \phi_L)$$ (4)

Consider a site labelled by $j$, away from the boundaries, so that there are no direct boundary effects. The question whether this local distribution is universal is the question whether this distribution depends on the boundary conditions only through physical variables such as $T$ and $\nabla T$. For fixed $T$, we have only the $\nabla T$ dependence whose behavior is similar but manifestly thermostat dependent. We can consider various possibilities regarding the significance of the results:
1. The behavior is universal if we consider relations involving variables other than $T$ and $\nabla T$. However, we note that quantities such as $\nabla^2 T$ can be reexpressed in terms of $\nabla T$, using perturbation theory in linear response theory\[8].

2. The behavior is non-universal; there is no way to remove this thermostat dependence and the results cannot be rephrased in a thermostat independent manner.

3. The behavior is a small size effect and large systems display different behavior that is universal. However, we have studied system sizes up to few hundred sites using deterministic thermostats and have found $L$ dependent behavior\[8] and also to some extent using stochastic thermostats.

We add here that the maximum Lyapunov exponent for the $\phi^4$ theory is another physical property of the distribution function that also depends explicitly on the thermostat type\[15].

In this work, we analyzed the microscopic properties of $\phi^4$ theory under thermal gradients, in steady state. The thermal gradients were created by stochastic thermostats placed at the ends of the system. The semi-quantitative non-equilibrium behavior of the system is identical to the behavior obtained using deterministic thermostats. Namely, not only global equilibrium but local equilibrium is broken by thermal gradients, which can be measured through the momentum cumulants. Also Fourier’s law does not hold far from equilibrium. The dependence of these deviations on the non-equilibrium nature can be described by $\sim (\nabla T/T)^2$ and their coefficients are of the same order independently of the thermostat type. So these properties are thermostat independent for $\phi^4$ theory. The exact coefficients of these deviations, however, have some thermostat dependence.

It would be interesting to find out how other theories behave microscopically in non-equilibrium and how the behavior depends on the thermostats, or perhaps more importantly, which parts do not. We believe that these questions are of import in understanding the nature of the non-equilibrium state from fundamental principles. We have also studied the FPU model and have found similar behavior, though numerical precision is harder to achieve.

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