Non-Equilibrium Steady States and Transport in the Classical Lattice $\phi^4$ Theory

Kenichiro Aoki* and Dimitri Kusnezov†

*Dept. of Physics, Keio University, 4–1–1 Hiyoshi, Kouhoku-ku, Yokohama 223–8521, Japan
†Center for Theoretical Physics, Sloane Physics Lab, Yale University, New Haven, CT 06520-8120

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We study the classical non-equilibrium statistical mechanics of scalar field theory on the lattice. Steady states are analyzed near and far from equilibrium. The bulk thermal conductivity is computed, including its temperature dependence. We examine the validity of linear response predictions, as well as properties of the non-equilibrium steady state. We find that the linear response theory applies to visibly curved temperature profiles as long as the thermal gradients are not too strong. We also examine the transition from local equilibrium to local non-equilibrium.

*E–mail: ken@phys-h.keio.ac.jp
†E–mail: dimitri@nst.physics.yale.edu
The understanding of the dynamics of non-equilibrium field theories is important to many areas in physical sciences, from processes in inflation or baryogenesis in the early universe, transport processes in condensed matter, to the possible states of hadronic matter in heavy ion collisions, such as quark–gluon plasma, disoriented chiral condensates and color superconducting states. However, many problems linger even in the basic understanding of non-equilibrium statistical mechanics and transport [1]. It is clearly desirable to address these problems regarding the non-equilibrium dynamics of field theories while making as few assumptions about the dynamics of the theory as possible. In this work, we study the steady state dynamics of classical massless φ⁴ lattice field theory in (d + 1) dimensions (d = 1, 3), under weak and strong thermal gradients. We study the classical field theory on a lattice since the problems are well defined and techniques are available to construct non-equilibrium states from first principles. It is not clear to us how to address the questions we pose in the full quantum theory without making some drastic assumptions. Our computations are non-perturbative. Furthermore, not only is the temperature within the system dynamical, but even the question of whether local equilibrium is achieved is not an assumption but is determined dynamically by the system. The equilibrium properties of classical φ⁴ theory have been studied in the past, including its ergodic properties [2,3]. Hamiltonian dynamics and phase transitions [4]. However, the kind of questions we address here have not been answered in the previous literature.

Near equilibrium, linear response theory supposedly holds; yet there is no means to address its regime of validity within the theory itself since the computation is performed in equilibrium. By explicitly constructing non-equilibrium steady states near equilibrium, we examine the validity of the linear response theory. We then construct steady states of the system under stronger thermal gradients and study their physical properties. Here, fundamental questions arise, such as under which conditions local equilibrium is achieved. Local equilibrium, an assumption that equilibrium concepts can be applied locally to a problem which might be globally non-equilibrium, is widely used [5]. In fact, thermalization is a concept which is assumed, often tacitly, in many applications of non-equilibrium physics. However, as a system moves away from equilibrium, what precisely constitutes ‘local equilibrium’ becomes unclear and it is of interest to understand what kind of deviations develop from it and why. These problems are also non-trivial from the statistical mechanical point of view; even small departures from equilibrium into non-equilibrium steady states (such as the those we study) already lead to peculiar behaviors including a divergent Gibbs entropy $S_G$ ($S_G \to -\infty$) and a multi-fractal steady state measure [6]. The steady-state distributions far from equilibrium are not well understood classically and very little is known concerning their quantum counterparts. We would like to see to what extent these peculiar statistical measures influence the steady state thermal profiles, $T(x)$.

Classical field theories are relevant to the high temperature dynamics of quantum field theories and have proved effective, for instance, in computing finite temperature properties of the standard model [7,8,9]. Furthermore, non-equilibrium dynamics of classical field theories is of interest in its own right, an understanding of which is essential to understanding the dynamics of the quantum theory. The approach we adopt here can be applied to classical lattice theories quite generally. Transport properties have been previously studied in scalar quantum field theory using linear response theory [10] and the theory is known to have a classical, finite temperature limit for correlation functions [10]. Yet the question of how to relate our results to those results is far from trivial and will not be pursued here.

We start with the Lagrangian

\[-\mathcal{L} = \frac{1}{2} \left( \frac{\partial \phi(\tilde{x})}{\partial \tilde{r}_\mu} \right)^2 + \frac{g^2}{4} \phi(\tilde{x})^4. \tag{1}\]

This model, when discretized, reduces to a model of lattice vibrations with quartic anharmonicity, with the following dimensionless Hamiltonian

\[H(\pi, \phi) = \frac{1}{2} \sum_r \left[ \pi^2_r + (\nabla \phi_r)^2 + \frac{1}{2} \phi^4_r \right]. \tag{2}\]

Here \(\pi = \partial \phi / \partial t\), \(r\) runs over all sites in the lattice, and the lattice derivative has components \(\nabla_k \phi_r \equiv \phi_{r+e_k} - \phi_r\) (\(e_k\) is the unit lattice vector in the \(k\)-th direction). The two theories are related by discretization and the rescalings, \(\phi_r(t) = a \tilde{\phi}(\tilde{r}, \tilde{t})\), \(t = \tilde{t} / a\), \(r = \tilde{r} / a\), where \(a\) is the lattice spacing. The equations of motion, \(\square \phi = -\phi^3\), are solved on a spatial grid, with two methods: fifth and sixth order Runge-Kutta, and leap-frog algorithms [1].

In order to generate a stationary non-equilibrium statistical ensemble, thermal boundary conditions are imposed on the equations of motion. Specifically, at \(x = 0\) and \(x = L\), we add two time-reversal invariant fields which act to dynamically thermalize these boundaries at given temperatures \(T_1\) and \(T_2\) [12] (a more detailed account will be given elsewhere). For \(d > 1\) we impose periodic boundary conditions on the other directions. Apart from the thermal boundary conditions, the system evolves according to the dynamics dictated by the Hamiltonian (2). We used from \(10^6\) to \(10^9\) time steps of \(dt\) from 0.1 to 0.001, with observables being sampled every \(\Delta t = 20 \sim 100 dt\). In \(d = 1\), the lattice size was varied from \(L = 20\) to 8000, while in \(d = 3\) it ranged from \(50 \times N \times N\) (\(N\) ranging from \(200\) to \(800\)).
from 3–20) to 1000 × 3 × 3. We have verified that when \( T_1 = T_2 \), these boundary conditions dynamically set all the temperatures inside the system to be equal to the boundary temperatures and reproduce the equilibrium canonical measure \( \rho_{eq}(\pi, \phi) \sim \exp[-H(\pi, \phi)/T_1] \) at all points.

By controlling \( T_1 \) and \( T_2 \) we can begin to explore the non-equilibrium steady state. One question we would like to address is how the temperature profile \( T(x) \) behaves. Near equilibrium one would expect a linear profile, but beyond that the shape is unknown. In our near equilibrium simulations, \( T_1 \lesssim T_2 \), we find a linear temperature profile and recover transport given by Fourier’s law, as shown in Fig. 1 (a). However, far from thermal equilibrium (\( T_1 \ll T_2 \)), the temperature profile develops significant curvature, seen in 1 (b),c for the ratio \( T_2/T_1 = 10, 20 \). It is of interest to understand the physics behind these temperature profiles. We would further like to understand until what point linear response and local equilibrium provide reasonable descriptions.

**Equilibrium: \( T_1 = T_2 \).** A standard approach to thermal conductivity utilizes equilibrium correlation functions to compute near-equilibrium transport. This linear response approach uses the Green–Kubo formula,

\[
\kappa(T) = \frac{1}{T^2} \int_0^\infty \! dt \int \! d\mathbf{r} \left\langle T^{0z}(\mathbf{r}, t)T^{0z}(\mathbf{r}_0, 0) \right\rangle_{eq},
\]

where the autocorrelation function is evaluated in the canonical ensemble, \( T_1 = T_2 \). For our lattice calculation, we replace \( \int \! d\mathbf{r} \) with a lattice sum. It is interesting to note that the integrand in (3) has been argued to develop a long time tail behavior of \( \sim t^{-d/2} \), leading to the divergence of (3) in \( d = 1 \) [13]. In Fig. 2 (top), a typical autocorrelation function for \((1+1)\) dimensions is plotted to several hundred times the mean free time, which is well into the regime where long-time tails would be evident. The time integral is given in Fig. 2 (bottom), showing that the integral (3) is finite, which we attribute to the ‘on-site’ nature of the \( \phi^4 \) interaction, in contrast to some of the other models [4]. Interestingly enough, we do find that the transient behavior of the Green–Kubo integrand is quite close to \( t^{-1/2} \) up to a few ten times the mean free time, after which it decays much faster. Consistent results are found in \( d = 3 \) as well. The computed \( \kappa(T) \) is shown in Fig. 3 (top).

**Near Equilibrium: \( T_1 \lesssim T_2 \).** Near equilibrium, we find that a linear temperature profile emerges dynamically. The thermal conductivity \( \kappa \) is then obtained through Fourier’s law:

\[
\kappa(T) = -\frac{\left\langle T^{0z} \right\rangle_{NE}}{\nabla T}, \quad T^{0z} = -\partial_t \phi \nabla \phi,
\]

where \( \left\langle T^{0z} \right\rangle_{NE} \) is the heat flux averaged over the non-equilibrium steady state. Attention is paid to verifying the linear response properties by varying the temperature difference \( |T_2 - T_1| \) around the same average temperature. \( T(x) \) is the local temperature defined through an ideal gas thermometer, by \( T(x) = \langle \pi^2(x) \rangle_{NE} \), where \( \pi(x) \) is the momentum density. This will serve as a convenient definition as long as local equilibrium is achieved and the momentum distributions are gaussian. Here \( \langle \cdot \cdot \cdot \rangle_{NE} \) indicates the ensemble average over the non-equilibrium steady state. To obtain the transport properties, each simulation is run long enough for observables such as \( T^{0z} \), the energy density as well as distribution functions to converge.

In Fig. 3 (top), we compile the Green-Kubo and direct measurements of \( \kappa \), plotted as a function of \( T \). We find that these independent computations are quite consistent with each other. \( \kappa \) is found to have a temperature dependence

\[
\kappa = AT^{-\gamma}, \quad \left\{ \begin{array}{ll}
\gamma = 1.38(2), & A = 2.72(4) \quad (1+1) \text{ dimensions} \\
\gamma = 1.64(4), & A = 9.1(2) \quad (3+1) \text{ dimensions}.
\end{array} \right.
\]

This behavior is similar to that of lattice phonons at high temperature [13]. We have also verified that a sensible bulk behavior exists, as shown in Fig. 3 (bottom): the thermal conductivity is independent of \( L \) when it is larger than the mean free path, which, on the lattice, is of order of the conductivity.

In trying to understand near equilibrium physics, one might be tempted to assign a statistical measure, such as \( \rho_{NE}(\pi, \phi) \sim \exp[-H(\pi, \phi)/T(x)] \) to the non-equilibrium stationary state, or similar measures which assume some form for \( T(x) \). Strictly speaking, this is not correct: the phase space measures which describe steady state non-equilibrium systems are multi-fractal (whether one studies shearing, heat flow and so forth), converging to smooth distributions (Boltzmann) only in the equilibrium limit [14]. An important consequence is that the dynamical space is necessarily of lesser dimension than the equilibrium phase space. This in turn results in additional correlations of \( \pi(x) \) and \( \phi(x) \). One can also see that the non-equilibrium measure is not locally Boltzmann since quantities such as \( \langle \pi(x)\phi(x') \rangle \neq 0 \) for \( x \neq x' \), which is also reflected in the non-zero energy flow, when \( \langle \pi(x) \rangle = 0 \) near and far from equilibrium.

**Far From Equilibrium: \( T_1 \ll T_2 \).** When the temperature gradients are larger and we are no longer in the linear regime, the temperature profile becomes visibly curved. An example of such a non–linear temperature profile are given in Fig. 1. It should be noted that inside the boundaries, the dynamics is that of only the \( \phi^4 \) theory and the temperature profile is determined by it. When the temperature varies substantially in the system, one cause for the
non-linearity is the temperature dependence of the thermal conductivity. If this were the only cause of non-linearity, the temperature profile can be determined within the region by integrating Eq. (4) (when $\gamma \neq 1$)

$$T(x) = T_1 \left[ 1 - \left( 1 - \left( \frac{T_2}{T_1} \right)^{1-\gamma} \right) \frac{x}{L} \right]^{\frac{1}{1-\gamma}}. \tag{6}$$

$T(x)$ is a function only of $x/L$ so that it is consistent with a smooth continuum limit. This expression for $T(x)$ provides very good descriptions of the measured profiles with significant curvature, as can be seen in Fig. 1 where Eq. (6) (dashes) is almost indistinguishable from the measured steady state profiles (solid). This indicates that linear response extends well beyond the regimes of small temperature differences, when applied locally. \textit{A priori}, this was not clear.

By continuing to increase the ratio $T_2/T_1$ in the simulation, we do eventually reach steady state situations where the linear response formula no longer works. At this point, we begin to see indications that the concept of local equilibrium also becomes more tenuous. To analyze these questions more concretely, we need a dimensionless measure of how strong the thermal gradient is. A natural choice we adopt is $\lambda \nabla T/T$, where $\lambda$ is the mean free path. In our model, the heat capacity per unit volume, $C$, and the sound speed, $c_s$, are of order unity, so that elementary kinetic theory suggests that the mean free path is $\lambda \sim d c_s$, where $d$ is the spatial dimension. To quantify the departures from the linear response formula, we plot in Fig. 4 (for one spatial dimension) the deviation of the measured heat flux to that obtained from linear response prediction using Eqs. (4) and (5) (denoted $\langle T^{0z} \rangle_{NE}$ and $\langle T^{0z} \rangle_{LR}$, respectively), as a function of the quantity $\kappa(T) \nabla T/T$. The figure includes different lattice sizes and temperatures. We see that for linear response theory holds quite well. This includes systems with significant curvature in $T(x)$ such as Fig. 1. Eventually, for sufficiently strong gradients, the measured heat flow begins to deviate from the linear response results; the system does not conduct heat as well as its linear response theory prediction. At this point, we observe simultaneously the departure of other quantities from a ‘local equilibrium’ characterized by gaussian momentum distributions. To see the departure from local equilibrium, we follow the behavior of various observables, which include the momentum cumulants, the steady-state momentum distributions $f$ and 2-body densities $f^{(2)}(\pi(x), \phi(x), \pi(x'), \phi(x'))$ in the non-equilibrium steady states, from $S_B^{(k)}(x) = - \int d\mu^{(k)} f^{(k)} \log f^{(k)}$. We find that $S^{(1)}$ does not shift noticeably from its equilibrium value regardless of how far the system is from equilibrium. Further, $S^{(2)} (\lesssim 2 S^{(1)})$ is only slightly less than its upper limit $2 S^{(1)}$ and remains so even far from equilibrium. So unlike $S_G (\lesssim V S_B^{(1)})$, $S_B$ is found to be rather insensitive to the non-equilibrium nature of the system. While this could be a manifestation of coarse graining, it does suggest that some local thermodynamic concepts might still be useful in making connections with non-equilibrium thermodynamics.

The behavior of scalar lattice field theory near and far from equilibrium has been explored, and the present study allows us to establish a number of features regarding the non-equilibrium stationary state. The bulk thermal conductivity and its dependence on the temperature over few decades was found. To our knowledge, such a computation from first principles, without assuming linear response, has not been performed previously. This was done using both linear response (equilibrium) and direct (near equilibrium) approaches. The $d = 1$ Green-Kubo integrals in our theory are non-divergent and agree with the direct computation, in contrast to some of the other models. We find that linear response theory is quite robust and works well even when the steady state thermal profile has significant curvature, and as a consequence we derive an analytic description for the profile. By driving the system farther from equilibrium, we are able to see when linear response breaks down. Surprisingly, this is found to be near the same point where local equilibrium becomes noticeably violated. A sufficient condition for noticeable departures from linear response and local equilibrium in $d = 1, 3$ seems to be $\lambda \nabla T/T \gtrsim 1/10$. It would be interesting to examine the dynamics of

\[ S_B^{(k)} = - \int d\mu^{(k)} f^{(k)} \log f^{(k)} \]

\[ S_G^{(1)} \]

\[ V S_B^{(1)} \]

\[ S_B \]

\[ S_G \]

\[ V \]
non-equilibrium phase transitions or explore dynamical cooling of boundary temperatures to provide a means to access more complex non-equilibrium environments, and in particular, the dynamics of ultrarelativistic heavy–ion collisions.

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FIG. 1. (a) Linear thermal profile (solid) near equilibrium for L=800, d = 1 compared to a linear fit (dashes). The temperature was sampled at Δt = 1 for 5 × 10⁶ points. (b) Sagging profile for a non-equilibrium steady state in (1+1) dimensions far from equilibrium (solid) compared to theoretical predictions (dashes), where \((T_1, T_2) = (0.1, 1)\). The temperature was sampled 10⁶ times every Δt = 0.25. (c) A curved profile in (3+1) dimensions (solid) with the theoretical fit (dashes) for a 1000 × 3 × 3 system with \((T_1, T_2) = (0.5, 10)\). The temperature was sampled 4 × 10⁶ times every Δt = 0.1. In both (b) and (c), the fits are virtually indistinguishable from the temperature profiles.

FIG. 2. (Top) Time dependence of \(|C(t)|\), where \(C(t) = \int dx \langle T^0_x(x, t)T^0_x(x_0, 0) \rangle_{EQ}/T^2\), for \(L = 100\), up to a time \(t = 2 \times 10^4\), well into the region where long-time tails should be evident. Inset: Short time decorrelation. (Bottom) Green-Kubo integral up to time \(t\), converging to \(\kappa\) in 1+1 dimensions.
FIG. 3. (Top) Thermal conductivity $\kappa$ obtained from direct (□ 1+1-d; ◦ 3+1-d) and Green-Kubo (∗) measurements for various lattice sizes $L$, and the power law fit (dashes,dots). (Bottom) $L$ dependence of $\kappa$ indicating bulk behavior for temperatures (upper to lower) $T = 1/10, 1/4, 1$ (solid, 1+1-d) and $T = 1$ (dashes, 3+1-d).

FIG. 4. Breakdown of the linear response theory: The deviation of the measured energy flow $\langle T^{0x} \rangle_{NE}$ from its linear response expectation, $\langle T^{0x} \rangle_{LR}$, is shown as a function of $\kappa \nabla T / T$ for $d = 1$ non-equilibrium steady states. As discussed in the text, local equilibrium fails simultaneously.