Classical $\phi^4$ Lattice Field Theory in Strong Thermal Gradients

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Abstract

The dynamics of classical $\phi^4$ theory under weak and strong thermal gradients is studied. We obtain the thermal conductivity of the theory including its temperature dependence. Under moderately strong thermal gradients, the temperature profiles become visibly non-linear, yet the phenomenon can be understood using the linear response theory. When we move further away from equilibrium, we find that the linear response theory eventually breaks down, and the concept of local equilibrium also fails.

1 Introduction

It is widely accepted that the non-equilibrium dynamics of field theories has many important but difficult issues yet to be understood. The motivation for considering such theories hardly needs to be stressed — non-equilibrium situations are ubiquitous — 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. These phenomena all involve the non-equilibrium dynamics in some essential manner.

The particular non-equilibrium problem we study is the behavior of a field theory when various temperature boundary conditions are imposed on the boundaries of the theory. The physical properties such as the temperature profile, $T(x)$, pressure or entropy inside the boundaries, are determined dynamically. It is at a priori not clear whether the system thermalizes when strong thermal gradients are present, and we would like to clarify the situation. It would be preferable to compute the physical properties of the theory within an analytic field theory, yet such an approach seems difficult: One can compute the transport coefficients within linear response theory, since such a computation is performed in equilibrium, yet even then, its region of applicability is unclear and in principle could even be null, as was found in some cases. Within the linear regime, we might try to approach the problem directly using thermofield dynamics, for instance, but it seems difficult to do so without imposing some assumptions on the dynamics of the theory. Beyond the linear regime, it seems fair to say that the problem is very difficult.

In this work, we impose various temperature boundary conditions on massless $\phi^4$ theory in (1+1) and (3+1) dimensions and study the behavior of the theory in the steady state. We make use of numerical methods to compute physical quantities of interest. We shall be interested in such questions as the validity of the linear response theory and the region of its applicability, or the possibility of the failure to achieve thermalization. Let us point out the limitations of our current approach: The theory we work with is classical and it is formulated on a lattice. However, apart from this, we make no assumptions on the dynamics of the theory and we compute physical observables from first principles. Also, it should be clear from our approach that our methods are applicable to other field theories as well, except perhaps for the need for more computational time in more complicated problems. We choose the $\phi^4$ theory since it is a prototypical field theory and it appears in various contexts in many areas of physics. It should also be pointed out that classical approximations to quantum field theories have been studied for some time and while far from trivial, a basic understanding of the relation of the classical theory to the quantum one for high temperatures does exist. In addition, the classical theory is of interest on its own right and we believe that the understating of its dynamics is essential, if not necessary, to the understanding of the quantum theory.

2 The model

The Lagrangian of the model we study, the massless $\phi^4$ theory, is in the continuum,

$$ L = \left( \partial \nu \tilde{\phi} \right)^2 + \frac{\tilde{g}^2 \tilde{\phi}}{4} $$

(1)

We may scale out the dimensionful variables and the coupling using the rescalings $r = \tilde{r}/a$, $t = \tilde{t}/a$, $\phi_r = a\tilde{g}\tilde{\phi}(\tilde{r}, \tilde{t})$ with $a$ being the lattice spacing. We obtain the Hamiltonian on the lattice, $H$,

$$ H = \sum_r \left\{ \frac{1}{2} a^2 + \frac{1}{2} (\nabla \phi)^2 + \frac{1}{2} \phi^4 \right\}, \quad 0 \leq x \leq L, 0 \leq y, z \leq L' $$

(2)

Here, $(\nabla_k \phi)_r = \phi_{r+e_k} - \phi_r$ where $e_k$ is the unit vector in the $k$-th direction.

We thermostat the boundaries at temperatures $T(x=0) = T_1^0$ and $T(x=L) = T_2^0$. In (3+1) dimensions, we impose periodic boundary conditions in the $y, z$ directions. In this manner, statistical averages of observables in equilibrium or non-equilibrium steady states are equivalent to time averages in the long-time limit. The dynamics of the system is purely that of the $\phi^4$ theory inside the boundaries $0 < x < L$. The thermostats are provided using the "global demons" of a non-Hamiltonian generalization of the Nosé–Hoover approach.
When the boundary temperatures are equal, $T_0^1 = T_2^0$, we recover the equilibrium ensemble, as we should. The temperature inside the system is the same as the boundary temperature, $T(r) = T_0^0 (0 < x < L)$ and the distribution of the momentum $\pi_x$ at any site is Maxwellian. As we make the boundary temperatures different, we find the linear regime and then the non-linear regime. We now discuss the behavior of the system under these conditions.

3 Weak Thermal Gradients: $T_1^0 \lesssim T_2^0$

When the boundary temperature difference is small, a linear temperature profile emerges. An example of such a profile is shown in Fig. 1. We find that the distributions of the momenta are thermal at any of the points inside and outside the boundaries. Thermalization of the region outside the boundaries is established through the direct coupling to the thermostats while the thermalization of the sites inside the boundaries is established dynamically.

![Figure 1: A linear temperature profile for $L = 8000, T_0^1 = 0.15, T_2^0 = 0.35$, compared to the linear fit (dashes).](image)

Using these types of linear profiles, we have obtained the thermal conductivity of the system for various temperatures and various lattice sizes. We expect that the linear region should be well described by Fourier’s law,

$$\langle \mathbf{T} \mathbf{T}^\dagger \rangle_{\text{NE}} = -\kappa(T) \nabla T,$$

where $\mathbf{T}^\dagger_k = -\pi_k (\nabla \phi)_k$, (3)

$\langle \cdots \rangle_{\text{NE}}$ is the non-equilibrium average, and $\mathbf{T}^\dagger$ is the heat flux in our theory. While it is quite possible to extract a value for the thermal conductivity from systems like the one shown in Fig. 1, we have extracted the thermal conductivity for a given temperature from systems obtained by varying the temperature difference around the given temperature. We find that the thermal conductivity has a well defined bulk limit. In other words, it remains constant when the lattice size is increased for moderately large lattices. The thermal conductivity we find is described by a power law as shown on Fig. 2 (both in $(1+1)$ ($\times$) and $(3+1)$ (+) dimensions:

$$\kappa(T) = \frac{A}{T^\gamma}, \quad \begin{cases} \gamma = 1.35(2), \quad A = 2.83(4) & (1+1) \text{ dimensions} \\ \gamma = 1.58(4), \quad A = 9.5(5) & (3+1) \text{ dimensions} \end{cases} (4)$$

![Figure 2: The temperature dependence of the thermal conductivity (left): The direct measurement in $(1+1)$-d ($\times$) and $(3+1)$-d (+) obtained through the application of Fourier’s law and the Green–Kubo predictions in $(1+1)$-d ($) are plotted. These two independent methods clearly lead to the same result. The volume dependence of the thermal conductivity in $(1+1)$-d for the temperatures 0.1 (+), 0.25 ($\times$), 0.5 (*) and 0.1 (□). The dashed lines denote the values of thermal conductivity predicted by Eq. (4). We see that the bulk limit is reached for reasonably small lattices in this temperature range.](image)
The thermal conductivity may also be computed in a completely different manner in equilibrium, by using the Green–Kubo formula for the thermal conductivity,

$$\kappa(T) = \frac{1}{T^2} \int dx \, dt \, \langle T^{01}(x_0, t_0) T^{01}(x, t) \rangle_{eq}.$$  

(5)

Applying the formula to our lattice theory, we obtain the thermal conductivity for various temperatures which agree well with our direct measurements, as we can see in Fig. 2 (left, +). While this might seem obvious, it should be pointed out that the integrands in the Green–Kubo formula have “long time tails” and the integrand was found to be divergent in various low dimensional systems. In our theory, the long time tails do exist in (1+1) dimensions up to \( \sim 10 \tau \), where \( \tau \) is the mean free time. These transient tails do have the expected behavior of \( t^{-1/2} \), which, if it continued, would lead to a divergent integral in the Green–Kubo formula. In our case, the long time tails are transient and the integrand decays much faster for \( t \gg 10 \tau \) leading to a finite transport coefficient.

4 Strong Thermal Gradients: \( T_1^0 \ll T_2^0 \)

In the regime where the two boundary temperatures are substantially different, the thermal profiles become visibly curved. An example of such a profile is shown in Fig. 3 as the solid curve (dashed curve will be explained later). Also, another feature that emerges is that jumps in the temperature arises at the boundaries; namely, the temperature obtained by extrapolating the temperature profile inside does not match the boundary thermostat temperatures. We would like to understand the physics behind these features.

The boundary temperature jumps can be understood quantitatively using kinetic theory ideas. We dispense with the details here which can be found in \cite{5}. We should point out, however, that these jumps are physical and are observed generically in real systems as well as simulations for systems that are far away enough from the equilibrium. In any case, it should be emphasized that as long as the boundary thermostats are thermalizing the degrees of freedom outside the boundaries — which we indeed do confirm — what happens within the boundaries is determined dynamically only by the degrees of freedom of the \( \phi^4 \) theory.

Let us now move on to the curved temperature profiles: We first note that even within the context of linear response theory, the temperature profile will become curved since the thermal conductivity is a non–trivial function of the temperature, as in Eq. (6). If we assume that this is the only cause of the non–linearity of the profile, we obtain

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

(6)

where \( T_{1,2} \) are the extrapolated boundary temperatures which in general can be different from the thermostat temperatures, \( T_{1,2}^0 \), due to the existence of the boundary temperature jumps. We find that as long as the temperature gradient is not too large, the temperature profile is well explained by this formula. An example of such a fit is shown in Fig. 3 (left) as a dashed curve — in fact, the fit is barely distinguishable from the observed thermal profile except at the boundaries. It should be noted that \( \gamma \) in Eq. (6) is determined independently from systems near and at equilibrium. We have also looked at the momentum distributions in these systems at various sites and find that they are quite close to their equilibrium gaussian distributions. To analyze this quantitatively, one may look at the higher order cumulants of \( \pi_k \),

$$\frac{\langle \pi_k^4 \rangle}{3(\langle \pi_k^2 \rangle)^2} - 1, \frac{\langle \pi_k^6 \rangle}{15(\langle \pi_k^2 \rangle)^3} - 1, \ldots, \quad k = 0, 1, \ldots L$$  

(7)
The spatial dependence of the fourth order cumulant is shown in Fig. 3 where we see that the deviation from
the equilibrium value, 0, is at a percent level. So in conclusion, there exists a regime where the thermal profiles
are curved, yet both the concept of local equilibrium and linear response theory apply quite well. A priori, this
needed not be the case.

Let us briefly discuss what happens when we make the temperature difference larger and larger. We find that
linear response predictions break down and that the profiles are no longer described by the equation Eq. (1).
It is tempting to interpret this as a “non-linear” response of the system involving higher order derivatives of
the temperature, such as $\nabla^3 T, \nabla T \nabla^2 T, ...$. However, before we apply these ideas, we should check that local
equilibrium is achieved and that the usual concept of temperature applies. In our approach, whether local
equilibrium is achieved or not is a dynamical question that can be answered unambiguously. We find that when
the linear response does not apply, neither does local equilibrium hold. So, in fact, the situation is much more
complicated; while non-linear response might indeed exist, at least for the theory at hand, the failure of local
equilibrium needs to be taken into account simultaneously.

5 Discussions

The dynamics of the classical lattice $\phi^4$ theory was studied under weak and strong thermal gradients from first
principles. In equilibrium, the Green–Kubo formula was applied to derive the thermal conductivity. This was
found to agree with that obtained using the Fourier’s law for the system under weak thermal gradients. To our
knowledge, this is the first time the non–trivial temperature dependence of the thermal conductivity computed
from first principles over a number of decades for any system. For moderately strong gradients, the linear response
theory was found to be quite applicable even though the thermal profiles were visibly curved. For even stronger
gradients, linear response theory ceases to hold and local equilibrium breaks down also at the same time. While
we did not have time to discuss this here, we have also studied other quantities in the theory, such as the heat
capacity, entropy and the speed of sound and have elucidated how they are related to each other, leading to a
comprensive understanding of the dynamics.[8]

Clearly, much remains to be done: It would be interesting to study the dynamics of the theory which exhibits
spontaneous symmetry breaking. In this case, the phase boundary will emerge dynamically and this can be
analyzed within the current approach. We would also like to understand the dynamics of other theories, such as
Yang–Mills theories under thermal gradients. Since our methods are not restricted to the steady state case,
another problem of import is that of transient phenomena, such as thermalization. An important point which
needs to be investigated is the relation of the physical quantities in the lattice theory to those in the continuum
theory. In a related question, we would like to understand the quantum effects and understand how the classical
theory can be “matched” to the classical theory. Work is in progress in these areas.

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