Quantifying Nonequilibrium Behavior with Varying Cooling Rates

Carmen J. Gagne and Marcelo Gleiser
Department of Physics and Astronomy, Dartmouth College, Hanover, NH 03755, USA
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We investigate nonequilibrium behavior in (1+1)-dimensional stochastic field theories in the context of Ginzburg-Landau models at varying cooling rates. We argue that a reliable measure of the departure from thermal equilibrium can be obtained from the absolute value of the rate of change of the momentum-integrated structure function, $\Delta S_{\text{tot}}$. We show that the peak of $\Delta S_{\text{tot}}$ scales with the cooling, or quench, time-scale, $\tau_q$, in agreement with the prediction by Laguna and Zurek for the scaling of freeze-out time in both over and under-damped regimes. Furthermore, we show that the amplitude of the peak scales as $\tau_q^{-6/8}$ independent of the viscosity.

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Due to the widespread role of symmetry breaking phase transitions in cosmology, condensed matter physics, and high energy physics, it is imperative that the nonequilibrium aspects of the dynamics of these phase transitions be better understood. In particular, the effect of the cooling rate is still a widely open topic of investigation. Since all but the simplest problems are notoriously difficult to handle analytically, most approaches assume one of two extreme limits: either one assumes a quasi-adiabatic (infinitely slow) cooling, or an instantaneous (infinitely fast) quench, often even in numerical studies. However, in reality all cooling occurs with a finite rate and, therefore, lies somewhere between these two extremes. Some notable exceptions are Wong and Knobler’s [1] and Binder’s [2] work on quenches within the one-phase region, Wong and Knobler’s [3] and Ruiz’s [4] work on double quenches, and Onuki’s [5] work on periodic quenches. For excellent reviews, see [6], [7] and [4] work on double quenches, and Onuki’s [5] work on

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Freezing rates on the dynamics of phase transitions, as well as other nonequilibrium situations that commonly arise in nonlinear field theories, requires much further study. Even if advances in computer technology in recent years have greatly facilitated numerical studies of phase transitions, some aspects of nonequilibrium dynamics of nonlinear field theories remain difficult to study numerically, as they necessarily require large lattices and/or long simulations. In particular, dynamical studies near the critical region of continuous phase transitions, or of nucleation in discontinuous phase transitions, require both long runs and large lattices.

Once we focus on dynamical issues, it is often desirable to observe how a system evolves towards its final equilibrium state. It is thus important to develop tools designed to quantify the nonequilibrium behavior of a system being cooled (or warmed up) in a way that is numerically efficient. With this goal in mind, in this letter we propose a possible measure to quantify the departure from equilibrium of a system coupled to a heat bath, which clearly correlates the approach to equilibrium with the relevant control parameters of the system, namely, the absolute value of the rate of change of the momentum-integrated structure function, $\Delta S_{\text{tot}},$ which will be defined below.

For simplicity of comparison, we chose to use Laguna and Zurek’s model of a linear pressure quench for a single classical real scalar field $\phi(x,t)$ in (1+1)-dimensions [9]. Although there is no phase transition in one dimension, we can still examine (local) symmetry breaking and phase ordering through the formation of kink-antikink pairs. The present work should be considered a further step in the quantification of nonequilibrium behavior, which can be extended to higher-dimensional systems. All quantities have been scaled appropriately to be dimensionless.

We implement linear cooling with the following potential (or, equivalently, the homogeneous part of the free-energy density for the order parameter $\phi$),

$$V(\phi) = \frac{1}{8} \left( 1 - 2\epsilon(t) \phi^2 + \phi^4 \right),$$

where $\epsilon(t) \equiv \min(t/\tau_q,1)$, and $t$ is measured from the “phase transition point” (when $V''(\phi = 0) = 0$), so that, when the potential is a single well, both $t$ and $\epsilon(t)$ are negative. $\tau_q$ is the cooling time-scale. Note that the potential stops changing when $\epsilon(t) = 1$, which, in a Ginzburg-Landau system, is the zero-temperature limit. We simulate the coupling of the scalar field $\phi$ to the thermal bath using a generalized Langevin equation,

$$\frac{\partial^2 \phi}{\partial t^2} = \frac{\partial^2 \phi}{\partial x^2} - \eta \frac{\partial \phi}{\partial t} - \frac{\partial V}{\partial \phi} + \xi(x,t).$$

The terminology “pressure quench” is justified by the fact that the temperature of the bath $T$, which is related to the viscosity $\eta$ and the stochastic force of zero mean $\xi(x,t)$ by the fluctuation-dissipation relation,

$$\langle \xi(x,t)\xi(x',t') \rangle = 2\eta T \delta(x-x')\delta(t-t'),$$
remains constant, while the quadratic coefficient of the potential changes linearly in time. This is equivalent to a pressure quench at constant temperature in the laboratory. An obvious extension of this work is to implement a true linear cooling, where the temperature of the bath changes linearly, and $\epsilon(t) = (T_c - T)/T_c$. We will leave this case for a future investigation. [See, however, Ref. 10.] Our main interest here is in proposing a measure for nonequilibration of classical fields, which can be adapted for several different situations, including those involving cooling through the bath temperature, as we show below.

Zurek, and Laguna and Zurek have studied the effect of different cooling rates on the density of zero crossings of the field. [A counting of the number of times the field goes through zero for a given lattice length), which provides the approximate kink density as a function of time $[5].$ In general, the field will attempt to keep up with the changing potential as best it can, that is, its modes will try to keep thermalized as the cooling occurs. Clearly, as the cooling rate is increased, we can envisage a situation where this will not be possible any longer, and the field becomes “frozen”, unable to maintain thermal equilibrium with the bath. According to Zurek’s conjecture, this freeze-out occurs when the dynamical relaxation time – given by $\tau_\phi \simeq |\phi/\dot{\phi}|$ for overdamped systems, and by $\tau_\phi \simeq |\phi/\dot{\phi}|^{1/2}$ for underdamped systems – is comparable to the time to (from) the phase transition. From this freeze-out condition, one can derive the scaling relationships for the freeze-out time, $\tau_\phi \propto \tau_0^{1/3}$ and $\tau_{\phi} \propto \tau_0^{1/2}$. Using these results, Zurek and Laguna find scaling laws for kink density, which they confirm with simulations and contrast with experimental results for pressure quenches. Here, we are mostly concerned with how to extend our knowledge of nonequilibrium properties of field theories. We will thus be using Zurek and Laguna’s model as a testing ground for our methods, comparing some of our results to theirs.

For any given moment during the evolution of the system, there will be local fluctuations around the space-averaged order parameter. These can be studied with the structure function $S_k(t)$, which tells us how different Fourier modes evolve in time. Its time derivative will thus give us information on the rate of change of the individual modes. (Notice that this is not the dynamic structure function, which is a Fourier transform in both space and time.) Integrating the time derivative of the structure function over wave number gives the net change of the fluctuations in the order parameter. (Notice that this is not the dynamic structure function, which is a Fourier transform in both space and time.) Integrating the time derivative of the structure function, which is a Fourier transform in both space and time. The integral is over the first Brillouin zone. Here is our main point: In equilibrium the field is in a steady state, and so $\Delta S_{\text{tot}} \approx 0$. Thus, values of $\Delta S_{\text{tot}}$ greater than zero can be used as a measure of nonequilibration of the system. $\Delta S_{\text{tot}}$ may be smoothed, if necessary, by sampling every few time steps, which is equivalent to averaging over the same number of time steps.

\[ \Delta S_{\text{tot}} = \int \frac{dk}{2} \frac{\partial S_k(t)}{\partial t} \] . \hspace{1cm} (4)

$S_k(t) = |u_k(t)|^2$, where $u_k(t)$ is the Fourier transform of the field fluctuations, $u(x, t) = \phi(x, t) - \bar{\phi}(t)$ and $\bar{\phi}(t)$ is the spatial average of the field. $\delta x$ is the lattice spacing and $L$ is the lattice size. The integral is over the first Brillouin zone. Here is our main point: In equilibrium the field is in a steady state, and so $\Delta S_{\text{tot}} \approx 0$. Thus, values of $\Delta S_{\text{tot}}$ greater than zero can be used as a measure of nonequilibration of the system. $\Delta S_{\text{tot}}$ may be smoothed, if necessary, by sampling every few time steps, which is equivalent to averaging over the same number of time steps.

\[ V(\phi) = \frac{1}{2} \phi^2 \]

\[ \Delta S_{\text{tot}} \]

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\[ \text{KED } (\text{sim. } T_0 = 0.01) \]

\[ \Delta S_{\text{tot}} \text{ (theo. } T_0 = 0.005) \]

\[ \Delta S_{\text{tot}} \text{ (sim. } T_0 = 0.005) \]

FIG. 1. $\Delta S_{\text{tot}}$ and the average kinetic energy for an instantaneous temperature quench in a time-independent potential.

As a first illustration, Figure 1 shows $\Delta S_{\text{tot}}$ and the kinetic energy density, $KED$, for a field in a time-independent potential, $V(\phi) = \frac{1}{2} \phi^2$. $\phi$ is initially thermalized to a temperature $T_0$ with viscosity $\eta$, which is equal to unity for both cases shown. At $t = 0$, the bath is instantaneously quenched to zero temperature. Notice how initially $\Delta S_{\text{tot}}$ is approximately zero because the field is thermalized ($KED = T_0/2$), but begins immediately to rise when the quench begins, reaches a maximum and returns to zero after the field thermalizes ($KED \to 0$). This case can be solved analytically for $\eta \leq 2$, if we take the ideal limits $\delta x \to 0$ and $L \to \infty$,

\[ \Delta S_{\text{tot}} \simeq \frac{\text{sign}(\omega_0 t) \pi N T_0 L e^{-\eta t}}{2} \left[ \frac{1 - D^2}{2} J_0(2\omega_0 t) + \omega_0 D \left[ 2 + D\eta - \frac{D}{t} \right] J_1(2\omega_0 t) + 2\omega_0^2 D^2 J_2(2\omega_0 t) \right] \]
\[ \eta t + \frac{\eta^2}{2} (1 + D)^2 I_1 F_2 \left[ \frac{1}{2}, \frac{3}{2}; 1 - \omega_0^2 t^2 \right] \] 

where \( \omega_0 = \sqrt{1 - \eta^2} \), \( J_0, J_1 \) and \( J_2 \) are Bessel functions of the first kind and \( I_1 F_2 \) is a hypergeometric function. \( N \) and \( D \equiv C^4 T_0 \), where \( C \) is the value of \( \frac{\partial S}{\partial t} \) at \( t = 0 \), are parameters that were varied to fit the data. This is shown for both initial temperatures, \( T_0 = 0.01 \) and \( T_0 = 0.005 \), as a line in Figure 1. The simulation data were fit using \( N = 0.82 \) and \( D = 0.65 \) for both \( T_0 = 0.01 \) and \( T_0 = 0.005 \). We have verified (not shown) that both the time, \( t_{\text{peak}} \), and amplitude of the peak, \( A_{\text{peak}} \), depend on the viscosity. Also, and this is very important, the amplitude increases linearly with temperature change, as can be seen in Figure 1; thus, the location of the peak gives a measure of the equilibration time-scale of the system, while its amplitude provides a measure of the departure from equilibrium.

FIG. 2. \( \Delta S_{\text{tot}} \) for different viscosities and cooling time-scales with the potential in Eq. 1. \( A_{\text{peak}} \) increases with increasing cooling time-scales and decreases with increasing viscosity. \( t_{\text{peak}}/\tau_q \) increases with decreasing cooling time-scale and viscosity.

In addition to testing our second order staggered leapfrog Langevin code for stability with the same parameters as \( L = 2048, \delta x = .125, \delta t = .025 \) and \( T = .01 \), we reproduced their defect density results to test our code. For a more thorough description of the algorithm used see [12]. We added the calculation of the structure function to our code using a FFT routine from Numerical Recipes [13] and the change in the structure function using a simple finite difference method, with the ability to average over a few time steps to smooth the data. We can then extract the amplitude and time (after the phase transition) of the peak. Figure 2 shows the variation in \( \Delta S_{\text{tot}} (t/\tau_q) \) with viscosity and cooling time-scale. \( t/\tau_q \) is used on the time axis for easier comparison between different cooling time-scales. The amplitude of the peak is higher the lower the viscosity and the shorter the cooling time-scale (faster cooling). Also, the peak occurs earlier for longer cooling time-scales (slower cooling). Those peaks that occur during the cooling show a plateau beginning after the peak and lasting until the cooling ends at \( \epsilon = 1 \). We were able to identify a peak up to \( \tau_q \sim 128 \) at which point the data becomes too noisy to distinguish the peak from the plateau. The fastest coolings (with \( \eta = 1 \) it happens for \( \tau_q \lesssim 16 \) ) actually peak \textit{after} the potential stops changing (\( \epsilon = t/\tau_q = 1 \)): the system remains out of equilibrium during the whole cooling process, which is thus equivalent to an instantaneous quench. For \( \tau_q \gtrsim 256 \), \( \Delta S_{\text{tot}} \simeq 0 \), and thus the system remains thermalized during the cooling; this is equivalent to an adiabatic cooling. It is between these two regimes that the cooling most dramatically affects the dynamics of the system.

The time and amplitude of the maximum in \( \Delta S_{\text{tot}} \) are plotted in Figure 3 and Figure 4 respectively as a function of \( \tau_q \) for several viscosities. From fig. 3 we note that the location of the peak scales with \( \tau_q \) in agreement to the scaling obtained in Ref. [9] for over- and under-damped freeze-out times as a function of \( \tau_q \) in agreement to the scaling obtained in Ref. [9] for the freeze-out time. Since this is the time after which the field is able to begin relaxing to its equilibrium state, this seems reasonable.

FIG. 3. Peak time vs. cooling time-scale for time-dependent potential with varying viscosity. The straight lines above and below the data show the variation in \( \Delta S_{\text{tot}} (t/\tau_q) \) with viscosity and cooling time-scale. The simulation data interpolates between these two extremes appropriately.
because the field is still changing after the cooling has ended, which, as we remarked above, approximates an instantaneous quench. We hope to report on the extension of this method to higher dimensional systems and on a in-depth analysis of the relevant parameter space in the near future.

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We found that the amplitude of the maximum universally scales as $\tau_q^{-p}$, where $p = 1.2 \pm .05$ for all but the fastest coolings. There are thus essentially three regimes: i) the field remains thermalized all through the cooling process, thus approximating an “adiabatic” cooling (for $\tau_q > 256$ with $\eta = 1$); ii) the field remains out of equilibrium through the complete cooling process, thus approximating an instantaneous quench (for $\tau_q < 16$ and $\eta = 1$); iii) the intermediate regime, where the field reaches thermalization during the cooling process, which is signaled by the appearance of a plateau in $\Delta S_{\text{tot}}$, which decreases in amplitude as $\tau_q$ is increased, until it cannot be differentiated from noise. The general picture can be described qualitatively as follows: the modes are initially thermalized, and their rate of change increases as they try to “catch up” with the changing potential (or, when appropriate, the changing environment). This may or may not happen during the cooling, determined by the value of $\tau_q$. As the quench proceeds at the steady rate of $\tau_q^{-1}$, $\Delta S_{\text{tot}}$ increases until the field begins to probe the bottom of the potential (the free-energy minima), when it has essentially “caught up” with the changing potential. If this happens while the potential is still changing, the field then changes at the same rate as the potential ($\Delta S_{\text{tot}}$ begins to plateau), until the potential stops changing and the field can fully thermalize ($\Delta S_{\text{tot}} \to 0$). In the fastest coolings ($\tau_q \lesssim 16$ for $\eta = 1$, the field is not able to “catch up” to the changing potential before the end of the cooling, and so $\Delta S_{\text{tot}}$ never plateaus; the amplitude of the peak does not obey the scaling in Figure

**FIG. 4.** Amplitude of peak vs. cooling time-scale for time-dependent potential with varying viscosity. For all but the fastest quench times, all viscosities studied satisfy the scaling $A_{\text{peak}} \propto \tau_q^{-6/5}$. All three fit lines have a slope of $-6/5$; the fit lines are labeled by their $y$-intercepts.

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