THERMAL MIXING OF PHASES:
NUMERICAL AND ANALYTICAL STUDIES

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Abstract

The dynamics of phase transitions plays a crucial rôle in the so-called interface between high energy particle physics and cosmology. Many of the interesting results generated during the last fifteen years or so rely on simplified assumptions concerning the complex mechanisms typical of nonequilibrium field theories. In particular, whenever first order phase transitions are invoked, the metastable background is assumed to be sufficiently smooth to justify the use of homogeneous nucleation theory in the computation of nucleation rates of critical bubbles. In this talk I present the results of numerical simulations which were designed to quantify “smoothness”; that is, how the contribution from nonperturbative subcritical fluctuations may spoil the homogeneity assumption of nucleation theory. I then show how the numerical results can be understood quantitatively in terms of a simple analytical model of subcritical thermal fluctuations. Encouraged by the success of the model in matching the numerical results, I apply it to the standard model electroweak phase transition.

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I. INTRODUCTION: HOMOGENEOUS NUCLEATION AND ITS ASSUMPTIONS

The fact that the gauge symmetries describing particle interactions can be restored at high enough temperatures has led, during the past 15 years or so, to an active research program on the possible implications that this symmetry restoration might have had to the physics of the very early Universe. One of the most interesting and popular possibilities is that during its expansion the Universe underwent a series of phase transitions, as some higher symmetry group was successively broken into products of smaller groups, up to the present standard model described by the product $SU(3)_C \otimes SU(2)_L \otimes U(1)_Y$. Most models of inflation and the formation of topological (and nontopological) defects are well-known consequences of taking the existence of cosmological phase transitions seriously.

One, but certainly not the only, motivation of the works addressed in this talk comes from the possibility that the baryon asymmetry of the Universe could have been dynamically generated during a first order electroweak phase transition. As is by now clear, a realistic calculation of the net baryon number produced during the transition is a formidable challenge. We probably must invoke physics beyond the standard model (an exciting prospect for most people), push perturbation theory to its limits (and beyond, due to the nonperturbative nature of magnetic plasma masses that regulate the perturbative expansion in the symmetric phase), and we must deal with nonequilibrium aspects of the phase transition. Here I will focus on the latter problem, as it seems to me to be the least discussed of the pillars on which most baryon number calculations are built upon. To be more specific, it is possible to separate the nonequilibrium aspects of the phase transition into two main subdivisions. If the transition proceeds by bubble nucleation, we can study the propagation of bubbles in the hot plasma and the transport properties of particles through the bubble wall. A considerable amount of work has been devoted to this issue, and the reader can consult the works of Ref. [4] for details. These works assume that homogeneous nucleation theory is adequate to investigate the evolution of the phase transition, at least for the range of parameters of interest in the particular model being used to generate the baryon asymmetry. This brings us to the second important aspect of the nonequilibrium dynamics of first order phase transitions, namely the validity of homogeneous nucleation theory to describe the approach to equilibrium. This is the issue addressed in this talk.

Nucleation theory is a well-studied, but far from exhausted, subject. Since the pioneering work of Becker and Döring on the nucleation of droplets in supercooled vapor, the study of first order phase transitions has been of interest to investigators in several fields, from meteorology and materials science to quantum field theory and cosmology. Phenomenological field theories were developed by Cahn and Hilliard and by Langer in the context of coarse-grained time-dependent Ginzburg-Landau models, in which an expression for the decay rate per unit volume was obtained by assuming a steady-state probability current flowing through the saddle-point of the free-energy functional. The application of metastable decay to quantum field theory was initiated by Voloshin, Kobzarev, and Okun, and soon after put onto firmer theoretical ground by Coleman and Callan. The generalization of these results for finite temperature field theory was first studied by Linde, and has been...
the focus of much recent attention \cite{12}.

The crucial ingredient in the evaluation of the decay rate is the computation of the imaginary part of the free energy. As shown by Langer \cite{7}, the decay rate $\mathcal{R}$ is proportional to the imaginary part of the free energy $\mathcal{F}$,

$$\mathcal{R} = \frac{|E_-|}{\pi T} \text{Im}\mathcal{F},$$

where $E_-$ is the negative eigenvalue related to metastability, which depends on nonequilibrium aspects of the dynamics, such as the growth rate of the critical bubble. Since $\mathcal{F} = -T \ln Z$, where $Z$ is the partition function, the computation for the rate boils down to the evaluation of the partition function for the system comprised of critical bubbles of the lower energy phase inside the metastable phase.

If we imagine the space of all possible field configurations for a given model, there will be different paths to go from the metastable to the ground state. We can think of the two states as being separated by a hill of a given “height”. The energy barrier for the decay is then related to the height of this hill. At the top of the hill, only one direction leads down to the ground state, the unstable direction. Fluctuations about this direction will grow, with rate given by the negative eigenvalue which appears in the above formula. All other directions are positively curved, and fluctuations about them give rise to positive eigenvalues which do not contribute to the decay rate. The path which will cost less energy is the one which will dominate the partition function, the so-called critical bubble or bounce. It is simply the field configuration that interpolates between the two stable points in the energy landscape, the metastable and ground state. The energy barrier for the decay is the energy of this particular field configuration.

For a dilute gas of bubbles only, the partition function for several bubbles is given by \cite{13,14},

$$Z \simeq Z(\varphi_f) + Z(\varphi_f) \frac{Z(\varphi_b)}{Z(\varphi_f)} + Z(\varphi_f) \frac{1}{2!} \left[ \frac{Z(\varphi_b)}{Z(\varphi_f)} \right]^2 + \ldots$$

$$\simeq Z(\varphi_f) \exp \left[ \frac{Z(\varphi_b)}{Z(\varphi_f)} \right],$$

where $\varphi_f$ is the metastable vacuum field configuration and $\varphi_b$ is the bubble configuration, the bounce solution to the $O(3)$-symmetric Euclidean equation of motion. We must evaluate the partition functions above. This is done by the saddle-point method, expanding the scalar field $\phi(x, \tau)$, such that $\phi(x, \tau) \to \varphi_f + \zeta(x, \tau)$ for $Z(\varphi_f)$, and $\phi(x, \tau) \to \varphi_b(x) + \eta(x, \tau)$ for $Z(\varphi_b)$, where $\zeta(x, \tau)$ and $\eta(x, \tau)$ are small fluctuations about equilibrium.

It is crucial to note that the saddle-point, or Gaussian, method only gives good results if indeed the fluctuations about equilibrium are sufficiently small that nonlinear terms in the fields can be neglected. Even though the method sums over all amplitude fluctuations, it does so by assuming that the functional integral is well approximated by truncating the expansion of the action to second order. The efficiency of the method relies on the fact that higher amplitudes will be suppressed fast enough that their contribution to the partition function
will be negligible. One can visualize this by comparing a sharp parabolic curve with a flatter one with minimum at \( x_0 \), and investigating when \( \int dx e^{-f(x)} \) will be well approximated by writing \( f(x) \simeq f(x_0) + \frac{1}{2}(x - x_0)^2 f''(x_0) \). For a sharp curve, larger amplitude fluctuations will be strongly suppressed and thus give a negligible contribution to the integral over all amplitudes. Clearly, this will not be the case for flatter curves.

Skipping details \[12\], using the saddle-point method one obtains for the ratio of partition functions, \( \frac{Z(\varphi_b)}{Z(\varphi_f)} \),

\[
\frac{Z(\varphi_b)}{Z(\varphi_f)} \simeq \left[ \frac{\det(-\Box_E + V''(\varphi_b))_\beta}{\det(-\Box_E + V''(\varphi_f))_\beta} \right]^{-\frac{1}{2}} e^{-\Delta S},
\]

(3)

where \( [\det(M)_\beta]^{-\frac{1}{2}} \equiv \int D\eta \exp \left\{ -\int_0^\beta d\tau \int d^3x \frac{1}{2} \eta[M] \eta \right\} \) and \( \Delta S = S_E(\varphi_b) - S_E(\varphi_f) \) is the difference between the Euclidean actions for the field configurations \( \varphi_b \) and \( \varphi_f \). [Note that \( S_E(\varphi) \), and hence \( \Delta S \), does not include any temperature corrections. It would if one had summed over other fields coupled to \( \varphi \).] Thus, the free energy of the system is,

\[
\mathcal{F} = -T \left[ \frac{\det(-\Box_E + V''(\varphi_b))_\beta}{\det(-\Box_E + V''(\varphi_f))_\beta} \right]^{-\frac{1}{2}} e^{-\Delta S}.
\]

(4)

Let me stress again the assumptions that go into computing the free energy. First, that the partition function is given by Eq. 2 within the dilute gas approximation, and second, that the partition function is evaluated approximately by assuming small fluctuations about the homogeneous metastable state \( \varphi_f \). It is clear that for situations in which there are large amplitude fluctuations about the metastable equilibrium state the above formula must break down. Thus the breakdown of the expression for the rate is intimately connected with the question of how well-localized the system is about the metastable state as the temperature drops below the critical temperature \( T_c \). Homogeneous nucleation, as its name already states, is only accurate when the metastable state is sufficiently homogeneous. In the presence of inhomogeneities, there is no reason to expect that the decay rate formula will apply. The question then is to quantify when does it breakdown.

In order to study the properties of the metastable background in the presence of thermal fluctuations, I have recently investigated the nonequilibrium dynamics of a (2+1)-dimensional model of a scalar field coupled to a thermal bath \[14\]. The nonlinear interactions were chosen to reflect the gross properties of the electroweak effective potential, although the model only deals with a real scalar field. These results were then extended to a (3+1)-dimensional simulation, in work done in collaboration with Julian Borrill \[15 \]. The results for two and three dimensions were qualitatively similar, showing how the amount of phase mixing is related to the parameters of the model. In particular, for the three-dimensional study we varied the strength of the scalar field’s quartic coupling, which for the electroweak model is related to the Higgs boson mass. In the next Section I review the results of this work. In Section 3 I present an improved treatment of the kinetics of subcritical bubbles which I then use to understand the results of the numerical simulations. The agreement between numerical experiment and analytical model is extremely satisfactory. The simplicity of the kinetic approach based on the dynamics of subcritical thermal fluctuations makes
it a useful tool in studying the properties of the thermal background. I then briefly apply the subcritical bubbles method to the simple 1-loop electroweak potential, showing that for Higgs masses above 60 GeV, the amount of phase mixing is such that homogeneous nucleation should not be used to study the dynamics of the transition. I conclude in Section 4 with a brief overview of the results and possible future work.

II. NUMERICAL SIMULATIONS OF THERMAL PHASE MIXING

The homogeneous part of the free energy density is written as

\[ U(\phi, T) = \frac{a}{2} \left( T^2 - T_2^2 \right) \phi^2 - \frac{\alpha}{3} T \phi^3 + \frac{\lambda}{4} \phi^4. \]  

(5)

This choice intentionally resembles the electroweak effective potential to some order in perturbation theory, although here \( \phi(x, t) \) is a real scalar field, as opposed to the magnitude of the Higgs field. The goal is to explore the possible dynamics of a model described by the above free-energy density, generalizing the results obtained in Ref. [14] to (3+1)-dimensions. The analogy with the electroweak model is suggestive but not quantitative.

Introducing dimensionless variables \( \tilde{x} = a^{-\frac{1}{2}} T_2 x, \tilde{t} = a^{-\frac{1}{2}} T_2 t, X = a^{-\frac{1}{2}} T_2^{-1} \phi, \) and \( \theta = T/T_2 \), the Hamiltonian is,

\[ \frac{H[X]}{\theta} = \frac{1}{\theta} \int d^2 \tilde{x} \left[ \frac{1}{2} \left\{ \nabla^2 X \right\}^2 + \frac{1}{2} \left( \theta^2 - 1 \right) X^2 - \frac{\tilde{\alpha}}{3} \theta X^3 + \frac{\tilde{\lambda}}{4} X^4 \right], \]

(6)

where \( \tilde{\alpha} = a^{-\frac{4}{3}} \alpha \), and \( \tilde{\lambda} = a^{-\frac{4}{3}} \lambda \) (henceforth we drop the tildes). For temperatures above \( \theta_1 = (1 - \alpha^2/4\lambda)^{-\frac{1}{2}} \) there is only one minimum at \( X = 0 \). At \( \theta = \theta_1 \) an inflection point appears at \( X_{\text{inf}} = \alpha \theta_1 / 2 \lambda \). Below \( \theta_1 \) the inflection point separates into a maximum and a minimum given by \( X_{\pm} = \frac{\theta_1}{2 \lambda} \left[ 1 \pm \sqrt{1 - 4 \lambda (1 - 1/\theta^2) / \alpha^2} \right] \). At the critical temperature \( \theta_c = (1 - 2 \alpha^2/9 \lambda)^{-\frac{1}{2}} \) the two minima, at \( X_0 = 0 \) and \( X_+ \), are degenerate. Below \( \theta_c \) the minimum at \( X_+ \) becomes the global minimum and the \( X_0 \)-phase becomes metastable. Finally, at \( \theta = 1 \) the barrier between the two phases at \( X_- \) disappears.

The coupling with the thermal bath will be modelled by a Markovian Langevin equation which, in terms of the dimensionless variables defined above, is

\[ \frac{\partial^2 X}{\partial t^2} = \nabla^2 X - \eta \frac{\partial X}{\partial t} - \frac{\partial U(X, \theta)}{\partial X} + \xi(x, t) \]

(7)

where \( \eta \) is the dimensionless viscosity coefficient, and \( \xi \) the dimensionless stochastic noise with vanishing mean, related to \( \eta \) by the fluctuation-dissipation theorem,

\[ \langle \xi(x, t)\xi(x', t') \rangle = 2 \eta \theta \delta(t - t') \delta^3(x - x') \]

(8)

A few comments are in order concerning our choice of equation. It is clear that we are assuming that \( X(x, t) \) represents the long-wavelength modes of the scalar field. Whenever
one discretizes a continuum system there is an implicit coarse-graining scale built in. We encapsulate information about the shorter-wavelength modes, which have faster relaxation time-scales, in the dissipation and noise terms. In principle it should be possible to derive an effective Langevin-like equation for the slow modes by integrating out the fast modes from the effective action. This is a complicated problem, and progress has been slow. Recent work indicates that one should expect departures from the Langevin equation written above [16], although details are sensitive to the particular model one starts with. For example, the noise may be colored (with more complicated correlation functions) and the coupling to the bath may be multiplicative, as opposed to the additive coupling chosen above. Here, we will adopt the above equation as a first step. We do not expect that the nature of the noise will change the final equilibrium properties of the system, but mostly the relevant relaxation time-scales. Furthermore, Gleiser and Ramos showed that for high enough temperatures the noise does become white [17]. Since the physical results here are related to the final equilibrium state of the system, we believe that they will not be affected by more complicated representations of the coupling of the field to the thermal bath. However, a more thorough examination of this question deserves further study.

A related topic is the choice of coarse-graining scale, which is embedded in the lattice spacing used in the simulations. It is well-known that any classical field theory in more than one spatial dimension is ultra-violet divergent, and that the lattice spacing serves as an ultra-violet cutoff. This being the case, one should be careful when mapping from the lattice to the continuum theory. If one is to probe physics at shorter wavelengths, renormalization counterterms should be included in the lattice formulation so that a proper continuum limit is obtained on the lattice within the validity of perturbation theory. This point has been emphasized in Ref. [18], where a (2+1)-dimensional study of nucleation was performed for a temperature-independent potential. Renormalization counterterms (of order $\theta \ln \delta x$ for lattice spacing $\delta x$) for a particular renormalization prescription were obtained, and the results shown to be lattice-space independent.

Here, due to the temperature dependence of the potential, the renormalization prescription of Ref. [18] does not work. Instead, we will use $\delta x = 1$ throughout this work. It turns out that for all cases studied the mean-field correlation length $\xi^{-2} = V''(X_0, \theta_c)$ is sufficiently larger than unity to justify this choice. Modes with shorter wavelengths are coupled through the noise into the dynamics of the longer wavelength modes, as described by Eq. 7 above. But it should be stressed that different choices of lattice spacing imply in different effective coarse-graining scales, and hence different results. In other words, although phase mixing will always be present to some degree, the exact quantitative results will depend on the coarse-graining scale.

I will skip details of how we implemented this simulation in a parallel machine, as well as the tests to make sure our results were independent of simulation parameters such as lattice length, time and spatial steps, and random number generator. The reader is referred to Ref. [13] for information on these issues. I will now proceed by describing the numerical experiments and our results.

As pointed out in the Introduction, the question of whether homogeneous nucleation theory is trustworthy to describe a first order phase transition boils down to how well localized in the metastable state the system is, as the temperature drops below the critical tem-
perature. In the jargon of condensed matter physics, nucleation should work for quenches deep into the metastable branch of the coexistence curve. In order to address this question, following the procedure of Ref. [14], we will study the behavior of the system at the critical temperature, when the two minima are degenerate. The reason for this choice follows naturally from the fact that we are interested on the way by which the system approaches equilibrium as the temperature drops below $T_c$. The detailed dynamics will depend on the relative fraction of the total volume occupied by each phase; if at $T_c$ the system is well localized about the $X = 0$ minimum, as the temperature drops the transition may evolve by nucleation and subsequent percolation of bubbles larger than a critical size. If, on the other hand, considerable phase-mixing occurs already at $T_c$, we expect the transition to evolve by domain coarsening, with the domains of the $X_+$ phase eventually permeating the whole volume.

Let us call the two phases the 0-phase and the $+$-phase, corresponding to the local equilibrium values $X = X_0 = 0$, and $X = X_+$, respectively. We can quantify the phase distribution of the system as it evolves according to Eq. 7, by measuring the fraction of the total volume in each phase. This is done by simply counting the total volume of the system at the left of the potential barrier’s maximum height (i.e., $X \leq X_- \equiv X_{\text{max}}$), corresponding to the 0-phase. Dividing by the total volume, we obtain the fraction of the system in the 0-phase, $f_0(t)$, such that

$$f_0(t) + f_+(t) = 1,$$

where, of course, $f_+(t)$ corresponds to the fractional volume in the $+$-phase. A further measure of any configuration is given by the volume-averaged order parameter, $\langle X \rangle(t) = V^{-1} \int dV X(t)$. A localized configuration ($f_0^\text{eq} > 0.5$) then corresponds to $\langle X \rangle^\text{eq} < X_{\text{max}}$, and a fully phase-mixed configuration ($f_0^\text{eq} \approx 0.5$) to $\langle X \rangle^\text{eq} = X_{\text{max}}$, where the super(sub)-script ‘eq’ refers to final ensemble-averaged equilibrium values of $f_0(t)$ and $\langle X \rangle(t)$, respectively. [Recall that in the presence of noise we must take an ensemble average of the physical quantities of interest in order to get smooth, sensible results. In practice, this amounts to changing the seed of the random number generator for each run, and averaging the results over many runs.]

We prepare the system so that initially it is well localized in the 0-phase, with $f_0(0) = 1$ and $\langle X \rangle(0) = 0$. These initial conditions are clearly the most natural choice for the problem at hand. If one has cosmology in mind, it is quite possible that as the system slowly cools down (we are not interested in phase transitions close to the Planck scale), fluctuations from the high temperature phase $X = 0$ to the $X_+$ phase are already occurring before $T_c$ is reached. (In this case, our arguments are even stronger.) However, we will adopt the best-case scenario for homogeneous nucleation to work, in which the system managed to reach the $X = 0$ phase homogeneously, so that the initial state is a thermal state with mean at $X_0$. If one has more concrete applications in mind, we can assume that we quenched the system to its critical temperature, making sure that the order parameter remains localized about the high-temperature phase. Since thermalization happens very fast in the simulations, the exact point by point initial conditions should not be important, and we can view the first few time steps as generating an initial thermal distribution with $f_0(0) \sim 1$ and $\langle X \rangle \sim 0$, so that
the average kinetic energy per lattice point satisfies the equipartition theorem, $\frac{1}{N}E_k = \frac{3}{2}T$. For simplicity we take $X = 0, \dot{X} = 0$ everywhere initially.

There are two parameters controlling the strength of the transition, $\alpha$ and $\lambda$. In the previous (2+1)-dimensional work, $\alpha$ was chosen to vary while $\lambda$ was kept fixed. It is really immaterial which parameter is held fixed, or if both are made to vary, but in order to keep closer to the spirit of the electroweak model we will fix $\alpha$ and let $\lambda$ vary. As is well-known, $\lambda$ is related to the Higgs mass, while $\alpha$ is related to the gauge-boson masses [2]. The connection with the electroweak model is straightforward. If we consider as an example the unimproved one-loop approximation, the effective potential is [2],

$$V_{\text{EW}}(\phi, T) = D \left( T^2 - T_0^2 \right) \phi^2 - E T \phi^3 + \frac{1}{4} \lambda_T \phi^4, \quad (10)$$

where $D$ and $E$ are given by $D = [6(M_W/\sigma)^2 + 3(M_Z/\sigma)^2 + 6(M_T/\sigma)^2]/24 \approx 0.17$ and $E = [6(M_W/\sigma)^3 + 3(M_Z/\sigma)^3]/12\pi \approx 0.097$, for $M_W = 80.6$ GeV, $M_Z = 91.2$ GeV, $M_T = 174$ GeV [19], and $\sigma = 246$ GeV. $T_2$ is given by,

$$T_2 = \sqrt{(M_H^2 - 8B\sigma^2)}/4D, \quad (11)$$

where the physical Higgs mass is given in terms of the 1-loop corrected $\lambda$ as $M_H^2 = (2\lambda + 12B)\sigma^2$, with $B = (6M_W^4 + 3M_Z^4 - 12M_T^4)/64\pi^2\sigma^4$, and the temperature-corrected Higgs self-coupling is,

$$\lambda_T = \lambda - \frac{1}{16\pi^2} \left[ \sum_B g_B \left( \frac{M_B}{\sigma} \right)^4 \ln \left( \frac{M_B^2/c_B T^2}{\sigma} \right) - \sum_F g_F \left( \frac{M_F}{\sigma} \right)^4 \ln \left( \frac{M_F^2/c_F T^2}{\sigma} \right) \right] \quad (12)$$

where the sum is performed over bosons and fermions (in our case only the top quark) with their respective degrees of freedom $g_B(F)$, and $\ln c_B = 5.41$ and $\ln c_F = 2.64$.

Thus, the correspondence with our (dimensionless) parameters is

$$\alpha = \frac{3E}{(2D)^2} = 0.065, \quad \text{and} \quad \lambda = \frac{\lambda_T}{(2D)^2} = 1.72 \lambda_T. \quad (13)$$

Once this is established, the numerical experiment proceeds as follows: i) Choose $\alpha = 0.065$; ii) Prepare the system in the initial state described above, and measure the value of $f_0(t)$ and $\langle X \rangle(t)$ for several values of $\lambda$, as the system evolves according to Eq. 7. I can now present the results of the simulations.

Based on the above discussion, we choose lattice length $L = 48$, lattice spacing $\delta x = 1$, time step $\delta t = 0.1$, and $\alpha = 0.065$ in all simulations. [For details as to why this choice of parameters is sensible, see Ref. [13].] The experiment then consists in measuring the fraction of the volume in the 0-phase as a function of time for several values of $\lambda$.

In Fig. 1 we show the evolution of the ensemble-averaged fraction $f_0(t)$ for several values of $\lambda$. It is clear that for small enough values of $\lambda$ the system remains well-localized in the 0-phase with $f_0^{\text{eq}} \sim 1$, while for larger values the two phases become completely mixed, with $f_0^{\text{eq}} \rightarrow 0.5$. Remarkably, the transition region between the two regimes is quite
narrow, centered around $\lambda \simeq 0.025$. This can be seen from Fig. 2 where we show $f_0(t)$ for $\lambda = 0.024$, 0.025, and 0.026. [The curves are noisier due to the fact that we must run for longer times in order to approach the equilibrium values of $f_0(t)$, being thus constrained to perform an ensemble average with fewer runs.]

**Figure 1:** The approach to equilibrium for several values of $\lambda$.

**Figure 2:** Fitting $f_0(\theta_c)$ to a power law at large times for $\lambda = 0.025$.

Note that for $\lambda = 0.026$, $f_0^{eq} \simeq 0.5$, while for $\lambda = 0.024$, $f_0^{eq} \simeq 0.72$. There is a pronounced change in the behavior of the system for $\lambda \simeq 0.025$. Furthermore, we find that the numerical curves can be fitted at all times by a stretched exponential,

$$f_0(t) = (1 - f_0^{eq}) \exp \left[ -\left( t/\tau_{eq} \right)^{\sigma} \right] + f_0^{eq}, \quad (14)$$

where $f_0^{eq}$ is the final equilibrium fraction and $\tau_{eq}$ is the equilibration time-scale. In Table 1 we list $\sigma$ and $\tau_{eq}$ for several values of $\lambda$. Note that for $\lambda = 0.025$ the fit is obtained at late times by a power law, (smooth curve in Fig. 5)

$$f_0(t) \mid_{\lambda=0.025} \propto t^{-k}, \quad (15)$$

with $k = 0.10(\pm 0.02)$. This slowing down of the approach to equilibrium is typical of systems in the neighborhood of a second order phase transition, being known as ‘critical slowing down’ [20]. This behavior is suggestive of a “phase transition” between two possible regimes for the system, one in which the system is well-localized in the $0$-phase, and the other in which there is a complete mixing between the two phases. Let us call these two regimes the ‘smooth’ and the ‘mixed’ regimes, respectively. [In Refs. [14] and [15] I used the terms “strong” and “weak”, respectively. The change is not to induce confusion, but simply to emphasize that the difference between the two regimes is in the amount of mixing present in the background. Strong and weak refer to the strength of the associated phase transition, although I consider the term weak first order transition a misnomer; the question is nucleation vs. spinodal decomposition and not weak vs. strong.] Before we explore this idea any further, I note that the final equilibrium fractions are insensitive to the viscosity parameter $\eta$, which reflects the coupling of the system to the thermal bath. For details,
I refer the reader to Ref. [13]. This is precisely what one expects, as the coupling to the bath should not influence the final equilibrium properties of the system, but only how fast it equilibrates.

Table 1: The values of the equilibration time-scales and the exponents for the exponential fit of Eq. [14] for several values of $\lambda$. Uncertainties are in the last digit.

Armed with these results, and invoking also the results in (2 + 1)-dimensions [14], we define the equilibrium fractional population difference

$$\Delta F_{\text{EQ}}(\theta_c) = f_0^{\text{eq}} - f_+^{\text{eq}}. \quad (16)$$

In Fig. 3 we show the behavior of $\Delta F_{\text{EQ}}$ as a function of $\lambda$. There is a clear qualitative analogy between the behavior of $\Delta F_{\text{EQ}}$ as a function of $\lambda$ and the behavior of the magnetization as a function of temperature in Ising models. Here, the order parameter is the equilibrium fractional population difference and the control parameter is $\lambda$. $\lambda_c \approx 0.025$ is the critical value for the parameter $\lambda$, which determines the degree of mixing of the system at $T_c$.

Figure 3: The fractional equilibrium population difference $\Delta F_{\text{EQ}}$ as a function of $\lambda$.

We stress that the idea here is to probe the assumption of localization within the 0-phase as the system cools to $T_c$. Our results show that if the time-scales for cooling are slower than the equilibration time-scales of the system, for $\lambda > \lambda_c$ there will be considerable phase mixing before the temperature drops below $T_c$. This result can be made quite transparent by comparing the equilibrium value of the volume-averaged field $\langle X \rangle_{\text{eq}}$, and the location of both the inflection point and the maximum of the potential with varying $\lambda$. As can be seen from Fig. 4, the narrow transition region is clearly delimited by

$$X_{\text{inf}} < \langle X \rangle_{\text{eq}} < X_{\text{max}}, \quad (17)$$

where $X_{\text{inf}}$ and $X_{\text{max}}$ are the inflection point and the maximum of the potential barrier, respectively. Note that for $\lambda \geq 0.026$, $f_0^{\text{eq}} = 0.5$ and $\langle X \rangle_{\text{eq}} = X_{\text{max}}$.  

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Recalling the information from Fig. 3, we conclude that there is a clear distinction between the ‘smooth’ and ‘mixed’ regimes. The fact that the mean-field potential used in the simulation has a barrier between the two phases does not imply that we can assume that the background is sufficiently smooth in order for homogeneous nucleation to be applicable. Thermal fluctuations, not included in the coarse-grained potential, change the character of the transition by promoting an efficient mixing between the two stable phases. In other words, the effective potential describing the true behavior of the system turns into a single-well potential with minimum at $X_{\text{max}}$ for $\lambda > \lambda_c$, even though the mean-field potential has a barrier between the two phases. Similar behavior exists in ferromagnets, where it is known that the true Curie temperature is below that predicted by mean-field theory. In order to improve on the mean-field results, one uses large N or $\varepsilon$-expansion methods, which sum over a larger class of diagrams incorporating leading infrared effects. It is possible that our results could be understood in part by using $\varepsilon$-expansion methods. However, in the next Section I will propose a different approach to studying phase mixing, based on a kinetic equation for subcritical nonperturbative fluctuations, which, I believe, are responsible for the mixing. This is a new version of the subcritical bubbles method proposed by Gleiser, Kolb, and Watkins in Ref. [21]. It will be shown that this method provides a simple and powerful way to study the background.

III. MODELING PHASE MIXING WITH SUBCRITICAL BUBBLES

As was stressed before, the computation of decay rates based on homogeneous nucleation theory assumes a smooth metastable background over which critical bubbles of the lower free energy phase will appear, grow and coalesce, as the phase transition evolves. However, as the results from the numerical simulation indicate, the assumption of smoothness is not always valid. To the skeptical reader, I point out that several condensed matter experiments indicate that homogeneous nucleation fails to describe the transition when the nucleation barrier ($\Delta S/T$) becomes too small. Furthermore, the agreement between theory and experiment has a long and problematic history [23]. Homogeneous nucleation has to be used with care, in a case by case basis. It is thus important to obtain a criterion which will allow us to specify the conditions when homogeneous nucleation theory does apply. Below I describe a simple method which does exactly that.

The basic idea is that in a hot system, not only small but also large amplitude fluctuations away from equilibrium will, in principle, be present. Small amplitude fluctuations are perturbatively incorporated in the evaluation of the finite temperature effective potential,
following well-known procedures. Large amplitude fluctuations probing the nonlinearities of the theory are not. Whenever they are important, the perturbative effective potential becomes unreliable. In an ideal world, we should be able to sum over all amplitude fluctuations to obtain the exact partition function of the model, and thus compute the thermodynamic quantities of interest. However, we can only to this perturbatively, and will always miss information coming from the fluctuations not included in its evaluation. If large amplitude fluctuations are strongly suppressed, they will not contribute to the partition function, and we are in good shape. But when are they important? We can try to approach this question avoiding complicated issues related to the evaluation of path integrals beyond the Gaussian approximation by obtaining a kinetic equation which describes the fraction of volume populated by these large amplitude fluctuations. In order to keep the treatment simple, and thus easy to apply, several assumptions are made along the way, which I believe are quite sensible. In any case, the strength of the method is demonstrated when the results are compared with the numerical experiments described before.

Large amplitude fluctuations away from equilibrium are modelled by Gaussian-profile spherically-symmetric field configurations of a given size and amplitude. They can be thought of as being coreless bubbles. Keeping with the notation of the numerical experiment, fluctuations away from the 0-phase, and into the 0-phase are written respectively as,

$$
\phi_c(r) = \phi_c e^{-r^2/R^2}, \quad \phi_0(r) = \phi_c \left(1 - e^{-r^2/R^2}\right),
$$

(18)

where $R$ is the radial size of the configuration, and $\phi_c$ is the value of the amplitude at the bubble’s core, away from the 0-phase. In previous treatments (cf. Refs. [21] and [22]), it was assumed that $\phi_c = \phi_+$, that is, that the configuration interpolated between the two minima of the effective potential, and that $R = \xi(T)$, where $\xi(T) = m(T)^{-1}$ is the mean-field correlation length. But in general, one should sum over all radii and amplitudes above given values which depend on the particular model under study. This will become clear as we go along.

Define $dn(R, \phi, t)$ as the number density of bubbles of radius between $R$ and $R + dR$ at time $t$, with amplitudes $\phi \geq \phi_c$ between $\phi$ and $\phi + d\phi$. By choosing to sum over bubbles of amplitudes $\phi_c$ and larger, we are effectively describing the system as a “two-phase” system. For example, in the numerical simulation above it was assumed that the 0-phase was for amplitudes $\phi \leq \phi_{\text{max}}$, and the +–phase was for amplitudes $\phi > \phi_{\text{max}}$. Clearly, for a continuous system this division is artificial. However, since the models we are interested in have two local minima of the free energy, this division becomes better justified. Fluctuations with small enough amplitude about the minima are already summed over in the computation of the effective potential. It is the large amplitude ones which are of relevance here. To simplify the notation, from now on I will denote by “+–phase” all fluctuations with amplitudes $\phi > \phi_c$ and larger. The choice of $\phi_c$ is model-dependent, as will be clear when we apply this formalism to specific examples.

The fact that the bubbles shrink will be incorporated in the time dependence for the
radius $R$. Here, I will only describe a somewhat simplified approach to the dynamics. More details are provided in the forthcoming paper by Gleiser, Heckler, and Kolb [25]. The results, however, are essentially identical.

The net rate at which bubbles of a given radius and amplitude are created and destroyed is given by the kinetic equation,

$$\frac{\partial n(R, t)}{\partial t} = -\frac{\partial n(R, t)}{\partial R} \left( \frac{dR}{dt} \right) + \left( \frac{V_0}{V_T} \right) \Gamma_{0\rightarrow+}(R)$$

$$- \left( \frac{V_+}{V_T} \right) \Gamma_{+\rightarrow0}(R) - \left( \frac{V_+}{V_T} \right) \Gamma_{TN}(R)$$

(19)

Here, $\Gamma_{0\rightarrow+}(R)$ ($\Gamma_{+\rightarrow0}(R)$) is the rate per unit volume for the thermal nucleation of a bubble of radius $R$ of $+-$phase within the 0-phase (0-phase within the $+-$phase). $\Gamma_{TN}(R) \simeq aT/\frac{4}{3}\pi R^3$ is the (somewhat ad hoc) expression used for the thermal destruction rate, with $a$ a constant related to the coupling to the thermal bath. $V_{0(+)0}$ is the volume available for nucleating bubbles of the $+(0)$-phase. Thus we can write, for the total volume of the system, $V_T = V_0 + V_+$, expressing the fact that the system has been “divided” into two available phases, related to the local minima of the free energy density. It is convenient to define the fraction of volume in the $+-$phase, $\gamma$, as

$$\frac{V_0}{V_T} \equiv 1 - \gamma .$$

(20)

In order to compute $\gamma$ we must sum over all bubbles of different sizes, shapes, and amplitudes within the $+-$phase, i.e., starting with $\phi_{\text{min}} \geq \phi_c$. Clearly, we cannot compute $\gamma$ exactly. But it turns out that a very good approximation is obtained by assuming that the bubbles are spherically symmetric, and with radii above a given minimum radius, $R_{\text{min}}$. The reason we claim that the approximation is good comes from comparing the results of this analytical approach with numerical simulations. The approximation starts to break down as the background becomes more and more mixed, and the morphology of the “bubbles” becomes increasingly more important, as well as other terms in the kinetic equation which were ignored. For example, there should be a term which accounts for bubble coalescence, which increases the value of $\gamma$. This term becomes important when the density of bubbles is high enough for the probability of two or more of them coalescing to be non-negligible.

As we will see, by this point the mixing is already so pronounced that we are justified in neglecting this additional complication to the kinetic equation. As a bonus, we will be able to solve it analytically. The expression for $\gamma$ is,

$$\text{Of course, the amplitude } \phi \text{ will also be time-dependent. However, its time-dependence is coupled to that of the radius, as recent studies have shown [24]. In order to describe the effect of shrinking on the population of bubbles it is sufficient to include only the time dependence of the radius.}$$
\[
\gamma \simeq \int_{\phi_{\text{min}}}^{\infty} \int_{R_{\text{min}}}^{\infty} \left( \frac{4\pi R^3}{3} \right) \frac{\partial^2 n}{\partial \phi \partial R} d\phi dR .
\]  

(21)

The attentive reader must have by now noticed that we have a coupled system of equations; \(\gamma\), which appears in the rate equation for the number density \(n\), depends on \(n\) itself. And, to make things even worse, they both depend on time. Approximations are in order, if we want to proceed any further along an analytical approach. The first thing to do is to look for the equilibrium solutions, obtained by setting \(\partial n / \partial t = 0\) in the kinetic equation. In equilibrium, \(\gamma\) will also be constant. If wished, after finding the equilibrium solutions one can find the time-dependent solutions, as was done in Ref. [22]. Here, we are only interested in the final equilibrium distribution of subcritical bubbles, as opposed to the approach to equilibrium.

The first approximation is to take the shrinking velocity of the bubbles to be constant, \(dR / dt = -v\). This is in general not the case (cf. Ref. [24]), but it does encompass the fact that subcritical bubbles shrink into oblivion. The strength of the thermodynamic approach is that details of how the bubbles disappear are unimportant, only the time-scale playing a rôle. The second approximation is to assume that the rates for creation and destruction of subcritical fluctuations are Boltzmann suppressed, so that we can write them as \(\Gamma = AT^4 e^{-F_{\text{sc}}/T}\), where \(A\) is an arbitrary constant of order unity, and \(F_{\text{sc}}(R, \phi_c)\) is the cost in free energy to produce a configuration of given radius \(R\) and core amplitude \(\phi_c\). For the Gaussian ansatz we are using, \(F_{\text{sc}}\) assumes the general form, \(F_{\text{sc}} = \alpha R + \beta R^3\), where \(\alpha = b\phi_c^2\) (\(b\) is a combination of \(\pi\)'s and other numerical factors) and \(\beta\) depends on the particular potential used. In practice, the cubic term can usually be neglected, as the free energy of small \((R \sim \xi)\) subcritical bubbles is dominated by the gradient (linear) term. We chose to look at the system at the critical temperature \(T_c\). For this temperature, the creation and destruction rates, \(\Gamma_{0 \rightarrow +}\) and \(\Gamma_{+ \rightarrow 0}\) are identical. Also, for \(T_c\), the approximation of neglecting the cubic term is very good (in fact it is better and better the larger the bubble is) even for large bubbles, since for degenerate vacua there is no gain (or loss) of volume energy for large bubbles. Finally, we use that \(V_+/V_T = \gamma\) in the \(\Gamma_{+ \rightarrow 0}\) term, and that \(V_+/V_T = n(R)V_+(R)\) in the \(\Gamma_{\text{TD}}\) term. This latter expression assumes that the distribution of bubbles is sharply peaked around the smallest bubbles considered, so that the sum over all radii is fairly well approximated by one term. A more sophisticated approach is presented in Ref. [25]. We can then write the equilibrium rate equation as,

\[
\frac{\partial n}{\partial R} = dn(R) - cf(R) ,
\]

(22)

where,

\[\text{§}\] This doesn’t mean that thermal activity in or between the two phases is frozen; equilibrium is a statement of the average distribution of thermodynamical quantities. Locally, bubbles will be created and destroyed, but always in such a way that the average value of \(n\) and \(\gamma\) are constant.
\[ d \equiv aT/v, \quad c \equiv (1 - 2\gamma)AT^4/v, \quad f(R) \equiv e^{-F_{sc}/T}. \]  

(23)

Integrating from \( R_{\text{min}} \) and imposing that \( n(R \to \infty) = 0 \), the solution is easily found to be,

\[ n(R) = \frac{c}{d + \alpha(\phi_c)/T} e^{-\alpha R/T}. \]  

(24)

Not surprisingly, the equilibrium number density of bubbles is Boltzmann suppressed. But we now must go back to \( \gamma \), which is buried in the definition of \( c \). We can solve for \( \gamma \) perturbatively, by plugging the solution for \( n \) back into Eq. 21. After a couple of fairly nasty integrals, we obtain,

\[ \gamma = \frac{g(\alpha(\phi_{\text{min}}), R_{\text{min}}))}{1 + 2g(\alpha(\phi_{\text{min}}), R_{\text{min}})}, \]  

(25)

where,

\[ g(\alpha(\phi_{\text{min}}), R_{\text{min}}) = \frac{4\pi}{3} \left( \frac{AT^4}{v} \right) \left( \frac{T}{\alpha} \right)^3 e^{-\alpha R_{\text{min}}/T} \left[ 6 + \left( \frac{\alpha R_{\text{min}}}{T} \right)^3 + 3 \frac{\alpha R_{\text{min}}}{T} \left( 2 + \frac{\alpha R_{\text{min}}}{T} \right) \right]. \]  

(26)

A. Comparison with the numerical simulations

We can now apply this formalism to any model we wish. The first obvious application is to compare \( \gamma \) obtained from the numerical experiment with the value obtained from the kinetic approach. From the definition of the equilibrium fractional population difference, Eq. 16,

\[ \Delta F_{\text{EQ}}(\theta_c) = 1 - 2\gamma. \]  

(27)

Thus, it is straightforward to extract the value of \( \gamma \) from the numerical simulations, as a function of \( \lambda \). Also, as we neglected the volume contribution to the free energy of subcritical bubbles, we have,

\[ F_{\text{sc}} = \alpha(\phi_c) R_{\text{min}} = \frac{3\sqrt{2}}{8} \pi^{3/2} X_-^2(\theta_c) R_{\text{min}}. \]  

(28)

where, as you recall, \( X_- \) is the position of the maximum of the mean-field potential used in the simulations. So, we must sum over all amplitudes with \( X \geq X_- \), and all radii with \( R \geq 1 \) (in dimensionless units), as we took the lattice spacing to be \( \ell = 1 \). That is, we sum over all possible sizes, down to the minimum cut-off size of the lattice used in the simulations. In practice, we simply substitute \( \phi_c = X_- \) and \( R_{\text{min}} = 1 \) in the expression for \( \gamma \). In Fig. 5, we compare the numerical results for \( \gamma \) (dots) with the results from the
analytical integration of the kinetic equation. We took $A/v = 1$, and the two curves are for $a/v = 0$ (no thermal destruction), and $a/v = 1$. Up to the critical value for $\lambda \simeq 0.025$, the agreement is very convincing. As we increase $\lambda$ into the mixed phase region of the diagram, the kinetic approach underestimates the amount of volume in the $\pm$-phase. This is not surprising, since for these values of $\lambda$ the density of subcritical bubbles is high enough that terms not included in the equation become important, as I mentioned before. However, the lack of agreement for higher values of $\lambda$ is irrelevant, if we are interested in having a measure of the smoothness of the background; clearly, the rise in $\gamma$ is sharp enough that homogeneous nucleation should not be trusted for $\lambda > 0.024$ or so, as the fraction of volume occupied by the $\pm$-phase is already around 30% of the total volume. Subcritical bubbles give a simple and quantitatively accurate picture of the degree of inhomogeneity of the background, offering a guideline as to when homogeneous nucleation theory can be applied with confidence.

**Figure 5**: Comparison between results from numerical simulations (dots) and the result from the kinetic equation.

### B. Thermal Phase Mixing in the Standard Electroweak Model

It is straightforward to compute $\gamma$ for the electroweak model. One can choose any effective potential, and simply plug the results into Eq. 25. Here, I will work with the simplest version of the model, the unimproved 1-loop potential, written in Eq. 10. Clearly, different effective potentials will give different values for $\gamma$. So, if we used instead the 2-loop potential of Ref. [26], we would obtain smaller values for $\gamma$, as the two-loop potential gives rise to a stronger transition. The point here is not to get into the problems of computing a reliable effective potential, but to apply the method just developed to a simple situation.

There have been several recent papers on applying subcritical bubbles to different effective potentials or exploring some of their properties [27]. In my view, there are two important points which seem to be overlooked in most (but not all) of these works. First, the importance of subcritical bubbles is sensitive to the parameters of the model. If one finds that subcritical bubbles are not relevant for a given range of parameters, this does not mean that they are ruled out as unphysical. It simply means that they will be relevant for a different range (usually higher Higgs masses if one is interested in the electroweak phase transition); hot systems fluctuate, even if our description of the physics through a perturbative effective potential may be inaccurate. For the particular case of the electroweak transition, we ea-
gerly await for lattice gauge simulations which will probe the regime of higher Higgs masses. Second, approaches that use a saddle-point evaluation of the partition function to compute, say, the dispersion of the field around the background, will miss the important contributions coming from large amplitude fluctuations. Thus, they will underestimate the amount of mixing. This is an advantage of the kinetic approach presented here.

Using the parameters for the electroweak model, we can express $\gamma$ in terms of the Higgs mass, as shown in Fig. 6. I took $R_{\text{min}} = \xi(T_c)$, and $\phi_c = \phi_+(T_c)$. Again, the results are sensitive to the choice of minimum radius and amplitude, but these values are certainly conservative. It is clear from the Figure that taking $v = 1$, $\gamma$ changes sharply from 0 to 0.5 for $60 < M_{\text{Higgs}} < 70$, the window where lies the present lower bound on the Higgs mass. Thus, these results appear to rule out nucleation for the unimproved 1-loop effective potential\footnote{There is a volume factor which suppresses $\gamma$ not included here; simply, not all of the subcritical bubble is in the $+$-phase, just a fraction of it. However, this suppression is compensated by taking the more realistic choice $\phi_c = \phi_{\text{max}}$, as opposed to the conservative choice $\phi_c = \phi_+$ we used.}. Mechanisms for baryogenesis based on homogeneous nucleation must take the mixing of the background due to subcritical fluctuations into account.

**Figure 6**: Thermal phase mixing for the minimal electroweak model as a function of the Higgs mass.

**IV. CONCLUDING REMARKS**

In this talk I presented the results of both numerical simulations and analytical modelling of phase mixing induced by thermal fluctuations. Although I stressed mostly the importance of these results in the context of homogeneous nucleation in finite temperature field theory, the ideas presented here can be adapted to a variety of different situations of interest also in laboratory applications, as long as the system in question can be described by a coarse-grained Ginzburg-Landau free energy with a non-conserved order parameter. For example, together with Andrew Heckler, a method to compute the influence of subcritical bubbles on the nucleation rate is presently being developed, which, we believe, is quite general\footnote{There is a volume factor which suppresses $\gamma$ not included here; simply, not all of the subcritical bubble is in the $+$-phase, just a fraction of it. However, this suppression is compensated by taking the more realistic choice $\phi_c = \phi_{\text{max}}$, as opposed to the conservative choice $\phi_c = \phi_+$ we used.}. **

**\footnote{There is a volume factor which suppresses $\gamma$ not included here; simply, not all of the subcritical bubble is in the $+$-phase, just a fraction of it. However, this suppression is compensated by taking the more realistic choice $\phi_c = \phi_{\text{max}}$, as opposed to the conservative choice $\phi_c = \phi_+$ we used.}
The basic idea is to include the available free energy in the gas of subcritical bubbles in the computation of the effective nucleation barrier. In practice, this is done by obtaining a new coarse-grained effective action which sums over fluctuations of subcritical size, in the spirit of the renormalization group. Comparing the results from our method to numerical simulations of nucleation in 2 dimensions (Ref. [18]) shows how subcritical fluctuations can account for a dramatic drop in the effective nucleation barrier which is observed close to degeneracy.

I hope it was clear from this talk that subcritical bubbles can provide a clear and quantitatively accurate description of the degree of homogeneity of a given background, metastable or not. It would be interesting to generalize the ideas presented here to quantum fluctuations as well, since we should expect them to be dominant at very low temperatures. Naively, we could think of quantum subcritical bubbles as nonperturbative violations of energy conservation, with a probability distribution suppressed by their Euclidean action. If present, these fluctuations could have many interesting consequences, from inflationary scenarios to nucleation of topological defects in systems with nontrivial vacuum topology.

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| $\lambda$ | $\tau_{EQ}$ | $\sigma$ |
|----------|-------------|---------|
| 0.015    | 25.0        | 1.0     |
| 0.020    | 45.0        | 1.0     |
| 0.022    | 60.0        | 1.0     |
| 0.024    | 110.0       | 0.80    |
| 0.026    | 220.0       | 0.50    |
| 0.028    | 120.0       | 0.75    |
| 0.030    | 100.0       | 0.80    |
| 0.035    | 55.0        | 0.80    |
| 0.040    | 40.0        | 0.90    |
