Coarse Graining and First Order Phase Transitions

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Abstract

We discuss the dependence of the coarse grained free energy and the classical interface tension on the coarse graining scale $k$. A stable range appears only if the renormalized dimensionless couplings at the critical temperature are small. This gives a quantitative criterion for the validity of computations within Langer’s theory of spontaneous bubble nucleation.

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The discussion of the dynamics of a first order phase transition \[1\] usually relies on the study of a non-convex potential or free energy. The decay of unstable minima is associated either with tunneling fluctuations through barriers in the potential \[2\], or, at non-zero temperature, with thermal fluctuations above them \[3\]. However, the effective potential \[4\], which seems at first sight a natural tool for such studies, is expected to be a convex quantity with no barrier. The resolution of this paradox lies in the realization that the effective potential is convex because the tunneling or thermal fluctuations are incorporated in it. These fluctuations are associated with low frequency modes, while the non-convex part of the potential is related to the classical potential and the integration of high frequency modes. A natural approach to the study of first order phase transitions separates the problem in two parts. First, the high frequency modes are integrated out, with the possible generation of new minima through radiative symmetry breaking \[3\]. Subsequently, the decay of unstable minima is discussed with semiclassical techniques \[2, 3\], in the non-convex potential that has resulted from the first step. This leads us to the notion of the coarse grained free energy, which is fundamental in statistical physics. Every physical system has a characteristic length scale associated with it. The dynamics of smaller length scales is integrated out, and is incorporated in the parameters of the free energy one uses for the study of the behavior at larger length scales.

The notion of coarse graining is absent in the perturbative approach to the calculation of the effective potential \[3\]. This is the main reason for the non-convergence of the perturbative series near the maxima of the classical potential, and the appearance of imaginary parts in the perturbative effective potential. Despite attempts to give a physical interpretation to these imaginary parts \[3\], a satisfactory discussion of tunneling must incorporate the notion of coarse graining. The Wilson approach to the renormalization group provides the appropriate framework \[7\]. We employ here the method of the effective average action \(\Gamma_k\) \[8\], which results from the integration of fluctuations with characteristic momenta larger than a given scale \(k\). The dependence of \(\Gamma_k\) on \(k\) is described by an exact renormalization group equation \[8, 9\]. For large values of \(k\) (of the order of the ultraviolet cutoff \(\Lambda\) of the theory) the effective average action is equal to the classical action (no fluctuations are integrated out), while for \(k \to 0\) it becomes the standard effective action (all fluctuations are integrated out). For non-zero \(k\) the effective average action has the properties of a coarse grained free energy. Its non-derivative part (the effective average potential \(U_k\)) is not necessarily convex. The coarse graining scale can be identified with \(k\).

In this letter we provide an explicit demonstration of how such a potential can be obtained starting from the microscopic or classical action of a field theory. We investigate the dependence of the effective average potential \(U_k\) and the ‘classical’ surface tension \(\sigma_k\) on the coarse graining scale \(k\) with special emphasis on the question of the validity of Langer’s theory of bubble formation. We study the first order phase transitions for the Abelian Higgs model and for a scalar matrix model in three dimensions. An application of the formalism to the case of the high temperature phase transitions for the Abelian and

\[1\] For related work see \[3, 4, 11\].
SU(2) Higgs models is given in ref. [12] and a discussion of the first order phase transition in matrix models can be found in ref. [13].

Near a phase transition, the three dimensional Abelian Higgs model describes the behavior of ordinary superconductors [14]. It can also be viewed as the effective theory resulting from the non-zero temperature four dimensional model near the critical temperature. The dependence of the effective average potential $U_k(\rho)$ and the running renormalized gauge coupling $e_R(k)$ on the coarse graining scale $k$ is governed by the evolution equations [9]

\[
\frac{\partial U_k(\rho)}{\partial t} = \int \frac{d^3q}{2(2\pi)^3} \frac{\partial P_k}{\partial t} \left( \frac{1}{P_k(q) + U_k'(\rho) + 2U_k''(\rho)\rho} \right.
\]

\[
+ \left. \frac{1}{P_k(q) + U_k'(\rho)} \right. + \frac{2}{P_k(q) + 2e_R^2(k)\rho},
\]

\[
\frac{de_R^2(k)}{dt} = \frac{0.84 e_R^4(k)}{6\pi^2} \frac{1}{k},
\]

where $t = \ln(k/\Lambda)$ (with $\Lambda$ the ultraviolet cutoff of the theory) and $\rho = |\phi|^2/2$ (with $\phi$ the complex order parameter). Primes denote derivatives with respect to $\rho$. The three terms on the r.h.s. correspond to the contributions of the radial and Goldstone scalar modes and the gauge field. The inverse propagator

\[
P_k(q) = \frac{q^2}{1 - \exp(-q^2/k^2)}
\]

provides for an infrared cutoff which acts like a mass term $\sim k^2$ for the modes with $q^2 \ll k^2$, while it leaves unaffected the modes with $q^2 \gg k^2$. The momentum integral on the r.h.s. of eq. (1) can be written in terms of dimensionless functions $l^3_0(w)$, whose arguments are given by the rescaled mass terms $(U_k'(\rho) + 2U_k''(\rho)\rho)/k^2$, $U_k'(\rho)/k^2$ and $2e_R^2(k)\rho/k^2$. These functions fall off for large values of $w$, following a power law. As a result they introduce threshold behavior, which leads to the decoupling of massive modes from the evolution equations [8, 15, 16]. The derivation of eq. (1) under some approximations, starting from the exact renormalization group equation for the effective average action, is given in ref. [9, 14, 12]. The approximations concern the omission of the anomalous dimension of the scalar field, the effective field dependence of the gauge coupling and the higher derivative terms in the action. The evolution starts at $k = \Lambda$, where the effective average potential is equal to the microscopic or classical one $U_\Lambda(\rho) = \frac{1}{2}\lambda_\Lambda(\rho - \rho_0\Lambda)^2$ and the running gauge coupling is equal to the bare coupling $\bar{e}_\Lambda$. In the opposite limit $k \to 0$, $U_k(\rho)$ becomes equal to the (convex) effective potential $U(\rho) = U_0(\rho)$ and the gauge coupling assumes its renormalized value $e_R = e_R(k = 0)$. Two algorithms for the numerical integration of eq. (1) have been presented in detail [17]. The phase transition is approached by fixing $\lambda_\Lambda$ and $e_R$ and tuning $\rho_0\Lambda$. The system exhibits a second order phase transition for $\bar{e}_\Lambda = 0$ which corresponds to the Wilson-Fisher fixed point of the $O(2)$ symmetric Heisenberg model. For large enough $\bar{e}_\Lambda^2/\lambda_\Lambda$ the phase transition is first order [18, 14, 12].
In fig. 1 we display the solution of eq. (1) for $\bar{\lambda} = 0.01\Lambda$, $\bar{\epsilon}^2 = 0.1\Lambda$ and $\rho_{0\Lambda} \simeq 0.867\Lambda$. All the quantities in the figures are expressed in units of the ultraviolet cutoff $\Lambda$. Initially the potential has only one minimum away from the origin, which evolves proportionally to the coarse graining scale $k$. At some point a new minimum appears at the origin. It is induced by the integration of fluctuations, through the generalization of the Coleman-Weinberg mechanism. The evolution slows down at the later stages, and for $k/\Lambda$ around 0.02 the potential converges towards a stable non-convex profile with two minima of equal depth. Around the minima the scale $k$ becomes smaller than the mass of the various massive modes, and this induces their decoupling. We have stopped the evolution at a non-zero $k_f$, for which the shape of the potential near the minima is stable. The presence of the non-convex part is explained by this non-zero value of $k$. We have not yet integrated out all the fluctuations, which should render the effective potential convex. More specifically, the fluctuations which interpolate between the two minima of fig. 1 are not included effectively in the non-convex potential. They are the ones that trigger the tunneling and drive the first order phase transition. If we continue the evolution all the way to $k = 0$, these interpolating configurations will be gradually integrated out. As a result, the height of the barrier will start getting smaller, until the region of the potential between the two minima becomes flat. The evolution of the characteristics of the potential is depicted in fig. 2. We plot the location of the minimum away from the origin $\rho_{\min}$, the value of the potential at the minimum $(U_k)_{\min}$, the location of the maximum $\rho_{\max}$, the value of the potential $(U_k)_{\max}$ and the curvature $(d^2U_k/d\phi^2)_{\max} = U''(\rho_{\max}) + 2p_{\max}U''_k(\rho_{\max})$ at the maximum. We observe that these parameters have almost constant values in the region $k/\Lambda \simeq 0.02 - 0.03$.

In fig. 3 and 4 we present the effective average potential and its characteristics for parameters corresponding to a weaker first order transition. For $\bar{\lambda} = 0.1\Lambda$, $\bar{\epsilon}^2 = 0.1\Lambda$ and $\rho_{0\Lambda} \simeq 0.171\Lambda$ the discontinuity in the scalar field expectation value is about nine times smaller than for fig. 1. The most important difference is that the potential never becomes relatively stable for a range of $k$. During the later stages of the evolution, its outer part (for scalar field values larger than the location of the minimum) starts approaching a stable profile, due to the decoupling of the massive modes in this region. However, in the same range of $k$ the non-convex part starts already becoming flatter, as configurations interpolating between the two minima are being integrated out. The negative curvature at the top of the barrier is expected to behave $\sim -k^2$ during this stage. This has been verified explicitly through the analytical integration of the evolution equation for the $O(N)$ symmetric scalar theory in the large $N$ limit. We clearly observe the onset of this behavior of $d^2U/d\phi^2$ in fig. 4 in a range of $k$ before $\rho_{\min}$ settles. Also the maximum of $U_k$ decreases before the minimum settles. In this case it is far from obvious which coarse graining scale $k$ should be chosen for a definition of important nucleation characteristics such as the interface tension.

The behavior of the coarse grained effective potential for a fluctuation induced first order phase transition, as considered above, is not particular to the Abelian Higgs model. For example, our discussion can be extended with minor modifications to the electroweak phase transition for the range of Higgs-scalar masses where it is first order. It also
can be observed in pure scalar theories. One may consider models with $U(N) \times U(N)$ symmetry with a scalar field in the $(\bar{N}, N)$ representation, described by a complex $N \times N$ matrix $\phi$. The cases $N = 2, 3$ have an interesting relation to high temperature strong interaction physics and chiral symmetry breaking and non-perturbative flow equations have been studied in this context. We will concentrate here on $N = 2$. The most general effective average potential $U_k(\rho, \tau)$ can then be expressed as a function of only two invariants, namely

$$\rho = \text{tr} \left( \phi^\dagger \phi \right), \quad \tau = 2 \text{tr} \left( \phi^\dagger \phi - \frac{1}{2} \rho \right).$$

(3)

The microscopic or classical potential $U_\Lambda$ for these models can be characterized by two quartic couplings $\bar{\lambda}_{1A}, \bar{\lambda}_{2A}$ and a mass term ($\bar{\mu}_A^2 > 0$),

$$U_\Lambda(\rho, \tau) = -\bar{\mu}_A^2 \rho + \frac{1}{2} \bar{\lambda}_{1A} \rho^2 + \frac{1}{4} \bar{\lambda}_{2A} \tau.$$

(4)

In the limit $\bar{\lambda}_{1A} \to \infty, \bar{\lambda}_{2A} \to \infty$ this also covers the model of unitary matrices. One observes two symmetry breaking patterns for $\bar{\lambda}_{2A} > 0$ and $\bar{\lambda}_{2A} < 0$ respectively. The case $\bar{\lambda}_{2A} = 0$ denotes the boundary between the two phases. In this special case the theory exhibits an enhanced $O(8)$ symmetry and one finds a second order phase transition. For the symmetry breaking pattern $U(2) \times U(2) \to U(2)$ ($\bar{\lambda}_{2A} > 0$) the phase transition is always first order. In this case the relevant information for the phase transition is contained in $U_k(\rho) \equiv U_k(\rho, \tau = 0)$. The discussion of the dependence of the effective average potential $U_k(\rho)$ on the coarse graining scale $k$ can be presented along the same lines as for the Abelian Higgs model and the relevant flow equations can be found in ref. [13]. Here the second quartic coupling $\bar{\lambda}_{2A}$ for the scalar model plays the role of the gauge coupling $\bar{e}_A^2$ in the Abelian Higgs model. In addition to the above treatment of the Abelian Higgs model, the employed approximation for the scalar model takes into account a $k$-dependent wave function renormalization constant $Z_k$ for the fields and the effective field dependence of the second quartic coupling.

In the following we will use the scalar matrix model to establish a quantitative criterion for the validity of the standard treatment of spontaneous bubble nucleation as described by Langer’s theory [1]. Langer’s approach relies, on the one hand, on the definition of a suitable coarse grained free energy $\Gamma_k$ with a coarse graining scale $k$ and, on the other hand, on a saddle point approximation for the treatment of fluctuations around the ‘critical bubble’. The problem is therefore separated in two parts: The first part concerns the treatment of fluctuations with momenta $q^2 \gtrsim k^2$ which are included in the coarse grained free energy. The second part deals with an estimate of fluctuations around the bubble, for which only fluctuations with momenta smaller than $k$ must be considered.

To be explicit we consider a spherical bubble where the bubble wall with thickness $\Delta$ is thin as compared to the bubble radius $R$, i.e. $\Delta \ll R$. In this thin wall approximation the bubble nucleation rate $\Gamma$, which describes the probability per unit volume per unit time for the transition to the new vacuum, can be written in the form [3, 2]

$$\Gamma = A_k \exp \left( -\frac{16\pi}{3} \frac{\sigma^2}{e^2} \right).$$

(5)
Here the ‘classical’ surface tension $\sigma_k$ is given in our conventions by

$$\sigma_k = 2 \int_0^\varphi d\varphi \sqrt{2Z_k U_k(\varphi)}$$

(6)

where $\varphi = (\rho/2)^{1/2}$ and $\varphi$ denotes the second zero of $U_k(\varphi)$ near the outer minimum at $\varphi_{\text{min}}$. For the difference in the free energy density $\epsilon$ we include fluctuations with arbitrarily small momenta,

$$\epsilon = \lim_{k \to 0} (U_k(0) - U_k(\varphi_{\text{min}})).$$

(7)

In contrast, the long wavelength contributions to the true surface tension are effectively cut off by the characteristic length scale of the bubble surface. For the free energy of the critical bubble the modes with $q^2 \gtrsim k^2$ are incorporated in $\Gamma_k^{(0)}=16\pi\sigma_k^2/3e^2$ (lowest order or classical contribution) and they influence $\sigma_k$. The modes with $q^2 \lesssim k^2$ contribute to the ‘fluctuation determinant’ $A_k$, which also contains dynamical factors. Here $A_k$ depends on $k$ through the effective ultraviolet cutoff for these fluctuations, which is present since fluctuations with momenta larger than $k$ are already included in $\Gamma_k^{(0)}$. A more general discussion which does not rely on the thin wall approximation or a saddle point approximation is given in ref. [13]. Langer’s formula for bubble nucleation amounts essentially to a perturbative one loop estimate of $A_k$. It is clear that $k$ is only a technical construct and for physical quantities like the bubble nucleation rate the $k$-dependence of $\ln A_k$ and $\Gamma_k^{(0)}$ must cancel. A strong dependence of $\sigma_k$ on the coarse graining scale $k$ is only compatible with a large contribution from the higher orders of the saddle point expansion. The $k$-dependence of $\sigma_k$ therefore gives direct information about the convergence of the saddle point approximation and the validity of Langer’s formula.

We consider in detail the dependence of the surface tension $\sigma_k$ on the coarse graining scale $k$ at the phase transition ($\epsilon = 0$) for three examples. They are distinguished by different choices for the quartic couplings $\lambda_1\Lambda$ and $\lambda_2\Lambda$ of the short distance potential $U_\Lambda$ given by eq. (4). The choice $\lambda_1\Lambda/\Lambda = 0.1$, $\lambda_2\Lambda/\Lambda = 2$ corresponds to a strong first order phase transition with renormalized masses not much smaller than the cutoff scale $\Lambda$. In this case the $k$-dependence of the effective average potential resembles the one presented in fig. 1. In contrast we give two examples where the dependence of $\sigma_k$ on the coarse graining scale becomes of crucial importance. The choice $\lambda_1\Lambda/\Lambda = 2$, $\lambda_2\Lambda/\Lambda = 0.1$ leads to a weak first order phase transition with small renormalized masses and the behavior of the effective average potential is similar to the one given in fig. 3. The coarse grained potential and the surface tension show a high sensitivity on the scale $k$. A more increased sensitivity on the scale $k$ can be observed for $\lambda_1\Lambda/\Lambda = 4$, $\lambda_2\Lambda/\Lambda = 70$ which corresponds to a relatively strong first order phase transition.

The $k$-dependence of the surface tension $\sigma_k$ is displayed in fig. 5. Here $\sigma_k$ is normalized to its maximum value $\sigma_*$ where $\sigma_*/\Lambda^2 = 1.67 \times 10^{-2}(8.41 \times 10^{-11})(1.01 \times 10^{-3})$ for $\lambda_1\Lambda/\Lambda = 0.1(2)(4)$, $\lambda_2\Lambda/\Lambda = 2(0.1)(70)$. The scale $k_f$ is given by $|m_{\text{max}}|$ with

$\sigma_k$ the true surface tension is a ‘measurable quantity’. It is independent of $k$ and all fluctuations must be included. It therefore differs, in general, from $\sigma_k$ which includes only part of the fluctuations.
\[ m_{\text{max}}^2 = 2Z^{-1} \rho_{\text{max}} (\partial^2 U_k / \partial \rho^2) (\rho_{\text{max}}) \] denoting the renormalized mass term at the top of the potential barrier \( \rho_{\text{max}} \). More precisely, we chose \((k_f^2 - |m_{\text{max}}^2(k_f)|)/k_f^2 = 0.01\). For \( \lambda_1/\Lambda = 0.1, \lambda_2/\Lambda = 2 \) the curve exhibits a small \( k \)-dependence around its maximum and \( \sigma_* \simeq \sigma_{k_f} \). For the second and the third example one observes that \( \sigma_{k_f} \) becomes considerably smaller than the maximum value due to a strong \( k \)-dependence. The coarse graining scale \( k \) should not be taken smaller than the inverse bubble wall thickness \( \Delta^{-1} \). This ensures that the detailed properties of the bubble are irrelevant for the computation of the ‘classical’ surface tension \( \sigma_k \). We estimate the bubble wall thickness \( \Delta \) by

\[ \Delta = 2Zk \rho_{\text{min}} / \sigma_k \tag{8} \]

where we have taken the gradient energy as half the total surface energy and approximated the mean field gradient at the bubble wall by \( \varphi_{\text{min}} / \Delta \). For the given examples we observe \( \Delta^{-1}(k_f) \simeq k_f/4 \). We choose \( k \simeq k_f \) as the coarse graining scale.

In order to quantify the differences between the three examples we have displayed some characteristic quantities in the table. The renormalized couplings

\[ \lambda_{1R} = Z k_f^{-2} \frac{\partial^2 U_{k_f}}{\partial \rho^2} (\rho_{\text{min}}), \quad \lambda_{2R} = 4Z k_f^{-2} \frac{\partial U_{k_f}}{\partial \tau} (\rho_{\text{min}}) \tag{9} \]

are normalized with respect to the mass term

\[ m_{\text{R}}^c = (2Zk \rho_{\text{min}} \lambda_{1R})^{1/2}. \tag{10} \]

In addition we give the mass term

\[ m_{2R}^c = (Zk \rho_{\text{min}} \lambda_{2R})^{1/2} \tag{11} \]

corresponding to the curvature of the potential in the direction of the second invariant \( \tau \). All couplings and masses are evaluated at the critical temperature (critical \( \rho_{0A} \)). In comparison with fig. 5 one observes in the vicinity of \( k_f \) a weaker scale dependence of \( \sigma_k \) for smaller effective couplings. In particular, a reasonably weak scale dependence of \( U_k \) and \( \sigma_k \) requires

\[ \lambda_{1R} / m_{\text{R}}^c \ll 1. \tag{12} \]

This establishes a quantitative criterion for the range where Langer’s theory can be used without paying too much attention to the precise definition of the coarse graining. In the table we also present \( k_f / \Lambda \) and the renormalized masses in units of \( \Lambda \), which indicate the strength of the phase transition. In particular, for the relatively strong phase transition of the third example with slightly larger effective couplings one observes an increased scale dependence as compared to the weak phase transition of the second example. This clearly shows that the ‘strength’ of the phase transition is, in general, not the primary criterion for the applicability of Langer’s theory.

In addition to the dependence on \( k \), the coarse grained free energy depends also on the precise shape of the infrared cutoff function or the inverse average propagator \( P_k(q) \).
given by eq. (2). Analytical studies in the Abelian Higgs model indicate [22] that this scheme dependence is rather weak for the effective potential and the surface tension.

In summary, we have shown that the coarse grained free energy cannot be defined without detailed information on the coarse graining scale $k$ unless the effective dimensionless couplings are small at the phase transition. For Abelian and non-Abelian gauge theories with a small gauge coupling at the scale $k = \Lambda$ this coincides with a relatively strong first order transition. Only for small couplings a range with a weak $k$-dependence of the classical surface tension appears. There is a close relation between the dependence of the coarse grained free energy on the coarse graining scale and the reliability of the saddle point approximation in Langer’s theory of bubble nucleation. For a strong $k$-dependence of $U_k$ a small variation in the coarse graining scale can induce large changes in the predicted nucleation rate in lowest order in a saddle point approximation. In this case the $k$-dependence of the prefactor $A_k$ has also to be computed. Therefore, for strong dimensionless couplings a realistic estimate of the nucleation rate needs the capability to compute $\ln A_k$ with the same accuracy as $16\pi \sigma_3^3/3\epsilon^2$ and a check of the cancelation of the $k$-dependence in the combined expression (3). Our observation that the details of the coarse graining prescription become less important in the case of small dimensionless couplings is consistent with the fact that typically small couplings are needed for a reliable saddle point approximation for $A_k$. 

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Figures

1. Evolution of the potential for a strongly first order phase transition.

2. Characteristics of the potential for a strongly first order phase transition in dependence on the coarse graining scale $k$.

3. Evolution of the potential for a weakly first order phase transition.

4. Characteristics of the potential for a weakly first order phase transition in dependence on the coarse graining scale $k$.

5. The normalized surface tension $\sigma_k/\sigma_*$ as a function of $\ln(k/k_f)$. The short distance parameters are (1) $\bar{\lambda}_{1A}/\Lambda = 0.1$, $\bar{\lambda}_{2A}/\Lambda = 2$, (2) $\bar{\lambda}_{1A}/\Lambda = 2$, $\bar{\lambda}_{2A}/\Lambda = 0.1$, (3) $\bar{\lambda}_{1A}/\Lambda = 4$, $\bar{\lambda}_{2A}/\Lambda = 70$.

Table

1. Effective dimensionless renormalized couplings $\lambda_{1R}/m_R^c$ and $\lambda_{2R}/m_R^c$ at the phase transition. The critical couplings and mass terms $m_R^c$, $m_{2R}^c$ are evaluated at the scale $k_f$.

| $\lambda_{1A}/\Lambda$ | $\lambda_{2A}/\Lambda$ | $\lambda_{1R}/m_R^c$ | $\lambda_{2R}/m_R^c$ | $m_R^c/\Lambda$ | $m_{2R}^c/\Lambda$ | $k_f/\Lambda$ |
|------------------------|------------------------|-----------------------|-----------------------|-----------------|-------------------|---------------|
| 0.1                    | 2                      | 0.228                 | 8.26                  | $1.55 \times 10^{-1}$ | $6.62 \times 10^{-1}$ | $1.011 \times 10^{-1}$ |
| 2                      | 0.1                    | 0.845                 | 15.0                  | $2.04 \times 10^{-5}$ | $6.10 \times 10^{-5}$ | $1.145 \times 10^{-5}$ |
| 4                      | 70                     | 0.980                 | 16.8                  | $6.96 \times 10^{-2}$ | $2.04 \times 10^{-1}$ | $3.781 \times 10^{-2}$ |
\[ \frac{\sigma_k}{\sigma_*} = \frac{\ln \left( \frac{k}{k_f} \right)}{1} (1) (2) (3) \]