Numerical analysis of bubble nucleation processes for first-order phase transitions within quantum fields
by David Adrian Samuel

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Physics
Montana State University

Abstract:
The well established links between statistical mechanics and quantum field theory have resulted in the extension of the theory of phase transitions to quantum fields. Within this framework first-order phase transition rates for quantum fields have traditionally been calculated via the Coleman "thin-wall" approximation. This approximation scheme is claimed to have validity in the situation where a first-order phase transition takes place between two nearly degenerate vacuum (ground) states.

It is the purpose of this dissertation to make a comprehensive study of the range of validity of the "thin-wall" approximation via a comparison of its results with exact results obtained numerically. It is found that both in the absence of gravity and the presence of gravity the "thin-wall" approximation has a very restricted range of validity, and that it characteristically overestimates the phase transition rate. A new approximation scheme is presented which considerably improves upon the original "thin-wall" approximation, yet requires roughly the same degree of calculation effort as the original "thin-wall". approximation.

The numerical analysis of first-order phase transitions within quantum fields is also extended to regimes not applicable to the "thin-wall" approximation in a search for new physical effects. An evolution from the "thin-wall" tunneling mode to the Hawking-Moss tunneling mode is observed for the decay from a de Sitter spacetime to a Minkowski spacetime. For the decay from Minkowski spacetime to an anti-de Sitter spacetime, the "thin-wall" approximation is seen to over-estimate the size of the "forbidden region" (predicted within the "thin-wall" approximation) in which the transition is not allowed.

The effect of gravitationally compact objects upon vacuum phase transitions is considered within a perturbative analysis. It is found that they may act as nucleation sites for first-order phase transitions. The nucleation rate is. maximized when the size of the gravitationally compact object is comparable to the size of the nucleating bubble associated with the phase transition.

Some astrophysical applications of first-order vacuum phase transitions are analyzed. In particular, the post-nucleation evolution of a bubble of "new" phase; together with a relationship between the number density of possible astrophysical nucleation sites within the Universe (e.g., microscopic black-holes) and the mass of fermions within the Standard Model.

NUMERICAL ANALYSIS OF BUBBLE NUCLEATION PROCESSES FOR FIRST-ORDER PHASE TRANSITIONS WITHIN QUANTUM FIELDS

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A thesis submitted in partial fulfillment
of the requirements for the degree

of

Doctor of Philosophy

in

Physics

MONTANA STATE UNIVERSITY
Bozeman, Montana

December 1991

APPROVAL

of a thesis submitted by

David Adrian Samuel

This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

18 December 1991
Date

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18 December 1991
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Approved for the College of Graduate Studies

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Date 18 December 1991

ACKNOWLEDGMENTS

I wish to express my appreciation to Dr. William Hiscock, my advisor. His helpfulness during my graduate studies at Montana State University has been unending. It is a position of privilege to have an advisor who allows one to have intellectual freedom but who can also provide direction when needed. I would also like to thank Dr. Hiscock for his financial support, through a research assistantship from his National Science Foundation grant.

My studies in relativity and quantum field theory, at the Physics Department of Montana State University, have also benefited from discussions with Dr. Lee Lindblom, Dr. John Mc.Laughlin, and Dr. Paul Anderson.

I am indebted to Dr. Lane Hughston for initially introducing me to quantum field theory and relativity, at Lincoln College, Oxford, and for his continued guidance and stimulating conversations over the past several years.

Finally, I would like to express gratitude to my wife, Julia, for enduring an increasingly absent husband during my writing of this dissertation !

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CHAPTER 1

INTRODUCTION

VACUUM - empty space; specifically, an enclosed space devoid of matter...

" The Encyclopedia Britannica"

How arid the vacuum used to be! Fortunately, the arrival of quantum field theory has brought with it a dynamic life for the vacuum. No longer do we think of the vacuum as empty space but rather as a sea of virtual particles, a medium capable of transition, and the stage for particle physics and cosmology. In some ways we may think of it as the long sought after "aether" of the nineteenth century.

Under the classical definition of the vacuum the question of stability was not an issue. How may one question the stability of emptiness? Perhaps this may be the subject for some esoteric philosophical argument but it is certainly not a physical issue. However, such a question has been thrown into the physicists' arena with the introduction of quantum field theory. Though the vacuum may be classically stable it is possible that it may undergo some form of quantum decay. The emission of an alpha particle from a radioactive nucleus provides us with a loose analogy here. Classically, the nucleus should be stable and the alpha particle bound to it by a potential barrier; however, quantum theory allows for tunneling through the barrier and the resultant escape of the alpha particle. Quantum field theory allows for the association of potentials with the various quantum fields in nature. Such potentials may also have "barriers" similar to those which bind alpha particles to nuclei, and quantum tunneling of the field through the potential barrier may then be a possibility.

Within the framework of quantum field theory, a vacuum is defined as being the ground state for the quantum fields, where the ground state is defined to be a local minimum of the associated field potential. Within this picture the "sea of virtual particles" may be thought of as the quantum fluctuations of the field about the ground state. If a potential has more than one local minimum then there are multiple ground states available to the field. Multiple ground states would mean, by definition, multiple vacuum states. Thus it is necessary for us to make some form of distinction between these possible multiple vacuum states. We shall refer to the vacuum state with the lowest potential energy as the "true vacuum". Under the assumption that the potential is bounded from below, the true vacuum will have absolute stability, i.e., stability against quantum decay as well as classical stability. The remaining vacuum states shall be referred to as "false vacua"; such vacua enjoy only classical stability. Figure 1 illustrates these ideas.

The picture of false vacuum states separated from the true vacuum by potential barriers, with the resultant decay of the false vacua, has a very close analogy in another branch of physics, notably the theory of first order phase transitions in thermodynamic systems. A first order phase transition may be associated with the presence of a potential barrier separating the two ground (vacuum) states within the transition. When this barrier is absent then the phase transition becomes second (or higher) order.

The condensation of gases to form liquids, the onset of ferromagnetism and even the everyday appearance of bubbles of carbon dioxide in a newly opened bottle of soda are examples of first order phase transitions. The important common characteristic here is that the transition occurs via nucleation of bubbles of the new phase within the medium of the old phase.

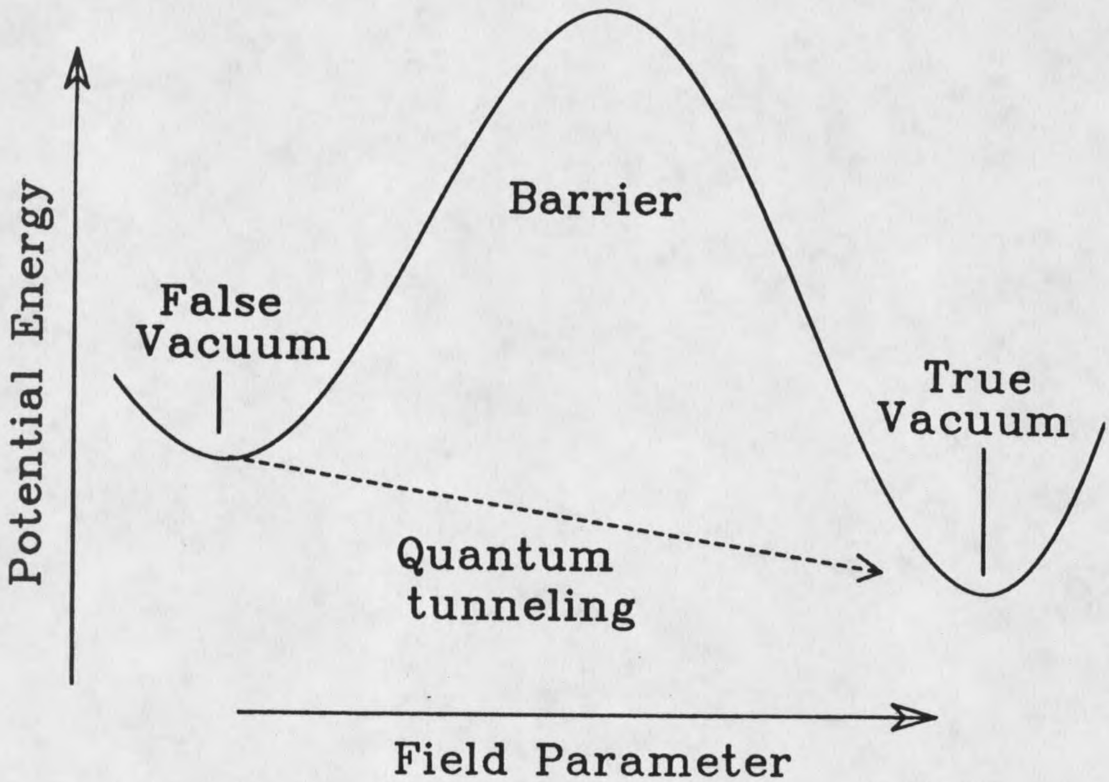

Figure 1 Decay from a false vacuum state to the true vacuum state. The potential barrier separating the false vacuum from the true vacuum allows for classical stability of the false vacuum, but quantum barrier penetration results in its eventual decay to the true vacuum state.

The links between quantum field theory and statistical mechanics are well established (see, for example, Allen (1986)). As a result, first order phase transitions for the decay of false vacua associated with quantum fields will proceed in a similar manner to first order phase transitions in everyday matter. Bubbles of new phase will be nucleated via quantum fluctuations rather than statistical fluctuations, but there will otherwise be very little difference.

When considering phase transitions in everyday matter we usually do not consider the effects of gravity. In the absence of gravity we are free to choose the zero level of our energy; the physics being sensitive only to energy differences and not to the absolute values of the energy. However, when considering phase transitions in quantum fields we are often faced with a cosmological setting. As gravity plays a fundamental role in most cosmological settings we are forced to consider its possible effects upon such phase transitions.

If gravity is included in the analysis then we no longer have the freedom of arbitrarily choosing a zero-level for the energy of the quantum fields. The energy density associated with the quantum fields will be a source for the gravitational field via the stress-energy tensor for the quantum fields. Thus, arbitrarily fixing zero levels for the energy of the quantum fields could have a drastic effect upon the evolution of a spacetime. General relativity predicts that if the energy density of the vacuum state for the quantum fields is positive, zero or negative then an otherwise empty universe will be described by a de Sitter, Minkowski or anti-de Sitter spacetime, respectively. As the properties of these are vastly different it is necessary to conclude that quantum fields may have an essential role to play in cosmology.

Today we find ourselves living in a universe described by a Robertson-Walker spacetime with zero vacuum energy density. The smallness of the present vacuum energy density is, in fact, the most accurately known quantity in the physical sciences at this time: The observational bound on the mass density of the universe is 10^{-28} g cm^{-3} ; while, for example, the characteristic mass density associated with the electroweak theory is 10^{26} g cm^{-3}. Thus, in dimensionless units the maximum vacuum energy density of the Universe is of the order of 10^{-54}, which for all practical purposes is zero!

If we are currently living in a false vacuum state then its decay would result in an anti-de Sitter spacetime, i.e., a spacetime corresponding to a negative vacuum energy density. Similarly, any first-order phase transition, with supercooling (i.e., where thermal excitations are insufficient to push the field over the potential barrier), which may have taken place in the past would have placed us into our current state from an initial de Sitter spacetime (i.e., a spacetime corresponding to a positive vacuum energy density). Such a scenario is commonly accepted because the inflation of the Universe during its de Sitter phase would solve many of the problems of present day cosmology; for example, the lack of magnetic monopoles, the flatness problem and the isotropy of the Universe.

Another interesting phenomenon associated with first order phase transitions is their ability to be nucleated by an inhomogeneity or some other form of nucleation site. An example of this is the preferential formation of rain drops around dust particles in the atmosphere. The presence of nucleation sites can considerably enhance the nucleation rate for a phase transition, and their absence can often result in the phenomenon of supercooling. One is therefore led to ask whether there are analogous nucleation sites for vacuum phase transitions. In particular, can inhomogeneities in the gravitational field act as nucleation sites for vacuum phase transitions? Such inhomogeneities may find their origin with black holes, boson stars or other gravitationally compact objects. Even density perturbations in the background metric associated with a hot early universe might act as nucleation sites.

The Higgs fields of the electroweak theory of Glashow (1961), Weinberg (1964), and Salam (1968) (hereafter referred to as GWS theory) provide the motivation for most of the study of vacuum phase transitions with quantum fields. The Higgs field provides an example of a quantum field in which vacuum phase transitions are believed to occur; there are also very compelling reasons to believe in the existence of the Higgs fields.

The "weak interaction" proved to be problematic for most of the early days of particle physics (non-renormalizable in a point-like interaction model, for example). The interaction is short ranged and must therefore be transmitted via a heavy (vector) boson. Fortunately, massive bosons may be generated quite naturally within gauge theories via the process of spontaneous symmetry breaking (SSB) of a continuous symmetry within the Lagrangian of the field theory. There is an added bonus in that such theories are also renormalizable. Within the GWS theory, the SSB is generated via the Higgs field (i.e., the broken symmetry vacuum state of the Higgs field does not respect the full symmetry of the Lagrangian for the theory). The required vector gauge-bosons, together with their masses and couplings, are predicted quite naturally within the theory; this is a compelling reason to believe in the theory.

The creation of the electroweak theory provided a unification of the electromagnetic and weak forces. This unification has been extended in various theories to include the strong interaction (Grand Unified Theories, or GUTs); and even grander unification schemes have been proposed. The motivation for these "unifications" are the numerous problems in particle physics and cosmology that they may solve (together, of course, with their aesthetic appeal). A characteristic of many of these grand unification schemes are the presence of Higgs fields.

An initial study of false vacuum decay, in the absence of gravity, was made by Coleman (1977) in which he formulated the "thin-wall" approximation scheme. Coleman showed that the "nucleating bubble profile" should be given by the solution to the Euclideanized field equations with appropriate boundary conditions. The number of nucleating bubbles per unit four volume within this analysis may be expressed by $\Gamma = A \exp(-B)$, where B is the difference between the Euclidean action for the spacetime with and without the bubble. The coefficient 'A' is a functional determinant associated with the field equation, and is typically of the order of the mass scale of the field to the fourth power.

The terminology "nucleating bubble profile" should be read with caution as it is misleading to think of the bubble field profile *at the moment of nucleation* to be given by the solution to the Euclideanized field equations. The reason for this is that at the moment of nucleation the quantum fluctuations in the field are comparable in "size" to the field profile of the nucleating bubble. Thus the notion of a "classical field profile" is misleading in this situation. However, the "classical field profile", to the exterior of the lightcone centered on the nucleation site, is at late times (i.e., at times much greater than m^{-1}, where m is the characteristic mass scale of the quantum field undergoing the phase transition) well represented by the solution to the Euclideanized field equations "rotated" into the Lorentzian sector. Thus, whenever the terminology "nucleating bubble profile" shall be used then the above qualifications will be understood to apply. We also note that the solutions to the Euclideanized scalar field equations are also used in the evaluation of the Euclidean action of the nucleating bubble.

The "thin-wall" model assumes that the bubble created as a result of quantum fluctuations has a well defined core of new phase, a very thin wall and an exterior of old phase. Such a bubble profile is an approximate solution to the Euclideanized field equations when there is a small vacuum energy density difference between the two vacuum states. This approximation scheme provides a straight forward and often an analytic way of determining bubble nucleation rates in a field theoretic context.

In a later paper Coleman and De Luccia (1980) extended the "thin-wall" approximation with the inclusion of gravity. Their analysis was specialized to the formation of O(4)-symmetric bubbles in the decay from de Sitter to Minkowski space and from Minkowski to anti-de Sitter space. Coleman, et. al. (1978), have shown that in the absence of gravity, O(4)-symmetric bubbles always have the least action and are therefore the dominant decay mode for first order vacuum phase transitions. Several proofs extending this result to the situation where gravity is present have been offered, but all have been shown to be flawed. Though no proof exists at this time to demonstrate that O(4)-symmetric bubbles will always have the lowest action when gravity is included, it is widely believed to be true.

Quantum fields have associated with them a stress-energy tensor and are therefore a source for the gravitational field, as given by the Einstein field equations. Thus the Coleman-De Luccia analysis required the approximate solution of the coupled Euclideanized field and Einstein equations in order to incorporate the effects of the self-gravity of the bubble. Their results showed an enhanced rate for vacuum decay from de Sitter to Minkowski space and a decreased rate for decay from Minkowski to anti-de Sitter space. This was associated with a decrease in the nucleating bubble size for the decay from de Sitter to Minkowski space and an increase in the nucleating bubble size for the decay from Minkowski to anti-de Sitter space as compared with the nucleating bubble in the absence of gravity. There was also a predicted forbidden region for the decay from Minkowski to anti-de Sitter space in which false vacuum decay was prohibited. This region corresponded to a small vacuum energy density difference between the two vacuum states.

As might be expected, the effect of self-gravity on the false vacuum decay rate is negligible unless the mass of the field concerned is close to the Planck mass. Thus for phase transitions at the electroweak energy scale (10^2 GeV), and even the GUT energy scale (of the order of 10^{16} GeV), the effect of self gravity is usually neglected (n.b., the Planck scale is of the order 10^{19} GeV). In such situations gravity would play a more dominant role in the later evolution of the bubble (i.e., on a cosmological scale) rather than in its formation. However, it is conceivable that either in the very early Universe, or even today, a phase transition could occur which is associated with a highly massive field.

The effect of gravitational nucleation sites upon false vacuum decay has been studied within the "thin-wall" approximation by Hiscock (1987), who considered the effect of black holes, and Mendell and Hiscock (1989) who considered the effect of gravitationally compact objects such as neutron stars. Their analysis proceeded via the solution of the Israel (1966) equations corresponding to the "patching" together of two spacetimes (and is therefore a "thin-wall" analysis). For example, in the analysis of the effect of a black hole upon false vacuum decay from a Schwarzschild spacetime to a Schwarzschild - anti - de Sitter spacetime, the solution of the Israel equations corresponding to the patching together of a bubble core of Schwarzschild-anti-de Sitter spacetime to an exterior of Schwarzschild spacetime is required. Their analysis showed that the gravitationally compact objects under consideration have the effect of reducing B, the difference between the Euclidean action for the spacetime with and without the bubble, and that these objects may therefore play the role of nucleation sites.

It is the purpose of this dissertation to make a study of bubble nucleation processes for first-order phase transitions in quantum scalar fields. This is to be achieved via the exact numerical solution of the relevant field equations, or in some instances where exact solutions are intractable, a perturbative numerical approach is adopted. The field of study is specialized to: O(4)-symmetric bubble nucleation without gravity, O(4)-symmetric bubble nucleation with gravity (for the decays from de Sitter to Minkowski space and Minkowski to anti-de Sitter space), and O(3)-symmetric bubble nucleation around gravitationally compact objects. In all of these instances a comparison is made of exact numerical results with those of the "thin-wall" approximation; this will allow us to estimate the range of validity of the "thin-wall" approximation in the various scenarios. A search is also made for new physical effects which may not be apparent from the "thin-wall" analysis.

Finally, some astrophysical aspects of the bubble nucleation processes are addressed in light of the exact numerical results. In particular, the evolution of the interior of the nucleating bubble is considered together with a model for placing bounds upon the number density of astrophysical nucleation sites. This bound shall be based upon the GWS electroweak theory in which a sufficiently massive top-quark may render our current vacuum state a false-vacuum (Politzer and Wolfram (1976), Flores and Sher (1983), Duncan et. al. (1985)).

The convention, c = G = h =1, shall be used throughout this dissertation, except for Chapter 3 which will use c=h=1, and $G=1/m_p^2$; where m_p is the Planck mass.

CHAPTER 2

FIRST - ORDER VACUUM PHASE TRANSITIONS IN THE ABSENCE OF GRAVITY

Motivation and Background

The theory of the decay of an apparent ground state to a deeper lying or absolute ground state of a physical system via some quantum process or statistical fluctuation has its roots in many branches of the physical sciences. It has recently found a stage for its action in the "marriage" of high energy and elementary particle physics with cosmology.

The advent of the electroweak theory of Glashow, Weinberg and Salam showed that the fundamental quantum fields of nature may play an important role in the evolution of the Universe. This is a result of a possible non-zero vacuum energy density associated with some of the quantum fields of the theory (the Higgs fields). A non-zero vacuum energy density has quite a dramatic effect on the evolution of a spacetime; a positive vacuum energy density may result in the exponential expansion of a spacetime, whereas a negative vacuum energy density may result in a spacetime in which the "Cauchy Problem" is not even well defined. Verification of the GWS electroweak theory, through the discovery of neutral currents and the W and Z particles, gave credibility to other unified models, for example the "Grand Unified Theories". Such theories also predict states for the quantum fields in which the vacuum energy density would be non-zero.

A characteristic of unified field theories is the presence of a temperature dependent (Higgs) field potential. The vacuum state corresponding to the Higgs field potential respects the symmetry of the Lagrangian at high temperatures. However, at low temperatures spontaneous symmetry breaking occurs, and the true vacuum state no longer has the symmetry of the Lagrangian. The true vacuum will lie at some non-zero value of the Higgs field, and may be separated from the false (symmetric) vacuum by a potential barrier. Figure 2 illustrates these ideas.

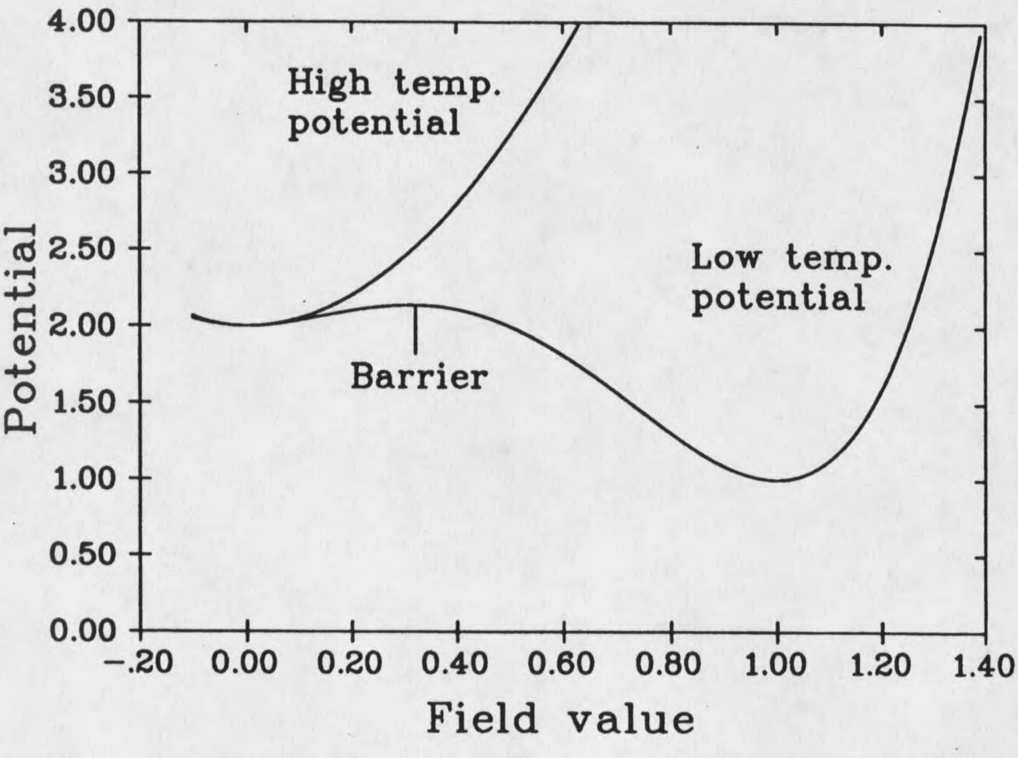

Figure 2 The temperature dependent field potential which is a characteristic of many unified field models.

In a cosmological setting, a "Hot Big Bang" would initially place the Higgs potential into its symmetric state due to the very high temperatures shortly after the Big Bang. Such a state would have a positive vacuum energy density as shown in Figure 2. The energy density of the Universe would initially be dominated by a "hot gas" of relativistic particles, and the evolution would be described by a Friedman-Robertson-Walker cosmological model. However, as the Universe expanded the energy density of the hot gas of particles would decrease and the temperature would fall. Eventually, some point would be reached where the vacuum energy density would dominate over that of the hot gas.

Within many of the grand unified models the quantum field that is driving the exponential expansion of the Universe will now find itself in a trapped false vacuum state. The evolution of the Universe would then be well modeled by a de Sitter spacetime in which the Universe undergoes an exponential expansion. Such an expansion will in a very short time, drop the temperature of the initially hot gas of particles to some value very close to zero. If the field behaved in a classical manner then this would be the end of the story (i.e., an exponentially expanding Universe). However, quantum fluctuations in the field allow it to escape from its trapped state, tunneling through the barrier and thus enabling it to reach the true vacuum state.

The quantum tunneling of a field through a barrier in the effective field potential is analogous to an order parameter of a thermodynamic system tunneling through a barrier in the free energy of the system as a result of statistical fluctuations. These processes are characteristic of first order phase transitions; such transitions being accomplished via the nucleation of bubbles of the new phase within the medium of the old phase.

Coleman (1977) has provided us with an analysis which shows that the field profile of the nucleating bubble, for a first order phase transition, is given by the solution of the Euclideanized field equations with appropriate boundary conditions. Additionally, the "bubble nucleation rate" is determined by the Euclidean action of the nucleating bubble.

The Coleman analysis goes further by providing us with an analytical approximation scheme, the "thin-wall" approximation, for the calculation of the Euclidean action of a nucleating bubble for a given field theory. This approximation scheme is valid in the situation where the energy density difference between the false vacuum (ground) state and the true vacuum (ground) state is small. When this is the case then the approximate solution to the Euclideanized field equations results in a nucleating bubble which has a well defined core of "new" phase, a thin-wall, in which there is a rapid transition from the "new" to the "old" phase, and an exterior of "old" phase. An example of a "thin-wall" nucleating bubble profile is shown in Figure 3.

In this chapter we shall review the "thin-wall" approximation for a particular "toy model" field theory (without the effects of gravity). We shall also obtain exact nucleating bubble profiles and Euclidean actions via the numerical solution of the Euclideanized field equations; this will allow us to critically analyze the "thin-wall" approximation and determine its range of validity. This analysis will eventually lead us to a new approximation scheme, which considerably improves upon the results of the original "thin-wall" approximation (these results have been reported in Samuel and Hiscock (1991[a])).

We shall consider first-order phase transitions for the decay of false vacua with quantum scalar fields, i.e., fields of zero intrinsic spin. It is conceivable that phase transitions processes may differ somewhat for fields of higher spin (e.g., possible