Quantum Statistical Metastability Revisited

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Abstract

We calculate the decay rate for a state prepared in a thermal density matrix centered on a metastable ground state. We find a rate that is intrinsically time dependent, as opposed to the constant rates of previous works. The rate vanishes at early times, rises to a maximum and eventually falls-off to zero as a consequence of unitary time evolution. Finally, we discuss extensions of this calculation to field theories and possible implications for both sphaleron mediated transitions and first order inflationary theories.
The analysis of the decay of metastable states has always been an important and interesting topic in physics. Recently, however, this subject has assumed even greater importance due to the discovery that there are field configurations in the standard model (so-called sphalerons\textsuperscript{1}) that mediate baryon number violating transitions which are \textit{unsuppressed} at high temperature. Needless to say, this has important implications for the evolution of baryon number in the early universe\textsuperscript{2}. Another reason why there has been a rekindling of interest in the evolution of metastable states in the early universe is due to the development of viable models of inflation (extended inflation\textsuperscript{3}) that go back to Guth’s\textsuperscript{4} idea of ending the inflationary era via false vacuum decay. In short, there are good reasons for making sure that the decay of metastable states at finite temperature is, in fact, well understood.

We will argue in this Letter that some aspects of the calculation of the decay rate of metastable states must be rethought. In particular, we will make the point that different choices of initial state can make for significant changes in the decay rate. We show that under realistic conditions, the decay rate \textit{must} be time dependent. This is consistent with some recent experimental data which we discuss below.

Two of the seminal works on this topic are those by Langer\textsuperscript{5} and Affleck\textsuperscript{6}. It will be instructive to review these calculations, since our results are quite different from theirs.

Langer develops a Fokker-Planck type equation for the probability of finding the system in a given configuration at time $t$. This probability obeys a continuity equation and the associated current gives the flow of probability in the configuration space. In a one dimensional system, this current, evaluated at the saddle point (which is the top of the barrier), is identified with the rate of activation of the system over the barrier.

To compute this current, Langer then constructs a \textit{steady state} solution to his Fokker-Planck equation. This is tantamount to setting up a steady state situation by continuously replenishing the metastable state at a rate equal to the rate at which it is leaking across
the activation energy barrier. This point is emphasized in Langer’s work.

In Affleck’s calculation, the rate is defined as the Boltzmann average of the probability current over a set of quantum states that, for energies less than the barrier height, are standing waves in the metastable well. For energies higher than the barrier height, these are waves incident from the left, reflected and transmitted at the barrier. The rate is then calculated as:

\[
\Gamma = Z_0^{-1} \int_0^\infty dE \rho(E) \Gamma(E) \exp(-\beta E),
\]

where \(\rho(E)\) is the density of states at energy \(E\), \(\Gamma(E)\) the decay rate for states with energy \(E\), \(\beta = 1/k_B T\). The rate is normalized using the partition function \(Z_0\) of a harmonic oscillator centered at the metastable state at \(x = x_0\) and whose frequency is just \(\omega_0^2 = V''(x_0)\). As in Langer’s calculation, this corresponds to a steady flow of particles across the barrier.

Both of these calculations (and those that have built on them) assume that the state under consideration is one in which probability is being fed continuously into the metastable well in order to replenish the probability that is flowing out and over the activation barrier, thus ensuring a steady state. However, we would argue that this is not a realistic initial state to use to compute a rate for processes relevant in the early universe, though there may be other physical situations for which such an initial state is appropriate.

Usually in inflationary models, say, one thinks of the field that will drive inflation as being “trapped” in the metastable minimum. This trapping arose due to the fact that the field was in thermal equilibrium with the ambient heat bath, and as the temperature dependent effective potential changed shape, the global minimum became separated from the local one by a barrier. We would thus expect that the appropriate description for the initial state of the field would correspond to a thermal density matrix, centered at
the metastable minimum. As long as the field remained in good thermal contact with the heat bath, the thermal character of the initial density matrix would be maintained.

This is a very different initial state from that considered by Langer and Affleck. In particular, there is no replenishing of probability by an outside source. Thus we expect the decay rate out of the metastable state to behave very differently than that found by Langer and Affleck. The rate thus obtained will be an intrinsically non-equilibrium quantity as the initial density matrix will evolve in time. It is to this calculation that we now turn to.

The procedure is straightforward. Consider a one dimensional quantum mechanical system for simplicity. Start with an initial density matrix $\rho(t = 0)$ and then evolve it in time via either the Liouville equation:

$$i\hbar \frac{\partial \rho(t)}{\partial t} = [H, \rho(t)],$$

or via the solution to this equation:

$$\rho(t) = \exp\left(-\frac{i}{\hbar}Ht\right)\rho(0) \exp\left(\frac{i}{\hbar}Ht\right).$$

Here $H$ is the Hamiltonian of the system: $H = p^2/2 + V(x)$, where we choose units so that the mass $m = 1$.

Given the density matrix as a function of time, we can look at its position space representation $\rho(x, x'; t) \equiv \langle x|\rho(t)|x'\rangle$. The current is then found via:

$$J(x, t) = \frac{\hbar}{2i} \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right) \rho(x, x'; t)|_{x=x'}.$$
initial thermal state given an arbitrary potential \( V(x) \), as well as of how to compute the required propagators. To circumvent these problems, we will use the following techniques. First, we will assume that for \( t < 0 \), the potential is just a quadratic centered around the metastable state at \( x = x_0 \). This then allows us to compute the initial density matrix as:

\[
\rho(x, x'; t = 0) = N(0) \exp \left\{-\frac{\omega}{2\hbar \sinh(\beta \hbar \omega)} \left[ ((x - x_0)^2 + (x' - x_0)^2) \cosh(\beta \hbar \omega)
- 2(x - x_0)(x' - x_0) \right]\right\}
\]

(5)

where the normalization factor \( N(0) = \sqrt{\frac{\omega \tanh(\beta \hbar \omega)}{\pi \hbar}} \) ensures that \( \text{Tr}(\rho(t = 0)) = 1 \). This was also the approach followed implicitly by Langer and Affleck when they normalized their rates.

We then use the sudden approximation and say that for \( t > 0 \), the potential consists of the barrier whose peak is at \( x = 0 \) (see fig. 1). Furthermore, since we are only interested in over the barrier activation, we use the quadratic approximation \( V(x) \approx V_0 - \frac{1}{2} \Omega^2 x^2 \) for the potential, where \( \Omega^2 \equiv -V''(x = 0) \) is positive, (since \( x = 0 \) is a maximum of \( V(x) \)) and \( V_0 \) is the height of the barrier.

The coordinate space expression for the time evolved density matrix is, for \( t > 0 \):

\[
\rho(x, x'; t) = \int dy \, dy' \langle x | \exp(-\frac{i}{\hbar} H_q t) | y \rangle \rho(y, y'; t = 0) \langle y' | \exp(\frac{i}{\hbar} H_q t) | x' \rangle
\]

(6)

where the effective Hamiltonian \( H_q \) is the quadratic approximation to \( H \) near the top of the barrier: \( H_q = p^2/2 + V_0 - 1/2 \Omega^2 x^2 \).

The propagators \( \langle x | \exp(\pm \frac{i}{\hbar} H_q t) | y \rangle \) are easy to evaluate by analytically continuing the propagator for a standard harmonic oscillator with real frequency:

\[
\langle x | \exp(\pm \frac{i}{\hbar} H_q t) | y \rangle = M(t) \exp(\pm \frac{i}{2\hbar \sinh(\Omega t)} \left[ (x^2 + y^2) \cosh(\Omega t) - 2xy \right]).
\]

(7)
with \( M(t) = (\pm \Omega/2\pi i\hbar \sinh(\Omega t))^{1/2} \). These propagators are solutions to the evolution equation with the proper boundary conditions. We can now compute the density matrix as a function of time, as well as the current. We have verified that the resulting density matrix is a solution of the Liouville equation (Eq. (2)) with the initial boundary condition given by Eq. (3), thus confirming that the analytically continued propagators give the correct answer.

Rather than write down the density matrix, we consider the probability density \( p(x, t) \equiv \rho(x, x; t) \):

\[
p(x, t) = \frac{1}{\sqrt{2\pi \sigma(t)}} \exp\left(-\frac{(x - x_0 \cosh(\Omega t))^2}{2\sigma(t)^2}\right)
\]

with

\[
2\sigma(t)^2 = \frac{\hbar}{\omega \tanh(\beta \hbar\omega/2)} (\cosh^2(\Omega t) + \frac{\omega^2}{\Omega^2} \sinh^2(\Omega t)).
\]

The rate \( \Gamma(t) = J(x = 0, t) \) is found to be:

\[
\Gamma(t) = \frac{\omega^2}{\Omega} \left[ \frac{\omega}{\pi \hbar} \tanh(\beta \hbar\omega/2) \right]^{1/2} |x_0| A(t) \exp[-\tanh(\beta \hbar\omega/2)B(t)]
\]

with

\[
A(t) = \frac{\sinh(\Omega t)}{\left[ \cosh^2(\Omega t) + \frac{\omega^2}{\Omega^2} \sinh^2(\Omega t) \right]^{3/2}}
\]

\[
B(t) = \frac{\omega x_0^2}{\hbar} \left[ 1 + \frac{\omega^2}{\Omega^2} \tanh^2(\Omega t) \right]^{-1}
\]

The first feature we should remark on is that both the probability density and the rate are time dependent! This is in marked contrast to both Affleck and Langer’s results where the rate had the generic form: \( \Gamma = A \exp(-B) \), with both \( A \) and \( B \) time independent. However, it is easy enough to argue that given our initial state, and the fact that the transition from the metastable state to the true ground state must be a non-equilibrium process, this time dependence was inevitable.
As the system activates over the barrier, there is loss of probability in the metastable well. Thus, as time goes on, we should expect to have less and less “initial state” to decay from. This is a consequence of unitary time evolution for the density matrix, and hence for the probability distribution. From this argument, we expect the rate to start at zero initially, and then rise to some maximum. After this, the rate should then decrease to zero at large times. This is exactly the behavior demonstrated by the rate we have calculated (fig. 2).

There are two competing effects that determine the behavior of the rate: the motion of the center of the probability distribution (Eq. (8)) and the spread, determined by $\sigma(t)$. The most important factor turns out to be the spread. This may be understood from the fact that the fluctuation $\langle (x - x_0(t))^2 \rangle = \sigma^2(t)$, where $x_0(t) = x_0 \cosh(\Omega t)$.

A remarkable result has been recently reported by Min and Goldburg concerning nucleation in a classical fluid under shear. They found a time dependent nucleation rate for this system that is strikingly similar in form to the rate obtained above and strongly dependent on the initial state. Though our quantum mechanical calculation does not apply to the classical fluid case, these results show that there are systems in which the nucleation rate is time dependent. These results cannot be explained by the steady-state homogeneous nucleation theory. While our quantum mechanical calculation only describes one degree of freedom, it may provide qualitative insight into the dynamics of the collective coordinate that describes the radius of a droplet. Thus the classical limit of our calculation may still provide a qualitative description of time dependent rates in macroscopic situations.

In previous calculations of an activation rate, a Boltzmann suppression factor of the form $\exp(-\beta V_0)$ usually appears. Our result above does not seem to have such a factor in it. However, a suppression factor of this type does in fact appear in our $\Gamma(t)$. It is encoded in the relationship between $\omega$ and $\Omega$. To see this, we need to consider a specific
potential \( V(x) \). Thus consider a cubic potential:

\[
V(x) = V_0(1 + 2x^3/x_0^3 - 3x^2/x_0^2)
\]  

where we take \( x_0 < 0 \). With this potential we have \( \omega^2 = \Omega^2 = 6V_0/x_0^2 \). If we now take the high temperature limit, we find that the exponential in the current becomes \( \exp(-3\beta V_0 f(t)) \), with \( f(t) = 1/2 \left( 1 + \text{sech}(2\Omega t) \right) \); note that \( f(t) \) varies from 1 to 1/2 as \( t \) varies from 0 to \( \infty \). Thus, we do get a suppression of the Boltzmann form, but it is larger than \( \exp(-\beta V_0) \). This extra suppression comes about due to the initial state we are using; since it is centered around \( x = x_0 \), only a fraction of the probability is near the saddle point at \( x = 0 \). In fact, \( p(x = 0, t) \propto \exp(-3\beta V_0 f(t)) \) in the high \( T \) limit. The extra suppression is then seen as a measure of how much (or how little!) support \( p(x, t) \) has near \( x = 0 \).

The next feature we examine is the temperature dependence of the rate. The prefactor in \( \Gamma(t) \) contains the factor \( \sqrt{\tanh(\beta \hbar \omega/2)} \) and so decreases at high enough temperature. However, the exponential is given by \( \exp(-\tanh(\beta \hbar \omega/2)B(t)) \), which \textit{increases} with temperature. Thus, there will be a temperature regime in which the rate increases with temperature. In the high \( T \) limit i.e. \( \beta \hbar \omega \ll 1 \), we can find this regime by computing \( \partial \ln \Gamma/\partial \beta \):

\[
\partial \ln \Gamma/\partial \beta = \frac{1}{2\beta}(1 - \beta \hbar \omega B(t))
\]  

Thus, \( \Gamma \) increases with \( T \) as long as \( 1 - \beta \hbar \omega B(t) < 0 \). For the case of the cubic potential above, this becomes \( 6\beta V_0 > 1 + \tanh^2(\Omega t) \). Now, in order to have a metastable state at all, we should require that the temperature be less than the barrier height \( V_0 \). Thus, to the extent that we have an initial state that can be thought of as trapped in the metastable well (which is to say, \( \beta V_0 > 1 \)), the rate will increase with temperature (fig.3).
requires $V_0 >> \hbar \omega$ as a consistency condition. This is also a required condition for the initial state to be thought of as metastable.

A valid point to raise at this time concerns the validity of our approximations. Certainly, if we quench the system quickly enough, it will settle into the metastable well. Furthermore, as long as $1/2 \hbar \omega < V_0$, we expect the harmonic oscillator approximation for the potential near $x = x_0$ to be reasonable. While our calculations were made within the sudden approximation, the fact that the density matrix and hence the rate will be time dependent will still remain even under more realistic time evolution. The reason for this is, again, the fact that the density matrix evolves in a unitary way.

The last truncation of the original theory was the use of the quadratic approximation for the potential near the top of the barrier. This gives rise to the motion of the center of the probability distribution as well as its spread as described in eq.(8). After a time $\tau \sim \Omega^{-1}$, however, we expect the effects of the non-quadratic terms of the potential to make themselves felt and modify our result. Thus, our expression for $\Gamma(t)$ can be trusted for time of order $\Omega^{-1}$. As can be seen from, Figure 2, however, this is sufficient time to see the rise of $\Gamma(t)$ to its peak value and to see the beginning of its decrease to zero. The fact that $\Gamma(t)$ will approach zero asymptotically is, as mentioned previously, just a consequence of unitary time evolution of $\rho(t)$ and hence can be trusted. However, the exact shape of the curve may be different than that shown in Figure 2.

We started this work by using examples such as first order inflationary models and baryon number violation via sphaleron mediated decays to motivate the discussion. What does our calculation say about these topics? In order to truly extract some information, we need to understand how our calculation should be generalized within the context of field theory. Some steps in this direction have already been taken. Boyanovsky and Aragão de Carvalho have considered the problem of thermal activation over a barrier in a $1+1$ dimensional scalar field theory. While their calculation involves some subtleties
not present in the quantum mechanical case (such as dealing with collective coordinates), the results are similar. They arrive at a rate that varies in time much like the rate we find here. We are also currently involved in calculations of decay rates in theories involving sphalerons using the real-time formalism developed here\cite{1}.

While we do not yet have all the answers we need to fully understand what changes the time dependence of the rate will bring, we may speculate. We have considered thermal activation here rather than under the barrier tunnelling. This makes the range of applicability of our calculation to inflationary models somewhat suspect. The reason for this is that once inflation sets in, the temperature of the heat bath will decrease rapidly, turning the problem into a zero temperature one. Even in this case, however, we should expect the rate to be time dependent. The basic change in our calculation is that the paths used to compute the propagators required to evolve the density matrix in time will be different. Essentially, one must do a WKB approximation of the propagators\cite{2}. Again, though, we would expect the rate to start at zero and approach zero asymptotically at large times. This implies the rate must peak at some time, just as our current calculation. Our work can therefore be used to provide some hints as to what might occur in the zero temperature case.

In the case of Guth’s original inflationary scenario, it seems to us that the time dependence of the rate just exacerbates the problems that led to its downfall. Recall that the problem had to do with the fact that the nucleation rate had to be small enough to keep the system in the false vacuum long enough to achieve a sufficient amount of inflation yet large enough so that the phase transition would be completed (these requirements can be quantified more explicitly\cite{3}). Our rate will start off being small and then grow to a maximum and finally tail off to zero. Thus, just when a large rate is needed to complete the phase transition, the rate is getting small. There may be ways to avoid this. For example, if the rate starts off small enough, there may be enough time before the rate
peaks to achieve the requisite 60 e-folds of inflation. The rate could still be growing past this time in a way that would allow the new phase to percolate.

The situation in extended inflationary models is somewhat trickier to assess, since the nucleation rate is already time dependent in most of these models due to the time evolution of the Jordan-Brans-Dicke field in them\textsuperscript{14}.

In the case of the sphaleron, the question of whether the sphaleron interactions are in thermal equilibrium (which is crucial in terms of determining whether a baryon asymmetry can be generated by these interactions), becomes more difficult to assess due to the time dependence of the rate. One could imagine that the rate of these interactions decreased sufficiently quickly so as to allow them to drop out of local thermal equilibrium thus allowing a net $B$ asymmetry to be generated. However, the answer to these and other questions will only be found when the field theoretic generalization of our calculation is completed.

It seems clear then that a \textit{real time} calculation of the rate of thermal activation of a metastable state will always yield a time dependent rate. This time dependence is completely missed in the standard equilibrium calculations due to a choice of initial state that is not realized in the situations these calculations are usually applied to. Furthermore, there are now experimental results that support our arguments and that \textit{cannot} be explained by the usual homogeneous nucleation theory. We believe that our methods will have wide applicability to a variety of problems in this branch of physics, not least of which is the understanding of some very important facets of early universe physics.

\textbf{Acknowledgements}

D.B. would like to thank David Jasnow and Walter Goldburg for useful discussions. D.B. and D-S.L were supported in part by NSF grant # PHY-8921311 as well as a Mellon
Pre-Doctoral Fellowship Award (D-S.L). R. H., J.S. and A.S. were supported in part by DOE grant # DE-FG02-91ER40682. The work of J.S. is also supported in part by the Portuguese JNICT, under CIENCIA grant # BD/374/90-RM.

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Figure Captions

Figure 1: The potential for a 1 dimensional metastable system

Figure 2: The thermal activation rate $\Gamma(t)$ as a function of $t$ at fixed temperature. Time is measured in units of $\Omega^{-1}$, while the rate is measured in arbitrary units.

Figure 3: Plots of $\Gamma(t)$ at different temperatures $T_1$, $T_2$, $T_3$, with $T_1 > T_2 > T_3$. The $T_i$ are taken so that the system can be thought of as metastable.