A Note on Thermal Activation

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Abstract

Thermal activation is mediated by field configurations that correspond to saddle points of the energy functional. The rate of probability flow along the unstable functional directions, i.e. the activation rate, is usually obtained from the imaginary part of a suitable analytic continuation of the equilibrium free energy. In this note we provide a real-time, non-equilibrium interpretation of this imaginary part which is analogous to the real-time interpretation of the imaginary part of the one-loop effective potential in theories with symmetry breaking. We argue that in situations in which the system is strongly out of equilibrium the rate will be time dependent, and illustrate this with an example.
The analysis of thermal activation has always been an important and interesting topic in different areas in physics. Recently, however, this subject has assumed even greater importance due to the observation that there are field configurations in the standard model (so-called sphalerons[1, 2, 3]) that mediate baryon number violating transitions which are unsuppressed at high temperature. Needless to say, this has important implications for the evolution of baryon number in the early universe[4]. 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[5]) that go back to Guth’s[6] 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 understood from as many different perspectives as possible.

The motivations for this note are twofold. First, we offer a real-time interpretation of the standard equilibrium calculation of the activation rate based on the imaginary part of an analytically continued free energy. Here we draw an analogy with the case of the imaginary part of the effective potential in theories with spontaneous symmetry breaking as studied by Weinberg and Wu[7]. Second, we will make the point that in an out of equilibrium situation, different initial states can make for significant changes in the activation rate. We show by an explicit example that in an out of equilibrium situation the activation rate must be time dependent.

Two of the seminal works on this topic are those by Langer[8] and Affleck[9]. It will be instructive to review the concepts and assumptions involved in these calculations, since our results will provide a different interpretation of these standard results, as well as an extension of them.

Langer[8, 10] develops a Fokker-Planck type equation for the probability of finding the system in a given configuration at time $t$. There are two terms in this Fokker-Planck
equation. The first term is deterministic in nature, corresponding to the Liouville time evolution in phase space. The other is a stochastic term and represents the diffusion or dissipation arising from the coupling to a heat bath. The probability density in phase space obeys a continuity equation and the associated current gives the flow of probability. In a metastable situation, there is a particular configuration that corresponds to a saddle point of the energy functional, and probability flows along the unstable direction from the metastable phase towards the stable phase. The activation (decay) rate is obtained as the total current passing over the saddle point along the unstable direction divided by the initial population of the metastable state[10].

There are two very important assumptions in Langer’s original work. The first is that a steady state solution is reached in which a source in the metastable state continually feeds probability (or particles) and a sink in the stable phase removes probability at a steady rate. Secondly, the metastable state is supposed to be in local thermodynamic equilibrium. This assumption implies that there is a wide separation between the equilibration (relaxation) time scale and the time it takes for the state to lose a significant amount of probability. This in turn translates into the statement that there is fairly strong dissipation[10]. Under these assumptions, there is no memory of the initial preparation of the metastable state.

Similar assumptions are implicit in Affleck’s calculation[9]. The rate is defined as the Boltzmann average of the decay rates of the 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:

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

(1)
where $\rho(E)$ is the density of states at energy $E$, $\Gamma(E)$ the decay rate for states with energy $E$, and $\beta = 1/T$. The rate is normalized using the partition function $Z_0$ of a harmonic oscillator centered at the metastable state. As in Langer’s calculation, this corresponds to a steady flow of probability 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. Alternatively, the assumption is that the system is in quasi-equilibrium and “slowly” leaking probability on timescales much longer than typical scales of the system. However, this implies that the system is looked at during times for which all transient effects arising from the initial preparation have died out and that the probability inside the metastable well has not been depleted appreciably. In particular the underlying assumption[10] is that the equilibration time inside the metastable well is much shorter than the inverse rate of depletion of the population in the well.

These authors showed that under these (implicit) assumptions, the rate obtained is the same as that obtained from the imaginary part of the analytically continued free energy:

$$\Gamma = \frac{\Omega}{\pi T} \text{Im} F$$

(2)

where $\Omega$ is the unstable frequency at the top of the barrier.

This description offers a fairly reliable method of calculation in a wide variety of experimental situations in macroscopic systems[10], in which there is a strong coupling to an environment (heat bath) and only a few degrees of freedom are relevant.

However, the setting we have in mind is that of a weakly coupled quantum field theory,
in which the separation between system and bath is somewhat blurred. In particular, at the onset of a first order phase transition, several time scales are relevant such as the equilibration rate, expansion rate (in a cosmological situation) and the activation rate.

Given that this calculation of the rate involves assumptions which in any typical quantum field theory will be extremely hard to justify at the microscopic level without invoking some phenomenological approximation, we want to investigate an alternative real-time description of the process of thermal activation. We also envisage situations in which the system may be strongly out of equilibrium, and in which some of the above assumptions are not likely to apply.

To illustrate our discussion with a definite example, consider the case of a scalar field theory described by a potential with a local metastable minimum and a global, stable minimum. In this case, there is a static spherically symmetric solution to the classical field equations that resembles a droplet of the stable phase immersed in a sea of the metastable phase[8, 17]. This solution is characterized by the following collective coordinates: translational ("zero modes") corresponding to the position of the droplet and another that represents the radius of this droplet (although technically speaking this latter does not correspond to a "zero mode"). The static solution to the field equation corresponds to a particular value of the radius of the droplet, the critical radius, at which the surface energy is balanced by the volume energy.

Fluctuations around this particular solution are characterized by zero frequency modes (corresponding to translational invariance), a negative eigenvalue corresponding to small fluctuations of the radius of the droplet, and a spectrum of positive frequencies. Thus this configuration corresponds to a saddle point in functional space. The unstable mode describes the instability towards collapse or growth of the droplet for radii smaller or larger than the critical radius, respectively, when either the surface energy or the volume energy start to dominate.
Quantization around the classical solution corresponds to treating the position of the droplet as a collective coordinate and expanding \[\Phi(\vec{r}, t) = \Phi_{cl}(\vec{r} - \vec{r}_o(t), R = R^*) + \sum_i Q_i(t) f_i(\vec{r} - \vec{r}_o(t), R = R^*), \] (3)

where \(\vec{r}_o\) is the position of the droplet, \(R\) is the radius and \(R^*\) is the critical radius for which the energy functional has an extremum. The mode functions \(f_i(\vec{r})\) are the eigenfunctions of the fluctuation operator around the static droplet configuration and are chosen to be orthogonal to the “zero modes” [15]. There is a coordinate \(Q_u\) associated with an unstable mode with mode function \(f_u(\vec{r}) \approx d\Phi_{cl}/dR|_{R=R^*}\) and negative frequency \(-\Omega^2\). To lowest order in the semiclassical expansion, the Hamiltonian operator becomes

\[H = E_{R^*} + \frac{\tilde{P}^2}{2M} + \frac{p^2}{2} - \frac{1}{2} \Omega^2 Q^2_u + \sum_i \left[ \frac{p_i^2}{2} + \frac{1}{2} \omega_i^2 Q_i^2 \right], \] (4)

with \(E_{R^*}\) being the energy of the critical droplet, \(M\) is given by the normalization of the zero modes and \(\omega_i\) are the stable frequencies. To this order in the semiclassical approximation, \(\tilde{P}\) is the total momentum of the system. When the radius of the droplet is much larger than the correlation length (thin wall approximation)

\[E(R) \approx 4\pi R^2 \sigma - \frac{4\pi}{3} R^3 \Delta \mathcal{E} \] (5)

with \(\sigma\) being the surface tension given by the gradient terms and \(\Delta \mathcal{E}\) the energy (or free energy) difference between the globally stable and the metastable lower energy (or free energy) states for the homogeneous configuration. In this case the radius of the critical droplet is given by

\[R^* \approx \frac{2\sigma}{\Delta \mathcal{E}} \] (6)

In a saddle point approximation of the equilibrium partition function, only two extremum configurations are usually considered. The first corresponds to the metastable
minimimun, while the second corresponds to the droplet configuration (saddle point). The partition function is thus written as the sum of these two independent terms.

Formally, the partition function evaluated at the saddle point corresponding to the droplet does not exist because of the presence of the unstable (negative frequency squared) oscillator. However, it may be defined via an analytic continuation, in which case it attains an imaginary part which in three spatial dimensions is given by:

\[
Z_{an} = \pm iV \left[ \frac{MT}{2\pi} \right]^{3/2} \frac{1}{2\sinh(\Omega/2T)} \prod_k \frac{1}{2\sinh(\omega_k/2T)},
\]

where the \( \pm \) arises from the direction of the analytic continuation. The volume factor \( V \) and the \( T^{9/2} \) factor arise from the “free particle” zero mode, the \( 1/\sin(\Omega/2T) \) from the unstable mode and the product over \( \ell \) is only for the stable modes. Writing the partition function \( Z \) as:

\[
Z = Z_s + Z_{an} = Z_s \left[ 1 + \frac{Z_{an}}{Z_s} \right] \approx Z_s \exp \left[ \frac{Z_{an}}{Z_s} \right]
\]

with \( Z_s \) the partition function of independent harmonic oscillators at the metastable minimum of the potential, choosing the negative sign for the analytic continuation (so as to obtain decaying exponentials), and using the identification (2) finally leads to the usual formula for the rate per unit volume:

\[
\frac{\Gamma}{V} = \left[ \frac{MT}{2\pi} \right]^{3/2} \frac{\Omega \exp\left[ -\frac{E(R^*)}{T} \right]}{2\pi \sin(\Omega/2T)} \prod_k \frac{2\sinh(\omega_k^*/2T)}{2\sinh(\omega^*/2T)}
\]

Here \( \omega_k^* \) are the frequencies at the metastable minimum and \( \omega^* \) are the stable frequencies in the perpendicular directions at the saddle point.

In functional space, the direction of steepest descent at the saddle point corresponds (locally) to the unstable coordinate \( Q_u \). For the purposes of analyzing the decay of a metastable state and activation over the barrier (near the top of the barrier), only
this quantum mechanical coordinate is important. Thus along this unstable direction, the problem becomes effectively that of a quantum mechanical inverted oscillator near the top of the barrier. This approximation implies that the temperature is such that \( \omega_k \ll T < E(R^*) \), where \( \omega_k \) are the typical frequencies at the metastable well.

Another situation in which the free energy (or ground state energy) acquires an imaginary part is in the calculation of the one-loop effective potential for homogeneous configurations either at zero or finite temperature in the case when the tree level potential \( V(\Phi) \) has a double well structure\(^7\). In this case the fluctuations of wave vectors \( \vec{k}^2 < V''(\Phi) \) are unstable since they see an inverted harmonic oscillator, just like the unstable coordinate above. These modes are treated via analytic continuation similar to the one performed above, giving rise to an imaginary part for the one-loop effective potential (or free energy) for homogeneous configurations\(^1\)\(^6\).

Weinberg and Wu\(^7\) argued that this imaginary part of the effective potential can be interpreted as the decay rate of a gaussian state peaked at the “top of the inverted oscillator” for these unstable modes. The rate of spread of this gaussian wave packet was identified with the imaginary part of the one-loop effective potential.

Further analysis\(^1\)\(^6\) shows that this rate also determines the rate of growth of fluctuations which is determined by the width of the gaussian state initially prepared to be centered at the top of the inverted parabola at the maximum of the tree level potential. This analysis was also carried out at finite temperature, in which case the analytically continued free energy has an imaginary part\(^1\)\(^6\). These unstable modes are responsible for the early stage dynamics of a second order phase transition and for the non-equilibrium evolution during the phase transition. The regions in which the field becomes correlated grow in time as the system becomes more and more correlated. Initially the unstable modes grow exponentially but eventually the non-linearities set in, slowing down the rate of growth. Finally, at a later time the growth stops. The system is now described as
having large correlated regions in which the field inside is close to one of the minima of the (effective) potential. This is the mechanism of “spinodal decomposition”[16]. Thus the imaginary part of the one-loop effective potential (or alternatively at finite temperature the free energy) disguises a time dependent situation. Trying to study this time dependent situation via an equilibrium description leads to treating the unstable modes via an analytic continuation and an imaginary part.

The physical difference between the mechanism of spinodal decomposition and thermal activation is that in the former there are no free energy barriers, and small amplitude long wavelength fluctuations become unstable and grow. By contrast, in thermal activation, there is a free energy barrier to be overcome. Thus, a large amplitude configuration must be present in the bath with a radius that is bigger than the critical radius. Once this configuration is created, however, it is the instability towards growth of this bubble that drives the phase transition. The probability of finding these configurations in the bath is determined by the Arrhenius-Kramer exponential factor explicit in \( Z_{an} \) above. When a critical bubble is formed, the system is found at the top of the barrier, that is at the saddle point. In the gaussian approximation, the situation corresponds to a gaussian density matrix (the thermal equivalent of the gaussian wave packet studied by Weinberg and Wu) centered at the top of the barrier, and for the unstable coordinate corresponds to an inverted harmonic oscillator. From this point onwards, the analysis of the evolution, is then similar to that of Weinberg and Wu[7] and Boyanovsky and de Vega[16], with the difference that the initial state is a thermal density matrix rather than a wavepacket.

We see then that the imaginary parts of the free energy and/or the effective potential usually found in the calculation of the decay rates are a signal of non-equilibrium, real-time evolution.

Thus motivated by the situation with the one-loop effective potential we now present
a real-time evolution of an initial state that corresponds to a one-dimensional quantum mechanical system describing the unstable coordinate $Q_u$. The reduction of the multidimensional problem to one collective coordinate is justified because this unstable coordinate determines (in a neighborhood of the saddle point) the direction of steepest descent in functional space. This is the direction along which probability will flow.

The procedure is straightforward. 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:

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

Here $H$ is the Hamiltonian for the unstable coordinate

$$H_u = \frac{p_u^2}{2} - \frac{1}{2}\Omega^2 Q_u^2,$$

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

$$J(Q_u, t) = \frac{\hbar}{2i}\left(\frac{\partial}{\partial Q_u} - \frac{\partial}{\partial Q'_u}\right)\rho(Q_u, Q'_u; t)|_{Q_u=Q'_u}.\quad (13)$$

Evaluating this current at the saddle point will then give us the transition rate (or activation rate) over the barrier.

Generalizing the analysis of Weinberg and Wu[7] and Boyanovsky et. al.[16], we will assume that the initial density matrix $\rho(t = 0)$ (only for the unstable coordinate) is that of an upright harmonic oscillator of frequency $\omega$ in thermal equilibrium at temperature $T = 1/\beta$ given by[18]:

10
\[
\rho(Q_u, Q'_u; t = 0) = \mathcal{N}(0) \exp \left\{ -\frac{\omega}{2\hbar \sinh(\beta \hbar \omega)} \left[ (Q_u^2 + Q'_u^2) \cosh(\beta \hbar \omega) - 2Q_u Q'_u \right] \right\} 
\]

(14)

\[
\mathcal{N}(0) = \sqrt{\frac{\omega}{2\pi \hbar \sinh(\beta \hbar \omega)}} 
\]

(15)

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

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

(16)

The propagators \( \langle x | \exp(\pm \frac{i}{\hbar} H_u t)|y \rangle \) are easy to evaluate by analytically continuing the propagator for a standard harmonic oscillator with real frequency[19]:

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

(17)

\[
N(t) = (\frac{\pm \Omega}{2\pi i \hbar \sinh(\Omega t)})^{1/2}. 
\]

It can be easily checked that 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 (10) with the initial boundary condition given by (14), thus confirming that the analytically continued propagators give the correct answer.

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

\[
p(Q_u, t) = \mathcal{N}(t) \exp(-Q_u^2/2\sigma(t)^2) 
\]

(18)

\[
\sigma(t) = \sqrt{\frac{\hbar}{2\omega \tanh(\beta \hbar \omega/2)}} \left[ \cosh^2(\Omega t) + \frac{\omega^2}{\Omega^2} \sinh^2(\Omega t) \right]^{1/2} 
\]

\[
\mathcal{N}(t) = \mathcal{N}(0) \left[ \frac{\sigma(0)}{\sigma(t)} \right] 
\]
Thus, at long times, the probability to find the density matrix of the unstable coordinate centered at the saddle point is
\[
p(0, t) \approx \frac{\mathcal{N}(0)}{[1 + \omega^2/\Omega^2]^{1/2}} \exp[-\Omega t]
\] (19)

At zero temperature this is similar to the result obtained by Weinberg and Wu\cite{7} for a particular unstable mode by identifying $\Omega$ with the unstable frequency for that particular mode.

The probability current (13) evaluated at the saddle is zero because the density matrix spreads symmetrically around the saddle point along the unstable direction. However, we may still define a rate as
\[
\Gamma_u = -\frac{d \ln[p(0, t)]}{dt} \approx \Omega.
\] (20)

This expression will be valid for $t \gg \Omega^{-1}$. Integrating this rate in all functional directions perpendicular to $Q_u$ to obtain the total probability at the saddle point and dividing by the partition function for the harmonic oscillators at the metastable well, we finally obtain an alternative definition for the rate per unit volume:
\[
\Gamma_u / V = \Omega \left[ \frac{MT}{2\pi} \right]^{3/2} \exp\left[-\frac{E(R^*)}{T} \right] \left[ \prod_k \frac{2 \sinh(\omega_k^*/2T)}{2 \sinh(\omega_k^*/2T)} \right]
\] (21)

which differs from (9) by the prefactor.

Each contribution to the rate above has a very simple and clear real-time interpretation. The situation considered corresponds to the system being described as a gaussian density matrix centered at the saddle point. Along the unstable direction the density matrix (similarly to a wave packet) spreads at a rate determined by the unstable frequency $\Omega$. Thus the rate (21) corresponds to the total rate of spread of the initial density matrix (integrated over all the perpendicular directions) divided by the total probability in the
metastable well. The underlying assumption here is that the system has reached the saddle point and remains there in quasi-equilibrium and that the depletion of probability at the saddle is a consequence of the spreading of the density matrix, although the statistical average of the collective coordinate (radius of the droplet) remains at the top of the barrier.

We may draw the following conclusion from this analysis. The calculation of the rate via the imaginary part of the free energy, which in Langer’s work is derived from a steady state assumption, corresponds to the assumption that the statistical density matrix is centered at the saddle point, and that the expectation value of the radius of droplet is the critical radius. Hence, just as in the case of the one-loop effective potential, the imaginary part of the free energy is disguising an intrinsically time dependent situation and it will determine the rate of growth of fluctuations (width of the gaussian density matrix)[7, 16]. This can be easily understood from the fact that the fluctuation in the unstable coordinate is given by

$$\langle Q_u^2(t) \rangle \propto \sigma^2(t)$$

(22)

We can apply the same analysis for a very different situation, that of the system initially away from the saddle and for which a steady state assumption is not applicable. Thus we now consider activation as an initial condition problem and look at the situation in which the average radius of droplets is smaller than the critical. This corresponds to an initial situation far from equilibrium and not in the steady state. Such a condition corresponds to the situation studied in a simplified 1 + 1 dimensional field theory model by Boyanovsky and de Carvalho[20].

Again we will only concentrate on the unstable coordinate $Q_u$, and consider the case in which the initial density matrix for this collective coordinate is that of an upright
harmonic oscillator of frequency $\omega$ that is displaced a distance $Q_{u_0} < 0$ from the origin at the initial time $t = 0$ and with zero average of the momentum conjugate to this coordinate:

$$
\rho(Q_u, Q'_u; t = 0) = \mathcal{N}(0) \exp \left\{ -\frac{\omega}{2\hbar \sinh(\beta \hbar \omega)} \left[ ((Q'^2 - Q^2_{u_0}) + (Q'^2_u - Q^2_{u_0})) \cosh(\beta \hbar \omega) 
- 2(Q_u - Q_{u_0})(Q'_u - Q_{u_0}) \right] \right\}
$$

with the same normalization factor as in (14).

We now solve the Liouville equation along the same steps used in the previous case using the real-time propagators. We obtain the probability as a function of time $p(Q_u; t) = \rho(Q_u, Q_u; t)$ as:

$$
p(Q_u, t) = \mathcal{N}(t) \exp \left[ -(Q_u - Q_{u_0} \cosh(\Omega t))^2 / 2\sigma(t)^2 \right]
$$

with $\sigma(t)$ and $\mathcal{N}(t)$ given by (18). The current (13) along the unstable direction evaluated at the saddle point ($Q_u = 0$) is found to be

$$
J_u(Q_u = 0; t) = \frac{\omega^2}{\Omega} \mathcal{N}(0) |Q_{u_0}| A(t) \exp \left[ -\tanh(\beta \hbar \omega / 2) B(t) \right]
$$

with

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

$$
B(t) = \frac{\omega Q^2_{u_0}}{\hbar} \left[ 1 + \frac{\omega^2}{\Omega^2} \tanh^2(\Omega t) \right]^{-1}
$$

The current is shown in figure 1. The probability evaluated at the saddle point is

$$
p(Q_u = 0, t) = \mathcal{N}(t) \exp \left[ -(Q_{u_0} \cosh(\Omega t))^2 / 2\sigma(t)^2 \right]
$$

with $\sigma(t)$ and $\mathcal{N}(t)$ given by (18). At times $t \gg \Omega^{-1}$, the rate
\[- \frac{d \ln[p(Q_u = 0, t)]}{dt} \approx \Omega \]

coincides with (20) and only reflects the spread of the initial density matrix. One can use this rate as an alternative definition in real time, leading again to the result (21) after integrating along all the perpendicular directions in functional space.

The depletion of probability at the saddle clearly reflects two physical effects. The first is the spread of the density matrix determined by \( \sigma(t) \), while the second is the “rolling” of the unstable coordinate down the inverted harmonic oscillator potential. The same features give the total current at the saddle. However, whereas the coordinate rolls down with a time dependence \( Q_u \cosh(\Omega t) \), the spread of the density matrix increases much faster and is given by \( \sigma(t) \). The two effects thus combine to give a positive current along the saddle point. We see then that despite the fact that bubbles with radii smaller than the critical radius collapse, they still contribute a positive current over the barrier. The total current along the unstable direction, evaluated at the saddle point is obtained by integrating the current (25) along all the perpendicular directions, and restoring the exponential Arrhenius factor. It is normalized by dividing by the partition function of the metastable well. This procedure then yields:

\[ \mathcal{J}_{T,u} = J_u(Q_u = 0; t) \left[ \frac{MT}{2\pi} \right]^{3/2} \exp[- \frac{E(R^*)}{T} \prod_k 2 \sinh(\omega^k / 2T) \prod_l 2 \sinh(\omega^l / 2T)] \]

where the factors were obtained as in (21) and \( J_u(Q_u = 0; t) \) is given by (25).

There are two questions that require an answer at this point: i) which one is a suitable definition of the rate, ii) what is the range of validity of the approximations involved in obtaining the results presented above. We answer these in turn:

i) We have seen that the definition of the rate given by (21) coincides (up to the prefactor) with the oft quoted result in the literature given by equation (2). This defi-
nition corresponds to describing the process of activation by assuming that the system is described by a gaussian density matrix in terms of the small fluctuations around the critical droplet, and that the activation rate is given by the rate of spread of the probability for a critical droplet integrated along all perpendicular directions in functional space. Although this seems a sensible definition of the rate, it is not the definition of the rate of change of probability for finding the system localized in the metastable state. This latter definition corresponds to calculating the total probability current at the saddle point as is obtained either from quantum mechanics or via the Fokker-Planck description[8, 10] and corresponds to the current (29) calculated above. The steady state assumption implicit in Langer's treatment thus leads to the identification of the two. However, we expect that in a strongly out of equilibrium situation, for which a steady state assumption is not valid, or during times for which the details of the initial state are important, the correct definition of the rate, that is, the probability current at the saddle, will yield a time dependent rate which will be sensitive to the initial conditions. In the case we have described above, this corresponds to sensitivity to the initial value of the coordinate $Q_u$.

There are several approximations invoked in this (and most other) analysis. First, the quadratic approximation around the critical droplet configuration. This approximation will be justified insofar as the higher order terms in the expansion (cubic and quartic in terms of the coordinates $Q_l$) can be neglected. Given that the imaginary part of the free energy describes a time dependent process in which the width of the probability distribution grows and therefore the fluctuations are growing, this approximation will break down at some time that will be given by the details of the particular problem, such as couplings and structure factors of the stable mode functions $f_l(\vec{r})$. In order to identify the rate (21) we had to assume that $t \gg \Omega^{-1}$, for small $\Omega$ (as is expected in the thin-wall approximation). This approximation may imply times longer than the regime of validity of the gaussian approximation, in which case the rate may depend on time.
A quantitative analysis of the validity of the approximations will require a more detailed knowledge of the potentials, mode functions couplings etc. and will have to be done for each particular problem individually.

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 on thermal activation. It is our impression that there is certain amount of discomfort and uneasy trust on the usual calculation of the activation rate via the imaginary part of an analytically continued equilibrium free energy. We have drawn the analogy between the case of thermal activation and the case of the one-loop effective potential for theories with spontaneous symmetry breaking at tree level. Both calculations involve gaussian approximations around unstable configurations (inverted harmonic oscillators) and both calculations obtain an imaginary part by analytically continuing the result for upright harmonic oscillators.

In both cases, the imaginary part of the free energy is associated with the growth of the width of an initially prepared gaussian state (density matrix) and signals the growth of fluctuations as a consequence of the instabilities.

We have shown that a real-time description of this process leads to a definition of the rate that, up to prefactors, is similar to that obtained via the recipe using the imaginary part of the free energy.

We also argued that in general, non-steady state or strongly out of equilibrium situations the correct definition of the rate, as the total probability current flowing across the saddle point along the unstable direction will lead to a rather different result which may in general be time dependent. We illustrated this situation with a non-equilibrium case with an initial situation in which the mean value of the collective coordinate representing the radius of the droplet has an expectation value which is smaller than the critical radius. Time dependent rates are common in activated events in condensed phases[21]
where transient behavior after an initial preparation is observed (see also[10]).

Although we cannot make general claims as to what is the correct rate in a given theory, our goal here was somewhat more restricted: to provide a dynamical, real-time interpretation of the imaginary part of the free energy and at the same time investigate scenarios for which a calculation of the rate based on this analytic continuation may not yield reliable results.

We are currently involved in calculations of decay rates in theories involving sphalerons using the real-time formalism developed here[22] as an initial condition problem. Specifically, if the phase transition occurs via a quench in such a way that the system does not have time to equilibrate around the minima, thermal activation will occur strongly out of equilibrium and dependence on the initial state and time dependent rates are expected.

The issue of thermalization in the wells requires a deeper understanding of the time scales involved, in particular in inflationary scenarios.

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[23].

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[24].

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 once a deeper understanding of the real-time dynamics of the process of thermal activation is understood in these systems.

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Figure Captions

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