Quantum field dynamics of the slow rollover in the linear delta expansion

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Abstract

We show how the linear delta expansion, as applied to the slow-roll transition in quantum mechanics, can be recast in the closed time-path formalism. This results in simpler, explicit expressions than were obtained in the Schrödinger formulation and allows for a straightforward generalization to higher dimensions. Motivated by the success of the method in the quantum-mechanical problem, where it has been shown to give more accurate results for longer than existing alternatives, we apply the linear delta expansion to four-dimensional field theory. At small times all methods agree. At later times, the first-order linear delta expansion is consistently higher than Hartree-Fock, but does not show any sign of a turnover. A turnover emerges in second-order of the method, but the value of $\langle \hat{\Phi}^2(t) \rangle$ at the turnover is larger than that given by the Hartree-Fock approximation. Based on this calculation, and our experience in the corresponding quantum-mechanical problem, we believe that the Hartree-Fock approximation does indeed underestimate the value of $\langle \hat{\Phi}^2(t) \rangle$ at the turnover. In subsequent applications of the method we hope to implement the calculation in the context of an expanding universe, following the line of earlier calculations by Boyanovsky et al., who used the Hartree-Fock and large-$N$ methods. It seems clear, however, that the method will become unreliable as the system enters the reheating stage.

1 Introduction

A period of inflation in the early universe could have the desirable consequence that a general initial condition will evolve towards the homogeneity, isotropy and flatness which we observe. Basic models require the slow evolution of a scalar field from an initial unstable vacuum state to a final stable state. Without knowing how to perform this inherently non-perturbative calculation exactly, approximation attempts must first prove themselves in the simpler situation of the quantum-mechanical slow roll. Though this simpler problem cannot be solved analytically, the degrees of freedom are sufficiently few that an exact numerical solution can be found. This allows us to test non-perturbative methods before proceeding to a calculation for the four-dimensional scalar field.

The quantum-mechanical slow roll was first treated by Guth and Pi [1], who considered the evolution of a Gaussian wave-packet initially centred at the top of a potential hill $V = -\frac{1}{2}m\omega q^2$. Following this, the Dirac time-dependent variational method was used for a potential $V = \lambda(q^2 - a^2)^2/24$, first by Cooper et al. [2], who used a Gaussian wave function ansatz, and

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later by Cheetham and Copeland [3], who included the second-order Hermite polynomial in their ansatz.

The work presented here is based on an alternative variational approach, the linear delta expansion (LDE), recently applied [4] to the quantum mechanical slow roll. The method was found to reproduce the exact time dependence for longer than any of the alternative methods.

In this paper we reformulate the LDE method in terms of a path integral rather than solving the Schrödinger equation with some wavefunction ansatz. Since we directly calculate expectation values without calculating the wavefunction, we save on calculational effort. More importantly, it is relatively straightforward to generalize to the generating functional formalism of quantum field theory in four space-time dimensions. This strategy is the same as that employed by Boyanovsky et al. in Ref. [5], who were able to generalize the Hartree method of Ref. [2]. Since the LDE method is more successful in the quantum mechanical case, we should expect it to be more accurate when applied to field theory.

We first consider the slow-roll phase transition in a one-dimensional field theory (quantum mechanics) with potential

\[ V = -\frac{1}{2} m \omega q^2. \]

This serves as a simple introduction to the path integral formulation of this problem. We then turn to a potential of the form \( V = \lambda (q^2 - a^2)^2 / 24 \) where we outline the LDE method. Finally we demonstrate the use of this method for a four-dimensional scalar field undergoing an instantaneous temperature quench.

In line with previous papers on the quantum-mechanical slow roll, we characterize the dynamical process by considering the expectation value of the field operator squared \( \hat{q}^2(t) \) (now working in the Heisenberg picture) with respect to an initial harmonic oscillator ground state. This is equivalent to the zero-temperature limit for an initial thermal distribution of states with Hamiltonian \( H = \frac{p^2}{2m} + \frac{1}{2} m \omega_i^2 q^2 \). We formulate the problem in this way in order to facilitate our transition to finite-temperature four-dimensional field theory. We have

\[
\langle 0 | \hat{q}^2(t) | 0 \rangle = \lim_{\beta \to \infty} \int dq' \langle q'; t_0 | \exp(-\beta \hat{H}) \hat{q}^2(t) | q'; t_0 \rangle \]

\[
= \lim_{\beta \to \infty} \int dq' \langle q'; t_0 - i\beta | \hat{q}^2(t) | q'; t_0 \rangle. \]

Green functions with respect to an initial field state at time \( t_0 \) and a final state at time \( t_0 - i\beta \) can be derived from a generating functional whose time contour \( c \) passes between these two points. The contour must also pass through the time \( t \) at which the \( \hat{q}^2(t) \) operator is inserted. The time contour typically passes from \( t_0 \) along the real time axis in the positive direction the point \( t \) or beyond it. It then passes back along the real time axis to \( t_0 \) before moving in the imaginary time direction to \( t_0 - i\beta \) (see Fig. 1).

The generating functional is

\[
Z[j] = \int Dq \exp \left\{ \frac{i}{\hbar} \int_c dt [L + \hbar j q] \right\}, \]

Figure 1: Complex time path.
The Lagrangian \( L \) must satisfy

\[
L(\text{Re}\{t\} = t_0) = -\frac{1}{2} q (m \partial_t^2 + m \omega_t^2) q
\]

in order to meet the initial conditions. At later times the form of the Lagrangian may change, modelling some external influence on the particle.

The field boundary conditions are fixed such that \( q(t_0) = q(t_0 - i\beta) \) and we derive general time contour ordered expectation values as follows:

\[
(0 \mid T_c \hat{q}(t_1) \hat{q}(t_2) \cdots \mid 0) = \frac{1}{Z[0]} \left[ \frac{\delta}{i\delta j(t_1)} \frac{\delta}{i\delta j(t_2)} \cdots Z[j] \right]_{j=0}
\]

where we take \( \beta \) to infinity in the quantum-mechanical slow roll, but in principal could choose any value representing some fixed initial temperature. This we do when considering the case of four-dimensional field theory. The method is known as the closed time path method for studying real time dependent Green functions. It was first conceived by Schwinger [6] and Keldish [7] (for a more recent account see [5]).

In section 2 we outline the closed time path method and apply it to the quantum-mechanical model. We reproduce previous results for the inverted harmonic oscillator. In section 3 we develop the LDE approximation method. In section 4 we apply these techniques to four-dimensional scalar field theory in both first and second order. For completeness we include an Appendix on the derivation of the propagator \( D(t, t') \), although this material can also be found in standard references ([8], [9]).

In the remaining pages we shall use units where \( \hbar = m = 1. \)

## 2 Inverted harmonic oscillator

In previous articles considering the quantum mechanical slow roll [11, 2, 3, 4], the particle begins at a time \( t = 0 \) when it is described by a Gaussian wave function, centred at the top of a potential hill. To reproduce this situation here, we consider the particle prepared at \( t < 0 \) in the ground state of an harmonic oscillator potential (corresponding to a Gaussian wave function). When \( t = 0 \) we suddenly change the Hamiltonian to one with a potential hill. Subsequent real time evolution of the particle sees it “rolling off” the top of the hill.

First let us consider a final potential of the form \( V = -\frac{1}{2} \omega_j^2 q^2 \). In terms of the Lagrangian we have

\[
L(t) = \frac{1}{2} q K(t) q
\]

\[
K(t) = -\partial_t^2 - \omega^2(t)
\]

\[
\omega^2(t) = \Theta(-t) \omega_1^2 - \Theta(t) \omega_2^2.
\]

where we define

\[
\Theta(t) = \begin{cases} 
1 & \text{Re}\{t\} > 0 \\
0 & \text{Re}\{t\} < 0 
\end{cases}
\]

To solve the field theory we begin by shifting the field variable \( q \) in Eq. (6) in order to complete the square

\[
q(t) \rightarrow q(t) - \int_c dt' D(t, t') j(t').
\]

The propagator \( D \) must satisfy \( K(t) D(t, t') = \delta_c(t, t') \), where the contour delta function \( \delta_c(t, t') \) is defined for a test function \( f(t) \) by \( \int_c dt' f(t') \delta_c(t, t') = f(t) \). This results in a generating functional of the form

\[
Z[j] = Z[0] \exp \left\{ -i \int_c dt' dt'' \left[ \frac{1}{2} j(t') D(t', t'') j(t'') \right] \right\}.
\]
Performing the functional derivatives in order to obtain $\langle \dot{q}^2(t) \rangle$ we find
\[
\langle \dot{q}^2(t) \rangle = \langle 0 \mid \dot{q}^2(t) \mid 0 \rangle = \frac{1}{Z[0]} \left[ -\frac{\delta^2}{\delta j^2(t)} Z[j] \right]_{j=0} = iD(t, t). \tag{10}
\]

In the zero temperature limit, the propagator is found to have the general solution (see appendix)
\[
iD(t_1, t_2) = \frac{1}{2\omega_i} \left[ \theta_c(t_1 - t_2)U^-(t_1)U^+(t_2) + \theta_c(t_2 - t_1)U^+(t_1)U^-(t_2) \right] \tag{11}
\]
where
\[
[\partial_t^2 + \omega^2(t)]U^\pm(t) = 0 \tag{12}
\]
and for $\text{Re}\{t\} < 0$ the two independent solutions are
\[
U^\pm(t) = \exp\{\pm i\omega_i t\}. \tag{13}
\]

The dynamical information of the theory is contained purely in the $U^\pm$-functions. The problem is essentially reduced to solving a second order differential equation. Fixing the boundary conditions such that
\[
U^\pm(0^+) = U^\pm(0^-) \tag{14}
\]
\[
\partial_t U^\pm(0^+) = \partial_t U^\pm(0^-) \tag{15}
\]
we find the general solution to Eq. (12):
\[
U^\pm(t) = \Theta(-t)e^{\pm i\omega_i t} + \Theta(t) \left( \cosh(\omega_f t) \pm i\frac{\omega_i}{\omega_f} \sinh(\omega_f t) \right). \tag{16}
\]

Putting Eqs. (10), (11) and (16) together we find
\[
\langle \dot{q}^2(t) \rangle = \Theta(-t)\frac{1}{2\omega_i} + \Theta(t) \left[ 1 + \frac{1}{2} \left( 1 + \frac{\omega_i^2}{\omega_f^2} \right) [\cosh(2\omega_f t) - 1] \right]. \tag{17}
\]

This is the standard harmonic oscillator result for $t < 0$. For $t > 0$ the expectation value begins to grow as the particle rolls off the top of the hill. The growth becomes exponential for large $t$:
\[
\langle \dot{q}^2(t) \rangle \rightarrow \frac{1}{8\omega_i} \left( 1 + \frac{\omega_i^2}{\omega_f^2} \right) \exp(2\omega_f t). \tag{18}
\]

This is in exact agreement with Guth and Pi after carefully comparing parameters.

### 3 Linear delta expansion

We next turn to the problem of a symmetry breaking potential described by a Lagrangian of the form
\[
L(t) = \frac{1}{2} q K(t) q - \frac{\lambda(t)}{24} q^4 \tag{19}
\]
\[
K(t) = -\partial_t^2 - \omega^2(t) \\
\omega^2(t) = \Theta(-t)\omega_i^2 - \Theta(t)\omega_f^2 \\
\lambda(t) = \Theta(t)\lambda.
\]

We could at this stage perform a perturbative expansion in powers of $\lambda$. However, we know that the particle is bound by the $q^4$ term to a region near to $q = 0$. If we perturb about the
Gaussian solution for $\langle \hat{q}^2(t) \rangle$, the perturbative correction must become large so as to prevent the exponential increase, and the philosophy of perturbation theory therefore breaks down.

The linear delta expansion (LDE) is a practical way of improving those aspects of a perturbative series which lead to its divergence [10, 11]. In toy models, where exact results are achievable, the LDE is known to produce convergent results and to do so much faster than alternatives. See, for instance, [12, 13] and references therein. The LDE has also been used successfully in many other situations, including studies of scalar theories [14].

In practice we substitute the Lagrangian with a new $\delta$-Lagrangian which is the same as the original upon setting $\delta$ equal to 1

$$L \rightarrow L_\delta = (1 - \delta)L_0 + \delta L.$$  \hspace{1cm} (20)

Here, $L_0$ is just taken to be the quadratic part of the Lagrangian, depending on some variational mass $\mu$,

$$L_0 = -\frac{1}{2} q(\partial_t^2 - \mu^2)q.$$  \hspace{1cm} (21)

The mass $\mu$ is treated as a constant for the purpose of performing any time integrals, and $\mu^2$ is taken to be equal to $-\omega_i^2$ for $\text{Re}\{t\} < 0$ so as not to interfere with the fixed initial conditions. We have

$$L(\text{Re}\{t\} < 0) = -\frac{1}{2} q(\partial_t^2 + \omega_i^2)q$$  \hspace{1cm} (22)

and

$$L_\delta(\text{Re}\{t\} > 0) = -\frac{1}{2} q(\partial_t^2 - \mu^2)q + \delta \left[ \frac{1}{2} q^2 - \frac{1}{24} q^4 + \frac{\lambda}{24} q^4 \right].$$  \hspace{1cm} (23)

Any given physical quantity is calculated as a perturbative expansion up to some given order in $\delta$. We then set $\delta$ equal to 1 and choose the value of $\mu$ according to the principle of minimal sensitivity (PMS). For $\langle \hat{q}^2(t) \rangle$ this is

$$\frac{d\langle \hat{q}^2(t) \rangle}{d\mu} = 0.$$  \hspace{1cm} (24)

The rationale for the PMS is that, although the exact value of the quantity in question can not depend on $\mu$, the expansion will have some residual $\mu$ dependence when truncated to some finite order. The stationary points have a special status, in that at such points this dependence is locally zero. At other points, where the dependence is non-zero, there is no reason to choose one over another. Apart from this logical justification, it has been rigorously proved in some simple models that the sequence of approximations provided by the PMS indeed converges (exponentially rapidly) to the exact answer [12, 13], in contrast to the perturbative expansion, where $\mu$ is fixed, which gives rise to an alternating divergent series. Apart from these proofs of convergence, it has been applied successfully, in a pragmatic way, to a large variety of problems in quantum mechanics and quantum field theory, both in the continuum and on the lattice [15, 16].

In some problems it is unfortunately the case that there is not a unique solution to the PMS condition, i.e. that there are several stationary points. In that event, some element of subjective judgement has to be exercised, such as the width of the maximum or minimum and continuity with known results or expected behaviour.

In the present problem the PMS criterion provides a different constraint on $\mu$ for each final time that we consider. Though $\mu$ will be different for different final times, it is not considered as a time dependent function in the evolution up to that final time. This is the simplest and most natural way to implement the LDE in a time-dependent problem.

The propagator is given as in Eq. (11); however, the mode functions are now dependent on $\mu$ and satisfy

$$[\partial_t^2 + \Theta(-t)\omega_i^2 - \Theta(t)\mu^2] U^\pm(t) = 0,$$  \hspace{1cm} (25)

where

\footnote{It is important to note that the LDE with PMS gives a sequence of approximations, rather than a conventional series, in which subsequent orders merely add additional terms to the series. Instead, subsequent orders also change the values of earlier terms.}
with solution
\[ U^\pm(t) = \Theta(-t)e^{\pm i \omega_i t} + \Theta(t) \left( \cosh(\mu t) \pm \frac{i \omega_i}{\mu} \sinh(\mu t) \right). \] (26)

At first order in \( \delta \), the relevant Feynman diagrams (Fig. 2) can be written out to give
\[
\langle \hat{q}^2(t) \rangle = iD(t,t) + \frac{\delta \lambda}{2} \int dt' \Theta(t')iD^2(t',t)iD(t',t') - \delta(\omega_i^2 - \mu^2) \int dt' \Theta(t')iD^2(t',t). \] (27)

Evaluating the integrals we have (for \( t > 0 \))
\[
\langle \hat{q}^2(t) \rangle = \frac{1}{2\omega_i} \left[ 1 + \frac{1}{2} \left( 1 + \frac{\omega_i^2}{\mu^2} \right) \cosh(2\mu t) - 1 \right] + \frac{\lambda}{16\omega_i^2 \mu^2} \left[ \frac{\omega_i^2}{\mu^2} \left( 1 - \frac{\omega_i^2}{\mu^2} \right) \cosh(2\mu t) - 1 \right] - 12 \left( 1 - \frac{\omega_i^2}{\mu^2} \right) \mu t \sinh(2\mu t) \left( 1 + \frac{\omega_i^2}{\mu^2} \right)^2 \cosh(4\mu t) - 1 \right] + \frac{(\omega_i^2 - \mu^2)}{4\omega_i \mu^2} \left[ \frac{\omega_i^2}{\mu^2} \left( 1 - \cosh(2\mu t) \right) + \left( 1 + \frac{\omega_i^2}{\mu^2} \right) \mu t \sinh(2\mu t) \right]. \] (28)

This is a remarkably simple, explicit form for \( \langle \hat{q}^2(t) \rangle \) compared with the complicated implicit expressions given in Ref. [4]. However, we have verified that these expressions do indeed reduce to Eq. (28).

To proceed, we find the optimum value of Eq. (28) according to the PMS criterion, Eq. (24). The result is the curve shown in Fig. 3. We have chosen \( \lambda = 0.01 \) and \( w_i^2 = \omega_i^2 = 25\lambda/6 \) (recall that \( w_i^2 \) appears with a different sign in the Lagrangian). These parameters coincide with those chosen in [1, 2, 3, 4] in order that we may easily compare our results. Also shown are the exact result, first-order perturbation theory, and the Hartree approximation of Ref. [2].

First-order perturbation theory is achieved upon setting \( \mu^2 = \omega_i^2 \) in Eq. (28), while the Hartree approximation amounts to taking \( \mu \) to be a time-dependent function given by \( \mu^2(t') = \omega_i^2 - (\lambda/2)iD(t',t') \). This results in a cancellation between the coupling correction and the mass insertion, and a self-consistent set of equations
\[
\langle \hat{q}^2(t) \rangle = iD(t,t) = \frac{1}{2\omega_i} U^-(t)U^+(t)
\left[ \partial_t^2 + \omega_i^2(t) + \frac{\lambda}{2} iD(t,t) \right] U^\pm(t) = 0. \] (29)

The LDE result is seen to track the exact result for a significantly longer time than the Hartree result. It then overshoots, signifying that the LDE result gives a much improved description of the inflationary period, but does not do so well during reheating.
In quantum mechanics it is possible to go to high order in the LDE by the use of recursion relations. The results of this exercise were given in Ref. [4], where the calculations were carried out to $O(\delta^7)$. It turns out that the second- and third-order calculations do not exhibit clear PMS points, but thereafter successive orders follow the true curve more and more accurately up to the turnover point, but diverge beyond that point. We can hope that in field theory in $(3+1)$ dimensions, the LDE will again give a good description of the initial slow-roll process. In field theory, however, it is not practical to go beyond second order.

4 Scalar field theory

Having developed our method for quantum mechanics, it remains to see how easily it can be implemented for the case of field theory. We consider a single real scalar field theory with time-dependent Lagrangian of the form

$$L(t) = \int d^3x \left\{ \frac{1}{2} \Phi \left(-\partial_t^2 + \nabla^2 - m^2(t)\right) \Phi - \frac{\lambda}{24} \Phi^4 \right\}$$

$$m^2(t) = \Theta(-t) m_i^2 - \Theta(t) m_f^2.$$  

With appropriate choice of the parameters, this model crudely describes a sudden temperature quench in which the field is driven through a phase transition at time $t = 0$.

Our interest is in determining the quantity

$$\langle \Phi^2(t) \rangle = \frac{1}{V} \int d^3x \langle \Phi^2(x, t) \rangle.$$
To perform the delta expansion we again define a $\delta$-Lagrangian by
\[ L \to L_\delta = (1 - \delta)L_0 + \delta L \] (33)
with
\[ L_0 = \int d^3x \left\{ \frac{1}{2} \Phi \left( -\partial_t^2 + \nabla^2 + \mu^2 \right) \Phi \right\}. \] (34)
We replace the original Lagrangian by our $\delta$-Lagrangian for $\text{Re}\{t\} > 0$. This gives
\[ L(\text{Re}\{t\} > 0) = \int d^3x \left\{ \frac{1}{2} \Phi \left( -\partial_t^2 + \nabla^2 + \mu^2 \right) \Phi \right\} + \delta \left[ \left( \frac{m_i^2 - \mu^2}{2} \right) \Phi^2 - \frac{\lambda}{24} \Phi^4 \right]. \] (35)
Switching to momentum space, the propagator now satisfies the relation
\[ K_p(t)D_p(t, t') = \delta_c(t, t'), \] (36)
where
\[ K_p(t) = -\partial_t^2 - \omega_p^2(t) \] (37)
and now
\[ \omega_{i\beta}^2 = p^2 + m_i^2 \] (39)
\[ \omega_{f\beta}^2 = \mu^2 - p^2. \] (40)
The propagator has the solution (see appendix)
\[ iD_p(t_1, t_2) = \theta_c(t_1 - t_2)iD_p^+(t_1, t_2) + \theta_c(t_2 - t_1)iD_p^-(t_1, t_2) \] (41)
where
\[ iD_p^+(t_1, t_2) = \frac{1}{2\omega_{i\beta}} \frac{1}{e^{\omega_{i\beta}t} - 1} \left[ U_p^+(t_1)U_p^-(t_2) + e^{\omega_{i\beta}t}U_p^-(t_1)U_p^+(t_2) \right] \] (42)
\[ iD_p^-(t_1, t_2) = \frac{1}{2\omega_{i\beta}} \frac{1}{e^{\omega_{i\beta}t} - 1} \left[ e^{\omega_{i\beta}t}U_p^+(t_1)U_p^-(t_2) + U_p^-(t_1)U_p^+(t_2) \right]. \] (43)
The mode functions satisfy
\[ \left[ \partial_t^2 + \omega_p^2(t) \right] U_p^\pm(t) = 0, \] (44)
with solutions
\[ U_p^\pm(t) = \Theta(-t)e^{\pm i\omega_p t} + \Theta(t) \left( \cosh(\omega_p t) \pm \frac{i}{\omega_p} \sinh(\omega_p t) \right). \] (45)

### 4.1 First order

The same diagrams which contributed to $\langle \dot{q}^2(t) \rangle$ in the previous section contribute to $\langle \dot{\Phi}^2(t) \rangle$ here. The essential difference from the quantum-mechanical case is that the propagators now depend on momentum and that any loops will involve an integration over loop momenta. The Feynman diagrams in Fig. 2 give
\[ \langle \dot{\Phi}^2(t) \rangle = \int_p iD_p(t, t) \]
\[ + \frac{\delta \lambda}{2} \int_c dt' \int_p iD_p^+(t', t) \int_k iD_k(t', t') \]
\[ - \delta (m_i^2 - \mu^2) \int_c dt' \Theta(t') \int_p iD_p^+(t', t) \] (46)
(cf. Eq. (27)) where we have used the notation

$$\int_p = \int \frac{d^3p}{(2\pi)^3}.$$  \hfill (47)

The momentum integrals are divergent and must be regularized. As in Ref. [5], we assume a scheme which leaves the contributions from stable modes ($p^2, k^2 > \mu^2$) being negligibly small. The dominant growth in $\langle \hat{\Phi}^2(t) \rangle$ is associated with the finite contribution of the unstable modes. In practice this means that we may perform momentum integrals in the finite range $p^2, k^2 < \mu^2$ to achieve finite results. We simply make the replacement

$$\int_p = \frac{1}{2\pi^2} \int_0^{\mu} p^2 dp.$$  \hfill (48)

The calculations are performed in the high-temperature limit, where $\beta \omega_{i;p} \ll 1$, so that

$$\coth \left( \frac{1}{2} \omega_{i;p} \beta \right) \sim \frac{2}{\beta \omega_{i;p}}.$$  \hfill (49)

In this limit the first term is found to be

$$\frac{1}{\beta} \int_p \frac{1}{\omega_{i;p}^2} \left[ 1 + \frac{1}{2} \left( 1 + \frac{\omega_{i;p}^2}{\omega_{f;p}^2} \right) \left[ \cosh(2\omega_{f;p}t) - 1 \right] \right],$$  \hfill (50)

the second is

$$-\frac{\lambda}{2\beta^2} \int_0^t dt' \int_p \frac{1}{\omega_{i;p}^2 \omega_{f;p}^2} \sinh \left[ \omega_{f;p}(t - t') \right]$$

$$\times \left[ \left( 1 + \frac{\omega_{i;p}^2}{\omega_{f;p}^2} \right) \cosh \left[ \omega_{f;p}(t + t') \right] + \left( 1 - \frac{\omega_{i;p}^2}{\omega_{f;p}^2} \right) \cosh \left[ \omega_{f;p}(t - t') \right] \right]$$

$$\times \int_k \frac{1}{\omega_{i;k}^2} \left[ 1 + \frac{1}{2} \left( 1 + \frac{\omega_{i;k}^2}{\omega_{f;k}^2} \right) \left[ \cosh(2\omega_{f;k}t') - 1 \right] \right],$$  \hfill (51)

and the third is

$$\frac{(m_f^2 - \mu^2)}{2\beta} \int_p \frac{1}{\omega_{i;p}^2 \omega_{f;p}^2} \left[ \omega_{i;p}^2 \left[ 1 - \cosh(2\omega_{f;p}t) \right] \right]$$

$$+ \left( 1 + \frac{\omega_{i;p}^2}{\omega_{f;p}^2} \right) \omega_{f;p}t \sinh(2\omega_{f;p}t).$$  \hfill (52)

In the second term, the time integral has not been performed explicitly since the result is rather involved.

Finally we impose the PMS constraint at each $t$ in order to find $\mu$ and evaluate $\langle \hat{\Phi}^2(t) \rangle$

$$\frac{d\langle \hat{\Phi}^2(t) \rangle}{d\mu} = 0.$$  \hfill (53)

For numerical calculations the units are chosen such that $\hbar = c = k_B = m_i^2 = 1$. The remaining parameters are then chosen in these units to be $m_f^2 = 1$, $T = 1/\beta = 4\sqrt{6/\lambda}$ (the initial temperature) and $\lambda = 10^{-12}$. These are chosen to coincide with those in Ref. [5]. The initial temperature has no particular meaning, it is simply twice the critical temperature. The coupling must be small for this type of model of inflation due to constraints from the spectrum of density fluctuations.
Examples of $\lambda\langle \hat{\Phi}^2 \rangle/2$ as functions of $\mu^2$ for various times are shown in Fig. 4. We observe a single stationary point, a maximum, which moves to the left and becomes sharper as $t$ increases. The motivation for the PMS criterion is that the exact answer is independent of $\mu$. In any finite order of the LDE this independence can only be achieved locally. A broad maximum indicates that the LDE is robust, but it becomes increasingly unreliable as the peak becomes sharper. From Fig. 4 we estimate that the first-order LDE can not be trusted beyond about $t=11$.

The position of the maximum versus time is shown in Fig. 5. At small times the dominant part of the action is the quadratic part, and the evolution is well described by perturbation theory, i.e. $\mu^2 \sim m_f^2 = 1$. At later times, as the fluctuations of the field grow, the quartic terms become more important. In the context of the LDE this is taken into account by smaller values of $\mu^2$ in the trial Lagrangian $L_0$ of Eq. (34).

The results for the evolution of the field are shown in Fig. 6 in the restricted range of $t$ where the different methods begin to diverge. Though we have no exact solution to compare with, the results display the same qualitative behaviour as in the quantum mechanical case studied in the earlier sections (Fig. 4).

First-order perturbation theory is achieved within the LDE framework by setting $\mu^2 = m_f^2$. As in the quantum-mechanical case, the Hartree result can be reproduced by considering $\mu$ to be a time-dependent function, this time given by

$$\mu^2(t') = m_f^2 - (\lambda/2) \int_p iD(t', t').$$

The resulting self-consistent set of equations are

$$\langle \hat{\Phi}^2(t) \rangle = \int_p iD(t, t) = \frac{1}{\beta} \int_p \frac{1}{\omega_{p_0}} U_p^-(t) U_p^+(t) \left[ \partial_t^2 + \omega_p^2(t) + \frac{\lambda}{2} \int_p iD(t, t) \right] U_p^+(t) = 0.$$
Figure 5: The PMS maximum $\mu^2$ versus $t$ in first-order LDE.

Figure 6: $\lambda\langle \Phi^2 \rangle/2$ versus $t$. The first-order LDE result is shown as a solid line. Also shown are the Hartree-Fock result of Ref. [5] (HF) and zeroth (PT$_0$) and first-order (PT$_1$) perturbation theory.
All methods give almost indistinguishable results up to $t \sim 9$. The Hartree and LDE methods remain close up to the classical spinodal region (where $V''(\Phi) < 0$, i.e., $\frac{1}{2}\langle \dot{\Phi}^2(t) \rangle > 1$). At later times the LDE method gives a larger value of $\langle \dot{\Phi}^2(t) \rangle$ than the Hartree method. Based on our experience of the quantum-mechanical case, we believe that the Hartree method turns over prematurely and that the LDE is closer to the exact result for longer. However, to this order it fails to give any indication of a turnover. As mentioned in relation to Fig. 4, the LDE becomes unreliable beyond $t \sim 11$, as the PMS peak becomes narrower.

### 4.2 Second order

To second order in the LDE there are altogether six additional graphs. These are exhibited in Eqs. (55–60), along with their analytic expressions, where the integrals along the time contour have not yet been performed. We have used a more compact notation for the $D$'s, whereby $D_p^{t''}t'$ stands for $D_p(t',t)$ and so on.

\begin{align}
\hat{\Phi}(t) &= -\frac{\delta^2}{4} \int_c dt' \int_c dt'' \int_p \left( i D_p^{t''}t' \right)^2 \int_{k_1} \left( i D_{k_1}^{t''}t' \right)^2 \int_{k_2} \left( i D_{k_2}^{t''}t' \right)^2 \\
&= -\frac{\delta^2}{4} \int_c dt' \int_c dt'' \int_p i D_p^{t''}t' i D_p^{t''}t' \int_{k_1} i D_{k_1}^{t''}t' \int_{k_2} i D_{k_2}^{t''}t' \\
&= -\frac{\delta^2}{6} \int_c dt' \int_c dt'' \int_p i D_p^{t''}t' i D_p^{t''}t' \int_{k_1} i D_{k_1}^{t''}t' \int_{k_2} i D_{k_2}^{t''}t' \\
&= \frac{\delta^2}{2} \int_c dt' \int_c dt'' \int_p \left( i D_p^{t'}t' \right)^2 \int_{k_1} \left( i D_{k_1}^{t'}t' \right) \int_{k_2} \left( i D_{k_2}^{t'}t' \right) \\
&= \frac{\delta^2}{2} \int_c dt' \int_c dt'' \int_p i D_p^{t''}t' i D_p^{t''}t' \int_{k_1} i D_{k_1}^{t''}t' \int_{k_2} i D_{k_2}^{t''}t' \\
&= -\frac{\delta^2}{2} (m_f^2 - \mu^2)^2 \int_c dt' \int_c dt'' \int_p i D_p^{t''}t' i D_p^{t''}t' \int_{k_1} i D_{k_1}^{t''}t' \int_{k_2} i D_{k_2}^{t''}t' \\
&= -\frac{\delta^2}{2} (m_f^2 - \mu^2)^2 \int_c dt' \int_c dt'' \int_p i D_p^{t''}t' i D_p^{t''}t' \int_{k_1} i D_{k_1}^{t''}t' \int_{k_2} i D_{k_2}^{t''}t'.
\end{align}

In performing the time integrals in $t''$, $t'$ over the contour of Fig. 1, the result is most easily expressed in terms of the real and imaginary parts of the $D$'s, or more precisely $F$ and $\rho$, defined by

\begin{align}
F &= \frac{1}{2} (iD^> + iD^<) \\
\rho &= i (iD^> - iD^<). \quad (61)
\end{align}

In the high-temperature limit, in which we are working, the imaginary parts are much smaller than the real parts:

\begin{align}
F_p^{t_1t_2} &= \frac{1}{\omega_{t_1t_2}^2} \left[ \cosh(\omega_{f,p}t_1) \cosh(\omega_{f,p}t_2) + \frac{\omega_{f,p}^2}{\omega_{f,p}^2} \sinh(\omega_{f,p}t_1) \sinh(\omega_{f,p}t_2) \right], \quad (62)
\end{align}

compared with

\begin{align}
\rho_p^{t_1t_2} &= \frac{1}{\omega_{f,p}} (\sinh(\omega_{f,p}t_1) \cosh(\omega_{f,p}t_2) - \cosh(\omega_{f,p}t_1) \sinh(\omega_{f,p}t_2)) \quad (63)
\end{align}
The resulting expressions for diagrams (55)–(60), having set δ = 1, are:

\[
\begin{split}
\bigcirc \quad & = \lambda^2 \int_0^t dt' \int_0^{t'} dt'' \int_p F'_{p+1} \rho'_{p-1} \int_k \int_k F''_{k-1} \rho''_{k+1} \\
\bigcirc \quad & = -\frac{\lambda^2}{4} \left\{ 2 \int_0^t dt' \int_0^{t'} dt'' \int_p \rho'_{p+1} F'_{p-1} \int_k \int_k F''_{k-1} \right. \\
\bigcirc \quad & \quad \quad \quad \left. - \int_0^t dt' \int_0^{t'} dt'' \int_p \rho'_{p+1} F'_{p-1} \int_k \int_k F''_{k-1} \right\} \\
\bigcirc \quad & = -\frac{\lambda^2}{24} \left\{ 2 \int_0^t dt' \int_0^{t'} dt'' \int_p \rho'_{p+1} F'_{p-1} \int_k \int_k \left( \frac{12 F'_{k-1} F''_{k-1} \rho'_{p-1} \rho''_{p-1}}{k_{k-1} - k_{k+1}} - \frac{12 F'_{k-1} F''_{k-1} \rho'_{p-1} \rho''_{p-1}}{k_{k-1} - k_{k+1}} \right) \\
\bigcirc \quad & \quad \quad \quad \left. + \int_0^t dt' \int_0^{t'} dt'' \int_p \rho'_{p+1} F'_{p-1} \int_k \int_k \left( \frac{12 F'_{k-1} F''_{k-1} \rho'_{p-1} \rho''_{p-1}}{k_{k-1} - k_{k+1}} - \frac{12 F'_{k-1} F''_{k-1} \rho'_{p-1} \rho''_{p-1}}{k_{k-1} - k_{k+1}} \right) \right\} \\
\bigcirc \quad & = -2\lambda(m^2 - \mu^2) \int_0^t dt' \int_0^{t'} dt'' \int_p F'_{p+1} \rho'_{p-1} \int_k \int_k F''_{k-1} \\
\bigcirc \quad & = \frac{\lambda(m^2 - \mu^2)}{2} \left\{ 2 \int_0^t dt' \int_0^{t'} dt'' \int_p \rho'_{p+1} F'_{p-1} \int_k \int_k \left( F'_{k-1} + \int_k F'_{k+1} \right) \\
\bigcirc \quad & \quad \quad \quad \left. - 2 \int_0^t dt' \int_0^{t'} dt'' \int_p \rho'_{p+1} F'_{p-1} \int_k \int_k \left( F'_{k-1} + \int_k F'_{k+1} \right) \right\} \\
\bigcirc \quad & = -(m^2 - \mu^2)^2 \left\{ 2 \int_0^t dt' \int_0^{t'} dt'' \int_p \rho'_{p+1} F'_{p-1} \int_k \int_k \left( F'_{k-1} + \int_k F'_{k+1} \right) \\
\bigcirc \quad & \quad \quad \quad \left. - \int_0^t dt' \int_0^{t'} dt'' \int_p \rho'_{p+1} F'_{p-1} \int_k \int_k \left( F'_{k-1} + \int_k F'_{k+1} \right) \right\} \\
\end{split}
\] (64) (65) (66) (67) (68) (69)

In most of the diagrams there are two terms involving an integral over t'' up to t and another up to t'. In the original forms of these expressions there were severe cancellations between the two integrals, which made accurate integration extremely difficult. In the present, equivalent, form the two integrals give roughly comparable contributions, posing no difficulty for numerical integration.

We have evaluated all the multidimensional integrals numerically, including the time integrals, using the NAG Fortran routine D01FCF. The most difficult diagram to evaluate is, of course, the “sunset” diagram of Eqs. (57) and (66). Because the integrand depends only on the magnitudes of the various momenta, there are two azimuthal integrations which can be trivially performed, leaving a seven-dimensional integral.

The result of these calculations is that the expectation value $\lambda(\hat{\Phi}^2)/2$ now develops a PMS minimum as a function of $\mu^2$. Examples of this behaviour are given in Fig. 7 for the same times as were previously shown at first order. The maximum appears to be a spurious stationary point, with a runaway behaviour for $\lambda(\hat{\Phi}^2)/2$.

The trend of the minimum as a function of $t$ is similar to that of the first-order maximum, decreasing slowly as $t$ increases, as shown in Fig. 8. The resulting plot of $\lambda(\hat{\Phi}^2(t))/2$ versus $t$ is shown in Figure 9 where in addition to the Hartree-Fock result we also show the result of the first-order large-$N$ calculation (with $N = 1$). We see that the second-order result now shows a turnover, but at a larger value of $\langle \hat{\Phi}^2(t) \rangle$ than that given by Hartree-Fock. This is the same feature that occurred in the quantum-mechanical problem, and we believe gives strong evidence that the Hartree-Fock method turns over too soon in $\langle \hat{\Phi}^2(t) \rangle$. In this case, where there is no symmetry breaking, the large-$N$ calculation differs from Hartree-Fock only in that the coefficient of $iD(t,t)$ in Eq. (54) is reduced by a factor of 3. This means that this term takes longer to
become important and produce a turnover, so that the maximum value is considerably greater. The same feature occurs in the quantum mechanical problem, where the large-$N$ approximation greatly overestimates the maximum value of $\langle \hat{q}^2(t) \rangle$.

Figure 7: $\lambda(\Phi^2)/2$ versus $\mu^2$ for $t = 10.5, 11, 11.5$ in second-order LDE.

Figure 8: The PMS minimum $\mu^2$ versus $t$ in second-order LDE.

We have seen that inclusion of the second-order diagrams leads to a turnover which does not occur in first order. It would be tempting to ascribe this turnover to the influence of the “sunset diagram”, the first diagram to include the important effects of rescattering\cite{17}. However, for
the present calculation it is not possible to single out this particular diagram from the others. Its distinctive role is rather to provide for dissipation and thermalization at later times (see e.g. [18, 19, 20]), where unfortunately the LDE is unreliable. The Hartree-Fock method, which in our language corresponds to a time-dependent $\mu$ with a particular selection criterion, provides an example where a turnover is achieved without the inclusion of this diagram.

5 Discussion

The main motivation for this work was to expand upon the available machinery for tackling out-of-equilibrium problems in field theory.

The linear delta expansion, applied to the quantum-mechanical equivalent of the slow-roll transition, has been shown to give a consistent improvement on other methods. However, the Schrödinger formulation of Ref. [4] can not immediately be generalized to field theory in higher dimensions. We have shown how to recast the problem in terms of the closed time-path formalism, which can be so generalized. This is an extension which has not been achieved in other treatments of the quantum-mechanical problem, with the exception of the Hartree method.

As noted in [5], the Hartree approximation cannot probe the non-linear regions of the potential. Moreover, the Hartree method is a one-off approximation, which is not capable of systematic improvement. To understand the later time behaviour and to probe the true vacuum, calculations must to go beyond Hartree. The LDE, a systematic expansion with a variational component, offers just this possibility, although for practical reasons, it would be extremely difficult to go beyond second order in quantum field theory.

The main result of the paper is the formalism outlined in section 4, and Fig. 9 which provides a demonstration of its use in the instantaneous quench approximation in four-dimensional field theory in flat space-time. The next obvious extension is to couple the field to the scale factor of an expanding Universe.
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Appendix

It is here demonstrated how to solve for the propagator $iD(t_1, t_2)$ in quantum mechanics. We shall need to impose constraints due to the commutation relations and the KMS boundary condition, but we begin by decomposing the propagator as

$$iD(t_1, t_2) = \theta(t_1 - t_2)iD^>(t_1, t_2) + \theta_c(t_2 - t_1)iD^<(t_1, t_2)$$  (70)

where $\theta(t - t') = \int_{t_0}^t dt''\delta_c(t', t'')$. Since $K(t)D(t, t') = \delta_c(t, t')$, it is straightforward to demonstrate that

$$K(t)D^{>(<)}(t, t') = 0.$$  (71)

We shall construct $D^{>(<)}$ from homogeneous solutions to the quadratic operator $K$, i.e. functions which satisfy $K(t)U^<(t) = 0$. For $t < 0$, these have the solution $U^<(t) = \exp\{\pm i\omega t\}$. Thus, the most general form for $D^{>(<)}$ is

$$iD^{>(<)}(t_1, t_2) = a^{>(<)}U^+(t_1)U^-(t_2) + b^{>(<)}U^-(t_1)U^+(t_2).$$  (72)

Other possible combinations of $U^\pm$ can be ruled out on imposing time translation invariance at early times. The parameters $a^{>(<)}$ and $b^{>(<)}$ are to be determined. To do this we begin by imposing the particle equal time commutation relation

$$[\hat{q}, \hat{p}] = i.$$  (73)

We make the free field identification $\langle T_c\hat{q}(t_1)\hat{q}(t_2)\rangle = iD(t_1, t_2)$ and further that $\hat{p} = \dot{\hat{q}}$. This leaves

$$\partial_{t_2}[iD^{>(<)}(t_1, t_2) - iD^{>(<)}(t_1, t_2)]_{t_1=t_2} = i$$  (74)

which constrains the free parameters as follows

$$a^<< - a^>> + b^>> - b^<< = \frac{1}{\omega_i}.  \tag{75}$$

A further symmetry requirement at equal time is that

$$iD^>(t, t) = iD^<(t, t)$$  (76)

which translates to

$$a^>> + b^>> = a^<< + b^<<.  \tag{77}$$

Finally we impose the KMS boundary condition

$$iD^<(t_0, t) = iD^>(t_0 - i\beta, t)$$  (78)

or

$$a^<< = \exp\{\omega_i\beta\}a^>> \tag{79}$$

$$b^<< = \exp\{-\omega_i\beta\}b^>>.  \tag{80}$$

Eqs. (70), (71), (72) and (78) constitute 4 constraints on our 4 parameters. The set of equations is easily solved yielding

$$a^>> = b^<< = \frac{1}{2\omega_i \exp\{\omega_i\beta\} - 1}$$  (81)

$$a^<< = b^>> = \frac{\exp\{\omega_i\beta\}}{2\omega_i \exp\{\omega_i\beta\} - 1}.  \tag{82}$$
We now have a general solution for the propagator at finite temperature. Taking the zero temperature limit we have

\[ iD^>(t_1, t_2) = \frac{1}{2\omega_i} U^-(t_1) U^+(t_2) \]  
\[ iD^<(t_1, t_2) = \frac{1}{2\omega_i} U^+(t_1) U^-(t_2). \]  

The field theory case is much the same, with mode functions satisfying

\[ K_p(t_1) D_p(t_1, t_2) = \delta_c(t_1, t_2) \]  

and

\[ \langle T c\hat{\phi}_p(t_1) \hat{\phi}_p(t_2) \rangle = ViD_p(t_1, t_2). \]  

The solution for an initial state described by a temperature $1/\beta$ is given in the main text.

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