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

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We apply the linear delta expansion to the quantum mechanical version of the slow rollover transition which is the principal feature of inflationary models of the early Universe. The method, which goes beyond the Gaussian approximation, gives results which stay close to the exact solution for longer than previous methods. It provides a promising basis for extension to a full field theoretic treatment.

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I. INTRODUCTION

Inflationary models of the early Universe rely on the slow evolution of an inflaton field φ from the initial unstable vacuum state in which $\langle \varphi \rangle = 0$ to the final stable vacuum in which $\langle \varphi \rangle = \pm a$, say. The effective potential $V_{\text{eff}}(\varphi_c)$ giving rise to this transition has the generic form of a gentle hill centered at $\varphi_c = 0$ with minima at $\varphi_c = \pm a$.

The transition can be discussed at various levels of sophistication. At the most naive level one can think classically in terms of a ball rolling slowly down the slope of the potential. The corresponding quantum-mechanical problem, which is the subject of the present paper, is the time development of a state whose wave function is initially concentrated around the position of the maximum of the potential. The full treatment of the problem must, of course, be formulated within the framework of quantum field theory.

The problem is inherently non-perturbative, so that the calculations are dependent on the use of one nonperturbative approximation method or another. To date, in the field theory context, the only methods available have been the large-N [1] and Hartree-Fock [2] approximations. The large-N method is notoriously difficult to extend beyond leading order, while the Hartree-Fock method involves a truncation whose accuracy is not obvious, and it may be that some of the results obtained are artifacts of the approximations. It would therefore be useful to have another method which in principle is capable of systematic extension to higher orders, and has proved successful in other, static contexts. Such a potential method is the linear delta expansion [3], which has had various successful applications [4] and can be shown rigorously to converge when applied to the finite-temperature partition function [5] or the energy levels [6] of the quartic anharmonic oscillator.

As a preliminary to the use of the linear delta expansion (LDE) in the full field-theoretic problem it is clearly desirable to check its applicability and compare it with the Hartree-Fock method in the simpler context of quantum mechanics, where we will indeed find that it is considerably more accurate.

The first treatment of the quantum mechanical problem

was given by Guth and Pi [7], who solved exactly the equation of motion for an initial Gaussian wave-function in an upside-down harmonic oscillator potential $V = -\frac{1}{2}kx^2$. This was followed by a paper by Cooper *et al.* [8], who used a Gaussian ansatz in the Dirac time-dependent variational principle for the standard symmetry-breaking potential $V = \lambda (x^2 - a^2)^2/24$. The resulting Hartree-Fock solution tracks the exact solution for a short time, but departs from it before the time at which $\langle x^2 \rangle$ reaches its first maximum. Several years later Cheetham and Copeland [9] went beyond the Gaussian approximation by using an ansatz which included a second-order Hermite polynomial. This represented an improvement on the Hartree-Fock approximation, but still did not reproduce the first maximum in $\langle x^2 \rangle$ of the exact wavefunction.

As mentioned above, we will use the quantum mechanical problem as a testing ground for the application of the linear delta expansion to time-dependent problems. The LDE is a method akin to perturbation theory, but with the crucial difference that the form of the unperturbed Hamiltonian H_0 is not fixed once and for all, but varied at each order in the expansion by some well-defined criterion. The role of the formal parameter δ is simply to keep track of the order of the expansion. The method has the great advantage that its generalization to field theory is straightforward. Its previous success with the static properties of the anharmonic oscillator encourage us to apply it to this dynamical problem.

The relevant Hamiltonian $(\hbar = 1)$ is

$$H = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \lambda (x^2 - a^2)^2 / 24 + \text{const}$$

= $-\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{2} m^2 x^2 + g x^4$, (1)

with $m^2 = \lambda a^2/6$ and $g = \lambda/24$, which we split according to

$$H = -\frac{1}{2} \frac{\partial^2}{\partial x^2} \pm \frac{1}{2} \mu^2 x^2 + \delta g(x^4 - \rho x^2), \qquad (2)$$

where $2g\rho = m^2 \pm \mu^2$. That is, we choose as bare mass term $\pm \frac{1}{2}\mu^2 x^2$. The sign of the term as well as the value of μ will be determined as functions of *t* after the perturbative expansion has been carried out to a given order (at which stage δ is set equal to 1) by the principle of minimal sensitivity (PMS) [10], namely that

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$$\frac{\partial \langle x^2 \rangle^{1/2}}{\partial \mu} = 0. \tag{3}$$

Note that for either sign of the new mass term, μ has a limited range. In case (i), when the mass term is $-\frac{1}{2}\mu^2 x^2$, we have $2g\rho = m^2 - \mu^2$. The essence of the delta expansion is that the extra term $-g\rho x^2$ in the interaction should compensate as far as possible the original term gx^4 , which means that ρ should be positive. Hence we require that $\mu^2 < m^2$. In case (ii), when the mass term is $+\frac{1}{2}\mu^2 x^2$, the same restriction will arise from the form of the zeroth-order solution and the initial wave function.

II. DELTA EXPANSION

The two cases need to be treated separately. Which of them is relevant at a given value of t is determined by the PMS criterion.

A. Case (i)

In this case the bare Hamiltonian is

$$H_0 = -\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{2} \mu^2 x^2.$$
 (4)

It is useful to scale x according to $x = y/\sqrt{\mu}$, so that

$$H_0 = -\frac{\mu}{2} \left(\frac{\partial^2}{\partial y^2} + y^2 \right). \tag{5}$$

Given that the initial wave function is a Gaussian of the form $\psi(t=0) = A \exp(-By^2)$, the zeroth-order equation of motion $H_0\psi_0 = i\partial\psi_0/\partial t$ can be solved exactly by a wave function of the same form with *A* and *B* becoming functions of *t*. The equations they have to satisfy are

$$i\dot{B}/\mu = 2B^2 + \frac{1}{2},$$
$$i\dot{A}/\mu = AB,$$
(6)

with solutions

$$B = \frac{1}{2} \tan(\eta_0 - i\mu t)$$
$$A = \mathcal{N}[\cos(\eta_0 - i\mu t)]^{-1/2}$$
(7)

where η_0 is determined by $B(t=0) = \frac{1}{2} \tan \eta_0$ and the normalization constant \mathcal{N} by $A(t=0) = \mathcal{N}(\cos \eta_0)^{-1/2}$. This is precisely the solution of Guth and Pi for the upside-down oscillator, with *m* replaced by μ .

To obtain a systematic perturbative expansion in powers of δ it is useful to write $\psi = \varphi \exp[-B(t)y^2]$. The equation for φ is then

$$i\dot{\varphi} = \mu \bigg[B\varphi + 2By\varphi' - \frac{1}{2}\varphi'' + \delta\tilde{g}(y^4 - \tilde{\rho}y^2)\varphi \bigg], \qquad (8)$$

where we have scaled g and ρ according to $g = \mu^3 \tilde{g}$ and $\rho = \tilde{\rho}/\mu$.

A general feature of perturbative expansions for a polynomial potential of degree *p* is that φ is also a polynomial, of degree *Np* in *N*th order of the expansion. Thus in the present case, expanding φ as $\varphi = \sum \delta^n \varphi_n$, the first-order part φ_1 is an (even) polynomial of degree 4, which we write as $\varphi_1 = a + by^2 + cy^4$. The equations of motion for the coefficients *a*, *b* and *c* are

$$i\dot{a}/\mu = Ba - b \tag{9}$$
$$i\dot{b}/\mu = 5Bb - 6c - \tilde{\rho}\tilde{g}A$$
$$i\dot{c}/\mu = 9Bc + \tilde{g}A,$$

which can be solved successively in reverse order, using the solutions for *A* and *B* previously determined. The initial conditions at t=0 are a=b=c=0. Thus *c* is given by

$$c = \frac{-i\tilde{g}\mathcal{N}/8}{(\cosh\tilde{\theta})^{9/2}} \left\{ 3\tilde{\theta} + 2\sinh 2\tilde{\theta} + \frac{1}{4}\sinh 4\tilde{\theta} - c_0 \right\}, \quad (10)$$

where $\hat{\theta} = \mu t + i \eta_0$ and $c_0 = 3i \eta_0 + 2i \sin 2\eta_0 + (i/4) \sin 4\eta_0$. Using this solution in the equation for *b* we obtain

$$b = \frac{-i\tilde{g}\mathcal{N}}{(\cosh\tilde{\theta})^{5/2}} \left\{ -\frac{1}{2}\tilde{\rho} \left(\tilde{\theta} + \frac{1}{2}\mathrm{sinh}2\,\tilde{\theta} \right) + b_0 + \frac{3i}{4} [3\,\tilde{\theta}\mathrm{tanh}\,\tilde{\theta} + \cosh^2\tilde{\theta} - c_0\mathrm{tanh}\,\tilde{\theta}] \right\}, \quad (11)$$

where

$$b_0 = \frac{i}{2} \tilde{\rho} \,\eta_0 + \frac{i}{4} \tilde{\rho} \sin 2 \,\eta_0 + \frac{9i}{4} \,\eta_0 \tan \,\eta_0 - \frac{3}{4} c_0 \tan \,\eta_0$$
$$- \frac{3i}{4} \cos^2 \eta_0 \,.$$

Finally, using this solution in the equation for a we obtain

$$a = \frac{\tilde{g}\mathcal{N}}{(\cosh\tilde{\theta})^{1/2}} \left\{ -\frac{1}{2}\tilde{\rho}\tilde{\theta}\tanh\tilde{\theta} + b_{0}\tanh\tilde{\theta} - a_{0} + \frac{3i}{4} \left[3\left(-\frac{1}{2}\tilde{\theta}\operatorname{sech}^{2}\tilde{\theta} + \frac{1}{2}\tanh\tilde{\theta} \right) + \tilde{\theta} + \frac{1}{2}c_{0}\operatorname{sech}^{2}\tilde{\theta} \right] \right\},$$
(12)

where

$$a_{0} = \frac{1}{2} \tilde{\rho} \,\eta_{0} \tan \,\eta_{0} + i b_{0} \tan \,\eta_{0} + \frac{3}{4} i \bigg[\frac{3}{2} (-i \,\eta_{0} \sec^{2} \eta_{0} + i \tan \,\eta_{0}) + i \,\eta_{0} + \frac{1}{2} c_{0} \sec^{2} \eta_{0} \bigg].$$

B. Case (ii)

The zeroth-order equations in this case are

$$i\dot{B}/\mu = 2B^2 - \frac{1}{2},$$

$$i\dot{A}/\mu = AB,$$
 (13)

with solutions

$$B = \frac{1}{2} \operatorname{coth}(\eta_0 + i\mu t)$$
$$A = \mathcal{N}[\sinh(\eta_0 + i\mu t)]^{-1/2}.$$
 (14)

As mentioned in the Introduction, the restriction on μ in this case comes from the form of B(t=0) and the form of the initial wave function, which, in all the papers quoted, is taken as a minimal wave packet appropriate to a positive mass term $+\frac{1}{2}m^2x^2$. In the present formulation this means that $B(t=0)=(1/2)(m/\mu)$. But since $B(t=0)=(1/2) \coth \eta_0 < 1/2$, we have the same restriction on μ , namely $\mu < m$, as in case (i).

The first-order equations for a, b and c are identical in form to Eq. (9), but the driving terms A and B are now different.

The solution for c is now

$$c = \frac{-i\tilde{g}\mathcal{N}/8}{(i\sin\tilde{\theta})^{9/2}} \left\{ 3\tilde{\theta} - 2\sin 2\tilde{\theta} + \frac{1}{4}\sin 4\tilde{\theta} - c_0 \right\}$$
(15)

where $c_0 = -3i \eta_0 + 2i \sinh 2\eta_0 - (i/4) \sinh 4\eta_0$ and in this case $\tilde{\theta} = \mu t - i \eta_0$.

Using this solution in the equation for b we obtain

$$b = \frac{\tilde{g}\mathcal{N}}{(i\sin\tilde{\theta})^{5/2}} \left\{ -\frac{i}{2}\tilde{\rho} \left(\tilde{\theta} - \frac{1}{2}\sin 2\tilde{\theta} \right) + b_0 - \frac{3}{4} \left[-3\tilde{\theta}\cot\tilde{\theta} + \cos^2\tilde{\theta} + c_0\cot\tilde{\theta} \right] \right\},$$
(16)

where

$$b_0 = \frac{1}{2} \tilde{\rho} \,\eta_0 - \frac{1}{4} \tilde{\rho} \sinh 2 \,\eta_0 - \frac{9}{4} \,\eta_0 \coth \,\eta_0 + \frac{3i}{4} c_0 \coth \,\eta_0 + \frac{3}{4} c_0 \coth \,\eta_0 + \frac{3}{4} \cosh^2 \eta_0.$$

Finally, using this solution in the equation for a we obtain

$$a = \frac{\tilde{g}\mathcal{N}}{(i\sin\tilde{\theta})^{1/2}} \left\{ \frac{1}{2} \tilde{\rho} \tilde{\theta} \cot\tilde{\theta} + ib_0 \cot\tilde{\theta} + a_0 - \frac{3i}{4} \left[\frac{3}{2} \tilde{\theta} \csc^2\tilde{\theta} + \frac{1}{2} \cot\tilde{\theta} - \tilde{\theta} - \frac{1}{2} c_0 \csc^2\tilde{\theta} \right] \right\}, \quad (17)$$

where

$$a_{0} = \frac{1}{2}\tilde{\rho} \,\eta_{0} \text{coth } \eta_{0} - b_{0} \text{coth } \eta_{0} - \frac{3}{4} \left[\frac{3}{2} \,\eta_{0} \,\text{cosech}^{2} \,\eta_{0} \right] \\ + \frac{1}{2} \text{coth } \eta_{0} + \eta_{0} - \frac{i}{2} \,c_{0} \,\text{cosech}^{2} \,\eta_{0} \right].$$

We have checked these solutions by numerical integration using the Runge-Kutta method. This reveals that in case (ii) care needs to be taken to ensure that we are on the appropriate branch of the square roots. At values of *t* where $\sin \theta = -1$, a naive numerical evaluation will stay on the first sheet, thus giving rise to a discontinuity, whereas the true solution is, of course, continuous.

In fact, as we shall see, the coefficient *a* is not needed in the calculation of $\langle x^2 \rangle^{1/2}$ to first order in δ , though it is, of course, needed in higher order.

III. VARIATIONAL ASPECT

The expressions we have obtained all depend on the parameter μ introduced in Eq. (2). The other essential aspect of the delta expansion is that such a parameter is determined by some non-perturbative criterion, most frequently the principle of minimal sensitivity, Eq. (3).

To that end we need an expression for $\langle x^2 \rangle$, which, given that the wave function is a (complex) Gaussian with polynomial corrections, can be written down in closed form in terms of the coefficients A, B, a, b, c. Thus to order δ ,

$$|\psi|^{2} = [|A|^{2} + 2\delta \operatorname{Re}\{A^{*}(a+by^{2}+cy^{4})\}]e^{-\alpha y^{2}}, \quad (18)$$

where $\alpha = 2 \operatorname{Re} B$, so that

$$\langle y^{2} \rangle = \frac{1}{2\alpha} \frac{1 + (2\delta/|A^{2}|)\operatorname{Re}\{A^{*}[a+3b/(2\alpha)+15c/(4\alpha^{2})]\}}{1 + (2\delta/|A^{2}|)\operatorname{Re}\{A^{*}[a+b/(2\alpha)+3c/(4\alpha^{2})]\}} = \frac{1}{2\alpha} \left[1 + \frac{2\delta}{|A^{2}|}\operatorname{Re}\left\{A^{*}\left(\frac{b}{\alpha}+\frac{3c}{\alpha^{2}}\right)\right\}\right].$$
(19)

It is an interesting feature of the structure of the perturbative equations that the wave-function is automatically normalized to the order we are working. That is, $\int \varphi_0^* \varphi_1 = 0$. Thus the

second equation is identical to the first, and not merely an O(δ) approximation to it. The expectation value we seek is obtained on scaling by μ , i.e. $\langle x^2 \rangle = \langle y^2 \rangle / \mu$.



FIG. 1. Graphs of $\langle x^2 \rangle^{1/2}$ versus $\sigma \mu^2$ for t=5, 9 and 13, where $\sigma = -1$ for case (i) and $\sigma = +1$ for case (ii).

At this stage we set $\delta = 1$ and apply Eq. (3). This has to be done for each time *t*, and the result is that the chosen value $\overline{\mu}$ of μ now becomes a function of *t*, even though μ was treated as a constant in the equations of motion. In the present case,



FIG. 2. $\sigma \overline{\mu}^2$ versus *t*. The changeover from case (i) to case (ii) occurs between t=11 and t=12.

since we are unable to go to very high orders in the expansion this is a more important property than the *N*-dependence of $\overline{\mu}$. The O(δ^0) calculation does not have such a stationary point.

In Fig. 1 we show graphs of $\langle x^2 \rangle^{1/2}$ for various values of t. The parameters chosen are those used in Refs. [8] and [9], namely a=5 and $\lambda=0.01$ (which corresponds to a "large" dimensionless coupling contant [8]). We include both cases by plotting $\langle x^2 \rangle^{1/2}$ as a function of $\sigma \mu^2$, where $\sigma = -1$ for case (i) and +1 for case (ii). There is a well-defined maximum which moves steadily to the right as t increases, crossing over from case (i) to case (ii) between t = 11 and t = 12. From these and similar graphs we extract the value of $\overline{\mu}(t)$, which is plotted in Fig. 2 (as $\sigma \overline{\mu}^2$). The way $\overline{\mu}$ develops in time makes very good intuitive sense. At small times the wave function is still concentrated near the origin, and the main influence is the downward sloping part of the potential, $-\frac{1}{2}m^2x^2$, but at later times, as it spreads out, the upward curving parts of the potential become more important and the positive mass squared term $+\frac{1}{2}\bar{\mu}^2 x^2$ represents a more reasonable starting point for the approximation.

Using these values of $\overline{\mu}(t)$ we can then calculate $\langle x^2 \rangle^{1/2}[\overline{\mu}(t),t]$ from Eq. (19) as a function of t. This is plotted in Fig. 3 along with the results obtained using the "Hartree-Fock" method of Ref. [8], the improved variational method of Ref. [9], the exact value of $\langle x^2 \rangle^{1/2}(t)$, obtained by Fourier transform and numerical integration [11], and finally the result of first-order perturbation theory. The latter corresponds to O(δ) of the delta expansion, but with μ fixed at *m* in case (i), and exemplifies the importance of the *t*-dependence of $\overline{\mu}$.

As can be seen, the delta-expansion result tracks the exact result for longer than either of the other variational calculations, essentially up to the point where $\langle x^2 \rangle^{1/2}$ reaches its maximum, but then overshoots. A similar degree of accuracy in quantum field theory would mean that, to this order of the expansion, the inflationary period would be very well described, but the reheating process less so.



FIG. 3. $\langle x^2 \rangle^{1/2}$ versus *t*. First-order linear delta expansion (LDE) compared with the exact result (Exact), the variational calculations of Ref. [7] (HF) and Ref. [8] (CC), and first-order perturbation theory (PT).

Figure 3 is the main result of this section, but it is also of interest to enquire how closely the calculated wave function agrees with the exact result, since a well-known feature of variational methods is that quite reasonable values for expectation values such as $\langle x^2 \rangle$ can be obtained with rather inaccurate wave functions. In fact our wave function agrees rather well with the true wave function up to $t \approx 6$, but begins to diverge from it thereafter, even though still giving good values for $\langle x^2 \rangle$. In Fig. 4 we plot the two values of $|\psi|^2$ versus x for t = 6 and 8.

IV. HIGHER ORDER

The simplicity of the method means that in quantum mechanics, if not in field theory, it is relatively easy to go to higher order in the delta expansion.

The general form of the *n*th-order wave function φ_n is

$$\varphi_n = \sum_{r=1}^{2n+1} a_{nr} y^{2(r-1)}, \qquad (20)$$

and the equation of motion of the coefficients is

$$i\dot{a}_{nr}/\mu = (4r-3)Ba_{nr} - r(2r-1)a_{n,r+1} + \tilde{g}(a_{n-1,r-2}) - \tilde{\rho}a_{n-1,r-1}),$$
(21)

with the understanding that a coefficient a_{ms} on the righthand side vanishes if the second index lies outside the range $1 \le s \le 2m+1$. In this new notation the first-order coefficients are $a=a_{11}$, $b=a_{12}$ and $c=a_{13}$.

It becomes increasingly impractical to solve these equations analytically, but numerical integration using the Runge-Kutta method presents no problem. As mentioned above, the structure of the equations is such that the wave function



FIG. 4. Graphs of $|\psi|^2$ versus x for t = 6 and 8. The solid line is the first-order LDE calculation and the dotted line is the exact result.

should remain normalized to each order in δ , which provides us with an important check on the accuracy of the calculation.

Altogether we have extended the method to order 7. In second and third order the PMS plots of $\langle x^2 \rangle$ versus μ exhibit either only a point of inflection or rather narrow maxima or minima. The results are an improvement on the first-order result for small *t*, but fare worse at larger *t*. The third-order result, improved by taking the Padé approximant P_{21} , is shown in Fig. 5. In order 4, however, the PMS plot exhibits a clean broad minimum, and the results show a dramatic improvement, up to the turnover point, where they diverge from the exact result. As we go to higher order the pattern is similar, with order 7 exhibiting a clean broad maximum, and a further improvement, again up to the turnover point but not beyond. These results are shown in Fig. 5, which focuses on the region near the turnover.

What emerges from these calculations is that there seems to be a barrier to the method at the turnover point. That is, successive orders can be expected to represent the true curve more and more closely up to that point, but then diverge



FIG. 5. $\langle x^2 \rangle^{1/2}$ versus *t*. Successive orders of the linear delta expansion compared with the exact result (Exact).

from it. The turnover exhibited by the first-order result, which seemed to mimic that of the exact result, now seems to have been fortuitous and unrepresentative of the method as a whole. In cosmological terms it appears that the delta expansion has a good chance of giving a reasonable description of the slow roll process, but not the subsequent reheating.

The fourth-order wave function is almost indistinguishable from the exact wave function at t=6. The fourth-order approximation to $|\psi|^2$ at t=8 is shown in Fig. 6. It is extremely close to the exact wave function for larger values of x, but differs somewhat at lower values of x. This feature is understandable in terms of the PMS procedure we have adopted, which is to optimize $\langle x^2 \rangle$. This measure is more sensitive to larger values of x. Hence, with a single variational parameter at our disposal the method will tend to optimize this part of the wave function, if necessary at the expense of the small-x behavior.

V. DISCUSSION

In the context of quantum mechanics a possible variant of the present treatment would be the use of the original delta expansion [12], whereby the x^4 term in the potential is written as $x^{2(1+\delta)}$ and expanded as $x^2(1+\delta \ln x^2+\cdots)$. This expansion is known to converge for the energy levels of the anharmonic oscillator, and the O(δ) calculation for the



FIG. 6. Graph of $|\psi|^2$ versus x for t=8. The solid line is the first-order LDE calculation, the dashed line the fourth-order calculation, and the dotted line is the exact result.

present problem should be tractable. However, the disadvantage of this method is that its extension to field theory beyond first order becomes extremely difficult.

In field theory the linear delta expansion is, apart from the crucial variational aspect, a modified form of perturbation theory, which includes mass insertions along with the fourpoint vertices. It is the variational aspect which takes one beyond perturbation theory, making the variational parameter a non-analytic function of the coupling constant, and, in the present context, a function of time as well. The importance of going beyond the Gaussian approximation has been emphasized in Refs. [9] and [13], and the LDE indeed provides a non-Gaussian alternative to the Hartree-Fock approximation. The superiority of the method in the simpler quantum mechanical problem encourages us to attempt to apply it to the full quantum field theory problem, which will be the subject of future research. We can be hopeful that the delta expansion will give a good reasonable description of the slow roll process, but it seems that the reheating process will require some more sophisticated ansatz.

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