# Exact and approximate dynamics of the quantum mechanical $O(N)$ model

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We study the dynamics of the quantum mechanical $O(N)$ model as a specific example to investigate the systematics of a $1/N$ expansion. The closed time path formalism melded with an expansion in $1/N$ is used to derive time evolution equations valid to order $1/N$ (next-to-leading order). The effective potential is also obtained to this order and its properties are elucidated. In order to compare theoretical predictions against numerical solutions of the time-dependent Schrödinger equation, we consider two initial conditions consistent with $O(N)$ symmetry, one of them a quantum roll, the other a wave packet initially to one side of the potential minimum, whose center has all coordinates equal. For the case of the quantum roll we map out the domain of validity of the large-$N$ expansion. We also discuss the existence of unitarity violation in this expansion, a well-known problem faced by moment truncation techniques. The $1/N$ results, both static and dynamic, are contrasted with those given by a Hartree variational ansatz at given values of $N$. A comparison against numerical results leads us to conclude that late-time dynamical behavior, where nonlinear effects are significant, is not well described by either approximation.

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## I. INTRODUCTION

Initial value problems in quantum field theory are of great interest in areas such as heavy ion collisions, dynamics of phase transitions, and early Universe physics. However, the solution of the corresponding functional Schrödinger equation is essentially impossible and one is forced to resort to approximate methods such as mean field approaches of the Hartree type or the large-$N$ expansion. The application of variational techniques such as the Hartree type is limited in scope since the errors are uncontrolled. While $1/N$ methods promise better error control since they are based on a systematic expansion, at next-to-leading order these methods can become extremely complicated and expensive to implement. The motivation for our work in this paper is to implement the $1/N$ expansion at the first nontrivial order in a quantum mechanical example. Not only does this simplify the analysis but it also opens the possibility of comparing the approximate results with numerical simulations of the time dependent Schrödinger equation, a luxury not available in the field theoretic case. However, it should be kept in mind that quantum mechanics and quantum field theory are very different. For example, in the quantum mechanics applications discussed below, the $O(1/N)$ corrections do not correspond to inter-particle collisions (as they do in field theory) since we are restricting ourselves to one-particle quantum mechanics. Nevertheless, as discussed in more detail below, quantum mechanical examples provide excellent testbeds for key issues such as positivity violation and late-time accuracy of the approximations.

The $O(N)$ model has been extensively employed in time independent applications in statistical physics and quantum field theory [1,2] and several recent applications have studied time-dependent phenomena. The dynamics of the chiral phase transition following the expansion of a quark-gluon plasma produced during a relativistic heavy ion collision has been modeled by an $O(4)$ $\sigma$ model at leading order in $1/N$ [3]. The nonequilibrium dynamics of an $O(N)$-symmetric $\lambda\phi^4$ theory, again treated at leading order, has been investigated in detail [4]. Even at leading order, the $1/N$ expansion captures the phase transition, but does not contain enough of the dynamics to allow for rethermalization, since direct scattering first occurs at next order. The $O(N)$ model has been used in inflationary models of the early Universe [5] with the scalar field often starting at the top of a hill in the potential and ''rolling'' down, giving rise to a quantum roll problem. It has also been applied to study primordial perturbations arising from defect models of structure formation [6].

The general method for obtaining the dynamical $1/N$ approximation via path integral techniques in quantum field theory was discussed earlier in Ref. [7] and applied later [8,9] to a quantum mechanical system of $N+1$ coupled oscillators, a one-dimensional truncation of scalar electrodynamics. Two different sets of approximate actions were considered, which differed by terms of order $1/N^2$, both of them being energy conserving. The first method in Ref. [9] was a perturbative expansion of the generating functional in pow-

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ers of $1/N$. The second method was to first Legendre transform the action to order $1/N$, and then find the equations of motion. When these two methods diverged from each other, they also diverged from an exact solution for the case $N=1$. However, because of computational restrictions, it was not possible to study numerically the accuracy of the approximation as a function of $N$. Remedying that deficiency is the main motivation of the present study, since for the quantum roll problem numerical solutions can be obtained for arbitrary $N$.

One of the subtle issues in expansions involving moment-based truncation schemes such as $1/N$, which is present both in quantum field theory and in quantum mechanics, relates to the imposition of constraints arising from the positivity of the underlying probability density function or functional. The importance of these constraints is well known in areas such as turbulence and beam dynamics [10]. In this paper, we show that possible violations of these constraints must be tamed in $1/N$ expansions if the approximation is at all expected to succeed at moderate values of $N$. This may be possible by using certain resummation schemes which will be discussed elsewhere.

In this paper we show that evolutions based on the naive next-to-leading order $1/N$ expansion violate unitarity (or, more generally, positivity of the density matrix) and that this violation is associated with a dynamical instability for $N$ less than some value $N_T$. We have numerical evidence for a sharp threshold at $N \sim N_T$, beyond which we have not been able to detect the instability. We also have evidence that this behavior is related to the nature of the effective potential at next-to-leading order: At this order, the (convex) effective potential has the property of not being defined everywhere for values of $N<N_c$, where $N_c$ depends on the values of the parameters specifying the potential. For $N>N_c$, the effective potential exists globally. What this means is that for $N<N_c$ one cannot associate a quantum state with the next-to-leading order $1/N$ expansion whereas such a state does exist for $N>N_c$. Even though this statement relates to a static property, our numerical results indicate that in fact $N_T \sim N_c$.

A comparison of the $1/N$ expansion and the Hartree variational method (appropriately generalized to the case of finite $N$) is of interest since both agree at infinite $N$. At finite $N$, the next-to-leading order large-$N$ and Hartree approximations differ and provide alternative routes to improving the leading order result which, for the quantum roll problem, consists of harmonic oscillations in $\langle r^2 \rangle$ where $r$ is the radial degree of freedom. At finite $N$, the inclusion of nonlinearities leads to amplitude modulation effects on top of the harmonic motion. The ability to capture this modulation is a good test for the next-to-leading order large-$N$ and Hartree approximations. Our numerical results provide evidence that neither of these methods is satisfactory at late times (relative to the oscillation time), though they work reasonably well at short to intermediate times.

Our results suggest that it is important to find ways to improve the naive $1/N$ expansion at next-to-leading order. Work using resummation schemes is in progress and short discussions of relevant issues are included in this paper.

The paper is organized as follows. In Sec. II we present the $O(N)$ model as it pertains to quantum mechanics and in Sec. III we derive equations of motion for the large $N$ approximation to order $1/N$. We derive the corresponding equations for the time dependent Hartree approximation (TDHA) in Sec. IV. In Sec. V we show how the same TDHA equations can be obtained from an equal-time Green's function approach which is computationally more attractive. The energies for the various approximations are calculated in Sec. VI. Section VII describes the two initial conditions which preserve the $O(N)$ symmetry, namely a quantum roll and the time evolution of an offset Gaussian centered at an $O(N)$ symmetric point. In Sec. VIII we determine the effective potential to both order $1/N$ and for the Hartree approximation. Numerical results and comparisons with the approximations are discussed in Sec. IX and our conclusions are stated and discussed in Sec. X.

## II. $O(N)$ MODEL

The Lagrangian for the $O(N)$ model in quantum mechanics is given by

$$L(x,\dot{x}) = \frac{1}{2}\sum_{i=1}^{N} \dot{x}_i^2 - V(r), \tag{2.1}$$

where $V(x)$ is a potential of the form

$$V(r) = \frac{g}{8N}(r^2 - r_0^2)^2, \quad r^2 = \sum_{i=1}^{N} x_i^2. \tag{2.2}$$

The time-dependent Schrödinger equation for this problem is given by

$$i\frac{\partial \psi(x,t)}{\partial t} = \left\{ -\frac{1}{2}\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + V(r) \right\} \psi(x,t). \tag{2.3}$$

For arbitrary initial conditions, given present computational constraints, these equations can be numerically integrated only for small $N \leqslant 4$. The initial conditions for the quantum roll problem allow a numerical solution for all $N$, and in this case we can attempt to study fully the behavior of the large-$N$ expansion. (For the shifted Gaussian initial conditions, however, this is not possible, and we used numerical solutions obtained for $N=1$ and 2 to benchmark the large-$N$ approximations and the TDHA solutions at short times.)

The symmetry of the quantum roll problem is such that only the radial part of the wave function is of interest. Assuming a solution of the form

$$\psi(r,t) = r^{(1-N)/2}\phi(r,t), \tag{2.4}$$

the time dependent Schrödinger equation for $\phi(r,t)$ reduces to [11]

$$i\frac{\partial \phi(r,t)}{\partial t} = \left\{ -\frac{1}{2}\frac{\partial^2}{\partial r^2} + U(r) \right\} \phi(r,t) \tag{2.5}$$

with an effective one dimensional potential $U(r)$ given by

$$U(r)=\frac{(N-1)(N-3)}{8r^2}+\frac{g}{8N}(r^2-r_0^2)^2. \tag{2.6}$$

It is further useful to make the rescaling

$$r^2=Ny^2, \quad r_0^2=Ny_0^2. \tag{2.7}$$

The potential (2.6) then becomes

$$u(y,N)=\frac{U(y)}{N}=\frac{(N-1)(N-3)}{8N^2y^2}+\frac{g}{8}(y^2-y_0^2)^2, \tag{2.8}$$

corresponding to the new Schrödinger equation

$$i\frac{\partial\phi(y,\tilde{t})}{\partial\tilde{t}}=\left\{-\frac{1}{2N^2}\frac{\partial^2}{\partial y^2}+u(y,N)\right\}\phi(y,\tilde{t}) \tag{2.9}$$

where $\tilde{t}=Nt$.

The method of choice to investigate the long-time behavior of the exact solution is the split-operator method, which has been presented in detail in Ref. [12]. The wave function is expanded as a Fourier series in the radial component, and the solution is obtained as the repeated application of a time-evolution operator in symmetrically split form. As a result, the use of a fast-Fourier transform algorithm is required. For the purpose of the present implementation, 256 radial grid points, a value of 20 for the radial grid boundary, and a time step size of 0.01 provide a conservation of the wave function unitarity to better than 9 significant figures. The accuracy of the method has been established by comparing results with a second method, where we first solve for the eigenvalues and eigenfunctions, and then use the expansion

$$\phi(r,t)=\sum_n C_n e^{-iE_nt}\phi_n(r), \tag{2.10}$$

where $C_n$ was determined from the initial conditions. Results from the two methods agreed in the cases where they were used together.

## III. LARGE-*N* APPROXIMATION

The large-$N$ approximation has been worked out for the $O(N)$ model in $1+3$ dimensions in Ref. [7]. The Lagrangian (2.1) with the potential function (2.2) is obtained from that paper by specializing to $0+1$ dimensions, and replacing $\phi_a(t)\to x_i(t)$, $v\to r_0$, and $\lambda\to g$.

To implement the large-$N$ expansion, it is useful [2] to rewrite the Lagrangian in terms of the composite field $\chi$ by adding a constraint term to Eq. (2.1), given by

$$\frac{N}{2g}\left[\chi-\frac{g}{2N}(r^2-r_0^2)\right]^2, \tag{3.1}$$

which yields an equivalent Lagrangian

$$L'(x,\dot{x},\chi)=\sum_i \frac{1}{2}(\dot{x}_i^2-\chi x_i^2)+\frac{r_0^2}{2}\chi+\frac{N}{2g}\chi^2. \tag{3.2}$$

The generating function $Z[j,J]$ is given by the path integral over the classical fields $x_i(t)$:

$$Z[j,J]=e^{iW[j,J]}=\int \mathrm{d}\chi\prod_i \mathrm{d}x_i \exp\{iS[x,\chi;j,J]\},$$

$$S[x,\chi;j,J]=\int_{\mathcal{C}}\mathrm{d}t\left\{L'+\sum_i j_ix_i+J\chi\right\}.$$

The effective action, to order $1/N$, is obtained by integrating the path integral for the generating functional for the Lagrangian (3.2), over the $x_i$ variables, and approximating the integral over $\chi$ by the method of steepest descent (keeping terms up to order $1/N$). A Legendre transform of the resulting generating functional then yields the effective action, which we find to be

$$\Gamma[q,\chi]=\int_{\mathcal{C}}\mathrm{d}t\left\{\frac{1}{2}\sum_i[\dot{q}_i^2(t)-\chi(t)q_i^2(t)]+\frac{i}{2}\sum_i \ln[G_{ii}^{-1}(t,t)]+\frac{r_0^2}{2}\chi(t)+\frac{N}{2g}\chi^2(t)+\frac{i}{2}\ln[D^{-1}(t,t)]\right\}, \tag{3.3}$$

where the integral is over the closed time path $\mathcal{C}$, discussed in Ref. [7] and $q_i(t)=\langle x_i(t)\rangle$. Here $G_{ij}^{-1}(t,t')$ and $D^{-1}(t,t')$ are the lowest order in $1/N$ inverse propagators for $x_i$ and $\chi$, given by

$$G_{ij}^{-1}(t,t')=\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2}+\chi(t)\right\}\delta_{\mathcal{C}}(t,t')\delta_{ij}\equiv G^{-1}(t,t')\delta_{ij},$$

$$D^{-1}(t,t')=-\frac{N}{g}\delta_{\mathcal{C}}(t,t')-\Pi(t,t'),$$

where

$$\Pi(t,t')=-\frac{i}{2}\sum_{i,j}G_{ij}(t,t')G_{ji}(t',t)+\sum_{i,j}q_i(t)G_{ij}(t,t')q_j(t'). \tag{3.4}$$

Here $\delta_{\mathcal{C}}(t,t')$ is the closed time path delta function.

The equations of motion for the classical fields $q_i(t)$, to order $1/N$, are

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}t^2}+\chi(t)\right\}q_i(t)+i\sum_j\int_{\mathcal{C}}\mathrm{d}t'G_{ij}(t,t')D(t,t')q_j(t')=0, \tag{3.5}$$

with the gap equation for $\chi(t)$ given by

$$\chi(t)=-\frac{g}{2N}r_0^2+\frac{g}{2N}\sum_i\left[q_i^2(t)+\frac{1}{i}\mathcal{G}_{ii}^{(2)}(t,t)\right]. \tag{3.6}$$

The next-to-leading order $x_i$ propagator $\mathcal{G}^{(2)}_{ij}(t,t')$ and self-energy $\Sigma_{ij}(t,t')$ to order $1/N$ turn out to be

$$\mathcal{G}^{(2)}_{ij}(t,t') = G_{ij}(t,t') - \sum_{k,l} \int_{\mathcal{C}} dt_1 \int_{\mathcal{C}} dt_2 G_{ik}(t,t_1) \times \Sigma_{kl}(t_1,t_2) G_{lj}(t_2,t'),$$

$$\Sigma_{kl}(t,t') = iG_{kl}(t,t')D(t,t') - q_k(t)D(t,t')q_l(t'). \tag{3.7}$$

These equations agree with (2.18)–(2.22) of Ref. [7]. We mention here that the actual equation for $\mathcal{G}$ which follows from the effective action differs from Eq. (3.7) in that the final $G$ in the integral equation is replaced by the full $\mathcal{G}$. This leads to a partial resummation of the $1/N$ corrections which which guarantees positivity of $\langle x^2(t)\rangle$ (this restricted result does not imply that the full positivity problem for the density matrix has been solved). However, it does not improve the long-time accuracy of the results [25].

In order to solve for $D(t,t')$, we first write

$$\frac{N}{g} D(t,t') = -\delta_{\mathcal{C}}(t,t') + \frac{N}{g} \Delta D(t,t'). \tag{3.8}$$

Then $\Delta D(t,t')$ satisfies the integral equation

$$\frac{N}{g} \Delta D(t,t') = \frac{g}{N} \Pi(t,t') - \int_{\mathcal{C}} dt'' \Pi(t,t'') \Delta D(t'',t'), \tag{3.9}$$

in agreement with (2.13)–(2.16) of Ref. [7].

We are now in a position to solve these coupled equations for the motion of $q_i(t)$ and $\chi(t)$ for given initial conditions. For the initial conditions discussed in Sec. VII, we find

$$G_{ij}(t,t')/i = \theta_{\mathcal{C}}(t,t')\,\delta_{ij} f(t) f^*(t'), \tag{3.10}$$

where $f(t)$ and $f^*(t)$ satisfy the homogeneous equation,

$$\left\{ \frac{d^2}{dt^2} + \chi(t) \right\} \begin{pmatrix} f(t) \\ f^*(t) \end{pmatrix} = 0, \tag{3.11}$$

with initial conditions

$$f(0) = \sqrt{G}, \quad \dot{f}(0) = 1/(2\sqrt{G}). \tag{3.12}$$

However, $\Delta D(t,t')$ cannot be factored into products of functions like $G_{ij}(t,t')$.

We solve Eqs. (3.5) and (3.6) simultaneously with Eqs. (3.7) and (3.9), using the Chebyshev expansion technique [13] of Appendixes A and B of Ref. [9].

## IV. TIME DEPENDENT HARTREE APPROXIMATION

It is useful to compare our results for the large-$N$ approximation to the time dependent Hartree approximation suitably formulated for the $O(N)$ problem. The static Hartree approximation is based on the idea of varying the parameters of a Gaussian wave function so as to minimize the energy (the generalization to the time-dependent case is given below). For the $O(N)$ problem this amounts to placing an $N$-dimensional Gaussian some (radial) distance away from the origin and then carrying out the minimization procedure. In contrast, the leading-order large-$N$ wave function is a Gaussian which is locked at the origin. At infinite $N$ the TDHA becomes exact and equivalent to the leading order large-$N$ approximation, a well-known result. (See, e.g., Refs. [14,15]. The TDHA being used here should not be confused with the Hartree approximation for $N=1$ which does differ from the leading-order large-$N$ approximation.) At finite $N$, the TDHA and the next-to-leading order large-$N$ approximation may be thought of as two competing schemes to improve on the leading-order result.

There are several ways of implementing the Hartree approximation: The most common is by using the time-dependent variational principle of Dirac [16–18]. This has the advantage of giving a classical Hamiltonian description for the dynamics of the variational parameters, which can be hidden in other formulations.

The idea behind this approach is that the variation of

$$\Gamma[\psi,\psi^*] = \int dt \langle \psi(t) | i\frac{\partial}{\partial t} - H | \psi(t) \rangle \tag{4.1}$$

is stationary for the exact solution of the Schrödinger equation, the time derivative acting in both directions. We consider Gaussian trial wave functions of the form

$$\psi(x,t) = \mathcal{N} \exp\left[ ip_i(t)z_i(t) - z_i(t)\left( \frac{G^{-1}_{ij}(t)}{4} - i\Pi_{ij}(t) \right) z_j(t) \right], \tag{4.2}$$

where $\mathcal{N}$ is the normalization constant, and we have set $z_i(t) = x_i - q_i(t)$. Here $q_i(t)$, $p_i(t)$, $G_{ij}(t)$ and $\Pi_{ij}(t)$ are time-dependent variational parameters, to be determined by minimizing the Dirac action. We note that $\Pi_{ij}(t)$, which is used only in this section, is conjugate to $G_{ij}(t)$ and is not to be confused with the self energy $\Pi(t,t')$ defined in Eq. (3.4).

The $n$-point functions can be calculated from the generating functional using the formula

$$\langle z_i z_j \cdots z_n \rangle = \left. \frac{\partial^n Z[j]}{\partial j_i \partial j_j \cdots \partial j_n} \right|_{j=0}, \tag{4.3}$$

where

$$Z[j] = \mathcal{N}^2 \int \prod_s dx_s \exp\left[ -\frac{1}{2} z_i(t) G^{-1}_{ij} z_j(t) + j_i z_i(t) \right] = \exp\left[ \frac{j_i G_{ij} j_j}{2} \right]. \tag{4.4}$$

The expectation value of the time derivative is given by

$$\left\langle i\frac{\partial}{\partial t} \right\rangle = p_i \dot{q}_i - G_{ij}\dot{\Pi}_{ij} \tag{4.5}$$

and the expectation value of the kinetic energy is

$$\left\langle -\frac{1}{2}\frac{\partial^2}{\partial x_i^2}\right\rangle = \frac{p_i p_i}{2}+\frac{1}{8}G_{ii}^{-1}+2\Pi_{ij}G_{jk}\Pi_{ki}. \qquad (4.6)$$

For the expectation value of $V$ we first expand the potential in a Taylor series about $z_i=0$,

$$V(q,z)=V(q)+V_i(q)z_i+\frac{1}{2}V_{ij}(q)z_iz_j+\cdots$$

where

$$V_i(q)=\frac{g}{2N}q_i(q_sq_s-r_0^2),$$

$$V_{ij}(q)=\frac{g}{2N}[\delta_{ij}(q_sq_s-r_0^2)+2q_iq_j],$$

$$V_{ijk}(q)=\frac{g}{N}(\delta_{ij}q_k+\delta_{ik}q_j+\delta_{jk}q_i),$$

$$V_{ijkl}(q)=\frac{g}{N}(\delta_{ij}\delta_{kl}+\delta_{il}\delta_{jk}+\delta_{ik}\delta_{jl}). \qquad (4.7)$$

Thus

$$V(q,z)=\frac{g}{8N}[(q_jq_j-r_0^2)^2+(z_iz_i)^2+4(z_iz_i)(z_jq_j)+4(z_iq_i)^2 +2(z_iz_i)(q_jq_j-r_0^2)+4(z_iq_i)(q_jq_j-r_0^2)].$$

Taking the expectation value, we obtain

$$\langle V\rangle=\frac{g}{8N}[(q_jq_j-r_0^2)^2+2G_{ii}(q_jq_j-r_0^2)+4G_{ij}q_iq_j+G_{ii}G_{jj} +2G_{ij}G_{ji}]. \qquad (4.8)$$

The Hartree equations of motion are Hamilton's equations for the variational parameters:

$$\dot{q}_i=p_i,$$

$$\dot{p}_i=-V_i-\frac{1}{2}V_{ijk}G_{jk},$$

$$\dot{G}_{ij}=2(G_{ik}\Pi_{kj}+G_{jk}\Pi_{ki}),$$

$$\dot{\Pi}_{ij}=\frac{1}{8}G_{ik}^{-1}G_{kj}^{-1}-2\Pi_{ik}\Pi_{kj}-\frac{1}{2}V_{ij}-\frac{1}{4}V_{ijkl}G_{kl}. \qquad (4.9)$$

Solutions of this set of equations determine the time-dependent Hartree approximation to the true solution of the Schrödinger equation.

## V. METHOD OF EQUAL-TIME GREEN's FUNCTIONS

Solutions of the TDHA equation (4.9) require computing the matrix inverse of $G_{ij}$. This can be difficult to carry out in practice for large $N$. Fortunately, the method of equal-time Green's functions provides a way to avoid this technical difficulty [19,14,20]. We begin by considering the time evolution of the one point functions,

$$\dot{q}_i=p_i,$$

$$\dot{p}_i=-V_i-\frac{1}{2}V_{ijk}G_{jk},$$

$$=-\frac{g}{2N}\{q_i(q_kq_k+G_{kk}-r_0^2)+q_k(G_{ik}+G_{ki})\} \qquad (5.1)$$

where $V_i$ and $V_{ijk}$ are given by Eqs. (4.7), as well as the evolution of the two-point functions:

$$G_{ij}(t)=\langle z_iz_j\rangle, \quad K_{ij}=\langle \dot{z}_i\dot{z}_j\rangle,$$

$$F_{ij}=\frac{1}{2}\langle[z_i\dot{z}_j+\dot{z}_jz_i]\rangle. \qquad (5.2)$$

Here we have again set $z_i(t)=x_i-q_i(t)$. All of the expectation values are taken with respect to the Gaussian trial wave function, Eq. (4.2). To obtain the equations of motion for the two-point functions, we use the exact equation of motion and the factorization resulting from the Gaussian approximation. This yields

$$\dot{G}_{ij}=F_{ij}+F_{ji}, \qquad (5.3)$$

$$\dot{F}_{ij}=K_{ij}-\left\langle z_i\frac{\partial V}{\partial x_j}\right\rangle, \qquad (5.4)$$

$$\dot{K}_{ij}=-\left\langle\left[\frac{\partial V}{\partial x_i}\dot{z}_j-\dot{z}_i\frac{\partial V}{\partial x_j}\right]\right\rangle. \qquad (5.5)$$

Here we have used the Lagrange equations of motion

$$\ddot{x}_i+\frac{\partial V}{\partial x_i}=0, \qquad (5.6)$$

where

$$\frac{\partial V}{\partial x_i}=V_{ij}z_j+\frac{1}{6}V_{ijkl}z_jz_kz_l+\text{terms with even powers of } z_i, \qquad (5.7)$$

and the fact that for our Gaussian wave packet, $\langle z_i\rangle=0$. The canonical commutation relations give

$$\langle z_i\dot{z}_j-\dot{z}_jz_i\rangle=\langle x_i\dot{x}_j-\dot{x}_jx_i\rangle=i\delta_{ij}, \qquad (5.8)$$

and we have

$$\langle z_iz_jz_kz_l\rangle=G_{ij}G_{kl}+G_{il}G_{jk}+G_{ik}G_{jl}, \qquad (5.9)$$

$$\langle z_iz_jz_k\dot{z}_l\rangle=G_{ij}F_{kl}+F_{il}G_{jk}+G_{ik}F_{jl} +i(G_{ij}\delta_{kl}+G_{jk}\delta_{il}+G_{ik}\delta_{jl})/2, \qquad (5.10)$$

$$\langle \dot{z}_i z_j z_k z_l \rangle = F_{ji} G_{kl} + F_{li} G_{jk} + F_{ki} G_{jl} - i(G_{kl}\delta_{ji} + G_{jk}\delta_{li} + G_{jl}\delta_{ki})/2. \quad (5.11)$$

Finally, from Eqs. (5.4) and (5.5) we get

$$\dot{F}_{ij} = K_{ij} - V_{jk} G_{ik} - V_{jklm}(G_{ik}G_{lm} + G_{im}G_{kl} + G_{il}G_{km})/6, \quad (5.12)$$

$$\dot{K}_{ij} = -V_{ik}F_{kj} - V_{jk}F_{ki} - V_{iklm}(G_{kl}F_{mj} + G_{lm}F_{kj} + G_{km}F_{lj})/6 - V_{jklm}(F_{ki}G_{lm} + F_{mi}G_{kl} + F_{li}G_{km})/6. \quad (5.13)$$

For Gaussian initial conditions, the equal-time Green's function method is assured to give the same result as the Hartree method, if $F_{ij}(0)$ and $K_{ij}(0)$ satisfy the requirements

$$F_{ij}(0) = 0, \quad K_{ij}(0) = G_{ij}^{-1}(0)/4.$$

Choosing $K_{ij}$ independently of $G_{ij}$ corresponds to a mixed initial density matrix, rather than a pure state. If we further choose $G_{ij}(0)$ to be diagonal and equal to the same number $G_0$,

$$G_{ij}(0) = \delta_{ij} G_0,$$

then $K_{ij}(0)$ is given by

$$K_{ij}(0) = \delta_{ij}/(4G_0).$$

For the initial conditions pertinent to the quantum roll, $q_i(t) = 0$ for all $t$. Then $G_{ij}(t)$, $F_{ij}(t)$, and $K_{ij}(t)$ are all proportional to the unit matrix, and have no off diagonal terms. For the offset initial condition, we choose large-$N$ symmetric initial conditions so that $q_i(0) = q_0$, and $p_i(0) = 0$, and $G_{ij}(0) = G_0 \delta_{ij}$. In that case, all the $q$'s and $p$'s are identical,

$$q_i(t) = q(t), \quad p_i(t) = p(t),$$

and the matrices $G_{ij}(t)$, $F_{ij}(t)$ and $K_{ij}(t)$ become off-diagonal in a simple way so that all the diagonal elements are equal and all the off-diagonal elements are equal. That is, we can write

$$G_{ij}(t) = G(t)\delta_{ij} + \overline{G}(t)(1-\delta_{ij}),$$

$$F_{ij}(t) = F(t)\delta_{ij} + \overline{F}(t)(1-\delta_{ij}),$$

$$K_{ij}(t) = K(t)\delta_{ij} + \overline{K}(t)(1-\delta_{ij}).$$

For this case, Eqs. (5.1), (5.3), (5.12), and (5.13) simplify to the following set of coupled equations:

$$\dot{q} = p,$$

$$\dot{p} = -\frac{g}{2N} q\{Nq^2 - r_0^2 + (N+2)G + 2(N-1)\overline{G}\},$$

$$\dot{G} = 2F, \quad \dot{\overline{G}} = 2\dot{\overline{F}},$$

$$\dot{F} = K - \frac{g}{2N}\{G[(N+2)(q^2+G) - r_0^2] + 2(N-1)\overline{G}(q^2+\overline{G})\},$$

$$\dot{\overline{F}} = \overline{K} - \frac{g}{2N}\{\overline{G}[(3N-2)q^2 + (N+4)G + 2(N-2)\overline{G} - r_0^2] + 2Gq^2\},$$

$$\dot{K} = -\frac{g}{N}\{F[(N+2)(q^2+G) - r_0^2] + \overline{F}2(N-1)(q^2+\overline{G})\},$$

$$\dot{\overline{K}} = -\frac{g}{N}\{\overline{F}[(3N-2)q^2 + (N+2)G + 2(N-2)\overline{G} - r_0^2] + F2(q^2+\overline{G})\}. \quad (5.14)$$

If we let $r_0^2 = N y_0^2$, and then take the limit $N \to \infty$, we recover the leading order in large $N$ result, as discussed in Refs. [19,14].

The equal time Green's function method is easier to implement numerically than the Hamiltonian system described by Eq. (4.9), since no matrix inversion is involved. However, if one wants to find the wave function or the energy, instead of just obtaining the Green's functions, matrix inversion is once again required.

## VI. ENERGY

It is important to note that even though the Hartree and large-$N$ approximations are truncations of the true dynamics, they are nevertheless energy conserving. In the large-$N$ approximation, to order $1/N$, the expectation value of the Hamiltonian is given by

$$E = \frac{1}{2}\sum_i [\langle \dot{x}_i^2(t)\rangle + \langle \hat{\chi}(t) x_i^2(t)\rangle] - \frac{r_0^2}{2}\langle \hat{\chi}(t)\rangle - \frac{N}{2g}\langle \hat{\chi}^2(t)\rangle. \quad (6.1)$$

We write these expectation values in terms of the closed time path (CTP) Green's functions. By definition, the disconnected two-point Green's functions are introduced as

$$D_{\rm dis}(t,t') = i\langle \mathrm{T}_{\mathcal{C}}[\hat{\chi}(t)\hat{\chi}(t')]\rangle = i\chi(t)\chi(t') + \mathcal{D}(t,t'), \quad (6.2)$$

$$G_{ij,\rm dis}(t,t') = i\langle \mathrm{T}_{\mathcal{C}}[x_i(t)x_j(t')]\rangle = i q_i(t) q_j(t') + \mathcal{G}_{ij}(t,t'), \quad (6.3)$$

where $\mathcal{D}$ and $\mathcal{G}_{ab}$ denote the *connected* two-point Green's functions:

$$\mathcal{D}(t,t') = \left[\frac{\delta^2 W[J,j]}{\delta J(t)\,\delta J(t')}\right]_{J,j=0},$$

$$\mathcal{G}_{ij}(t,t')=\left[\frac{\delta^2 W[J,j]}{\delta j_i(t)\,\delta j_j(t')}\right]_{J,j=0}. \tag{6.4}$$

To obtain the energy from Eq. (6.1), we require the expectation values

$$\langle\hat{\chi}(t)\rangle=\chi(t),$$

$$\langle\hat{\chi}^2(t)\rangle=\chi^2(t)+D(t,t)/i,$$

$$\langle x_i^2(t)\rangle=q_i^2(t)+\mathcal{G}_{ii}(t,t)/i,$$

$$\langle\dot{x}_i^2(t)\rangle=\dot{q}_i^2(t)+\left.\frac{\partial^2\mathcal{G}_{ii}(t,t')/i}{\partial t\,\partial t'}\right|_{t=t'},$$

$$\langle\hat{\chi}(t)x_i^2(t)\rangle=\chi(t)[q_i^2(t)+\mathcal{G}_{ii}(t,t)/i]-K_{ii}(t,t,t),$$

where $K_{ij}(t_1,t_2,t_3)$ is the 3-point Green's function defined as

$$K_{ij}(t_1,t_2,t_3)=-\int_{\mathcal{C}}dt G_{ik}(t_1,t)G_{kj}(t_2,t)D(t,t_3).$$

The energy for the next-to-leading order large-$N$ approximation is then given by

$$E=-\frac{r_0^2}{2}\chi(t)-\frac{N}{2g}\{\chi^2(t)+\Delta D(t,t)/i\}+\frac{1}{2}\sum_i\left\{\dot{q}_i^2(t)+\left.\frac{\partial^2\mathcal{G}_{ii}(t,t')/i}{\partial t\,\partial t'}\right|_{t=t'}\right\}+\frac{1}{2}\sum_i\{\chi(t)[q_i^2(t)+\mathcal{G}_{ii}(t,t)/i]-K_{ii}(t,t,t)\}. \tag{6.5}$$

Using the equations of motion, we can show directly that Eq. (6.5) is conserved.

It is easy to evaluate the energy at $t=0$ for the quantum roll problem using the initial conditions (3.12). The result for the leading and next-to-leading order large-$N$ approximation is

$$\frac{E}{N}=\epsilon_0+\frac{1}{N}\epsilon_1+\cdots$$

where

$$\epsilon_0=\frac{1}{8G}+\frac{1}{8}gy_0^4-\frac{1}{4}gGy_0^2+\frac{1}{8}gG^2,$$

$$\epsilon_1=\frac{1}{4}gG^2. \tag{6.6}$$

Our initial wave function was chosen to be Gaussian, so that the parameters of the Hartree approximation agree exactly with the energy and parameters of the exact wave function at $t=0$. However, the leading order in the large-$N$ approximation for the same value of $G$ will disagree with the exact energy by $\epsilon_1$. This discrepancy disappears when we include the $1/N$ corrections.

Since the Hartree approximation leads to a canonical Hamiltonian dynamical system, the corresponding energy in that approximation is also a constant of the motion. It is given by

$$E=\frac{1}{2}p_i^2+\frac{1}{8}G_{ii}^{-1}+2\Pi_{ij}G_{jk}\Pi_{ki}+V(q)+\frac{1}{2}V_{ij}G_{ij}+\frac{1}{4!}V_{ijkl}(G_{ij}G_{kl}+G_{il}G_{jk}+G_{ik}G_{jl}). \tag{6.7}$$

We used this expression to check the accuracy of our numerical solutions. As with the next-to-leading order $1/N$ expression, for the quantum roll initial condition, Eq. (6.7) agrees with the exact result.

## VII. INITIAL CONDITIONS

### A. Quantum roll

We wish to study initial conditions which are consistent with $O(N)$ symmetry. This implies immediately that all the $x_i(t)$ have to be identical, with $x_i(0)=0$, and $G_{ij}(t)$ must be diagonal. The quantum roll problem is defined by a Gaussian initial wave function that is centered on the origin:

$$\psi_0(r)=\frac{1}{(2\pi G)^{N/4}}\exp\left\{-\frac{r^2}{4G}\right\}. \tag{7.1}$$

In this section, $G\equiv G(0)$.

One of the difficulties in studying the systematics of the $1/N$ expansion is the fact that, at next to leading order, every different value of $N$ (with all other parameters held constant) defines a different initial value problem. In this sense one cannot naively compare individual solutions, exact or approximate, at different values of $N$. In effect one has to tune the parameters of the problem at each $N$ in order to maintain certain invariance properties which allow different $N$ evolutions to be compared to each other. This parameter tuning process is described below.

Since the infinite $N$ limit has very precise properties, several technical issues arise when one wants to approach this limit starting at $N=1$ in a uniform manner. To study the large-$N$ limit it is convenient to make a rescaling to the $y$ variables, given in Eqs. (2.7). At very large $N$, the potential energy $u(y,N)$ is, as given earlier in Eq. (2.8):

$$u(y,N)=\frac{(N-1)(N-3)}{8N^2y^2}+\frac{g}{8}(y^2-y_0^2)^2\sim\frac{1}{8y^2}+\frac{g}{8}(y^2-y_0^2)^2. \tag{7.2}$$

In this limit, $u(N,y)$ has a minimum which is independent of $N$, and the large-$N$ limit consists of harmonic oscillations about this minimum [the reason for this is that the large-$N$ limit also corresponds to an effectively large mass limit in the Schrödinger equation (2.9)].

One way to uniformly study the motion of a wave packet as a function of $N$ is to choose initial conditions so that there is a uniform overlap of the initial wave function with the set of eigenfunctions of the Hamiltonian in the $N\to\infty$ limit. We can obtain this constant overlap if we allow the coupling constant $g$ to be a slowly varying function of $N$. This can be done in several ways that differ by terms of order $1/N^2$. The method presented below leads to uniform results even at $N=1$ as we change the parameters with $N$. Our method is to keep the distance between the centers of the initial wave function and the position of the minimum of the potential a constant as $N$ is varied.

Using Eq. (7.1), we define $\tilde{r}$ by

$$\tilde{r}=\langle r\rangle=\sqrt{2G}\left[\frac{\Gamma((N+1)/2)}{\Gamma(N/2)}\right], \tag{7.3}$$

and $G_\infty$ by the variance

$$\frac{G_\infty}{2}=\langle r^2\rangle-\langle r\rangle^2=G\left\{N-2\left[\frac{\Gamma((N+1)/2)}{\Gamma(N/2)}\right]^2\right\}.$$

Solving the above equations for $G$, we have

$$G(N)=\frac{G_\infty}{2N-4[\Gamma((N+1)/2)/\Gamma(N/2)]^2}. \tag{7.4}$$

Substitution of this expression into Eq. (7.3) yields

$$\tilde{r}(N)=\sqrt{\frac{G_\infty}{N[\Gamma(N/2)/\Gamma((N+1)/2)]^2-2}}. \tag{7.5}$$

In the limit when $N$ goes to infinity, we have

$$G(N)\to G_\infty, \quad \tilde{r}(N)\to\tilde{r}_\infty=\sqrt{(N-1)G_\infty},$$

which defines $\tilde{r}_\infty$, and agrees with the asymptotic form of the rescaled version of the initial wave function (7.1):

$$\phi_0(r)=\frac{1}{(2\pi G)^{N/4}}\exp\left\{-\frac{r^2}{4G}+\frac{N-1}{2}\ln r\right\}$$
$$\approx\frac{1}{(2\pi G)^{N/4}}\exp\left\{-\frac{(r-\tilde{r}_\infty)^2}{2G_\infty}+O(1/\sqrt{N})\right\}.$$

In order to ensure that the initial wave function has a finite overlap with the energy eigenfunctions of the Schrödinger equation at large $N$, we will keep the value of $G_\infty$ (and not $G$) fixed in our simulations.

Another quantity that should be kept constant is the basic oscillation frequency. In order to do this, we first find the Gaussian oscillations about the minimum of the one dimensional potential, defined by Eq. (2.6). We expand $U(r)$ as

$$U(r)=U(\bar{r})+\frac{1}{2}\bar{m}^2(r-\bar{r})^2+\cdots, \tag{7.6}$$

where $\bar{r}$ is given by the solution of the equation

$$\frac{(N-1)(N-3)}{4\bar{r^4}}=\frac{g}{2N}(\bar{r^2}-r_0^2), \tag{7.7}$$

and $\bar{m^2}$ by

$$\bar{m^2}=\frac{3(N-1)(N-3)}{4\bar{r^4}}+\frac{g}{2N}(3\bar{r^2}-r_0^2)=\frac{g}{N}(3\bar{r^2}-2r_0^2). \tag{7.8}$$

The frequency of oscillation is determined by $\bar{m}$, and this is the quantity to be kept fixed as $N$ is changed.

The last technical issue is to keep the distance between the center of the initial wave function, $\tilde{r}$, and the minimum of the potential, $\bar{r}$, a constant as we vary $N$. That is, we keep

$$\delta r=\bar{r}-\tilde{r}$$

constant for all $N$.

With this strategy of keeping $G_\infty$, $\bar{m}$ and $\delta r$ fixed, we can now determine how the coupling constant must vary with $N$. We first define $m^2$ to be the second derivative of $V(r)$ evaluated at $r=\bar{r}$,

$$m^2=\left.\frac{\mathrm{d}^2V(r)}{\mathrm{d}r^2}\right|_{r=\bar{r}}=\frac{g}{2N}(3\bar{r^2}-r_0^2). \tag{7.9}$$

Then, Eq. (7.8) becomes

$$m^2(N)=\bar{m^2}-\frac{3(N-1)(N-3)}{4\bar{r^4}}. \tag{7.10}$$

Solving Eq. (7.9) for $r_0$, substituting into Eq. (7.7) and solving for $g$ gives

$$g(N)=\frac{N}{\bar{r^2}}\left\{\bar{m^2}-\frac{(N-1)(N-3)}{\bar{r^4}}\right\}, \tag{7.11}$$

with $\bar{r}=\tilde{r}+\delta r$. The value of $r_0^2$ is then determined by Eq. (7.7):

$$r_0^2(N)=\bar{r^2}-\frac{2N}{g(N)}\frac{(N-1)(N-3)}{4\bar{r^4}}. \tag{7.12}$$

Thus, for *fixed* values of $G_\infty$, $\bar{m}$ and $\delta r$, Eqs. (7.4), (7.5), (7.11), and (7.12) determine values for $G(N)$, $\tilde{r}(N)$, $g(N)$, and $r_0(N)$ at all values of $N$.

In the limit, $N\to\infty$, we find that

$$g(\infty)=\frac{1}{G_\infty}\left(\bar{m^2}-\frac{1}{G_\infty^2}\right), \tag{7.13}$$

$$m^2(\infty)=\bar{m^2}-\frac{3}{4G_\infty^2}. \tag{7.14}$$

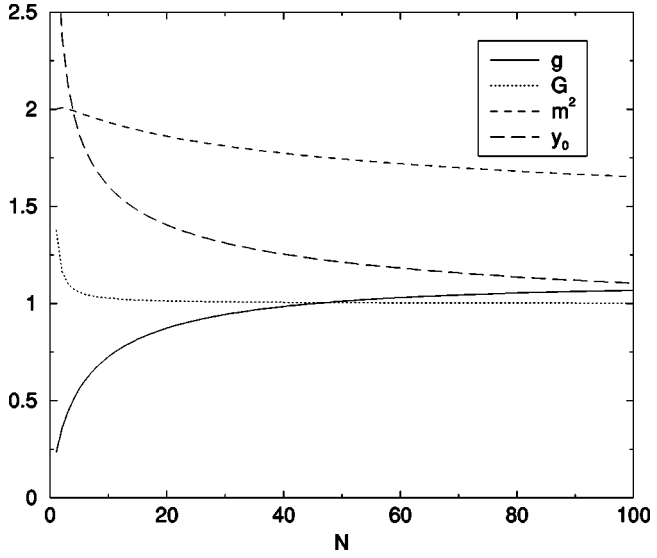


FIG. 1. Potential parameters as a function of $N$.

To summarize, in order to establish appropriate initial conditions for the quantum roll problem, we have kept the variance $G_\infty$ constant instead of $G$, and have allowed the parameters describing the potential function $g$ and $r_0$ to change with $N$ in order to compare solutions that have close to the same oscillation frequencies. In our numerical runs, we chose the values

$$G_\infty = 1, \quad \overline{m^2} = 2, \quad \delta r = 2, \quad g(\infty) = 1. \tag{7.15}$$

Figure 1 displays the variation of the potential parameters with $N$.

### B. Shifted Gaussian initial conditions

The second $O(N-1)$ invariant initial condition we investigated had a wave function localized in a wave packet near the center of the valley of the classical potential at $r = r_0$. For $N=1$ this would be the standard double-well tunneling problem; for higher values of $N$, tunneling is avoided by going around the barrier. Therefore this initial condition is qualitatively different from the roll problem and provides a different arena for testing approximations. However, since this initial condition violates the $O(N)$ symmetry of the potential, numerical solution is at present possible only for very small $N$.

We take the initial wave function to be a shifted Gaussian of the form

$$\psi_0(x) = \frac{1}{(2\pi G)^{N/4}} \exp\left\{ -\sum_i \frac{(x_i - r_0/\sqrt{N})^2}{4G} \right\}. \tag{7.16}$$

The energy $E$ of this state can be determined from Eq. (6.7) by the substitutions

$$G_{ij} \to \delta_{ij} G, \quad q_i \to r_0/\sqrt{N}, \quad p_i \to 0, \quad \Pi_{ij} \to 0,$$

from which we find

$$E = \frac{N}{8G} + \frac{g}{8N}\{N(N+2)G^2 - 2NGr_0^2 + r_0^4\}. \tag{7.17}$$

On the other hand, the height of the classical potential barrier is given by

$$E_b = \frac{g}{8N} r_0^4. \tag{7.18}$$

For $N=1$, the necessary requirement for tunneling is that $E < E_b$.

In the general case (arbitrary $N$), we have

$$M^2 = \left. \frac{\partial^2 V(r)}{\partial r^2} \right|_{r_0} = \frac{g}{N} r_0^2 \quad \text{or} \quad r_0^2 = \frac{N}{g} M^2. \tag{7.19}$$

If the initial state is close to the ground state of a harmonic potential that approximates the potential at the bottom of the well, then the width $G$ of the wave function is, approximately,

$$G = \frac{1}{2\sqrt{M^2}}, \tag{7.20}$$

which can be combined with Eq. (7.17) to give the desired energy of the initial state in terms of the values of $N$ and $g$.

We are interested in initial conditions where the energy per oscillator does not increase as a function of $N$. To implement this we fix $M^2 = 1$, which corresponds to $G = 1/2$ for the initial width. The barrier height is then given by

$$E_b = \frac{N}{8g} \tag{7.21}$$

and the total energy by

$$E = \frac{N+1}{4} + \frac{N+2}{32} g. \tag{7.22}$$

We explored three cases: $E = 0.5E_b$, $E = E_b$, and $E = 2E_b$. For each of these cases, Eqs. (7.21) and (7.22) determine $g$ for each $N$. In all cases we took $x_i(0) = r_0/\sqrt{N}$, $\dot{x}_i = 0$, $G_{ij}(0) = G\delta_{ij}$, and $\dot{G}_{ij}(0) = 0$. As a consequence, all of the oscillators $x_i(t)$ move identically.

## VIII. EFFECTIVE POTENTIAL

It is well known that the static effective potential is not always a useful guide to the true dynamics of the system (see, e.g., Ref. [4]). Nevertheless, one may seek to gain qualitative insight into some aspects of quantum dynamics this way, though care is certainly indicated (see, e.g., Ref. [21] for the Gaussian effective potential). Indeed, there appears to be an interesting connection with the properties of the effective potential at next-to-leading order and with the corresponding dynamical evolution (discussed in the next section).

The effective potential in the large-$N$ approximation has

been previously obtained by Root [22] to order $1/N$; we recalculate it here using our equations. When $x_i$ and $\chi$ are independent of time, we can ignore the closed time path ordering and use Fourier transforms, passing the poles by using the Feynman contour. Then, from the action given in Eq. (3.3), we find

$$V_{\rm eff}^{[1]}(r,\chi)=\frac{N\chi}{g}\left(\mu^2-\frac{\chi}{2}\right)+\frac{1}{2}\chi r^2+\frac{N}{2}\int\frac{dk}{2\pi i}\ln[\tilde{G}^{-1}(k)]+\frac{1}{2}\int\frac{dk}{2\pi i}\ln[\tilde{D}^{-1}(k)], \tag{8.1}$$

where $\chi$ satisfies the requirement

$$\frac{\partial}{\partial\chi}V_{\rm eff}(r,\chi)=0. \tag{8.2}$$

In this section to make contact with Root [22], we have $\mu^2=-gr_0^2/(2N)<0$. In order to examine the large-$N$ limit, we again rescale Eqs. (2.7) to the $y$ variables. Then for the Green's functions, we find

$$\tilde{G}^{-1}(k)=-(k^2-\chi),$$

$$\tilde{D}^{-1}(k)=-\frac{N}{g}-Ny^2\tilde{G}(k)+\frac{iN}{2}\int\frac{dp}{2\pi}\tilde{G}(p)\tilde{G}(k-p)$$

$$=-\frac{N}{g}\left\{1-g\frac{y^2}{k^2-\chi}-\frac{g}{2\sqrt{\chi}}\frac{1}{k^2-4\chi}\right\}$$

$$=-\frac{N}{g}\frac{(k^2-m_+^2)(k^2-m_-^2)}{(k^2-4\chi)(k^2-\chi)},$$

where $m_\pm^2=b\pm\sqrt{b^2-c}$, with

$$b=\frac{5}{2}\chi+\frac{g}{2}\left(y^2+\frac{1}{2\sqrt{\chi}}\right)$$

$$c=4\chi^2+g\left(4y^2\chi+\frac{1}{2}\sqrt{\chi}\right).$$

For the Feynman contour, we have

$$\int\frac{dk}{2\pi i}\ln(k^2-\chi)=\sqrt{\chi}+\text{constant terms}. \tag{8.3}$$

Thus the effective potential (8.1) becomes

$$\frac{V_{\rm eff}^{[1]}(y,\chi)}{N}=\frac{\chi}{2}(y^2-y_0^2)-\frac{\chi^2}{2g}+\frac{\sqrt{\chi}}{2}+\frac{1}{2N}(m_++m_--3\sqrt{\chi}). \tag{8.4}$$

The gap equation which determines $\chi$ follows from Eq. (8.2):

$$\chi=\frac{g}{2}(y^2-y_0^2)+\frac{g(N-3)}{4N\sqrt{\chi}}+\frac{g}{2N}\frac{\partial(m_++m_-)}{\partial\chi}. \tag{8.5}$$

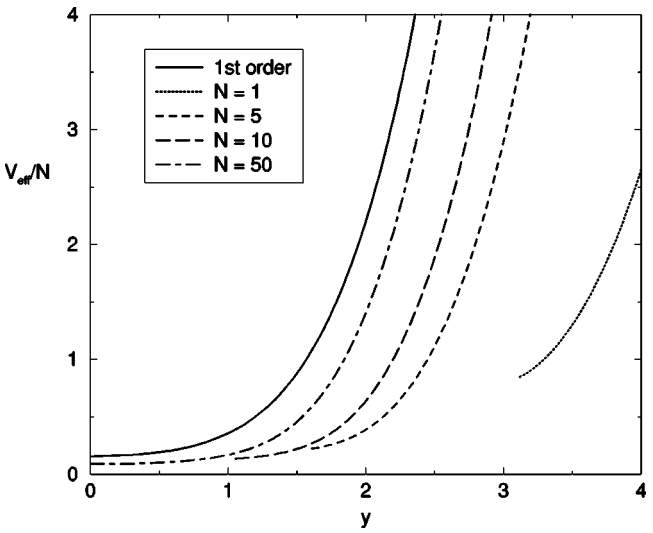


FIG. 2. $V_{\rm eff}/N$ vs $y=r/\sqrt{N}$ for the leading and next-to-leading order large-$N$ approximation for different values of $N$.

To leading order in the large-$N$ expansion, Eqs. (8.4), (8.5) reduce to the parametric set

$$\frac{V_{\rm eff}^{[0]}(\chi)}{N}=\frac{\chi^2}{2g}+\frac{\sqrt{\chi}}{4},$$

$$y^2(\chi)=y_0^2+\frac{2}{g}\chi-\frac{1}{2\sqrt{\chi}}. \tag{8.6}$$

Equations (8.4) and (8.5) agree with Root; however he used the leading order expression for $\chi$ in Eq. (8.6), rather than the full $\chi$ of Eq. (8.5).

There exist two real solutions of Eq. (8.5) for $\chi$ with $y$ greater than some minimum value $y_{\rm min}$. The next-to-leading order large-$N$ effective potential, from Eq. (8.4), is therefore double valued for $y>y_{\rm min}$, and does not exist for smaller values of $y$. The physical solution branch corresponds to the one that matches on to the leading order result; the other branch is an unphysical solution. Since it follows from a Legendre transformation, the effective potential (at any order in $1/N$) has to be a convex function. The nonexistence of the effective potential at $y<y_{\rm min}$ implies that no quantum state can be associated with the next-to-leading order large-$N$ approximation in this range.

In Fig. 2, we plot the physical branch of the effective potential as a function of $y$, for values of $N$ from 1 to 100, for the case $g=1$ and $y_0=2$. For comparison, we also show in this figure the leading order potential function from Eq. (8.6), which is single valued and finite for all $y$. (In contrast to the next-to-leading order case we can always associate a Gaussian wave function with the leading order approximation.)

In the case of the Hartree approximation, one can define an ''effective potential'' as the expectation value of the Hamiltonian using the variational wave function (4.2) for

static configurations [21,15]. Setting $p_i(t)=0$ and $\Pi_{ij}(t)=0$, and putting $\Sigma_i q_i^2 = r^2$ and $G_{ij}=\delta_{ij}G$ in Eqs. (4.6) and (4.8), we find

$$\frac{V_{\rm eff}^{[H]}(y,G)}{N}=\frac{1}{8G}+\frac{g}{8}(y^2-y_0^2)^2 + g\frac{N+2}{4N}\left(y^2+\frac{1}{2}G\right)G-\frac{g}{4}y_0^2G. \quad (8.7)$$

The value of $G$ is fixed by the requirement that

$$\frac{\partial V_{\rm eff}^{[H]}(y,G)}{\partial G}=0,$$

which gives the gap equation for the Hartree approximation:

$$\chi=\frac{g}{2}(y^2-y_0^2)+\frac{g}{N}\left(y^2+\frac{1}{2\chi}\right)+\frac{g}{4\sqrt{\chi}}, \quad (8.8)$$

where we have set $G=1/2\sqrt{\chi}$. Parametric equations for the Hartree effective potential are then given by

$$\frac{V_{\rm eff}^{[H]}(\chi)}{N}=\frac{1}{2g}\left(\frac{N}{N+2}\right)^2\chi^2-\frac{N}{(N+2)^2}y_0^2\chi+\frac{N+4}{4(N+2)}\sqrt{\chi} + \frac{g}{2(N+2)^2}y_0^4+\frac{g}{4(N+2)}\frac{y_0^2}{\sqrt{\chi}}-\frac{g}{16N}\frac{1}{\chi}$$

$$y^2(\chi)=\frac{N}{N+2}\left(y_0^2+\frac{2}{g}\chi-\frac{1}{2\sqrt{\chi}}\right)-\frac{1}{(N+2)\chi}. \quad (8.9)$$

Note that in the limit $N\to\infty$, Eq. (8.9) reduces to Eq. (8.6), the leading order large-$N$ result. Note also that the Hartree effective potential is not derived from a Legendre transform and hence is not subject to a convexity constraint.

In Fig. 3, we plot the Hartree effective potential from Eq. (8.9) as a function of $y$, for our chosen parameters $g_\infty=1$ and $y_0=2$, for different values of $N$. In contrast to the smooth behavior exhibited by the large-$N$ effective potentials, the Hartree effective potential shows a ''first-order transition'' in the placement of the minimum of the potential as a function of $N$.

The minimum of the effective potential corresponds to a determination of the ground state energy. In Fig. 4, we show values of the minimum energies of the large-$N$ and Hartree effective potentials as a function of $N$. For $N\geqslant 2$, the Hartree minimum is generally greater than that for the next-to-leading order large-$N$ approximation. Since the Hartree approximation is a variational ansatz, it gives an upper bound to the minimum energy. The fact that the next-to-leading order large-$N$ results are lower than this bound is encouraging, although no guarantee of absolute accuracy.

It is interesting to ask the question how the point $y_{\rm min}$, below which the next-to-leading order large-$N$ effective potential does not exist, changes as a function of $N$. We know that at ''infinite $N$'' (leading order), $y_{\rm min}=0$, but it is important to know how this limit is reached. For instance, is there a finite value of $N$ beyond which $y_{\rm min}=0$? In Fig. 5, we plot $y_{\rm min}$ as a function of $N$, for the Hartree and next-to-leading order large-$N$ approximations. As already stated, the Hartree approximation displays a first order phase transition between the broken and unbroken symmetry solutions at $N=6.2$, whereas for the next-to-leading order large-$N$ approximation a different type of behavior is found: for $N\leqslant 18.6$, $y_{\rm min}$ is finite, but for $N\geqslant 18.6$, it hits the origin. Thus for $N\geqslant 18.6$, we can associate a quantum state (though not known explicitly) with the next-to-leading order approximation.

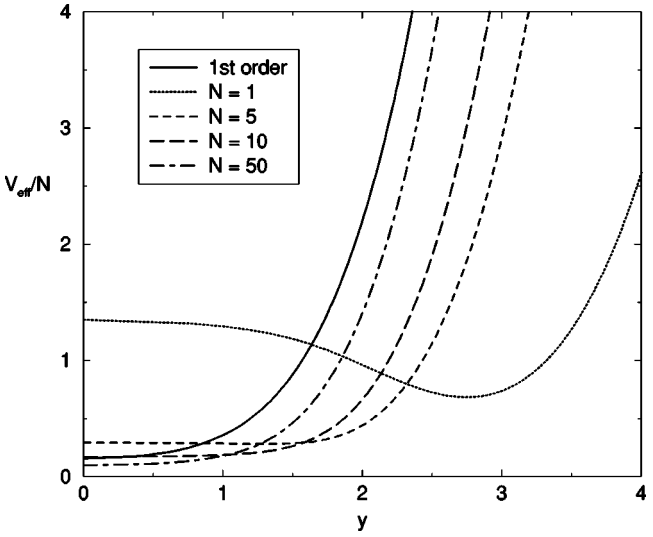


FIG. 3. $V_{\rm eff}/N$ vs $y=r/\sqrt{N}$ for the Hartree approximation using the parameters found in Eq. (7.15).

The critical value of $N$ is fixed by the value of $\chi$ at the gap equation at the inflection point. If we write the gap equation (8.5) as

$$f(\chi,y^2,N)=f_0(\chi,y^2)+\frac{1}{N}f_1(\chi,y^2)=0, \quad (8.10)$$

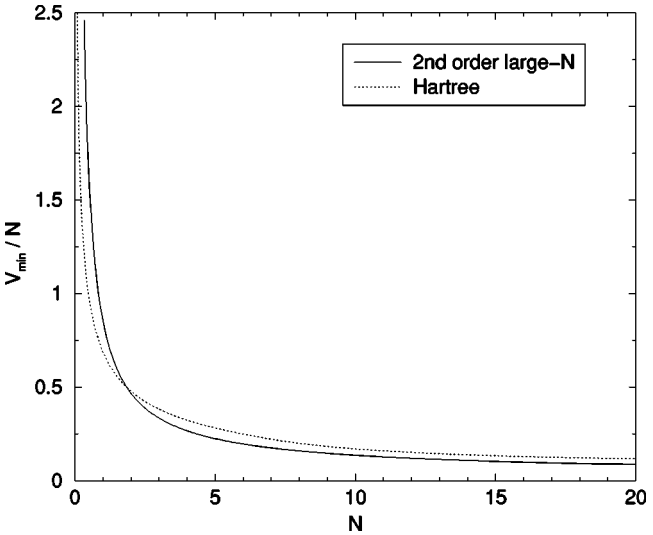


FIG. 4. $V_{\rm eff}/N$ at the minimum for the Hartree and 2nd order large-$N$ effective potentials, as a function of $N$, for the same set of parameters as in Fig. 3.

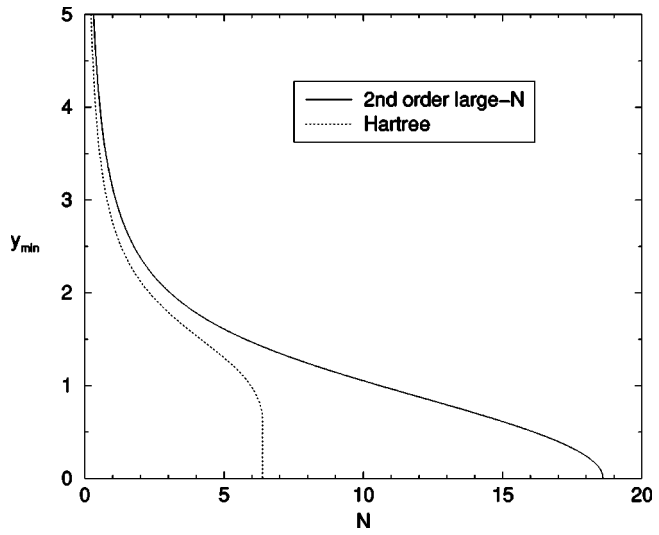


FIG. 5. The value of $y$ at the minimum of the effective potential for the Hartree and 2nd order large-$N$ approximation, as a function of $N$, for the same set of parameters as in Fig. 3.

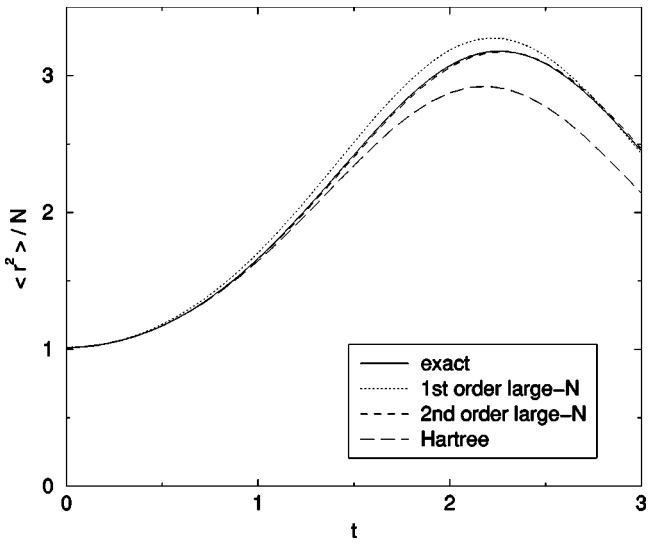


FIG. 6. $\langle r^2\rangle/N$ for $N=20$, for the exact, leading and next-to-leading order large-$N$, and Hartree approximations for short times.

where

$$f_0(\chi,y^2)=\frac{g}{2}(y^2-y_0^2)+\frac{g}{4}\frac{1}{\sqrt{\chi}}-\chi,$$

$$f_1(\chi,y^2)=-\frac{3g}{4}\frac{1}{\sqrt{\chi}}+\frac{g}{2}\frac{\partial(m_++m_-)}{\partial\chi},$$

then the critical point is determined by

$$N_c=-\frac{f_1(\bar{\chi},0)}{f_0(\bar{\chi},0)}=-\frac{\partial f_1(\bar{\chi},0)/\partial\bar{\chi}}{\partial f_0(\bar{\chi},0)/\partial\bar{\chi}}, \tag{8.11}$$

where $\bar{\chi}$ is given by the solution of this system of equations. For the parameters of Eq. (7.15), we find numerically that $N_c=18.60$, in excellent agreement with the results shown in Fig. 5.

## IX. NUMERICAL RESULTS

### A. Quantum roll

We begin with a discussion of our results for the quantum roll problem. We first examine the short time behavior, $0<t<3$, to see if the next-to-leading order large-$N$ approximation gives an improvement over the leading order solutions. In Fig. 6, we plot the values of $\langle r^2\rangle/N$ from the numerical solution, the leading and next-to-leading order large-$N$ approximations, and the Hartree approximation, for $N=20$. The next-to-leading order large-$N$ approximation is clearly better than the leading order solution and also better than the Hartree results. Similar behavior is seen for other values of $N$ (we also ran $N=50$, 80, and 100).

The long time behavior of these approximations is typically of much more interest. We examined behavior over times $0<t<100$ to see how long the approximations remained viable. Figure 7 displays $\langle r^2\rangle/N$ for the numerical solution, the leading and next-to-leading order large-$N$ approximations, and the Hartree approximation for $N=20$ and 100. The next-to-leading order large-$N$ approximation for $N=20$ blows up at $t\sim 84$. This instability is connected to a violation of unitarity in the particular implementation of this approximation and will be discussed in greater detail below. In general, at these moderate values of $N$, the approximations track the numerical solutions reasonably well though they do get out of phase as time progresses. As $N$ is increased, the phase errors are considerably reduced as is apparent in the results for $N=100$.

The energy of the next-to-leading order large-$N$ and Hartree approximations is the same as the exact one, but the energy of the leading order large-$N$ approximation differs from it by terms of order $1/N$. (This is because we need to keep the initial values of the parameters the same.) To make a comparison between the approximations this difference has to be compensated for; we do this by rescaling time by a constant multiplicative factor so as to match the last oscillation maxima. This effect is of order $1/N$. For $N=100$, we find that for $0<t<100$, the next-to-leading order $1/N$ approximation is always more accurate than the leading order; however, when comparing the next-to-leading order with the Hartree, although less accurate for $t<50$, the Hartree approximation starts becoming more accurate at $t\sim 50$ (however, the errors are very similar in magnitude, of the order of a few percent).

We now return to a discussion of the blowups first encountered in the $N=20$ case discussed above. The failure of truncation schemes (of which $1/N$ is an example) to maintain a rigid connection with the existence of a probability distribution function is a well-known problem in nonequilibrium statistical mechanics. It is often the case that, when this connection is lost (failure of reality or positivity conditions), instability soon follows. In our case, the violation of unitarity is manifest in that positive expressions such as $\langle r^2\rangle/N$ can turn out to be negative. Note that since both the Hartree and leading order $1/N$ approximations are variational in nature,

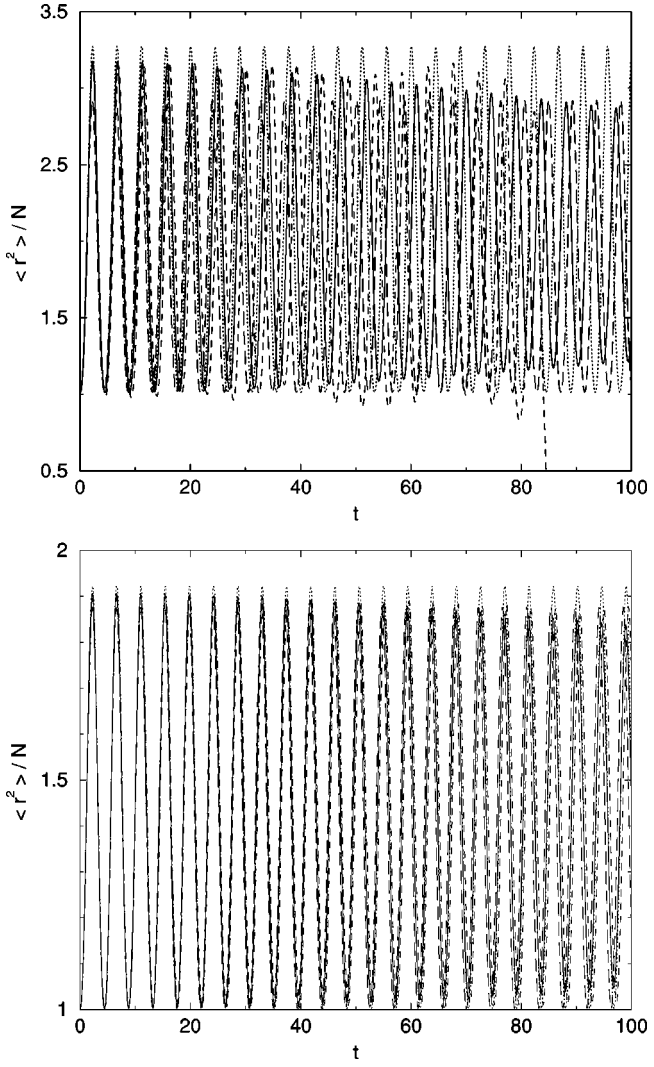


FIG. 7. $\langle r^2\rangle/N$ for the exact, leading and next-to-leading order large-$N$, and Hartree approximations for long times. The top figure is for $N=20$ while the bottom figure is for $N=100$. The labeling conventions are the same as in the previous figure.

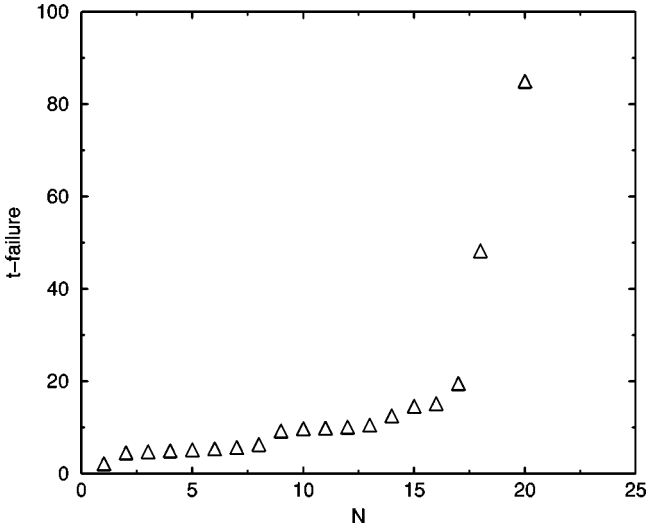


FIG. 8. Failure time for the next-to-leading order large-$N$ approximation, as a function of $N$, for the same set of parameters as in Fig. 3. Here failure time is defined as the time at which $\langle r^2\rangle/N$ becomes negative.

they can never violate unitarity. In Fig. 8, we show the blowup or failure time for the next-to-leading order large-$N$ approximation as a function of $N$, the failure time being defined as the time at which $\langle r^2\rangle/N$ becomes negative. It is interesting to note that for values of $N$ near the critical value $N_c=18.60$ where the effective potential extends down to the origin, the failure time starts to increase rapidly (consistent with our interpretation of the connection of the static effective potential to an associated quantum state). For values of $N$ greater than 21, we could not find failure for $t<150$. Thus, it may well be that above a certain value of $N$, the unitarity violation is pushed out to times of no practical significance, or may even disappear altogether.

We discussed previously how to choose initial conditions so as to reach the large-$N$ limit in a controlled manner. Starting with these initial conditions, we show in Fig. 9 results from numerical solutions of the Schrödinger equation for the time evolution of $\langle r^2\rangle/N$. In the strict large-$N$ limit one expects pure harmonic oscillations about the minimum of the infinite-$N$ effective potential. For any finite value of $N$, however, at sufficiently large times the pure harmonic motion is overcome by nonlinear effects, and interesting behavior is found, as shown in Fig. 10, indicating the presence of a very non-Gaussian wave function. The ability to capture this long time behavior is an important test of $1/N$ methods.

In order to test whether Hartree or the next-to-leading order approximation incorporate nonlinearities correctly so as to capture the late time modulation behavior, we ran a comparison against the numerical results for $N=21$, the results being displayed in Fig. 11. It is clear that both approximations do not give satisfactory results. This provides additional motivation for the development of alternative $1/N$ expansions which would incorporate selective resummations in order to reduce the coefficient of the error term at late times.

### B. Shifted Gaussian initial conditions

We now discuss the time evolution of a quantum state having an initial wave function given by Eq. (7.16). For this problem, because of the lack of symmetry, exact solutions were only obtained for $N\leqslant 2$. For $N=1$, depending on whether the energy is above or below the barrier height, one observes either slow tunneling with rapid oscillations in one well or slower oscillation in the complete range. At these low values of $N$, the large-$N$ expansion breaks down quickly, as in the quantum roll, but even here at $N=1$, the $1/N$ corrections improve the short time accuracy of $q(t)$.

A more relevant comparison is to consider larger values of $N$ at which the approximations have a better chance of capturing the exact behavior. In the next figure, we compare the Hartree with the leading and next-to-leading order large-$N$ approximation for $q(t)$, at $N=50$. Figure 12 displays the results for a run with $E>E_b$ using the equal time Green's function approximation (see Sec. V) method for obtaining the Hartree results. Unlike the situation for the roll initial

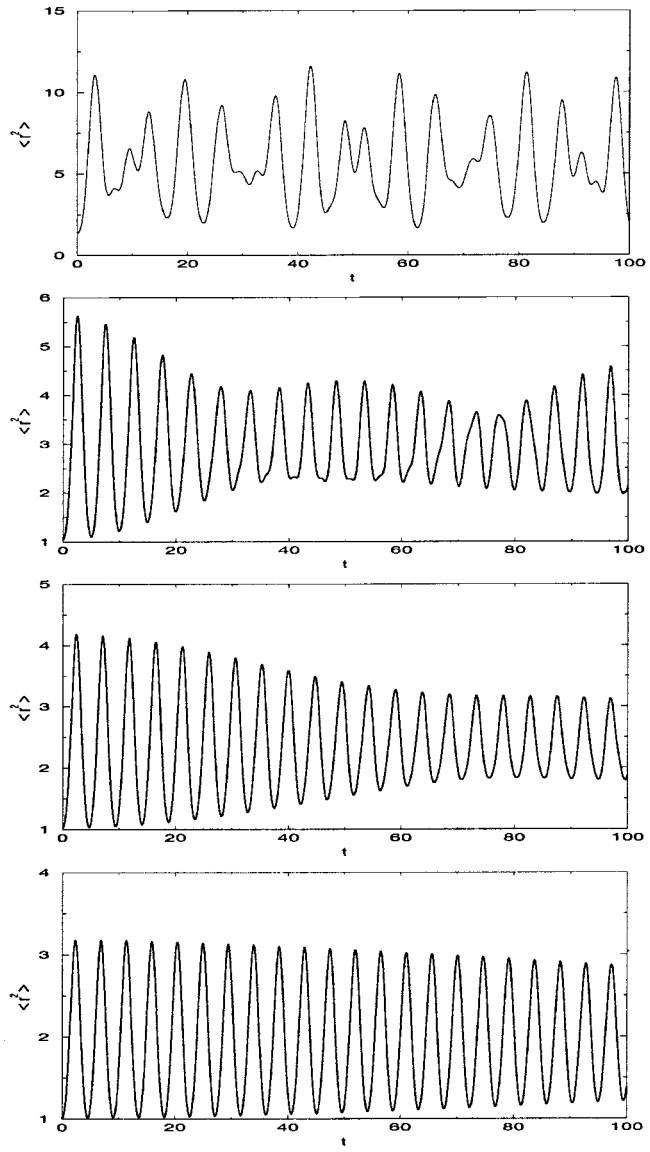


FIG. 9. Exact solutions for $\langle r^2 \rangle / N$ as a function of time. From top to bottom, $N=1$, 5, 10, and 20.

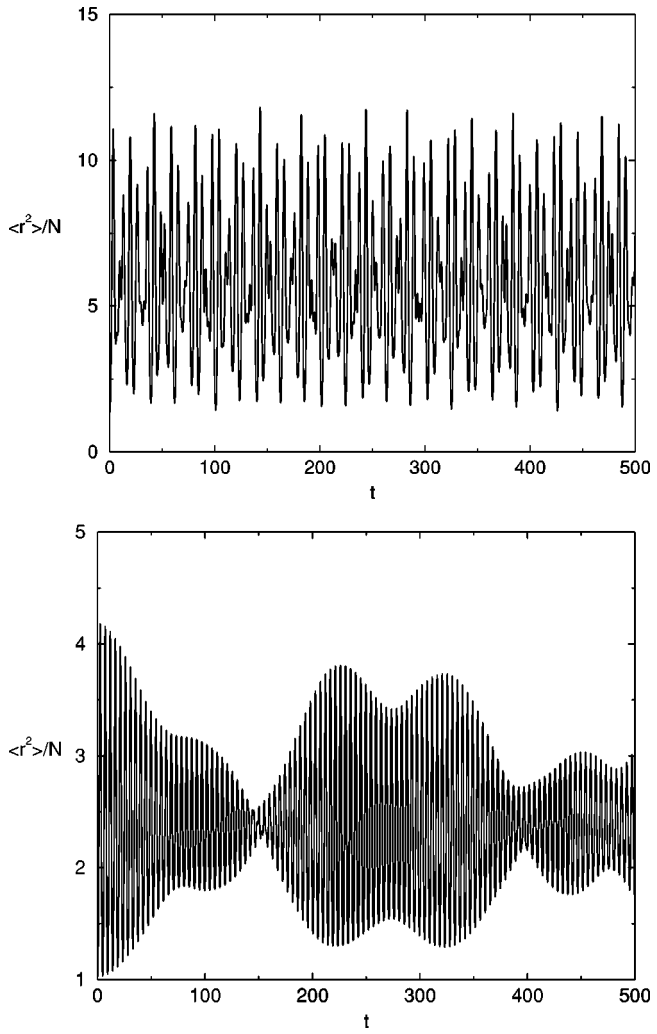


FIG. 10. Very long-time behavior of the exact results for $\langle r^2 \rangle / N$ for $0 \leqslant t \leqslant 500$. The top figure is for $N=1$ and the bottom figure for $N=10$.

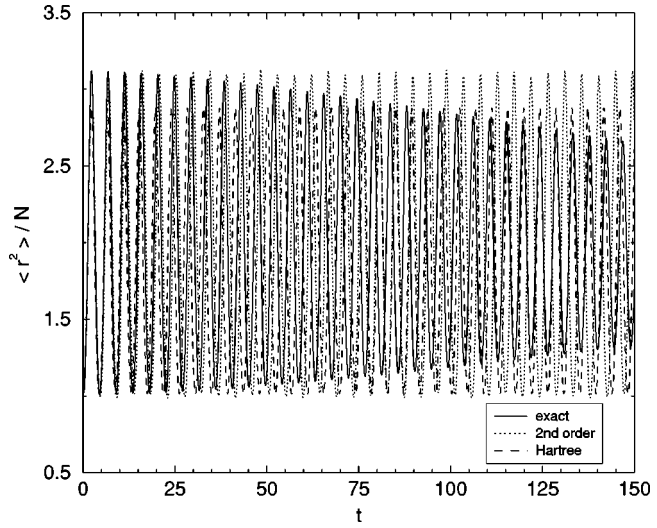


FIG. 11. $\langle r^2 \rangle / N$ for $N=21$, for the exact, next-to-leading order large-$N$, and Hartree approximations for late times.

condition where the Hartree and next-to-leading order large-$N$ results are not dramatically different, here the qualitative behavior is quite dissimilar (whereas the Hartree and leading order results are in fact very close).

## X. CONCLUSIONS

Testing the $1/N$ approximation in quantum mechanics has already enabled us to arrive at some useful conclusions. In order to interpret our results, it is important to keep in mind that $1/N$ approximations are a form of resummed perturbation theory and are therefore only valid at weak coupling. Thus for couplings of order unity, it is unrealistic to expect the approximation to give good results for small values of $N$. Our results have shown that at sufficiently large $N$ the next-to-leading order approximation is a clear improvement over the leading order approximation; however, at late times this approximation (as well as Hartree) fails to capture the non-

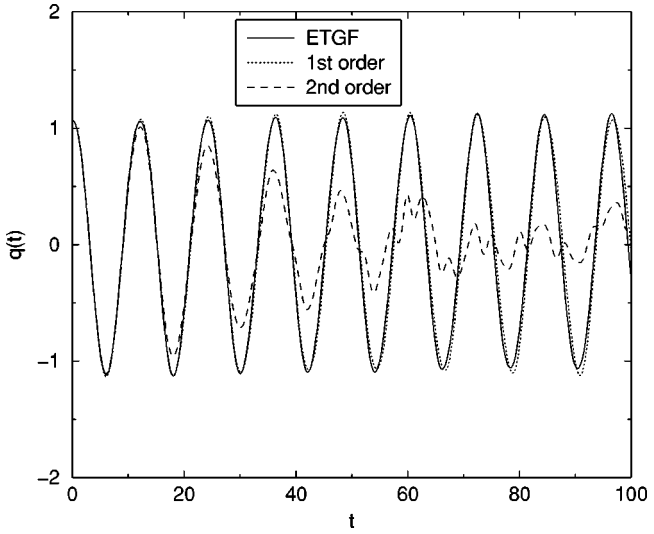


FIG. 12. Plot of $q(t)$ vs $t$ for $E>E_b$ with $N=50$.

linear effects that lead to nontrivial amplitude modulation of the radial oscillations in the quantum roll problem.

The main conclusions presented here are for radially invariant initial conditions. While other initial conditions can certainly be entertained (e.g., the off-centered Gaussians we considered above), the difficulty is that whereas results from the approximations can be more or less easily obtained, they cannot be benchmarked against numerical solutions at even moderate values of $N$ (for more general initial conditions, one needs to solve an $N$-dimensional Schrödinger equation for which the memory cost rises as $l^N$ where $l$ is the number of grid points in a single dimension). Moreover, it is unlikely that our (pessimistic) conclusions will be changed by making the exact evolution more, rather than less, complicated.

We have noted the presence of a finite-time breakdown in the evolution given by the next-to-leading order approximation. This result is related to the fact that the large-$N$ expansion for the expectation values does not necessarily correspond to a positive semi-definite density matrix when truncated at any finite order in $1/N$. (At lowest order, the $1/N$ approximation is equivalent to a Gaussian variational ansatz for the density matrix and does not have this problem.) This last aspect is already clear even in static situations such as the lack of a real effective potential for all $N$ in the next-to-leading order approximation. This type of finite-time breakdown induced by unitarity and positivity violation has also been noted in simulations of quantum systems where the coupled equal time Green's function approach was truncated at fourth order [23] or where high order cumulant expansion methods were used [24].

Two aspects of this breakdown deserve further mention: First, the time at which breakdown occurs appears to be strongly connected to the behavior of the effective potential. For values of $N$ not very much bigger than the critical value $N_c$ (beyond which the effective potential exits over the entire range of $y$), the breakdown time increases extremely steeply and may even be pushed to times long enough to be no longer an obstacle to practical calculations (this still needs to be demonstrated). Second, it is important to point out that avoiding the breakdown via a partial resummation does not automatically guarantee better late time accuracy (or convergence) since such a scheme is also only next-to-leading order accurate. However, it will help in the sense that one may carry out simulations at smaller values of $N$, thus making it easier to compare against the late-time numerical solutions of the corresponding Schrödinger equation.

One possible way of correcting the problem of a manifestly positive operator such as $\langle r^2 \rangle$ becoming negative is to solve for the full Green's function $\mathcal{G}_{ij}(t,t')$:

$$\mathcal{G}_{ij}(t,t') = G_{ij}(t,t') - \sum_{k,l} \int_{\mathcal{C}} dt_1 \int_{\mathcal{C}} dt_2 G_{ik}(t,t_1) \times \Sigma_{kl}(t_1,t_2)\mathcal{G}_{lj}(t_2,t'), \tag{10.1}$$

rather than the next-to-leading order one as in Eq. (3.7). This equation is the exact equation one obtains by varying the effective action and it contains terms of all orders in $1/N$ (thus, strictly speaking, one is no longer truncating at some fixed order).

However, just making this correction does not increase the time period during which the approximation is accurate. In order to extend the accuracy of the $1/N$ approximation to late times, it appears necessary to use a more robust approximation based on the Schwinger-Dyson equations. Several approximations of this sort are possible, which may both cure the positivity problem as well as lead to accurate results at late times. These will be discussed separately [25].

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