Evolution of the macroscopically entangled states in optical lattices

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We consider dynamics of boson condensates in finite optical lattices under a slow external perturbation which brings the system to the unstable equilibrium. It is shown that quantum fluctuations drive the condensate into the maximally entangled state. We argue that the truncated Wigner approximation being a natural generalization of the Gross-Pitaevskii classical equations of motion is adequate to correctly describe the time evolution including both collapse and revival of the condensate.

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I. INTRODUCTION

Recent advances in experimental realization of Bose-Einstein condensates (BECs) in optical lattices [1–3] make this field particularly interesting for theoretical analysis. One of the most striking features about these condensates is the possibility to observe directly effects of quantum fluctuations at zero temperature. For example, as was predicted theoretically [4] and shown experimentally [2], the zero- point motion can drive the system from the superfluid to the Mott insulating state. The other direct manifestation of quantum effects was reported in Ref. [3], where it has been shown that bosons can live in the superposition of number states even in the absence of tunneling. On the other hand, in the superfluid regime the quantum fluctuations are suppressed and either classical Gross-Pitaevskii (GP) or Bogoliubov's approach is often adequate for the description of both static and dynamic properties of the condensates (see, e.g., Refs. [5,6]). However, there is an interesting possibility, wherein the system is superfluid but neither of these approaches is good. Suppose that the initially stable condensate is driven to the regime of instability. This can be achieved either by applying a certain phase shift to the condensate with repulsive interactions [7–9] or by switching the sign of the interaction to the negative value using Feshbach resonance [10,11]. The main difficulty with standard approaches arises because near the instability all the fluctuations including quantum exponentially grow and cannot be treated as a small perturbation. To be more specific, suppose that for time $t \leqslant 0$ the periodic system of condensates in a lattice was in a superfluid ground state, i.e., the interaction was relatively weak. Then a phase imprint, i.e., a certain phase difference between the adjacent wells, was imposed. Experimentally this can be achieved by, e.g., applying a short (compared to a single tunneling time) pulse of an external field to the system. A case of special interest will be when there is a relative π phase shift between neighboring wells [12]. For the two wells with equal number of bosons and relatively small interaction, this state is metastable [7,12] (this is also the case for even number of wells and periodic boundary conditions). However, if the interaction increases and becomes larger than a critical value, this equilibrium becomes unstable and the bosons spontaneously form a ''dipole'' state [9,12–14] in which most of them occupy one of the two wells. Upon accounting for quantum fluctuations in a system with a finite number of bosons, the state obtained is a superposition of the two dipole states so that the inversion symmetry is preserved. Clearly in the case of infinite number of wells, the translational symmetry is always broken. For example, in Ref. [15] a similar instability but for the case of a Mott insulator in a strong electric field was shown to drive the system into a dipole state.

Related to this instability is a very interesting possibility of forming a ''Schrödinger cat'' (macroscopic quantum interference) state [16]. If the interaction slowly increases in the π state, then as we just mentioned, at certain point the system becomes unstable. Classically the bosons will remain in this unstable state forever unless there is some noise present either dynamical or in the initial conditions. As we will show below such a noise will drive all the bosons into one spontaneously chosen well. However, apart from classical fluctuations, which are always there but relatively weak in the condensates, there is also a quantum zero-point motion, which comes from the uncertainty relation between the number of bosons and their phase, so that the state where both are defined is simply impossible. This quantum noise will also cause the classical trajectories to move apart from the unstable equilibrium. However, as we mentioned above, the quantum fluctuations do not break translational invariance so the resulting state must be macroscopically entangled. Let us give a simple analogy with a ball laying on the top of the hill. Without fluctuations it will remain there forever. However, because of the uncertainty principle this ball will move down along different classical paths. The quantum effects will be manifested only in certain phase relations between these paths but will not affect the motion itself. This analogy suggests that a good way to describe these situations is to take into account fluctuations yielding some probability distribution of the number and the phase at $t=0$ and evolve the fields according to the classical equations of motion. In the literature this approach is known as the truncated Wigner approximation (TWA) [17–22]. In the Appendix we will show that TWA naturally arises in the path-integral derivation of the evolution equations. In Sec. III we will numerically test the results on the exactly solvable model of two

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condensates. We show how to go beyond TWA in a separate publication [27].

Let us also briefly mention a few other alternatives for generalization of the classical dynamics of the BECs existing in the literature. One of them relies on the idea of incorporating the interaction between the superfluid component of the condensate and excited bosons into GP equations [23,24]. This approach was successfully applied to the description of the condensate evaporation after a sudden change in the scattering length. Recently, there has been developed a different class of methods based on the exact stochastic reformulation of the time evolution of interacting bosons [18,25,26]. These ideas look very promising, however, near the classical instability, the convergence might be an issue.

Throughout this paper we will explicitly consider a one-dimensional array of coupled condensates. However, the results are quite general and should not depend on the dimensionality.

The standard Bose-Hubbard Hamiltonian we are going to employ reads

$$\mathcal{H}=\sum_j -J(a_j^\dagger a_{j+1}+a_{j+1}^\dagger a_j)+\frac{U}{2}a_j^\dagger a_j(a_j^\dagger a_j-1). \quad (1)$$

Here a_j is the canonical Bose annihilation operator on sites of the optical lattice (wells) labeled by an integer j, J is the tunneling amplitude between neighboring lattice sites, $U>0$ is the repulsive interaction energy between bosons in the same well. Another important parameter in the problem is the mean number of bosons per lattice site N. In this paper we will consider the case of large N, since it corresponds to the nearly classical limit. A dimensionless measure of the strength of interactions between the bosons is the coupling [12]

$$\lambda\equiv\frac{UN}{J}. \quad (2)$$

Hereafter, except otherwise specified, we set $\hbar=1$ and $J=1$ so that all the energies are given in the units of J and time has units of $\hbar/J$. As we noted in Ref. [12], $\lambda\sim 1$ corresponds to the crossover from weakly to strongly interacting superfluid and $\lambda\sim N^2$ corresponds to the quantum phase transition to the Mott insulating phase. We will be interested only in the superfluid regime and assume that $\lambda\ll N^2$. Note that Hamiltonian (1) clearly has a time-reversal invariance. Besides, the equations of motion

$$i\frac{da_j}{dt}=-[\mathcal{H},a_i] \quad (3)$$

are invariant under the transformation: $t\to -t$, $\lambda\to-\lambda$, and $a_j\to(-1)^j a_j$. So in the absence of energy relaxation, which would break the time-reversal symmetry, a π phase shift between neighboring sites is equivalent to the change of the sign of the interaction from repulsive to attractive. This equivalence is very useful for qualitative understanding of the resulting instabilities.

II. SEMICLASSICAL EVOLUTION OF THE PHASE MODULATED STATE

As we discussed in detail in Ref. [12], in the classical description of the two coupled condensates, the effective motion of the number difference is equivalent to that of a classical particle with a unit mass in the effective potential:

$$U_{eff}=2n^2(1+\lambda\sqrt{1-n_0^2}\cos\theta_0)+\lambda^2 n^2\left(\frac{n^2}{2}-n_0^2\right)=0, \quad (4)$$

where the ''coordinate'' n represents the number difference between the left and the right sites, θ is the relative phase; $n_0\equiv n(t=0)$ and $\theta_0\equiv\theta(t=0)$ are the initial conditions. In particular, if $n_0=0$ and $\theta_0=\pi$ then

$$U_{eff}=2n^2(1-\lambda)+\frac{\lambda^2 n^4}{2}. \quad (5)$$

Clearly the equilibrium with $n=0$ becomes unstable if $\lambda>\lambda_c=1$.

In a more general case of multiple wells a similar analysis can be done. Because there are now many degrees of freedom, a simple representation of the motion using the effective potential becomes impossible. Instead let us return to the GP version of Eq. (3),

$$i\frac{d\psi_j}{dt}=-(\psi_{j+1}+\psi_{j-1})+\lambda(t)\psi_j^*\psi_j^2, \quad (6)$$

where $\psi_j(t)$ is the semiclassical field corresponding to the expectation value of the operator $a_j(t)$. Here we let the interaction λ explicitly depend on time. Clearly the π modulated state is a stationary solution for any interaction:

$$\psi_j(t)=(-1)^j e^{i\Theta(t)}. \quad (7)$$

The unimportant global phase $\Theta(t)$ is given by

$$\Theta(t)=-2t-\int_0^t\lambda(\tau)d\tau. \quad (8)$$

Similarly to the two-well case, this state becomes unstable when the interaction exceeds a certain critical value [7,12]:

$$\lambda_c=2\sin^2\frac{\pi}{M}, \quad (9)$$

where M is the number of the lattice sites in the array. The origin of the instability becomes intuitively clear if we use a dynamical symmetry mentioned above: $\lambda\to-\lambda$, $\psi_j\to(-1)^j\psi_j^*$. So a strong repulsive interaction for the π state is equivalent to a strong attractive interaction for the symmetric state. The instability for the attractive interaction is naturally expected [10,11]. To get more quantitative results we consider a time evolution of fluctuations around the π state:

$$\psi_j(t)=(-1)^j e^{i\Theta(t)}[1+\xi_j(t)+i\eta_j(t)], \quad (10)$$

with ξ_j and η_j being small real deviations from the exact π solution found above. Substituting Eq. (10) into Eq. (6) and linearizing the resulting equations we obtain

$$\frac{d\xi_j}{dt} = \eta_{j+1} + \eta_{j-1} - 2\eta_j, \tag{11}$$

$$-\frac{d\eta_j}{dt} = \xi_{j+1} + \xi_{j-1} - 2\xi_j + 2\lambda(t)\xi_j. \tag{12}$$

In the Fourier space this system is equivalent to a set of decoupled second-order differential equations

$$\frac{d^2\xi_q}{dt^2} = -16\sin^4\frac{q}{2}\xi_q + 8\lambda(t)\sin^2\frac{q}{2}\xi_q \tag{13}$$

and

$$\eta_q = -\frac{1}{4\sin^2\frac{q}{2}}\frac{d\xi_q}{dt}. \tag{14}$$

In the case of adiabatically changing interaction we can write

$$\xi_q(t) = \xi_{0q}e^{i\phi_q(t)} \tag{15}$$

and neglect by the second derivative of ϕ_q. Here ξ_{0q} is the initial amplitude of fluctuations. Substituting Eq. (15) into Eq. (12) we get

$$\frac{d\phi_q}{dt} = \pm 4\sin^2\frac{q}{2}\sqrt{1-\frac{\lambda(t)}{2\sin^2\frac{q}{2}}}. \tag{16}$$

For simplicity we assume that the interaction increases in time as

$$\lambda(t) = \frac{\lambda_0}{1-\delta t}, \tag{17}$$

where δ is the parameter of adiabaticity and λ_0 is the initial interaction, which we assume to be small. This type of $\lambda(t)$ dependence, in fact, corresponds to the tunneling exponentially decreasing in time $[J(t) = J_0 e^{-\delta t}]$ with $t \to t/J(t)$. It is straightforward to solve Eq. (16) analytically and the result is

$$\begin{aligned}\phi_q(\lambda) = \pm\frac{2\sin^2(q/2)}{\delta}\Bigg[&\frac{\left(4-\frac{2\lambda_0}{\sin^2(q/2)}\right)^{1/2}}{\lambda_0} \\ &- \frac{\left(4-\frac{2\lambda}{\sin^2(q/2)}\right)^{1/2}}{\lambda} \\ &+ \ln\frac{1+\left(1-\frac{\lambda}{2\sin^2(q/2)}\right)^{1/2}}{1-\left(1-\frac{\lambda}{2\sin^2(q/2)}\right)^{1/2}} \\ &- \ln\frac{1+\left(1-\frac{\lambda_0}{2\sin^2(q/2)}\right)^{1/2}}{1-\left(1-\frac{\lambda_0}{2\sin^2(q/2)}\right)^{1/2}}\Bigg].\end{aligned} \tag{18}$$

Assuming that $\lambda_0 < 2\sin^2 q/2$ we see that in the limit $\lambda \to \infty$ the imaginary part of the phase ϕ_q goes to

$$\mathrm{Im}\,\phi_q(\infty) = \pm\frac{2\pi}{\delta}\sin^2\frac{q}{2}. \tag{19}$$

So if δ is large enough then the instability cannot develop in time and the phase remains essentially real. In the opposite limit the fluctuations become large and we have to study the nonlinear regime of GP equations. More specifically the relation

$$|\xi_{0q}|e^{\mathrm{Im}\,\phi_q(\infty)} = 1 \tag{20}$$

defines the boundary between the regimes of small and large fluctuations. Using the estimate of $\xi_{0\,q}$ (see the following section for the details),

$$\xi_{0\,q} \sim \frac{1}{\sqrt{N}}, \tag{21}$$

we derive that the instability for a given momentum mode will evolve into the nonlinear regime given that

$$\delta \leqslant \frac{2\pi\sin^2 q/2}{\ln N}. \tag{22}$$

This tells us that in order to get to the regime of strong fluctuations, the interaction should indeed change slowly in time (at least near the onset of instability) and so justifies the

adiabatic limit we used. The lowest-energy mode corresponds to the momentum $q=2\pi/M$ so the lower boundary for δ becomes

$$\delta_1=\frac{2\pi}{\ln N}\sin^2\frac{\pi}{M}, \tag{23}$$

and the upper boundary is

$$\delta_2=\frac{2\pi}{\ln N}. \tag{24}$$

If $\delta<\delta_1$ then all the modes have enough time to get into the nonlinear regime and, as we will show below, then classically all the bosons will go into a single well. On the contrary, if $\delta>\delta_2$ then the fluctuations around GP state will remain small. In the intermediate regime $\delta_1<\delta<\delta_2$ some of the momentum modes will exhibit small fluctuations and some will become strongly enhanced.

III. QUANTUM FLUCTUATIONS

A. Truncated Wigner approximation

In this section we will examine the role of quantum fluctuations. Before doing actual calculations, let us give some qualitative discussion. As we already mentioned we are interested in the regime, where N is large and interactions are relatively weak $\lambda\ll N^2$ so that the system is far from the Mott insulating transition and the quantum fluctuations are intrinsically small. This means that normally it is possible to use the GP approach or at most the Bogoliubov extension. However, this is not the case for our problem. Indeed, near the classical instability the starting point of unstable equilibrium for the Bogoliubov expansion of the uniform condensate becomes bad. The other way to describe this is to note that the Bogoliubov equations are nothing but the quantized version of the linearized equations (11) and (12), which can predict the onset of the instability but fail to describe the nonlinear regime. On the other hand, we can anticipate that the quantum fluctuations will remain weak until we cross the instability point. After that they will force the system to evolve into the superposition of unstable classical trajectories and become unimportant again, when those trajectories will be relatively far from each other.

These ideas, known as a truncated Wigner approximation [17], have been recently applied to the description of BECs [18–22]. The usual method of deriving this scheme is based on the cubic Fokker-Planck equations of motion for the density matrix written in the Wigner representation. In the Appendix we will show how the TWA naturally arises from the path-integral formulation of the dynamics and emphasize the key difference between the present derivation and that of the conventional Keldysh technique [28]. Moreover, in Ref. [27] we will show that within this derivation, it is straightforward to go beyond TWA perturbatively including quantum effects on the classical trajectories themselves. We will also argue there that the TWA gives the exact short-time asymptotical behavior of the evolution of *any* system. The time when it breaks down, however, depends on the details of the particular process (see Sec. III B).

The whole idea of the TWA is that the expectation value of any given operator Ω at time t is equal to the corresponding classical observable $\Omega_{cl}(t)$ evaluated according to standard GP equations and averaged over an ensemble of initial conditions distributed according to the Wigner transform of the initial density matrix (see Appendix for the details of the derivation):

$$\Omega(t)=\int d\psi_0^*\ d\psi_0\ p(\psi_0,\psi_0^*)\Omega_{cl}(\psi(t),\psi^*(t),t), \tag{25}$$

where p is defined as

$$p(\psi_0,\psi_0^*)=\int d\eta_0^*\ d\eta_0\left\langle \psi_0-\frac{\eta_0}{2}\middle|\rho_0\middle|\psi_0+\frac{\eta_0}{2}\right\rangle \times e^{-|\psi_0|^2-(1/4)|\eta_0|^2}e^{(1/2)(\eta_0^*\psi_0-\eta_0\psi_0^*)}. \tag{26}$$

In the equation above $|\psi_0\pm\eta_0/2\rangle$ denote coherent states. We use the following measure:

$$d\psi_0\ d\psi_0^*\equiv\prod_j\frac{d\,\mathrm{Re}\,\psi_{0\,j}\,d\,\mathrm{Im}\,\psi_{0\,j}}{\pi}, \tag{27}$$

with the product taken over continuous or discrete spatial indices, which we suppressed in Eqs. (25) and (26) to shorten the notations. The interpretation of $p(\psi_0,\psi_0^*)$ as a probability is not very precise because the Wigner transform does not have to be positive. To get the function $\Omega_{cl}(\psi,\psi^*,t)$ we need to rewrite the quantum operator Ω in the fully symmetrized form and substitute field operators a and $a^\dagger$ by their classical counterparts ψ and ψ^*. In particular, the relation between Ω_{cl} and a more familiar version of the classical counterpart of the normal-ordered operator Ω usually appearing in the functional integrals is

$$\Omega_{cl}(\psi,\psi^*)=\langle\Omega(\psi^*+\eta^*/2,\psi-\eta/2)\rangle, \tag{28}$$

where the average is taken over η with the weight $\exp(-|\eta|^2/2)$.

Let us now give general comments on the validity of Eq. (25). If the Hamiltonian is noninteracting, then this expression is exact. So TWA includes the Bogoliubov approximation and goes beyond. To recover the latter we just need to linearize the classical GP equations of motion while evaluating $\psi(t)$. This statement is not surprising since the noninteracting evolution is always identical to classical [21,29,30]. If there are nonlinear interactions then, in general, there will be corrections to the equations of motion themselves. We consider them in Ref. [27]. Let us only note here that for the two coupled condensates we showed in Ref. [12] (see also Sec. III B) that the time where GP breaks down in the worst possible scenario with the least classical initial state having completely undefined phase is equal to $t_c\approx N/\lambda=J/U$. We expect that the scaling with N is generic [33] and therefore Eq. (25) should be valid at least for the times shorter than t_c. In the following section we will see that if there are no sud-

den perturbations, so that a small fraction of quantum levels is populated, then the time scale of the validity of TWA becomes much longer.

B. Two coupled condensates: Comparison with the exact solution

The main purpose of this section is to test the truncated Wigner approximation on a simple example of two coupled condensates, where it is straightforward to obtain the exact solution. The two-well version of Hamiltonian (1) reads

$$\mathcal{H}(t) = -Ja_\alpha^\dagger \tau_x^{\alpha\beta} a_\beta + \frac{U(t)}{2} a_\alpha^\dagger a_\alpha (a_\alpha^\dagger a_\alpha - 1), \qquad (29)$$

where $\alpha,\beta = L,R$ denote the right or the left well, respectively, $\tau_a^{\alpha\beta}$, $a = x,y,z$ are the Pauli matrices. As usually we imply an implicit summation over repeated indices. Because of the total number conservation, Eq. (29) is equivalent to a more familiar version of the spin Hamiltonian

$$\tilde{\mathcal{H}}(t) = -Ja_\alpha^\dagger \tau_x^{\alpha\beta} a_\beta + \frac{U(t)}{4} (a_\alpha^\dagger \tau_z^{\alpha,\beta} a_\beta)^2. \qquad (30)$$

A convenient choice of the observable is

$$\Omega = \frac{1}{N^2} (a_\alpha^\dagger \tau_z^{\alpha\beta} a_\beta)^2 = \frac{1}{N^2} :(a_\alpha^\dagger \tau_z^{\alpha\beta} a_\beta)^2: + \frac{2}{N}, \qquad (31)$$

where semicolons denote the normal order. The operator Ω is nothing but the scaled variance of the relative number distribution. Let us consider several examples of the evolution: (i) the initial state is symmetric and the interaction increases with time, (ii) the initial state is antisymmetric and the interaction increases with time, and (iii) the initial state is the Fock state and the interaction does not change in time. Situation (ii) is directly relevant to the macroscopic quantum superposition (''cat'') state dynamics we consider in this paper, but we also look to the other possibilities to check the validity of this approach in a more general case.

The classical function $\Omega_{cl}(\psi,\psi^*,t)$ can be either found from the normal-ordered form of the operator Ω according to Eq. (28) or by direct symmetrization of the latter. In our particular case it reads

$$\Omega_{cl}(\psi^*,\psi) = (\psi_\alpha^* \tau_z^{\alpha\beta} \psi_\beta)^2 + \frac{2}{N} - \frac{2}{N} - \frac{1}{8N^2}$$

$$= (\psi_\alpha^* \tau_z^{\alpha\beta} \psi_\beta)^2 - \frac{1}{8N^2}. \qquad (32)$$

The final step is to find the probability function $p(\psi_0,\psi_0^*)$ according to Eq. (26). This will depend on the details of the state $|O\rangle$, therefore we have to study different initial configurations explicitly.

1. Symmetric or antisymmetric initial state

Suppose that at $t=0$ the interaction was negligible. Then the products of symmetric and antisymmetric wave functions give the ground and the most excited stationary states. They

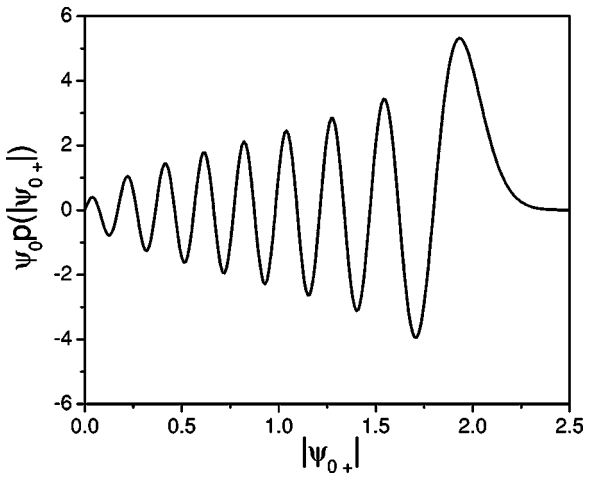

FIG. 1. Distribution of the GP initial conditions vs $|\psi_{0+}|$ for the symmetric state with eight noninteracting bosons per well.

can be also represented as a superposition of products of the two coherent states with equal or shifted by π phases,

$$|0\rangle = (4\pi N)^{1/4} e^{-N} \int \frac{d\theta}{2\pi} e^{-2i\theta N} |\sqrt{N} e^{i\theta}\rangle_L |\sqrt{N} e^{i\theta + i\pi\sigma}\rangle_R, \qquad (33)$$

where $\sigma = 0,1$ for the symmetric or antisymmetric state, respectively. The integral over the global phase θ ensures the particle number conservation. Before proceeding with further analysis let us look into a simpler example of just a product of the two coherent states, where the global phase symmetry is broken and θ takes some particular value. Then after straightforward calculation one can show that

$$p(\psi_0,\psi_0^*) = 4 \exp\left[-2 \sum_\alpha |\psi_{0\alpha} - \sqrt{N} e^{i\pi\sigma}|^2 \right]. \qquad (34)$$

We see that in this case the probability distribution of ψ_0 is just a Gaussian centered near the classical value with the relative variance of fluctuations of the order of $1/\sqrt{N}$. This is completely reasonable and we indeed recover GP picture having a single initial state in the limit $N \to \infty$. Now let us look closer to the wave function (33). After a simple calculation the final expression for the probability p reads

$$p(\psi_0,\psi_0^*) = 4 e^{-|\psi_{0+}|^2 - |\psi_{0-}|^2} L_{2N}(2|\psi_{0+}|^2), \qquad (35)$$

where $\psi_{0\pm} = \psi_{0L} \pm \psi_{0R}$ in the symmetric state, and we should interchange ψ_{0+} and ψ_{0-} for the π state, $L_{2N}(x)$ is the Laguerre's polynomial. This expression is a Gaussian in terms of $|\psi_{0-}|$, however, it has a nonlocal behavior as a function of $|\psi_{0+}|$. Moreover, $p(\psi_0,\psi_0^*)$ is not positively defined. This leads to interesting consequences. For example, while the average of $|\psi_{0+}|^2$, computed with help of Eq. (35) gives the expected classical result, the variance of $|\psi_{0+}|^2$ is *negative*. In Fig. 1 we plot the normalized function $|\psi_{0+}|\, p(|\psi_{0+}|)$ for the situation with 8 bosons per well. The extra factor of $|\psi_{0+}|$ comes from the integral measure

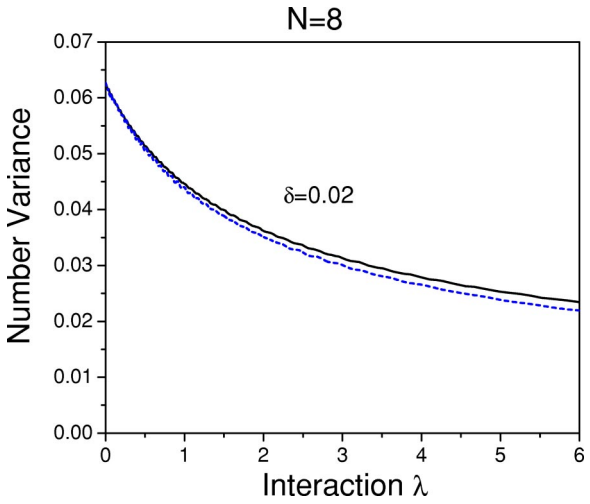

FIG. 2. Dependence of the number variance on the interaction changing with time according to Eq. (37) for initial symmetric state and 8 bosons per well. Dashed and solid lines show semiclassical and exact solutions, respectively.

$$\int_0^\infty |\psi_{0+}| p(|\psi_{0+}|) d|\psi_{0+}| = 1. \tag{36}$$

For convenience we rescaled the fields $\psi_0 \to \sqrt{N}\psi$ so that the classical expectation value of $|\psi_{0+}|$ is 2. In the limit $N \to \infty$ we again recover the classical result (for the rescaled fields) $\psi_{0L,R}=1$ or $|\psi_{0+}|=2$, $|\psi_{0-}|=0$, but in a peculiar way. The contributions from $|\psi_{0+}|<2$ will cancel each other because of fast oscillations of the probability p, and only the small interval around $|\psi_{0+}|=2$ will give the contribution to the final result. We might think, that if the observable is a smooth function of the initial parameters, then the details of the distribution $p(\psi_0, \psi_0^*)$ are not important and we can substitute it by some Gaussian function with appropriate mean and variance. However, as we pointed out before the variance given by distribution (35) is negative, so at least this is not very straightforward to do.

Now let us assume that the interaction increases with time according to

$$\lambda(t) = \frac{\tanh(\delta t)}{1-\delta t}, \tag{37}$$

where $\delta \ll 1$ is the adiabatic parameter. This dependence is somewhat different from what we used in the preceding section. But the resulting instability is still there, and besides the main purpose of this section is to test our approximation scheme rather than to do some particular calculations. The resulting graphs for both symmetric and antisymmetric initial states are plotted in Figs. 2 and 3. Note that even for the eight particles per well the agreement between the exact and the TWA solutions is remarkable. For 32 particles there is a small discrepancy for the intermediate value δ. Apparently the semiclassical curve does not capture the small oscillations very well. But note that both in the limit of large and small δ the oscillations disappear and the agreement becomes perfect.

Notice that the steady state for the initial antisymmetric conditions is exactly the maximally entangled Schrödinger cat state, where all the bosons occupy either left or right well:

$$|\Psi_f\rangle = \frac{1}{\sqrt{2}}(|LLL\ldots\rangle + |RRR\ldots\rangle). \tag{38}$$

The ultimate reason for this is that, as we mentioned above, the π shifted state is in the classical equilibrium for any interactions λ, however this equilibrium becomes unstable for $\lambda > \lambda_c$. So any fluctuation will cause a classical trajectory to end up either in the left or in the right well and the quantum zero-point motion gives us these fluctuations. On the other hand, quantum mechanically we do not break the

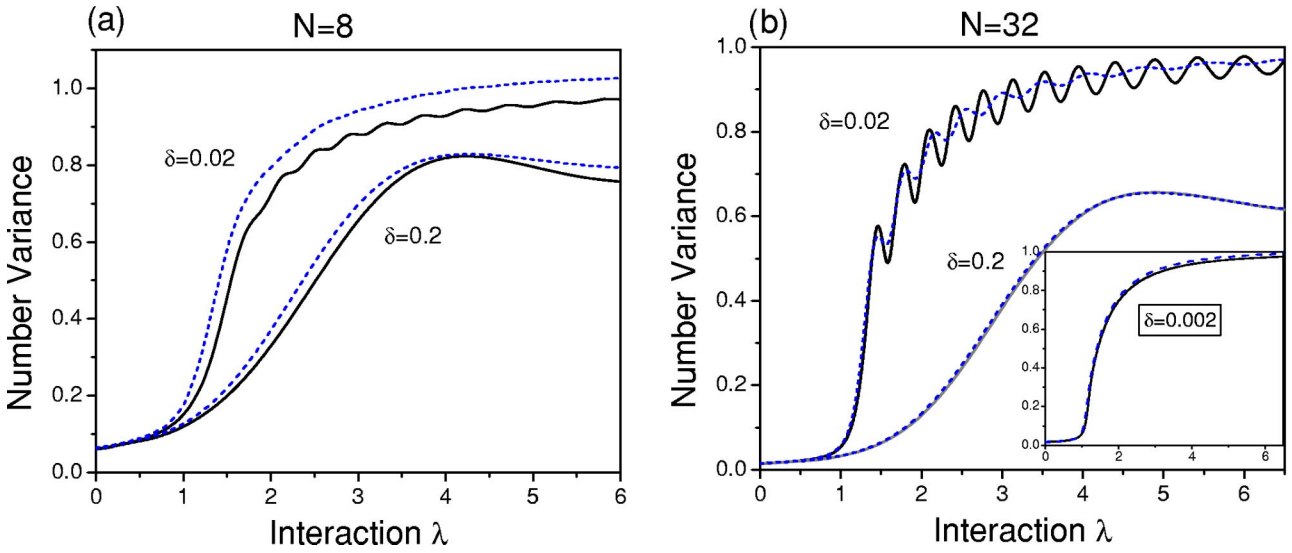

FIG. 3. Same as in Fig. 2 but for the initial antisymmetric state. The graphs (a) and (b) correspond to 8 and 32 bosons per well, respectively . The inset on the graph (b) shows the slowest evolution.

left-right symmetry because it is the property of the full Hamiltonian. The only way to reconcile these two results is to have the final configuration in the coherent superposition of the left and the right states. This statement can be also verified numerically.

2. Initial number state

Here we revisit our results derived earlier [12] assuming the two condensates are initially uncoupled and their wave function is just a product of the two number (Fock) states. Then at $t=0$ the tunneling is suddenly turned on and the number variance starts to experience some oscillatory behavior [12]. Repeating the same analysis as in the preceding section we find

$$\langle [a_\alpha^\dagger(t)\tau_z^{\alpha,\beta}a_\beta(t)]^2\rangle = \int_0^\infty \int_0^\infty \int_0^{2\pi} dn_L\, dn_R\, d\theta\, p_{num}(n_L) \times p_{num}(n_R)[\psi_\alpha^*(t)\tau_z^{\alpha,\beta}\psi_\beta(t)]^2, \tag{39}$$

where $n_{L,R}=|\psi_{L,R}(t=0)|^2$, θ is the initial phase difference between ψ_L and ψ_R. So in the Fock state the phases in the two wells are indeed uncorrelated as we argued in Ref. [12]. However, the number of bosons is distributed according to $p_{num}(n)$ given below and not fixed at $n=N$ as we might naively think. In Eq. (39) we ignored an additive $1/8N^2$ correction [see Eq. (32)]. The probability of having the initial occupation n in either well is [30]

$$p_{num}(n)=2e^{-2n}L_N(4n), \tag{40}$$

where as before $L_N(x)$ stands for Laguerre's polynomial of the order N. The function p_{num} is very similar to its counterpart defined in Eq. (35) in the sense that it also has an oscillatory behavior for $n<N$ and exponentially decays for $n>N$. In Ref. [12] we showed that the simple GP picture (i) gives a multiplicative error of $(1+1/N)$ in the number variance even in the noninteracting limit and (ii) it is valid for a finite period of time shorter than some characteristic scale determined by interactions: $t<t_c\approx J/U=N/\lambda$. For longer times the GP result starts to deviate strongly from the exact solution due to recurrence occurring in a quantum system. We might guess that the agreement between the semiclassical and the quantum results can be improved upon including quantum fluctuations at initial time according to Eq. (40). This is indeed the case for $t<t_c$, i.e., the discrepancy in the prefactor completely disappears. However, as we can see from Fig. 4, these fluctuations do not affect the time t_c itself so that the correct result can be recovered only if we also include quantum scattering, or in other words deviations of the trajectories from the classical ones. Finally, we would like to note that the initial number state is the worst possible from the classical point of view, because the phase is completely undefined there. So we expect that, in general, t_c gives the lower boundary of the applicability of TWA.

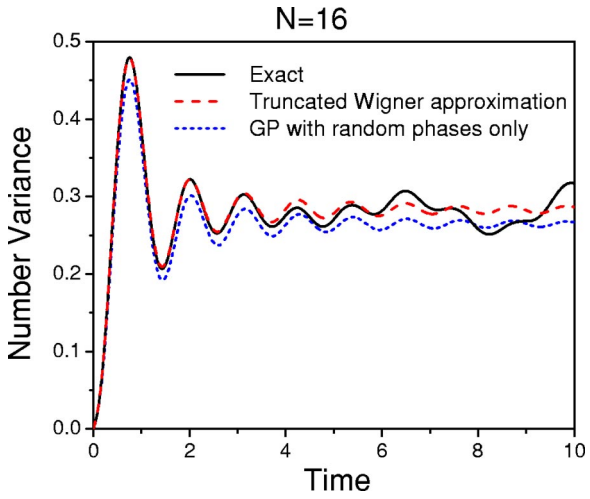

FIG. 4. Time dependence of the number variance for the initial number state and 16 bosons per well. The interaction strength is $\lambda=1$. Note that here and elsewhere in this paper time is measured in the units of $\hbar/J$.

IV. NUMERICAL RESULTS FOR MULTIPLE WELLS

Having established a general framework and checked its validity let us move on to the main subject of the paper. First, following the analysis given in Sec. II, we will study the temporal behavior of bosons in a periodic array of wells which were initially in the π state. Then we will consider a case of a harmonic trapping potential.

A. Periodic array

The straightforward generalization of Eq. (33) for the π state in a periodic chain of M coupled condensates with N bosons per well (we assume M to be even) is

$$|0\rangle=(4\pi NM)^{1/4}e^{-NM/2}\int\frac{d\theta}{2\pi}e^{-i\theta NM}\prod_{j=1}^{M}|\sqrt{N}e^{i\theta+i\pi j}\rangle_j, \tag{41}$$

where $|\cdots\rangle_j$ stands for the coherent state in the jth well. This is an eigenstate of the noninteracting Hamiltonian and apart from the global phase θ, which conserves the total number of bosons, it is just a product of coherent states with alternating phases. Ignoring the integral over θ, results in a Gaussian probability distribution of the initial state [compare with Eq. (34)]

$$p(\psi_0,\psi_0^*)=2^M\prod_{j=1}^{M}\exp[-2|\psi_{0j}-\sqrt{N}e^{i\pi j}|^2], \tag{42}$$

while the correct result for Eq. (41) reads

$$p(\psi_0,\psi_0^*)=2^M\exp\left[-2M\sum_k|\hat{\psi}_{0k}|^2\right]L_{NM}(4M|\hat{\psi}_{00}|^2), \tag{43}$$

where $\hat{\psi}_{0k}$ stands for the discrete Fourier transform of ψ_{0j},

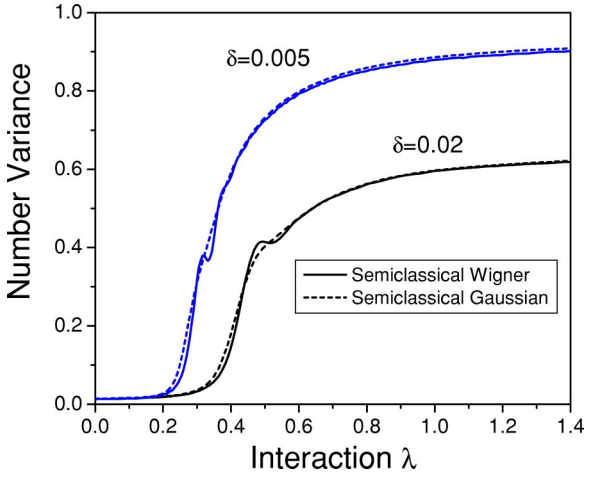

FIG. 5. Number variance as a function of the interaction for the case of ten wells with eight bosons per well. The solid and the dashed lines correspond to the distributions given by Eqs. (43) and (42), respectively. The upper curves correspond to a slower increase of the interaction with time.

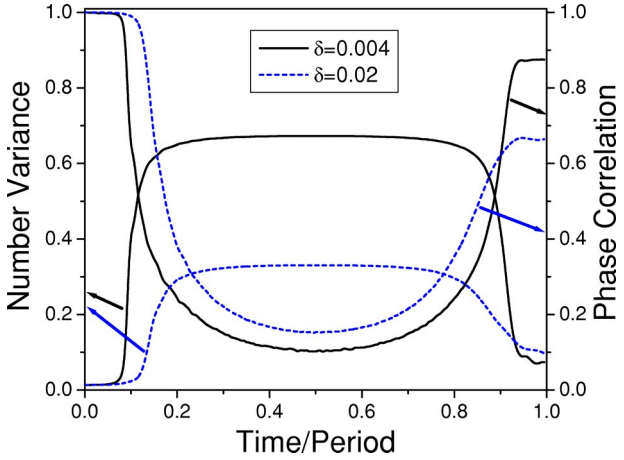

FIG. 6. Number variance and phase correlation as a function of time divided by the period of interaction ($T=1/\delta$) for ten wells and eight bosons per well. The interaction changes with time according to Eq. (48). For smaller δ the phase restoration is almost complete, which proves the coherence of the dynamics.

$$\hat{\psi}_{0k}=\frac{1}{M}\sum_j \psi_{0j}e^{-ikj}. \tag{44}$$

Clearly as $M\to\infty$ the difference between Eqs. (42) and (43) should vanish. Next let us define the operator Ω, which would be a good measure of the instability:

$$\Omega=\frac{1}{N^2M(M-1)}\sum_j (a_j^\dagger a_j-N)^2. \tag{45}$$

This is just a normalized sum of number variances over the different wells. We have chosen the prefactor so that $\langle\Omega\rangle \leqslant 1$, with 1 corresponding to the state with all the bosons located in any single well. It is easy to verify that the classical counterpart of Ω is

$$\Omega_{cl}(\psi,\psi^*)=\frac{1}{N^2M(M-1)}\sum_j\left(\psi_j^*\psi_j-N-\frac{1}{2}\right)^2 - \frac{1}{4N^2(M-1)}. \tag{46}$$

It is reasonable to expect that as the number of wells increases the global phase becomes less and less important and therefore Eq. (42) becomes more and more accurate.

Next, we consider several specific examples. First let us take the interaction to be monotonically increasing in time according to Eq. (37). In Fig. 5 we plot the resulting evolution of the state for the case of ten wells with 8 bosons per well. The solid and the dashed lines correspond to the probability distributions given by Eqs. (43) and (42), respectively. Clearly there is no significant difference between them. Note that the upper curves corresponding to smaller δ, i.e., to the adiabatic limit, saturate at $\Omega\approx 1$, which shows that *all* the bosons appear in a single well, i.e., the resulting steady state $|F\rangle$ is

$$|F\rangle=\frac{1}{\sqrt{M}}(|111\ldots\rangle+|222\ldots\rangle+\ldots|MMM\ldots\rangle). \tag{47}$$

The whole procedure of driving the system into the maximally entangled state described here is conceptually very similar to that recently suggested in Ref. [31], where the tunneling was assumed to decrease by the spatial drag of the double-well condensate through a beam splitter. The important difference, however, is that here we are not limited by a double-well system and can consider larger arrays, so that our entangled cat occupies more than two macroscopic states.

There is an important issue, which was completely obscured in the preceding analysis. Indeed, studying the number variance alone, it is impossible to distinguish the cat state from the collapsed condensate. While the collapse is often very well reproduced using GP equations, it is much harder to describe the recovery within this framework. To examine this issue let us consider the interaction, which is periodic in time

$$\lambda(t)=\lambda_0\sin^2(\pi\delta t), \tag{48}$$

where the parameter δ as in Eq. (37) determines the adiabaticity of the process. If δ is small then we expect complete restoration of the initial state after one period of oscillation $T=1/\delta$. With decreasing period we gradually lose adiabatic limit and the evolution of the system is no longer expected to be periodic. Figure 6 summarizes this discussion and the graphs are in perfect agreement with our expectations. The phase correlation in this figure is defined in a usual way as

$$-\frac{1}{2NM}\sum_j \langle a_j^\dagger a_{j+1}\rangle+\text{c.c.}$$

and the "$-$" sign is inserted for the sake of convenience because we start from the π state.

So far we considered examples where the initial state was a noninteracting π-phase-shifted condensate and then the interaction was slowly ramped up (or equivalently tunneling was ramped down). This rather hypothetical situation is certainly suitable for the theoretical analysis, but hardly applicable to any real experimental realization, where the interactions between the bosons is always present. So the initial wave function is not a simple product of coherent states but a more complicated object. One way to proceed with this issue is to write down an approximate wave function, which can be obtained using either Bogoliubov's Hamiltonian (valid for $\lambda \ll N^2$) or variational methods, and then find its Wigner transform according to Eq. (26). This would be a tractable but lengthy calculation. Instead, we can do a simple trick, demonstrating the advantage of the present approach. Namely, we can start from a noninteracting ground state, then adiabatically increase λ to the desired value, and finally apply the π phase shift following the subsequent evolution. In this scheme there is no need to do any additional analytic calculations, both ''fake'' and the real dynamics are described within the same scheme. Moreover, the computational time does not increase much because of the extra fake evolution towards the true ground state. Indeed, the classical motion is stable before the π phase shift is applied so that GP equations can be efficiently integrated. To be more specific, assume that we start from the interacting condensate with $\lambda = \text{const}(t)$, then at $t=0$ suddenly apply a π phase shift and follow the subsequent appearance of the cat. Clearly if $\lambda > \lambda_c$ [see Eq. (9)] the system becomes unstable and the quantum fluctuations force it into the entangled state. Without any calculations, it is obvious that the final state will not be maximally entangled as described in Fig. 5 because of the energy conservation. Indeed, the state with all the bosons occupying one well costs a huge interaction energy which cannot be compensated unless there is an external pumping resulting in the time dependence of the Hamiltonian. From the same considerations it is obvious that the maximum possible entanglement within this scheme can be achieved at some intermediate values of λ. Thus if $\lambda < \lambda_c$, there is no instability to begin with and so no entanglement in the final state. On the other hand, for the large λ any significant number fluctuations will cost a strong increase in the interaction energy, which cannot be compensated by a limited decrease in the hopping energy. We plot the resulting number variance as a function of time for the periodic array of ten wells in Fig. 7. The critical value of the interaction for this case is $\lambda_c = 2\sin^2(\pi/10) \approx 0.19$. Clearly for λ getting closer to λ_c the oscillations become slower and the steady state is achieved later. We would like to point out that this type of dynamics corresponds to a sudden perturbation discussed in Sec. III B 2. Therefore, we expect a finite ergodic time for a full quantum solution so that there is no true steady state for the finite number of bosons. So to achieve a stable stationary entangled state it is preferable to drive the system adiabatically towards the instability, i.e., apply a π phase shift at smallest possible λ and then slowly ramp up the interaction.

B. Harmonic trap

The effect of a harmonic trap can be mimicked by adding a quadratic potential term to the Hamiltonian of system (1)

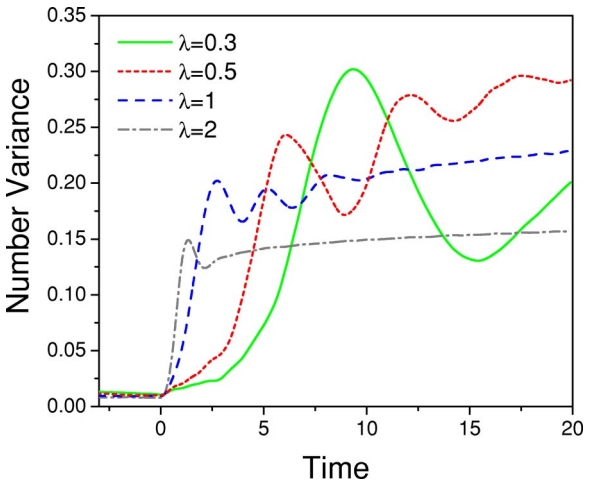

FIG. 7. Number variance as a function of time for ten wells and 8 bosons per well. The interaction remains constant in time in this example but at $t=0$ a sudden π phase shift is applied to the system.

$$V_j = \frac{J\omega_t^2}{4} j^2. \tag{49}$$

Here ω_t is the trapping frequency.

As before let us assume that initially the interactions were suppressed and the system was in the ground state:

$$|O\rangle = \left(\sum_j \alpha_j a_j^\dagger \right)^{N_{tot}} |Vac\rangle, \tag{50}$$

where $|Vac\rangle$ denotes a vacuum state with no particles, N_{tot} is the total number of bosons in the system, and

$$\alpha_j \approx \frac{\sqrt{2}}{(\pi\omega_t)^{1/4}} e^{-(\omega_t^2/4)j^2} \tag{51}$$

is the ground-state wave function of a single boson in the harmonic trap in the coordinate representation. The state $|O\rangle$ can be also written as

$$|O\rangle = \int \frac{d\theta}{2\pi} e^{i\theta(n_1+n_2+\cdots-N_{tot})} |\sqrt{N_{tot}}\alpha_1\rangle_c |\sqrt{N}_{tot}\alpha_2\rangle_c, \ldots, \tag{52}$$

where as usual $|\alpha\rangle_c$ stands for the coherent state, $n_j = |\alpha_j|^2$. If the number of populated wells is not small, then we can ignore the global phase and use an approximate expression

$$|O\rangle \approx \prod_j |\sqrt{N_{tot}}\alpha_j\rangle_c. \tag{53}$$

As in the previous discussion we assume that at initial time the phases in the adjacent wells were uniformly shifted by some phase ϕ. However, we will not consider only the case with $\phi = \pi$, because the π phase shift in the nonuniform potential does not give a stationary solution, although it still preserves the inversion symmetry. Also the number variance

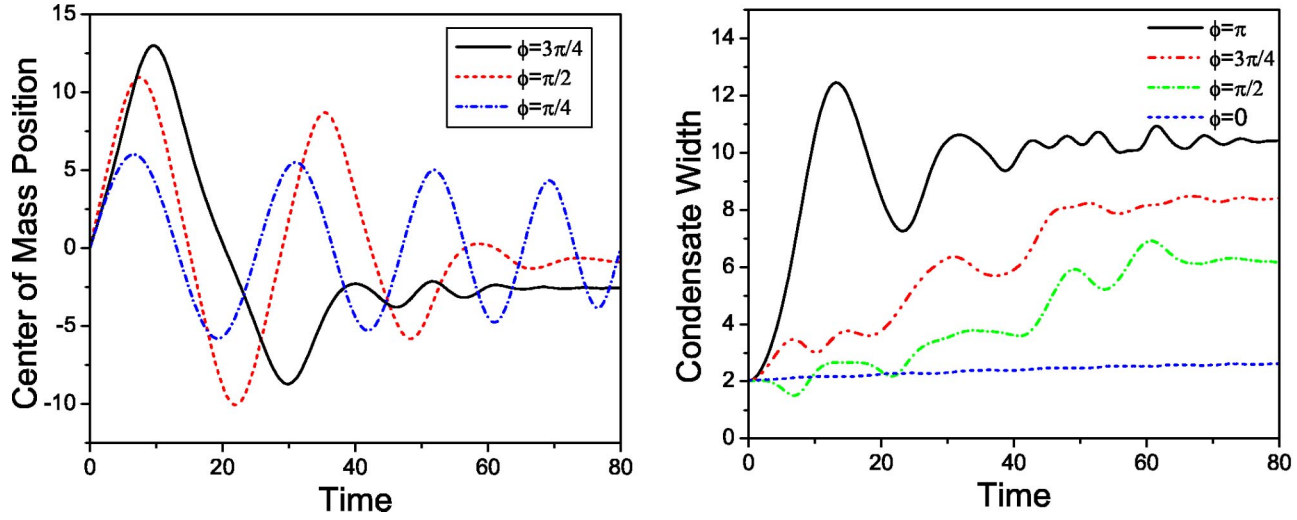

FIG. 8. Center-of-mass position and the condensate width as a function of time for the interaction and trapping frequency increasing in time according to Eq. (56) with $\delta=0.01$, $\omega_t^2(0)=0.03$, and the total number of bosons $N_{tot}=100$.

is no longer a convenient measure of the instability because the distribution is not uniform even in the initial state. Instead, let us introduce two other quantities: coordinate of the center of mass and the condensate width:

$$X=\frac{1}{N}\left\langle \sum_j j a_j^\dagger a_j \right\rangle, \quad W=\sqrt{\frac{1}{N}\left\langle \sum_j j^2 a_j^\dagger a_j \right\rangle - X^2}. \tag{54}$$

The semiclassical operators can be trivially obtained from Eq. (54). For example,

$$X_{cl}=\frac{1}{N}\left\langle \sum_j j(\psi_j^*\psi_j - 1/2) \right\rangle. \tag{55}$$

Let us assume that both the interaction and the trap frequency increase in time:

$$\lambda(t)=\frac{\tanh \delta t}{1-\delta t}, \quad \omega_t^2(t)=\frac{\omega_t^2(0)}{1-\delta t}. \tag{56}$$

We define λ according to Eq. (2) with $N=N_{tot}|\alpha_0|^2$ being the number of bosons in a central well. Note that with $\omega_t \neq 0$ there are two degrees of freedom: λ/J and ω_t/J. If we want to reflect the experimentally relevant case of vanishing tunneling rather than increasing interaction we have to keep the ratio λ/ω_t^2 constant. Extra multiplier "$\tanh \delta t$" in the interaction term is taken only for convenience purposes and it does not qualitatively change any of the results.

The two graphs in Fig. 8 show the condensate width and the center-of-mass position vs time for different initial phase imprints. Note that if the phase shift is equal to π, there is no center-of-mass oscillation because of the inversion symmetry. However, the width oscillations are very large and pronounced in this case. They also die very fast away from the π phase shift, however the steady-state condensate width depends on ϕ rather smoothly. It is also interesting to note that the center-of-mass oscillations decay faster for larger angles. This is in the direct agreement with the previous predictions of self-trapping at large phase gradients [7]. We would like to point out that the trapping is real in our case because of the rapidly increasing interaction (or equivalently vanishing tunneling).

There is, however, a major difference between the results for a periodic array and a harmonic trap. In the classical limit, the π state is an eigenstate in a periodic array for any strength of the interaction, therefore the motion is completely driven by the quantum-mechanical fluctuations, while in a harmonic trap the π state is classically unstable (that is why we plot our observables versus interaction for the periodic array and vs time for the parabolic trap). The classical instability makes quantum effects unimportant if the number of bosons is large. To further elucidate this point let us compare the results for a single Gross-Pitaevskii trajectory, i.e., a simple classical limit, with the TWA result. The two dependences are shown in Fig. 9 and they are clearly very alike. This proves that the resulting instability has a simple classi-

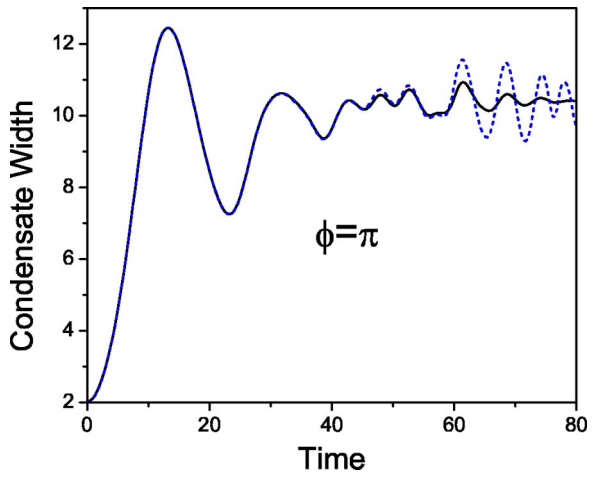

FIG. 9. Condensate width as a function of time for the same conditions as in Fig. (8). The dashed line is the simple Gross-Pitaevskii result and the solid line is the improved calculation according to Eq. (25).

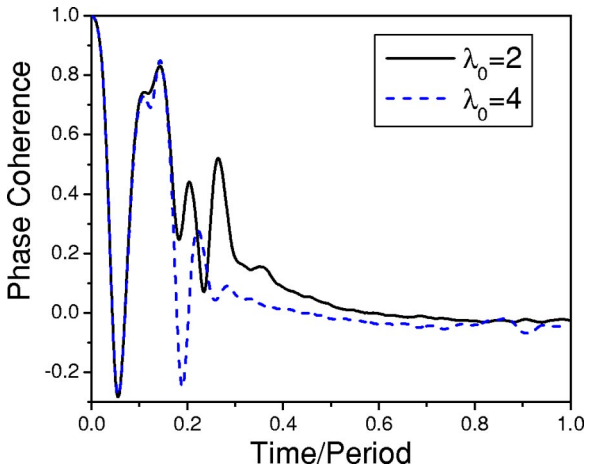

FIG. 10. Phase coherence as a function of time for the periodic interaction (48) with $\delta=0.004$. The total number of bosons $N_{tot}=100$, the trap frequency $\omega_t^2=0.03$, and the initial phase shift $\phi=\pi$. Clearly the dynamics is completely irreversible as opposed to Fig. 6.

cal nature and does not give a cat state, rather the condensate simply has large amplitude breathing modes. Such an outcome should not be very surprising. In order to get to the macroscopical entanglement one has to prepare a classically equilibrium but unstable state, which can be driven away via quantum fluctuations. This can be achieved by a simple phase shift only in a uniform periodic lattice.

We can also check the reversibility of the evolution for the periodic in time interaction (48). And clearly (see Fig. 10), the dynamics is completely irreversible. This result is also not surprising given that the initial state is not stationary even without interactions, so the π phase shift looks as a sudden perturbation applied at $t=0$ and even if the interactions change with time slowly the system is not in the adiabatic regime.

V. DISCUSSION

In the previous sections we adopted a truncated Wigner approximation allowing us to treat dynamical evolution of classical instabilities due to quantum fluctuations. We completely ignored the classical noise, which may come from various sources, e.g., fluctuations of the laser intensity or wavelength, fluctuations of the magnetic field creating the trap, collisions with external atoms, triple interactions leading to the loss of the atoms from the condensate, etc. All these sources are generally quite weak, otherwise no beautiful experiments would ever be possible. On the other hand, cat states are very fragile to any kind of classical noise. For example, in a double well in equilibrium, the noise required to destroy the coherence exponentially scales with the mass (or equivalently the number of particles), so that heavy objects are always localized in one of the classical minima. However, this is not the case in our situation. Indeed, the system is far from the equilibrium and the cat state is not a ground state. Let us crudely estimate the limits set on the noise. Assume that the classical fluctuations result in a random external potential with a usual correlator $\langle Y(t)Y(t')\rangle = Y_0\delta(t-t')$ and consider the case of two wells for simplicity. Then the relative phase flow due to fluctuations will be $\delta\theta\sim NY_0\sqrt{t}$. On the other hand, the minimum time required to get to the cat state is (see Sec. II) $t\sim\delta^{-1}\sim\ln N$. Requiring that the total phase accumulated during the evolution is less than one, we get the upper bound for the noise which does not destroy the coherence : $Y_0\sim 1/N\sqrt{\ln N}$. This result is encouraging, because instead of exponential we get a much weaker scaling of the noise with the number of particles. Clearly, in the multiwell case there will be an extra scaling with the number of wells and of course no cat state is possible in the thermodynamic limit. However, the scaling will be again weak and tractable. Another possibility to observe macroscopic cat states experimentally is to use a modulated hopping between the sites in a large array effectively splitting the condensate into pairs of sites, so the effects of the classical noise become weaker.

The other two constraints used in our analysis that the number of bosons is large and the condensate is one dimensional are also not essential. We used the large number of bosons rather to satisfy the formalism than to explain the effect. The instability is there even in the fully quantum-mechanical treatment of the problem and the resulting maximally entangled state is clearly independent of N. The only thing is that the evolution of macroscopically entangled states with a large number of atoms is more interesting from the experimental prospect. Concerning higher dimensions we would like to point out that, although we did not perform actual calculations, it is extremely unlikely that any of the results will qualitatively change. The instability will clearly survive in any dimensions and the π state can be implemented, at least theoretically, in square lattices of arbitrary dimensionality.

In conclusion, we showed that it is possible to create macroscopically entangled Schrödinger cat states in bosonic systems in optical lattices with finite number of sites. We justified and used truncated Wigner approximation generalizing a simple GP approach by the exact treatment of quantum fluctuations at initial time of the evolution. Using a solvable model of two coupled condensates we found a very good agreement of TWA with the exact results. At the end we presented some numerical simulations for the multiple-well condensates and argued that it is possible to create a cat state with more than two possible outcomes.

ACKNOWLEDGMENTS

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APPENDIX: MICROSCOPIC DERIVATION OF THE TRUNCATED WIGNER APPROXIMATION

Let us assume that at the initial time of evolution $t=0$ the system is described by a density matrix ρ_0,

$$\rho_0=\sum_\chi P(\chi)|\chi\rangle\langle\chi|, \tag{A1}$$

where $|\chi\rangle$ represents some basis state and $P(\chi)$ is the probability to occupy it (for the coherent basis $P(\chi)$ coincides with the Glauber P function commonly used in quantum optics [17]). If the initial state is pure, the sum contains only single term. According to the standard quantum-mechanical formulas, the expectation value of an arbitrary normal-ordered operator Ω at time t is given by

$$\Omega(t)=\mathrm{Tr}\left\{\rho_0 T_{K\tau}\exp\left[i\int_0^t\mathcal{H}(\tau)d\tau\right]\Omega \times\exp\left[-i\int_0^t\mathcal{H}(\tau)d\tau\right]\right\}, \tag{A2}$$

where $T_{K\tau}$ is the time-ordering operator along the Keldysh contour going from 0 to t and then returning back to 0 so that the operators corresponding to a later time are placed closer to Ω, $\mathcal{H}$ is the Hamiltonian of the system, e.g., Eq. (1) in our case. In the same way one can define correlation functions of products of operators. The conventional trick to deal with expressions such as (A2) is to rewrite them in the path-integral form using the coherent-state representation [32]. The only difference with a more usual equilibrium case is that there are two exponents containing $\mathcal{H}$. So it is convenient to introduce two fields a_f and a_b propagating forward and backward in time [28]. Then instead of Eq. (A2) we can write

$$\begin{aligned}\Omega(t)=\int Da_f Da_b\langle a_{b0}|\rho_0|a_{f0}\rangle &\times e^{-a^*_{f0}a_{f0}+a^*_{f0}a_{f1}+i\mathcal{H}(a^*_{f0},a_{f1})\Delta\tau}\ldots\\ &\times e^{-a^*_{fQ}a_{fQ}}\Omega(a^*_{fQ},a_{bQ},t)\\ &\times e^{a^*_{fQ}a_{bQ}}e^{-a^*_{bQ}a_{bQ}+a^*_{bQ}a_{bQ-1}-i\mathcal{H}(a^*_{bQ}a_{bQ-1})\Delta\tau}\ldots\\ &\times e^{-a^*_{b0}a_{b0}},\end{aligned} \tag{A3}$$

where $\Delta\tau=t/Q$ and $Q\to\infty$, $\Omega(a^*_f,a_b,t)$ is the normal-ordered operator Ω with the fields $a^\dagger(t)$ and $a(t)$ substituted by complex numbers $a^*_f(t)$ and $a_b(t)$. The expression above is intentionally written in a discrete form to take care of the boundary effects. In the classical limit the evolution is deterministic, so that $a_{fcl}(\tau)=a_{bcl}(\tau)$. On the other hand, because of quantum fluctuations the two trajectories may be different. Therefore, instead of the forward and backward fields it is natural to introduce their classical (ψ) and quantum (η) combinations [28]: $a_f=\psi+\eta/2$, $a_b=\psi-\eta/2$. So that in the classical limit ψ should correspond to the solution of the GP equations and η should be simply equal to zero. Now we can take a continuum limit in Eq. (A3) sending $\Delta\tau\to 0$:

$$\begin{aligned}\langle\Omega(t)\rangle\approx\int D\eta(\tau)D\psi(\tau)&\left\langle\psi_0-\frac{\eta_0}{2}\right|\rho_0\left|\psi_0+\frac{\eta_0}{2}\right\rangle\\ &\times\Omega\left(\psi(t)^*+\frac{\eta(t)^*}{2},\psi(t)-\frac{\eta(t)}{2}\right)\\ &\times e^{-|\psi_0|^2-(1/4)|\eta_0|^2-(1/2)|\eta(t)|^2}e^{(1/2)(\eta_0^*\psi_0-\eta_0\psi_0^*)}\\ &\times\exp\left[\int_0^t d\tau\ \eta^*(\tau)\mathcal{L}[\psi,\psi^*,\tau]\right.\\ &\left.-\eta(\tau)\mathcal{L}^*[\psi,\psi^*,\tau]\right]\exp\left[i\int_0^t d\tau\frac{\lambda(\tau)}{4N}\right.\\ &\left.\times[\psi^*(\tau)\eta(t)+\psi(\tau)\eta^*(\tau)]|\eta(\tau)|^2\right],\end{aligned} \tag{A4}$$

where $\mathcal{L}[\psi,\psi^*,\tau]$ stands for the classical (GP) differential operator acting on the field $\psi(t)$:

$$\mathcal{L}_j[\psi,\psi^*,\tau]\equiv\frac{d\psi_j}{d\tau}-i(\psi_{j+1}+\psi_{j-1})+i\lambda(\tau)\psi_j^*\psi_j^2. \tag{A5}$$

Note that $\mathcal{L}$ as well as the fields ψ and η have spatial indices which we suppressed in Eq. (A4) to simplify notations, the products such as η^*L in Eq. (A4) stand for the sum over j: $\Sigma_j\eta_j^*L_j$. A closer look to Eq. (A4) shows that there are linear, quadratic, and cubic terms in the quantum field η, the latter appearing only due to interactions. It is intuitively clear that in the classical limit $\eta(\tau)$ should be small in some sense. Thus, if we ignore completely all nonlinear terms in η, then the functional integral over the quantum field becomes a trivial product of δ functions enforcing GP equations on the classical field ψ. The next approximation will be to leave quadratic corrections but ignore cubic. From Eq. (A4) it is clear that the quadratic corrections affect only the initial and the final times of the evolution, that is why it was important for us to start from a discrete version of the path integral and be careful about the boundaries. The integral over $\eta(t)$ transforms the operator Ω into Ω_{cl} according to Eq. (28). It is a simple exercise to check that Ω_{cl} is obtained by first symmetrizing Ω and then substituting the operators a and $a^\dagger$ by the c numbers ψ and ψ^*. For example, if

$$\Omega=a^\dagger a=\tfrac{1}{2}(a^\dagger a+aa^\dagger)-\tfrac{1}{2}, \tag{A6}$$

then

$$\Omega_{cl}=\langle\psi^*+\eta^*/2,\psi-\eta/2\rangle=\psi^*\psi-\tfrac{1}{2}, \tag{A7}$$

whereas it follows from Eq. (A4), the average over η is taken with the weight $\exp(-|\eta|^2/2)$.

The second quadratic contribution originates from the field η_0 corresponding to the initial time of evolution. Because of the coupling to ψ_0 in Eq. (A4), these fluctuations introduce a probability distribution for the classical initial conditions given by Eq. (26). If we ignore the corrections to the classical equations of motion coming from the third

power of the quantum field η, then the time dependence of the observable Ω will be given by Eq. (25).

Let us now give general comments on validity of Eqs. (25) and (26). If the Hamiltonian is noninteracting, then these expressions are exact. If there are nonlinear interactions, then, in general, there will be corrections to the action involving terms proportional to all odd powers of η: η^3 in our case [see Eq. (A4)] or higher in general. Those terms will affect the time evolution, which will not be described by the GP equations any longer. In Ref. [27] we show that the corrections to the GP dynamics arise in the form of the quantum scattering events, which are equivalent to the nonlinear response to the infinitesimal perturbation of the field ψ along its classical path. We only note here that these corrections are always of the form $f(t)/N^2$ with $f(t)$ being some time-dependent function satisfying $f(t)\to 0$ at $t\to 0$, and $1/N$ is our semiclassical parameter. So the TWA given by Eqs. (25) and (26) always gives the exact short-time asymptotical behavior of the evolution. As we discuss in Sec. III B, the time when TWA breaks down depends on the details of a particular process and becomes longer under slow perturbations, where only a limited number of quantum levels are excited.

Another point we would like to make is that though the expansion in powers of $1/N$ is clearly around the classical solution, there is no $\hbar$ present anywhere. This should not be surprising since here and quite often in the atomic physics the Planck's constant either completely absorbed into energies, which are measured in hertz, or into time. In conventional units $\hbar^{-1}$ appears as the prefactor in the action justifying the saddle-point or classical approximation. In the same way, the number of bosons per site N appears as a prefactor in the exponent of Eq. (A4) after rescaling $\psi \to \sqrt{N}\psi$ and $\eta\to\sqrt{N}\eta$. So in general any expansion in powers of η is in fact the expansion in powers of $\hbar$.

Let us finally spend a few words discussing the difference between the present derivation and that of the conventional Keldysh technique. The key point in our discussion is that we ascribed the time dependence to the operator Ω itself, while leaving the density-matrix time independent. This allowed us to completely separate initial quantum fluctuations, which entered in the form of the Wigner distribution of the initial conditions for classical trajectories Eq. (26), from the quantum dynamical effects (which we consider in Ref. [27]). On the other hand, in the Keldysh technique the density matrix acquires time dependence and the initial density matrix is absorbed into the quantum propagator [28]. While it is still possible to derive GP equations in the saddle-point approximation, integrating out quantum fields in the lowest order gives a complicated self-interacting classical action [28], which is hardly possible to deal with except perturbatively or using stochastic methods. This should not be surprising since any diagrammatic technique uses a noninteracting Gaussian limit as a starting point. Therefore, to get just a classical GP dynamics in the Keldysh technique, it is necessary to sum all diagrams with classical vertices (three classical fields and one quantum) [28], which looks virtually impossible.

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