Splitting a trap containing a Bose-Einstein condensate: Atom number fluctuations

Juha Javanainen
Department of Physics, University of Connecticut, Storrs, Connecticut 06269-3046

Misha Yu. Ivanov
Steacie Institute for Molecular Sciences, National Research Council of Canada, 100 Sussex Drive, Ottawa, Ontario, Canada K1A 0R6

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We theoretically study atom number fluctuations between the halves of a double-well trap containing a Bose-Einstein condensate. The basic tool is the two-mode approximation, which assumes that only two one-particle states are involved. An analytical harmonic-oscillator-like model is developed and verified numerically for both stationary fluctuations in the ground state of the system, and for the fluctuations resulting from splitting of a single trap by dynamically erecting a barrier in the middle. With increasing strength of the atom-atom interactions and/or increasing height of the potential barrier, the fluctuations tend to evolve from Poissonian to sub-Poissonian. Limits of validity of the two-mode model and its relations to the phase-atom-number approach of Leggett and Sols [A. J. Leggett and F. Sols, Found. Phys. **21**, 353 (1991)] are discussed in detail. [S1050-2947(99)07809-9]

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I. INTRODUCTION

The recent experimental observations of Bose-Einstein condensates (BEC's) have, among other things, reinvigorated theoretical studies of condensates in double-well traps. The most often cited goal is to understand the analog of the Josephson effect [1] in this type of system. Broadly speaking, there are two main approaches capable of dealing with quantum fluctuations in this variant of the Josephson effect [2]. Authors with a quantum optics background tend to favor models in which two boson modes are involved [3–6]. Recently a numerical simulation has been presented that even takes into account both decoherence due to noncondensate atoms, and the detection of the atoms [7]. The second category of theories is based on using the differences of condensate phases and atom numbers between the two sides of the trap as conjugate quantum variables [8–10].

The two quantum approaches have not coexisted entirely without friction. There has been a difference in opinion about the state of the system after a condensate is split in two by raising a potential barrier in the middle of a trap containing a condensate [11,12]. This exchange serves as the point of departure for the present paper. We address two specific questions. First, what would the two-mode approach say about the state of the split trap? Second, more generally, what is the relationship between the two-mode and the phase-atom-number pictures?

We present and solve, for the most part analytically, a two-mode description for the splitting of the trap. Unfortunately, this analysis proves quantitatively accurate only in the limit of a weakly interacting gas. On the other hand, it also turns out that in the limit of a weakly interacting gas, the phase-atom-number approach does not correctly describe the unsplit trap. The two methods agree in the tunneling limit when the barrier is high enough. However, we contend that a reliable quantitative treatment of splitting of a trap that contains a strongly interacting condensate is yet to be devised [12].

In Sec. II we review the quantum-optics-style two-mode approach. The ground state and the fluctuations in atom number between the sides of the double trap is the subject of Sec. III. We develop simple harmonic-oscillator and perturbation theory expansions that cover the ground-state properties of the two-mode model for all relevant problem parameters, and verify the results against numerical computations. In Sec. IV we analyze adiabaticity when the trap is split using the harmonic-oscillator approximation, and again validate the results with numerical computations. The limitations of the two-mode approach in the case of a strongly interacting gas are discussed in Sec. V. A detailed comparison between the prevalent phase-atom-number approach and the two-mode approximation is the subject of Sec. VI. Whereas the two-mode picture has problems in the limit of a strongly interacting gas, the phase-atom-number picture is questionable for a weakly interacting gas and for modest atom numbers. Remarks in Sec. VII conclude the paper.

II. TWO-MODE MODEL

We begin by reviewing the two-mode approximation. We are following a well-traveled path; in addition to numerous publications that deal directly with the double trap [3–7], there are numerous other BEC publications that resort to one form or another of the two-mode model [13–17].

In a symmetric double-well potential, the ground state of a single particle is represented by an even wave function ψ_g that belongs equally to both wells of the potential. Provided the barrier between the halves of the potential is tall enough so that the tunneling rate between the potential wells is small, nearby lies an excited odd state ψ_e that likewise belongs to both halves of the double well. The superpositions $\psi_{l,r}=(1/\sqrt{2})(\psi_g\pm\psi_e)$ represent states in which the particle

lies predominantly on either the ''left'' or ''right'' side of the barrier. These are not stationary states: a single particle prepared in the left-localized state ψ_l slowly oscillates between the halves of the potential, tunneling to the right-localized state ψ_r and back.

Let us next consider interacting bosons. In the mean-field approximation one writes down the Gross-Pitaevskii equation (GPE) [18–20]. The interpretation of the GPE is that its stationary solution gives a one-particle state such that putting all N bosons in this state gives a (variational) approximation to a stationary state of the interacting many-particle Hamiltonian. One may check the validity of this description by using Bogoliubov theory. If the noncondensate fraction proves sufficiently small [21], the GPE presumably is useful.

It is intuitively obvious, and we have also checked this numerically, that for a symmetric double-well potential with a high middle barrier, the GPE similarly has nearly degenerate even and odd solutions ψ_g and ψ_e. However, since the GPE is nonlinear, it does not readily tell us about the dynamics of a boson prepared in the left- or right-localized states $\psi_{l,r}=(1/\sqrt{2})(\psi_g\pm\psi_e)$. Our central questions are the following: how should one think about states in which the atoms live in the left and right halves of the double well in the presence of atom-atom interactions, and how do the atom-atom interactions modify the simple single-particle tunneling between the wells?

Our basic assumption is that we take only two one-particle states ψ_g and ψ_e to be available to the N bosons. We adopt the usual two-particle contact interaction $U(\mathbf{r}_1,\mathbf{r}_2)=(4\pi\hbar^2a/m)\,\delta(\mathbf{r}_1-\mathbf{r}_2)$, where a is the s-wave scattering length and m is the atomic mass. Given the restricted state space of precisely two one-particle states, the many-particle Hamiltonian is

$$\begin{aligned}H=&\tfrac{1}{2}(\epsilon_e+\epsilon_g)(a_e^\dagger a_e+a_g^\dagger a_g)+\tfrac{1}{2}(\epsilon_e-\epsilon_g)(a_e^\dagger a_e-a_g^\dagger a_g)\\&+\kappa_{ee}a_e^\dagger a_e^\dagger a_e a_e+\kappa_{gg}a_g^\dagger a_g^\dagger a_g a_g\\&+\kappa_{eg}(a_e^\dagger a_e^\dagger a_g a_g+a_g^\dagger a_g^\dagger a_e a_e+4a_e^\dagger a_g^\dagger a_e a_g).\end{aligned}\tag{1}$$

Here, and from here on, we set $\hbar\equiv1$, and correspondingly use the terms energy and (angular) frequency interchangeably. In Eq. (1) a_g and a_e are the boson operators for the ground and excited wave functions. The constants ϵ and κ are the one- and two-particle matrix elements

$$\begin{aligned}\epsilon_e&=\int d^3r\,\psi_e(\mathbf{r})\left[-\frac{1}{2m}\nabla^2+V(\mathbf{r})\right]\psi_e(\mathbf{r}),\\\kappa_{ee}&=\frac{2\pi a}{m}\int d^3r\,|\psi_e(\mathbf{r})|^2|\psi_e(\mathbf{r})|^2,\\\kappa_{eg}&=\frac{2\pi a}{m}\int d^3r\,|\psi_e(\mathbf{r})|^2|\psi_g(\mathbf{r})|^2,\ldots.\end{aligned}\tag{2}$$

$V(\mathbf{r})$ is the symmetric double-well binding potential. Without restricting the generality, we assume that the wave functions $\psi_{e,g}$ are real. By virtue of the inversion symmetry of the wave functions, there are no off-diagonal one-particle matrix elements in this basis. The same symmetry also removes a number of two-particle matrix elements.

Physically, there are two key parameters in this many-body problem. First, there is the energy of one-particle excitations in the absence of atom-atom interactions,

$$\delta=\epsilon_e-\epsilon_g.\tag{3}$$

It also characterizes the single-particle tunneling rate between the left and right wells. The second parameter is the many-body interaction energy per atom. The expectation value of the Hamiltonian when all N atoms are in the state g is given by $E(N)=\epsilon_gN+N(N-1)\kappa_{gg}$. In the limit $N\gg1$ the chemical potential is therefore

$$\frac{dE}{dN}=\epsilon_g+2N\kappa_{gg}\equiv\epsilon_g+\mu.\tag{4}$$

The second term, which is the excess over the chemical potential of the noninteracting system, determines the many-body interaction energy per atom. Since the zero-point energy ϵ_g is somewhat trivial here, in what follows we drop it and refer to $\mu=2N\kappa_{gg}$ as the chemical potential. It is intuitively clear, and is confirmed by the analysis below, that the departure of the true many-body dynamics from simple single-particle tunneling picture, valid in the noninteracting limit, is determined by the relative magnitudes of δ and μ.

To simplify the discussion a bit further, we note that when the trap is nearly split in two halves, the absolute squares of the even and odd wave functions,

$$|\psi_{g,e}|^2=\tfrac{1}{2}(|\psi_l|^2+|\psi_r|^2\pm2\psi_l\psi_r),\tag{5}$$

should be nearly equal since the overlap $\psi_l\psi_r$ is small. For the time being, we therefore set

$$\kappa_{eg}=\kappa_{ee}=\kappa_{gg}\equiv\kappa.\tag{6}$$

This approximation is lifted in Sec. V.

To discuss physics in terms of left- and right-localized states, we introduce the corresponding boson operators

$$a_l=\frac{1}{\sqrt{2}}(a_g+a_e),\quad a_r=\frac{1}{\sqrt{2}}(a_g-a_e),\tag{7}$$

and rewrite the Hamiltonian (1) in terms of $a_{l,r}$. Notice that we may freely add or drop powers of the conserved particle number $N=a_e^\dagger a_e+a_g^\dagger a_g$ in the Hamiltonian. For a fixed total atom number, this kind of a variation will never have any dynamical consequences, although the zero of the energy scale may vary in an N-dependent manner. The development we pursue thus runs as follows:

$$H \simeq \frac{\delta}{2}(a_e^\dagger a_e - a_g^\dagger a_g) + \kappa(a_e^\dagger a_e^\dagger a_e a_e + a_g^\dagger a_g^\dagger a_g a_g + a_e^\dagger a_e^\dagger a_g a_g + a_g^\dagger a_g^\dagger a_e a_e + 4 a_e^\dagger a_g^\dagger a_e a_g)$$

$$= \frac{\delta}{2}(a_e^\dagger a_e - a_g^\dagger a_g) + \kappa\{a_e^\dagger a_e^\dagger a_g a_g + a_g^\dagger a_g^\dagger a_e a_e - a_e^\dagger a_e^\dagger a_e a_e - a_g^\dagger a_g^\dagger a_g a_g + 2[(a_e^\dagger a_e + a_g^\dagger a_g)^2 - (a_e^\dagger a_e + a_g^\dagger a_g)]\}$$

$$\simeq \frac{\delta}{2}(a_e^\dagger a_e - a_g^\dagger a_g) + \kappa\{a_e^\dagger a_e^\dagger a_g a_g + a_g^\dagger a_g^\dagger a_e a_e - a_e^\dagger a_e^\dagger a_e a_e - a_g^\dagger a_g^\dagger a_g a_g\}. \quad (8)$$

Now, substituting the expressions for $a_{l,r}$, and again ignoring a function of the conserved particle number, we obtain

$$H = -\frac{\delta}{2}(a_l^\dagger a_r + a_r^\dagger a_l) - 4\kappa a_l^\dagger a_l a_r^\dagger a_r . \quad (9)$$

The Hamiltonian, whether in the form of Eq. (8) or (9), involves two modes, and in addition the particle number is conserved. This means that the state space for the system may be spanned with the $N+1$ vectors

$$|n\rangle \equiv |n\rangle_l |N-n\rangle_r , \qquad n = 0, \ldots, N , \quad (10)$$

where the subscripts denote the number states for the left and right boson operators. Writing the state vector as a linear combination of $|n\rangle$, the action of Hamiltonian (9) is

$$H\sum_n c_n |n\rangle = \sum_n \left[-\frac{\delta}{2}(\sqrt{n(N-n+1)}\, c_{n-1} + \sqrt{(n+1)(N-n)}\, c_{n+1}) - 4\kappa n(N-n)\, c_n \right] |n\rangle . \quad (11)$$

The meaning of the operators $a_{l,r}$ as left- and right-trap operators is unambiguous only in the limit of a completely split trap, but we nevertheless use them as our primary description of the double-trap states. Of course, the state space of the system is not affected by substitutions (7).

We next turn to the analysis of the Hamiltonian as in Eq. (11). The key aspect is that H is tridiagonal in a suitable basis. For notational simplicity, from now on we always assume that the atom number N is even. We also introduce k, the difference between the number of atoms in the wells, and the average number $N/2$: $n \equiv N/2 + k$.

III. GROUND STATE OF DOUBLE TRAP

Our first objective is to analyze the ground state and its number fluctuations for Hamiltonian (8) or (9); specifically, fluctuations of atom number between the left and right sides of the trap. Modification of the atom-number fluctuations with increasing atom-atom interaction will answer the key question of how does the atom-atom interaction affect tunneling between the wells.

Two limiting cases are handled easily. First, suppose that atom-atom interactions totally dominate, so that the Hamiltonian is

$$H = -4\kappa a_l^\dagger a_l a_r^\dagger a_r . \quad (12)$$

The states $|k\rangle \equiv |N/2+k\rangle_l |N/2-k\rangle_r$ from Eq. (10) are the eigenstates in this limit, and their corresponding eigenenergies are $\omega_k = \kappa(4k^2 - N^2)$. The ground state is $k=0$, with atoms split evenly between the wells. Obviously, there are no fluctuations in atom number between the sides of the trap for any of these states.

Second, suppose there are no atom-atom interactions at all:

$$H = \frac{\delta}{2}(a_e^\dagger a_e - a_g^\dagger a_g). \quad (13)$$

The ground state is the one with all N atoms in the state g. Raising another atom to the upper state always costs the energy δ.

As in the previous case, the ground state has an equal number of atoms in each well. The difference is in the coherence between the wells, which shows up in atom number fluctuations between the sides of the trap (absent in the first case $\delta = 0$). A simple calculation shows that, for the noninteracting case, the ground state in the $l-r$ basis is

$$\frac{1}{\sqrt{N!}}(a_g^\dagger)^N |\mathrm{vac}\rangle = \frac{1}{\sqrt{N!}}\left(\frac{a_l^\dagger + a_r^\dagger}{\sqrt{2}}\right)^N |\mathrm{vac}\rangle = \frac{1}{2^{N/2}} \sum_{n=0}^{N} \sqrt{\binom{N}{n}}\, |n\rangle . \quad (14)$$

Hence, in the limit $\kappa = 0$, the atom number statistics is binomial in the $l-r$ basis, and the difference between particle numbers in the left and right sides has the standard deviation $\sqrt{N}/2$.

To see how tunneling is changed by the atom-atom interaction, we develop a more refined picture, valid when both atom-atom interactions and tunneling are present simultaneously. To this end, we have to diagonalize the matrix in Eq. (11). We start with a simple approximate analytical procedure, and then check it numerically.

Let us assume that the expansion coefficients $c_n \equiv C(k)$ ($n \equiv N/2 + k$) change little from k to $k \pm 1$, and expand $c_{n\pm1} \equiv C(k \pm 1)$ in Eq. (11) as Taylor series [13]:

$$c_{n\pm1} \equiv C(k \pm 1) = C(k) \pm C'(k) + \tfrac{1}{2} C''(k) + \cdots . \quad (15)$$

We also assume the limit $N \gg 1$, and expand all the coefficients in Eq. (11) in powers of $1/N$. In the ensuing expression we pick and choose terms as follows. First, in the coefficient of C'', which is proportional to δ, we keep only the leading order in $1/N$, which is $\propto \delta N^1 k^0$. Second, the coefficient of C'

similarly is $\propto \delta k^1 N^{-1}$. Third, on the account that they simply make a trivial shift in energy, in the coefficient of C we ignore all contributions that are independent of k. Some of the remaining terms are proportional to δ, others to κ. We keep the leading order in $1/N$ for both these type of terms, $\propto \delta k^2 N^{-1}$ and $\propto \kappa k^2$. These choices lead to the time-independent Schrödinger equation

$$\left[\frac{-N\delta}{4}\frac{d^2}{dk^2}+\frac{\delta k}{N}\frac{d}{dk}+\left(\frac{\delta}{N}+4\kappa\right)k^2\right]C(k)=\epsilon\, C(k). \tag{16}$$

Suppose that the typical k scale for the solution is given by Δn. Then we estimate $k\sim\Delta n$, $d/dk\sim 1/\Delta n$. Hence the first-derivative term has an estimate $O(1/N)$, and is always much smaller than the other two terms in Eq. (16) (it transpires shortly that $\Delta n\lesssim\sqrt{N}$ is a reasonable estimate). We therefore ignore the first derivative altogether, and write our final result as

$$\left[\frac{-N\delta}{4}\frac{d^2}{dk^2}+\left(\frac{\delta}{N}+4\kappa\right)k^2\right]C(k)=\epsilon\, C(k). \tag{17}$$

Equation (17) is nothing but the Schrödinger equation for the simple harmonic oscillator. In the ground state the root-mean-square fluctuations of the variable k, and hence of the variable n, are simply

$$\Delta n=\sqrt{\frac{N}{2}}\left(\frac{\delta}{\delta+4N\kappa}\right)^{1/4}. \tag{18}$$

The frequency of the oscillator is

$$\omega=\sqrt{\delta(\delta+4N\kappa)}. \tag{19}$$

The state of a double condensate was studied in Ref. [17] using an angular-momentum representation along with the projection of the Bloch sphere into a plane. Equation (18) agrees with a result given in Ref. [17]. We believe that, even though the approaches seem quite different, the present method and the method of Ref. [17] in the end are functionally equivalent.

Naturally, Eq. (18) agrees with the known limiting cases both for $\kappa\to 0$ and $\delta\to 0$, although in the latter case partly for the wrong reasons; with $\delta\to 0$ we have $\Delta n\to 0$, and expansion (15) eventually fails. We will rectify this shortcoming momentarily. Meanwhile, we emphasize the main message of our results: In the limit of large N, the key comparison of the parameters is between δ and $N\kappa$, essentially the tunneling rate and chemical potential. As the chemical potential μ increases and exceeds the tunneling coupling between the wells, tunneling is suppressed, and the atom number fluctuations decrease.

Let us now return to the case with $\Delta n\lesssim 1$, whereupon expansion (15) becomes dubious. We study this case using standard time-independent perturbation theory. The zeroth-order states are the eigenstates of Eq. (12), and the rest of Eq. (9) acts as the perturbation. In this way we find, to the leading order in $1/N$, the fluctuations

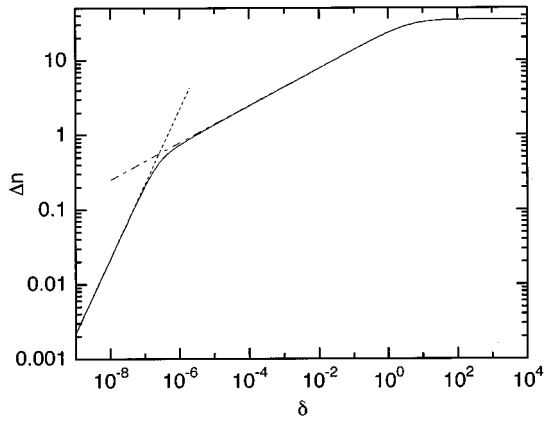

FIG. 1. Atom number fluctuations Δn between the left and right sides of a split trap as a function of the tunneling rate δ in the ground state of the double trap. The fixed parameters are particle number $N=5000$ and the parameter characterizing atom-atom interactions, $\kappa=0.0002$. Exact numerical results are plotted as a solid line. Also shown as dotted and dot-dashed lines are the small- and large-δ limits from the respective equations (20) and (18). Here, and elsewhere in this paper, the unit of frequency is arbitrary, though naturally the same for all frequencies.

$$\Delta n=\frac{1}{8\sqrt{2}}\frac{\delta N}{\kappa}. \tag{20}$$

The transition between the forms of fluctuations (18) and (20) occurs approximately where the same Δn is obtained from both expressions. In the limit of large N, this happens when

$$\delta=\frac{2^{8/3}\kappa}{N}. \tag{21}$$

In this case both Eqs. (18) and (20) give $\Delta n=0.56$, which is comfortably close to unity.

We have checked our arguments numerically. Standard algorithms from *Numerical Recipes* [22] were used to find the eigenvalues of the tridiagonal Hamiltonian. However, to compute particle number fluctuations, one also needs the lowest-energy eigenvector. With N approaching a couple of hundred, the attendant algorithms for finding eigenvectors start sputtering on roundoff error. We find the ground-state eigenvector by inverse iteration [22] instead.

The computed fluctuations Δn are shown in Fig. 1 as a function of the tunneling rate δ. In this figure the fixed parameters are $N=5000$ and $\kappa=0.0002$, so that $N\kappa=1$. There clearly are three different physical regimes in this graph. First, for the largest values of δ, we are in the regime with $\Delta n=\sqrt{N}/2$. When δ is decreased, at $\delta\simeq\kappa N\simeq\mu\simeq 1$, the dependence of fluctuations on atom-atom interactions kicks in as in Eq. (18). Finally, at about $\delta\simeq\kappa/N\simeq 10^{-7}$, expansion (15) and the harmonic-oscillator model fail, and the system enters the regime of Eq. (20). We also show the analytical results from Eqs. (18) and (20). They agree with the numerical data where they should.

Summarizing, within the two-state model, we have a complete analytical picture of atom number fluctuations in a

double-well system for the limit $N \gg 1$. The analytical arguments have been verified by comparisons with direct numerical computations. Large atom-atom interactions $\mu \simeq \kappa N > \delta$ suppress atom number fluctuations between the sides of the well, partially ''freezing'' the tunneling.

IV. ADIABATICITY IN SPLITTING OF TRAP

Suppose next that the double-well system starts out in its ground state, and subsequently the potential barrier in the middle is ramped up, decreasing the tunneling rate δ. The particle number fluctuations would also decrease [see Eq. (18)]. The question is, how close to zero can one take the fluctuations [11]?

Let us assume that there is a time scale τ to the decrease of δ, and that the harmonic-oscillator expansion (15) is valid. The system's ability to adjust its ground state, that is, the coefficients $C(k)$, to the changing potential is determined by the frequency ω [Eq. (19)]. As long as $\tau \gg 1/\omega$, the change of the potential is adiabatic, and the oscillator of Eq. (17) remains in its ground state. Adiabaticity breaks down when δ has decreased to the point where [11]

$$\omega = \sqrt{\delta(\delta + 4N\kappa)} = \frac{1}{\alpha\tau}. \tag{22}$$

Here α is a numerical parameter of the order of unity, which our crude argument can not determine. Below this point, the state can no longer follow the decreasing tunneling rate δ, and fluctuations that prevail at the time of the decoupling of the wells will be seen thenceforth.

We solve Eq. (22), and insert the result into Eq. (18). This gives the fluctuations once the wells are decoupled,

$$\Delta n_\infty = \sqrt{\frac{N}{2}} \left(\frac{\sqrt{1 + (2N\alpha\kappa\tau)^2} - 2N\alpha\kappa\tau}{\sqrt{1 + (2N\alpha\kappa\tau)^2} + 2N\alpha\kappa\tau} \right)^{1/4}. \tag{23}$$

Clearly, the time scale to which τ should be compared is $(2N\kappa)^{-1} = \mu^{-1}$. In the limit of slow ramp, $\tau \gg \mu^{-1}$, Eq. (23) becomes

$$\Delta n_\infty \simeq \frac{1}{4\sqrt{\alpha\kappa\tau}}. \tag{24}$$

In the opposite limit of fast ramp, $\tau \ll \mu^{-1}$, we obtain

$$\Delta n_\infty \simeq \sqrt{\frac{N}{2}}\ (1 - N\alpha\kappa\tau). \tag{25}$$

The analytical expressions (22)–(25) come with a substantial dose of heuristics. A comparison against numerical results is thus in order. We start by choosing δ_0 large enough to be firmly in the adiabatic limit, and find the stationary solution for this δ_0. Next we integrate the time-dependent Schrödinger equation starting from this initial ground state, letting δ decrease exponentially as $\delta(t) = \delta_0 e^{-t/\tau}$. As we go along, we compute the fluctuations Δn as a function of time.

As before, the Hamiltonian is tridiagonal in the basis $|n\rangle$, but now we are faced with a genuinely time-dependent integration. It turns out that standard general-purpose differential equations solvers quickly fail on roundoff error by the time a few hundred atoms are employed. Instead, we resort to an adaptation of the Crank-Nicholson method [22]. Basically, a time step from t to $t+h$ is carried out as follows:

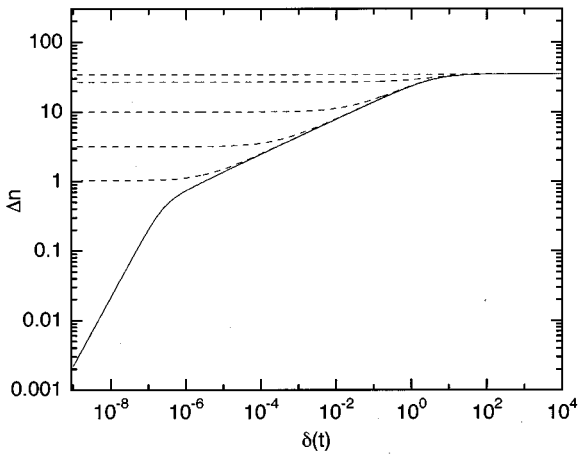

FIG. 2. Atom number fluctuations Δn as a function of time-dependent tunneling rate $\delta(t)$ when the tunneling rate is decreased exponentially as $\delta(t) \propto e^{-t/\tau}$. The fixed parameters are $N = 5000$ and $\kappa = 0.0002$. The solid line gives the steady state fluctuations corresponding to $\tau = \infty$, the dashed lines from top to bottom are for $\tau = 0.01$, 0.1, 1, 10, and 100.

$$|\psi(t+h)\rangle = \frac{1 - \frac{1}{2} ihH(t+h/2)}{1 + \frac{1}{2} ihH(t+h/2)} |\psi(t)\rangle. \tag{26}$$

The operator inversion entails solving a set of linear equations, but this set is tridiagonal. Algorithm (26) is unitary, i.e., it preserves the norm of the state vector, and therefore does not permit runaway roundoff errors. Moreover, we amend the algorithm by writing

$$|\psi(t+h)\rangle = \frac{1 - \frac{1}{2} ih[H(t+h/2) - \langle\psi(t)|H(t+h/2)|\psi(t)\rangle]}{1 + \frac{1}{2} ih[H(t+h/2) - \langle\psi(t)|H(t+h/2)|\psi(t)\rangle]} |\psi(t)\rangle. \tag{27}$$

Here we subtract from the Hamiltonian its expectation value, and thus arrest any rapid time evolution that would ensue from an inopportune choice of the zero of energy. Of course, mathematically, adding any (even a time-dependent) scalar to the Hamiltonian only amounts to modifying the overall phase of the wave function, and has no effect on the physics. To integrate the wave function over any fixed finite time interval, we simply keep on halving the step size h until convergence.

Results from our computations are shown in Fig. 2. Here we again choose $N = 5000$, $\kappa = 0.0002$, and thus $N\kappa = 1$. The figure shows the size of the fluctuations Δn as a function of the value of the parameter $\delta(t)$ reached while the time runs on. The solid line is the stationary value of Δn as in Fig. 1. Formally, it corresponds to the choice $\tau = \infty$. The various dashed lines depict $\Delta n(\delta)$ for the ramping time scales $\tau = 0.01$, 0.1, 1, 10, and 100. One clearly sees how the width first decreases adiabatically as δ is decreased, then decouples

and freezes to a constant value. The faster δ is decreased, the sooner nonadiabaticity sets in, i.e., the smaller the ramping time scale τ is.

We have compared the final widths with expression (23). It turns out that, after setting $\alpha=2\pi$, the analytical prediction works at the level of 1% for all of the data in Fig. 2. This agreement validates our analytical argument.

In summary, at least while the fluctuations satisfy $\Delta n \gtrsim 1$, and therefore the harmonic-oscillator expansion (15) remains useful, we have an accurate analytical description for the adiabaticity, or lack thereof, as a barrier is raised to split the double well in two. The basic conclusion is that, starting from the case $\delta \gg N\kappa$ and thus from fluctuations of the order $\sqrt{N}/2$, the key time scale is $\mu^{-1}=(2N\kappa)^{-1}$. If the time scale of adjusting the well τ is shorter than this, the fluctuations cannot be reduced substantially from their initial value $\sqrt{N}/2$. For slow variation of the tunneling rate δ, the fluctuations are brought down to a magnitude that scales as $\tau^{-1/2}$.

V. LIMITATIONS OF THE TWO-MODE MODEL

We have adopted two basic approximations in our reasoning; that only two one-particle states are relevant, and that the assumption about the matrix elements $\kappa_{ee}=\kappa_{gg}=\kappa_{eg}=\kappa$ [see Eq. (6)] holds. We shall discuss the validity of our model, paying attention to both of these assumptions.

In preparation, we note that there will be two major limiting cases, weakly interacting gas and strongly interacting gas. The watershed is the condition that $N\kappa_{gg}\sim\omega_0$, where ω_0 is the natural frequency of the unsplit trap. Let us correspondingly denote the length scale of the unsplit trap by l, whereupon the formulas for a harmonic oscillator give the estimate

$$\omega_0 \sim \frac{1}{ml^2}. \tag{28}$$

On dimensional grounds, one estimates that $\kappa_{gg}\sim a/ml^3$. Using estimate (28), the condition $N\kappa_{gg}\sim\omega_0$ then becomes $Na\sim l$. In most current BEC experiments, $Na\gg l$, which implies that the gas is strongly interacting.

Nonetheless, let us begin with the case of weakly interacting gas, $N\kappa_{gg}\ll\omega_0$. In this limit and for the unsplit trap, the very existence of the excited state is immaterial, and all atoms are in the single-particle state ψ_g. As we split the trap by increasing the barrier in the middle, the atom-atom interaction becomes essential. When $\delta\simeq N\kappa\simeq\mu$, the ground state is no longer obtained by simply depositing all atoms in the state ψ_g. For weak atom-atom interactions, this happens when $\delta\ll\omega_0$. Then the states ψ_g and ψ_e are close to one another in energy but well separated from the other states, and the two-mode approximation is justified. If our second approximation $\kappa_{ee}=\kappa_{gg}=\kappa_{eg}=\kappa$ is already valid at this point, all previous results are quantitatively correct.

If the matrix elements are not equal, a more refined treatment is required. In the Hamiltonian (1), we keep the various matrix elements κ with the notations

$$\kappa\equiv\kappa_{eg}, \quad K_g\equiv\kappa_{gg}-\kappa_{eg}, \quad K_e\equiv\kappa_{ee}-\kappa_{eg}. \tag{29}$$

While the left and right states $(\psi_g\pm\psi_e)/\sqrt{2}$ may not be sufficiently well localized in this case, there is nothing in the mathematics that would prevent us from introducing their annihilation operators exactly as in Eq. (7). We proceed to do so. Of course, since we still have only two one-particle states to deal with, the state space is once more spanned by the vectors (10). We may look for the ground state in terms of these basis states and the corresponding expansion coefficients c_n.

As before, in the limit of large N we expand the coefficients c_n as in Eq. (15). It turns out that, since $K_g\neq 0$, the Hamiltonian is no longer tridiagonal, and c_n are also coupled to $c_{n\pm 2}$. Therefore, we also use the expansion

$$c_{n\pm 2}\equiv c(n\pm 2)=c(n)\pm 2c'(n)+2c''(n)+\cdots. \tag{30}$$

Proceeding exactly as we did on going from Eq. (15) to Eq. (17), we obtain the effective Schrödinger equation for $C(k)\equiv c_{N/2+k}$:

$$\left\{-\frac{1}{4}N(\delta-2NK_g)\frac{d^2}{dk^2}+\left[\frac{1}{N}(\delta-2NK_g)+4\kappa\right]k^2\right\}C(k) = \epsilon\, C(k). \tag{31}$$

This result is equivalent to the previous result [Eq. (17)] with the simple replacement $\delta\to\delta-2NK_g$. Hence the root-mean-square fluctuations of particle number and the characteristic excitation frequency are simply

$$\Delta n=\sqrt{\frac{N}{2}}\left(\frac{\delta-2NK_g}{\delta-2NK_g+4N\kappa}\right)^{1/4}, \tag{32}$$

$$\omega=\sqrt{(\delta-2NK_g)(\delta-2NK_g+4N\kappa)}. \tag{33}$$

One might wonder why the coefficient characterizing the ground-state atom-atom interactions K_g appears in these expressions, yet not the corresponding excited-state coefficient K_e. After all, Hamiltonian (1) treats the ground and excited states exactly equally. The explanation is that the state vectors with slowly varying coefficient c_n have a preference for the ground state already built in. If nearly all atoms were in the excited state, the proper slowly varying expansion coefficients should be defined as $\overline{c_n}=(-1)^n c_n$. All of this follows from the choice of where to put the $+$ and $-$ signs in Eqs. (7).

Consider now the limit of strong atom-atom interactions, $N\kappa\gtrsim\omega_0$. The major weakness of our previous arguments in this case is not the validity or lack thereof of the equality (6), but instead the jitters of the two-mode assumption. Atom-atom interactions are a major part of the entire structure of the excitations, and of the stationary states lying far from the ground state that involve a large fraction of the atoms, such as vortices. As anyone who has attempted to solve the Bogoliubov theory numerically knows, one has to include possibly a large a number of wave functions to arrive at a reasonably accurate description of the elementary excitations. Alternatively, one has a multitude of excited solutions to the GPE available. As long as the system is not in a regime in which the GPE has two nearly degenerate solutions, there simply is no outstanding single candidate for use as the excited-state wave function ψ_e.

We thus propose a heuristic model that hides as much of our ignorance about the excited state as possible. First, we take the frequency (33) to represent the actual, observed, frequency of the lowest elementary excitation in the system. Second, we rewrite the particle number fluctuations (32) in terms of this frequency and the chemical potential $\mu = 2N\kappa_{gg}$, using the substitution $2N\kappa = (\kappa/\kappa_{gg})2N\kappa_{gg} \rightarrow \beta\mu$:

$$\Delta n = \sqrt{\frac{N}{2}}\left(\frac{\omega}{\beta\mu + \sqrt{(\beta\mu)^2+\omega^2}}\right)^{1/2}. \tag{34}$$

Here β is a semiempirical parameter. In the limit of the split trap, where there is a dominant excited-state wave function satisfying $|\psi_e|^2 \simeq |\psi_g|^2$, $\beta \simeq 1$. In the unsplit trap, $|\psi_e|^2$ should be something akin to particle density in the excited states of the GPE, or the (zero-temperature) density profile of noncondensate atoms. Either way, $|\psi_e|^2$ would be more spread out than the ground state, reducing the overlap between $|\psi_g|^2$ and $|\psi_e|^2$. Our best guess is that $\beta < 1$, maybe even $\beta \ll 1$.

Since we are back to the harmonic-oscillator model, our previous considerations about adiabatic ramping of the potential barrier remain valid with minor modifications. When the barrier is ramped up and the excitation frequency decreases on a time scale τ, adiabatic following ceases by the time $\omega(t) \simeq 1/(2\pi\tau)$, giving the final particle number fluctuations

$$\Delta n = \sqrt{\frac{N}{2}}\left(\frac{1}{2\pi\beta\mu\tau + \sqrt{1+(2\pi\beta\mu\tau)^2}}\right)^{1/2}. \tag{35}$$

If the system has landed deep in the tunneling regime to make $\beta = 1$, it may be verified easily that Eqs. (35) and (23) agree. Unfortunately, we have no general prediction for the parameter β other than $\beta \lesssim 1$.

VI. COMPARISONS WITH MODELING OF LEGGETT AND SOLS

A. General features

There is a long-standing tradition to describe a Josephson junction in terms of the particle number difference between the sides and the phase difference across the junction. A particularly well-known line of thought of this type has been put forward by Leggett, Sols, and their co-workers [8–10]. We refer to this as the Leggett-Sols approach (LSA). We now examine the similarities and differences between the LSA and our modeling in detail.

In order to avoid various clashes in notation, we write the basic Hamiltonian of the LSA as

$$H_{\rm LS} = -E_J \cos\phi + E_C(\Delta N)^2/2. \tag{36}$$

Here E_J is called the Josephson coupling energy, and E_C the capacitive energy. ΔN is the difference in particle number between the sides of the junction, and ϕ is the phase canonically conjugate to ΔN.

In order to compare with our approach, we first note that eigenstates of the relative phase between the sides of the trap may be chosen, in the notation of the present paper, as [23,5]

$$|\phi_p\rangle = \frac{1}{\sqrt{N+1}} \sum_{n=0}^{N} e^{in\phi_p}|n\rangle. \tag{37}$$

As there is only a finite number of relative-number states $|n\rangle$, there is only a finite number of phase eigenstates as well. Here we choose them as $\phi_p = 2\pi p/(N+1)$, with $p = -N/2, -N/2+1, \ldots, N/2$. The vectors $|\phi_p\rangle$ make an orthonormal basis in the same Hilbert space as the vectors $|n\rangle$. The phase operator is then written

$$\phi = \sum_p |\phi_p\rangle \phi_p \langle\phi_p|. \tag{38}$$

In the basis $|n\rangle$, the difference-in-particle-number operator is evidently

$$\Delta N = \sum_n (2n-N)|n\rangle\langle n|. \tag{39}$$

Equations (38) and (39) do not define canonical conjugate operators. As a matter of fact, it may be shown that, within the two-mode picture and for any finite number of particles N, there cannot exist an operator conjugate to ΔN. If such a ϕ existed, we would have the nonsensical chain of reasoning

$$\begin{aligned} -i &= \langle N/2|[\Delta N, \phi]|N/2\rangle \\ &= (\langle N/2|\Delta N)\,\phi|N/2\rangle - \langle N/2|\phi\,(\Delta N|N/2\rangle) \\ &= 0. \end{aligned} \tag{40}$$

The familiar position and momentum operators x and p_x get past an analogous objection because the variable x is continuous, an escape that is not available in the present case.

Since there are, strictly speaking, no canonical number difference and phase operators within the two-mode model, a comparison with the LSA is by necessity somewhat ambiguous. In the absence of any better alternatives we plug in the operators (39) and (38) to Eq. (36). The spectral representation of the two-mode version of the LSA Hamiltonian (36) is then

$$\begin{aligned} H_{\rm LS} = &-\tfrac{1}{2}E_J \sum_k (|N/2+k+1\rangle\langle N/2+k| + \text{H.c.}) \\ &+ 2E_C \sum_k k^2 |N/2+k\rangle\langle N/2+k|. \end{aligned} \tag{41}$$

We once more use a summation index k such that $n = N/2 + k$. The motivation is to facilitate comparison with our form of the Hamiltonian from Eq. (9),

$$\begin{aligned} H = -\frac{\delta}{2}\sum_k \Bigg(&\sqrt{\left(\frac{N}{2}+k+1\right)\left(\frac{N}{2}-k\right)}|N/2+k+1\rangle \\ &\times\langle N/2+k| + \text{H.c.}\Bigg) + 4\kappa\sum_k k^2 |N/2+k\rangle\langle N/2+k|. \end{aligned} \tag{42}$$

The difference is small. When acting on a state vector $\Sigma_n c_n|n\rangle$ such that only expansion coefficients $c_{N/2+k}$ with

$|k| \ll N$ are materially nonzero, Hamiltonians (41) and (42) produce approximately the same results, provided we make the identifications

$$E_J \leftrightarrow \frac{N\delta}{2}, \quad E_C \leftrightarrow 2\kappa. \tag{43}$$

To make the assertion $|k| \ll N$ somewhat more quantitative, we derive the time-independent Schrödinger equation from Hamiltonian (41) following exactly the same steps that we took going from Eq. (15) to Eq. (17). Using identifications (43), instead of Eq. (17) we have

$$\left(\frac{-N\delta}{4} \frac{d^2}{dk^2} + 4\kappa k^2 \right) C(k) = \epsilon\, C(k). \tag{44}$$

A stiffness term $\propto (\delta/N)k^2$ is missing here, the term that would limit particle number fluctuations to be at most of the order $\sqrt{N}$ when $\delta \gg N\kappa$.

We have carried out a detailed comparison by restricting the LSA to two boson modes. However, the basic features of the comparison are generic, and apply no matter what the microscopic meanings of the operators ϕ and ΔN are in Eq. (36). In our approach there are three independent parameters, N, κ, and δ, while in the LSA there are only two, basically $N\delta$ and κ. The difference shows in the limit of a weakly interacting gas. As a matter of fact, in the LSA particle number fluctuations then diverge. The LSA does not have a counterpart of the ground state g built in.

B. Fluctuations in a split trap

There has recently been some discussion about fluctuations of the particle number after a trap has been split. With the remark that ''at the moment we have no proof to this effect, but at least in the limit of weak interactions the assumption is clearly valid,'' we have assumed [5] that the fluctuations are of the order $\sqrt{N}$. Leggett and Sols criticized this assumption [11]. They applied basically the same adiabaticity argument to their Hamiltonian that we have adopted here for our model. Our response was [12] that the question cannot be regarded as closed, because the model of Leggett and Sols does not seem to apply to the unsplit trap.

In the present paper we have given a description of the events that take place when the trap is split. Unfortunately, our model describes the splitting of the trap from the beginning to the end in a quantitatively reliable manner only for a weakly interacting gas. In this case we see from Eq. (24) that, inasmuch as the barrier is raised on a time scale no longer than $\tau \sim \mu^{-1} \gtrsim \omega_0^{-1}$, where μ is the change in the chemical potential due to atom-atom interactions, $\sqrt{N}$ fluctuations apply at the end of the splitting.

As we have already noted, the descriptions of the splitting of the trap as in Eqs. (23) and (35) both apply and agree (even if the atom-atom interactions are strong) if the trap manages to make it far enough into the tunneling regime with the atoms in the (many-body) ground state. This happens if the trap is split slowly enough. We write the splitting time scale as $\tau = 1/(\lambda\omega_0)$, where ω_0 is the trap frequency and at the same time the frequency scale for the elementary excitations of the (unsplit) condensate, and the numerical parameter λ is as small as it takes to make it deep into the tunneling regime. For strong atom-atom interactions we invariably have $N\kappa \gg \delta$, and so, from Eq. (24) we have the result

$$\Delta n_\infty = \sqrt{\frac{N}{2}} \frac{1}{2} \sqrt{\frac{\lambda\omega_0}{\pi\mu}}. \tag{45}$$

In the Thomas-Fermi limit [19,20] the chemical potential of $N/2$ atoms in a spherically symmetric potential well is

$$\mu = \xi^{2/5}\omega_0, \quad \xi = \frac{15Na}{2^{7/2}l}, \tag{46}$$

where a is the scattering length and $l = \sqrt{1/m\omega_0}$ is the characteristic length scale of the trap. Inserting this into Eq. (45), we have

$$\Delta n_\infty = \sqrt{\frac{N}{2}} \frac{1}{2\sqrt{\pi}} \frac{\sqrt{\lambda}}{\xi^{1/5}}. \tag{47}$$

Equation (47) displays exactly the same parameter dependences as the result of Leggett and Sols in Ref. [11]. The difference from $\sqrt{N}$ is important as a matter of principles. However, according to Leggett and Sols, ''the fluctuations are ... by no means of the order of $\sqrt{N}$, but much smaller'' [11]. Given that we do not know how large the parameter λ could be, and that the parameter ξ even in the most extreme of the present alkali experiments only reaches up to about $\xi \simeq 10^5$, such a statement may be overly categorical.

For a strongly interacting gas, we have not been able to come up with a quantitatively reliable description of splitting of the trap, or even of the left-right fluctuations in the ground state of the unsplit trap. Leggett and Sols went even further, in that they denied us the unsplit ground state altogether; their ''argument ... does not depend on the (incorrect) assumption that [the many-particle state with all atoms in the ground state of the GPE] describes the unsplit well'' [11]. However, as they do not elaborate, we do not know what this statement is intended to mean or imply. We have to regard the question of splitting a strongly interacting gas as unsolved, just as it was when we began the present work.

VII. CONCLUDING REMARKS

It is relatively easy to discuss both atom number fluctuations and adiabaticity of the splitting of the trap in a two-mode description, as we have done in this paper. The problem is that the two-mode description is, generally speaking, valid only for either a weakly interacting gas, or when the condensate has already been split in two. As most of the current BEC experiments operate in the limit of strong interactions, a major gap remains in the understanding of the condensate.

Besides questions about the process of splitting, the limit of an unsplit trap containing a strongly interacting condensate leads to another even more basic question. The operational meaning of the left and right annihilation operators may be vague, but what the left and right sides of the trap are is not; more generally, one might inquire about particle number fluctuations in any part of the condensate [6]. If Eq. (34)

could be relied on, one would expect sub-Poissonian local fluctuations. Given that the coherence properties of a condensate analogous to the coherence properties of light are likely to be a major focus in the discussion of condensates and atom lasers, the case of a strongly interacting gas will presumably have to be solved in the end. As another future development, we anticipate that the loss of phase coherence in multiple traps, i.e., atomic tunnel arrays [24], will furnish an interesting topic of study already in the experimental case [24] of a weakly interacting gas.

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