Role of Excited States in the Splitting of a Trapped Interacting Bose-Einstein Condensate by a Time-Dependent Barrier

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An essentially exact approach to compute the wave function in the time-dependent many-boson Schrödinger equation is derived and employed to study accurately the process of splitting a trapped condensate. As the trap transforms from a single to double well the ground state changes from a coherent to a fragmented state. We follow the role played by many-body excited states during the splitting process. Among others, a ''counterintuitive'' regime is found in which the evolution of the condensate when the splitting is sufficiently slow *is not* to the fragmented ground state, but to a low-lying excited state which is a coherent state. Experimental implications are discussed.

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The first realizations of Bose-Einstein condensates (BECs) in ultracold dilute gases have boosted the community to explore matter-wave phenomena and how to manipulate and utilize them. One of the most popular ''screenplays'' studied is splitting of BECs by deforming a single well to a double well; see [1–5] for experimental and [6–11] for theoretical works. In such scenarios, the system is often prepared in the ground state of a harmonic trap and a central barrier is ramped-up to a certain fixed height. As the trap transforms from harmonic to double-well geometry the system continuously changes its localization from the center of the initial trap to two separated parts localized around the minima of the double well. Side by side, it can also change its character—from condensed to a twofold fragmented state [8]. Attacking the splitting process, much attention has been paid to understanding when it is adiabatic [6–8], demonstrating that the slower the barrier is ramped-up (to a certain fixed height), the closer the BEC is to the ground state of the bosons in the double well.

Here we study the many-body dynamics of splitting a BEC beyond the presently available theoretical and computational approaches. We develop and report on an essentially exact and numerically efficient approach for the solution of the time-dependent many-boson Schrödinger equation, which we term multiconfigurational time-dependent Hartree method for bosons (MCTDHB). Applying the MCTDHB method to the problem of splitting a BEC, we follow the many-boson wave function throughout the splitting process and identify the role and impact of many-body *excited states*. Among others, we identify a new ''counterintuitive'' regime where the evolution of the condensate when the barrier is ramped-up sufficiently slow *is not* to the ground state of the double well which is a fragmented BEC, but to a low-lying excited state which is a coherent BEC.

Our starting point is the many-body Hamiltonian describing N interacting bosons in a trap, $\hat{H} = \sum_{k=1}^{N}[\hat{T}(\mathbf{r}_k) + V(\mathbf{r}_k, t)] + \sum_{k>l=1}^{N} U(\mathbf{r}_k - \mathbf{r}_l)$. Here, $\mathbf{r}_k$ is the coordinate of the kth particle, $\hat{T}(\mathbf{r})$ and $V(\mathbf{r}, t)$ stand for the kinetic energy and trap potential, respectively, and $U(\mathbf{r}_k - \mathbf{r}_l)$ describes the pairwise interaction between the kth and lth atoms. To solve the time-dependent Schrödinger equation $\hat{H}\Psi = i\frac{\partial\Psi}{\partial t}$ we write the many-body wave function Ψ as a linear combination of *time-dependent* permanents

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) = \sum_{\vec{n}} C_{\vec{n}}(t)\Phi_{\vec{n}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t). \quad (1)$$

In the representation (1), the time-dependent permanents $\Phi_{\vec{n}}$ are constructed by distributing the N bosons over $j = 1, \ldots, M$ *time-dependent* orbitals $\{\phi_j(\mathbf{r}, t)\}$, and the summation runs over all possible occupations $\vec{n}$ preserving the total number of bosons N.

To proceed, we utilize the Dirac-Frenkel variational principle [12] and after some lengthy but straightforward algebra obtain a set of coupled nonlinear, generally integro-differential equations for the coefficients $C_{\vec{n}}(t)$ and orbitals $\{\phi_j(\mathbf{r}, t)\}$, for all $\vec{n}$ and $j = 1, \ldots, M$,

$$\hat{\mathbf{P}}\left[\{\hat{T}(\mathbf{r}) + V(\mathbf{r}, t)\}\phi_j(\mathbf{r}, t) + \sum_{qksl}\{\boldsymbol{\rho}(t)\}^{-1}_{jq}\rho_{qksl}(t)U_{kl}(\mathbf{r}, t)\phi_s(\mathbf{r}, t)\right] = i\frac{\partial\phi_j(\mathbf{r}, t)}{\partial t}, \qquad \sum_{\vec{n}'}\langle\Phi_{\vec{n}}|\hat{H}|\Phi_{\vec{n}'}\rangle C_{\vec{n}'}(t) = i\frac{dC_{\vec{n}}(t)}{dt}. \quad (2)$$

The quantities $\boldsymbol{\rho}(t) = \{\rho_{qs}(t)\}$ and $\rho_{qksl}(t)$ appearing in (2) are the matrix elements of the reduced one- and two-body densities of Ψ, $\rho(\mathbf{r}_1|\mathbf{r}_1'; t) = \sum_{qs}^{M}\rho_{qs}(t)\phi_q^*(\mathbf{r}_1', t)\phi_s(\mathbf{r}_1, t)$ and $\rho(\mathbf{r}_1\mathbf{r}_2|\mathbf{r}_1', \mathbf{r}_2'; t) = \sum_{qksl}^{M}\rho_{qksl}(t)\phi_q^*(\mathbf{r}_1', t)\phi_k^*(\mathbf{r}_2', t)\times\phi_s(\mathbf{r}_1, t)\phi_l(\mathbf{r}_2, t)$, respectively. The local time-dependent potentials $U_{kl}(\mathbf{r}, t) = \int\phi_k^*(\mathbf{r}', t)\hat{U}(\mathbf{r} - \mathbf{r}')\phi_l(\mathbf{r}', t)d\mathbf{r}'$ originate from the two-body interaction. Finally, the operator $\hat{\mathbf{P}} = 1 - \sum_{k=1}^{M}|\phi_k(\mathbf{r}, t)\rangle\langle\phi_k(\mathbf{r}, t)|$ appearing on the left-hand-side of

Eq. (2) is a projection operator which ensures that the orbitals remain orthogonal to one another throughout the propagation in time. Full details of the derivation and numerical implementation of equations of motion (2) and their uniqueness are given in [13]. It is gratifying to mention that the present many-body propagation theory adapts to identical bosons the multiconfigurational time-dependent Hartree approach routinely used for multidimensional dynamical systems consisting of distinguishable particles [14].

To study the dynamics of splitting a repulsive BEC we consider $N = 200$ ^{87}Rb atoms initially prepared in an elongated, quasi-one-dimensional harmonic trap of longitudinal $\omega_{\parallel} = 2\pi \times 44.7\,\mathrm{Hz}$ and transverse $\omega_{\perp} = 2\pi \times 1.1\,\mathrm{kHz}$ frequencies. At time $t = 0$ a barrier of Gaussian shape is ramped-up linearly in time to a height of $V_{\max}$ and with ramp-up time of T_{ramp}. Introducing a convenient length scale of $L = 1\ \mu$m, we translate to dimensionless units in which the kinetic energy reads $\hat{T}(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}$, the time-dependent trap potential is $V(x,t) = \frac{x^2}{2\sigma^2} + V_{\max}\exp(-\frac{x^2}{2\sigma^2}) \times \{t/T_{\mathrm{ramp}}, t \le T_{\mathrm{ramp}}; \text{or } 1, t > T_{\mathrm{ramp}}\}$, and the effective atom-atom interaction is $U(x - x') = \lambda_0 \delta(x - x')$, where the transverse confinement is properly accounted for [15]. The values of the parameters are $\sigma = 2.6$ and $V_{\max} = 30$, corresponding to an interwell separation of 13.6 μm at the end of the ramping-up process, and $\lambda_0 = 0.1$. For this final double-well potential the ground state is (totally) twofold fragmented. Finally, time is expressed in units of $\frac{mL^2}{\hbar} = 1.37$ msec, where m is the mass of ^{87}Rb atom, and energy in units of $\frac{\hbar^2}{mL^2} = 116$ Hz.

We begin our investigations by ramping-up the barrier during a time of $T_{\mathrm{ramp}} = 1000$ until the final double well is achieved. Since visualization of the time-dependent many-body wave function is quite cumbersome, we prescribe its natural occupation numbers, i.e., eigenvalues of the corresponding reduced one-particle density $\rho(x|x';t) = \sum_j^M \rho_j(t)\phi_j^{*\mathrm{NO}}(x',t)\phi_j^{\mathrm{NO}}(x,t)$, at each point in time [8,16]. We have found that for the range of parameters considered here, MCTDHB with two orbitals accurately describes the many-body dynamics. The corresponding $\rho_j(t)$ are plotted in Fig. 1(a) as a function of time. The initial state is a slightly depleted BEC, $\rho_1(0) = 99.62\%$ and $\rho_2(0) = 0.38\%$, as at $t = 0$ only one natural orbital is macroscopically occupied. As the barrier is ramped-up, $\rho_2(t)$ increases with time, i.e., the many-body wave function becomes more and more depleted. At approximately one third of the ramping-up time $\rho_1(t) = \rho_2(t)$, indicating that the system is momentarily twofold fragmented. From now on and although the barrier is ramped-up further, $\rho_1(t)$ and $\rho_2(t)$ oscillate around this totally fragmented configuration, as has been obtained in [8]. It is worth noticing, however, that an oscillatory behavior of the occupation numbers exists during all the splitting process with different amplitudes and frequencies, see Fig. 1(a).

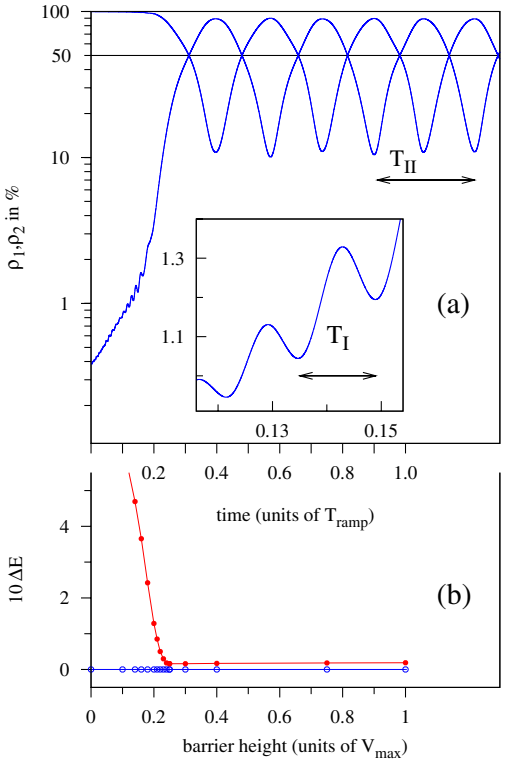

FIG. 1 (color online). Splitting a trapped condensate of $N = 200$ bosons (^{87}Rb atoms) with interaction strength $\lambda_0 = 0.1$ during a ramp-up time of $T_{\mathrm{ramp}} = 1000$. (a) Natural occupation numbers $\rho_1(t)$ and $\rho_2(t)$ as a function of time on a logarithmic scale [initial conditions: $\rho_1(0) = 99.62\%$, $\rho_2(0) = 0.38\%$]. During the splitting process the many-body wave function evolves from a condensed towards a twofold fragmented state. Inset shows oscillatory behavior of $\rho_2(t)$ around $0.14T_{\mathrm{ramp}}$. (b) Energy difference ΔE between the many-body ground state (○; taken as reference energy) and first excited state (●) as a function of barrier height of the time-dependent trap potential $V(x,t)$; see text for more details. Time is expressed in units of $\frac{mL^2}{\hbar} = 1.37$ msec and energy in units of $\frac{\hbar^2}{mL^2} = 116$ Hz.

The oscillations of $\rho_j(t)$ in time signify that the system *is not* in the ground state of the time-dependent trap [for this state ρ_1 (ρ_2) decreases (increases) monotonically with barrier height, see, e.g., [16]]. To investigate which many-body excited states contribute to these oscillations, we compute via imaginary time propagation of MCTDHB several low-lying many-body eigenstates of the static system at different barrier heights along the ramping-up path. The energy difference ΔE between the ground and first excited state is plotted in Fig. 1(b) as a function of barrier height. Since the barrier height increases linearly with time we can measure the evolution in the units of either ramping-up times or barrier heights. Next, we compute the inverse frequencies $T = \frac{2\pi}{\Delta E}$ and compare them with the corresponding oscillation periods of $\rho_j(t)$ at different barrier heights.

Here we present a comparison at two different times: at $t_{\mathrm{I}} = 0.14T_{\mathrm{ramp}}$ and $t_{\mathrm{II}} = T_{\mathrm{ramp}}$. In the inset of Fig. 1(a) we

plot on an enlarged scale the oscillations of $\rho_2(t)$ around t_{I}. The period of oscillations deduced from this inset is $T_{\mathrm{I}} = 13.7$. Since the ramping-up process is linear, t_{I} corresponds to the barrier height of $V_{\mathrm{I}} = 0.14V_{\max}$. The corresponding energy difference $\Delta E_{\mathrm{I}} = 0.47$ gives the value of $T = \frac{2\pi}{\Delta E_{\mathrm{I}}} = 13.4$, which is close to the observed oscillation period of $\rho_2(t)$ for this time point. Analogously, at t_{II} the observed oscillation period of $T_{\mathrm{II}} = 317.9$ agrees with the respective value of $T = 333.5$ obtained from $\Delta E_{\mathrm{II}} = 0.0188$. We obtain reasonable agreement between corresponding inverse frequencies and oscillation periods for other times as well. This analysis indicates an adiabatic character of the studied ramping-up process, and that only one many-body excited state is primarily involved in the many-body dynamics.

Let us now analyze the amplitudes of the oscillations of the natural orbitals. From Fig. 1(a) we see that oscillations are very modest at the beginning of the ramping-up process and substantial at the end of the process (notice the logarithmic scale). This is in accord with the decreasing many-body energy difference ΔE depicted in Fig. 1(b). As expected, an ideal adiabatic ramping-up along the ground-state trajectory is favored by a large ΔE. It is achieved for ramping-up times T_{ramp} large compared to the inverse frequency $T = \frac{2\pi}{\Delta E}$.

To study quantitatively the adiabatic character of the ramping-up process, we repeat the computation for several T_{ramp}. The results for $T_{\mathrm{ramp}} = 25$, 3000, 10 000 are presented in Fig. 2. From this figure a significant suppression of the amplitudes of the oscillations with growing ramping-up times is clearly seen. For the studied system of $N = 200$ bosons, a ramping-up procedure as long as of $T_{\mathrm{ramp}} = 10\,000 = 13.7$ sec still leads to 10.7% fluctuations of the final state. We see that even for such a long ramping-up time, which is of the order of the lifetime of a BEC [5], the final state deviates noticeably from the respective eigenstate and the ramping-up process is still away from being "ideal adiabatic."

In the above example the properties of the ground state and lowest-excited state change smoothly with barrier height. For small barrier heights these states are condensed, the excited state being more depleted than the ground state. As the barrier grows, these states become twofold fragmented and the first excited state results from the ground state by a transfer of a boson from one fragment to another. However, this simple scenario can vary strongly with the number of particles and with their interaction strength [16,17].

To proceed, we consider the same experiment as before, but with a three-times stronger interaction strength $\lambda_0 = 0.3$. This is achieved by a tighter confinement of $\omega_\perp = 2\pi \times 3.3$ kHz. Again, the ground state of the final double well for this system is fully twofold fragmented. In Fig. 3(a) we plot $\rho_j(t)$ for the durations $T_{\mathrm{ramp}} = 75$ and $T_{\mathrm{ramp}} = 500$ of the ramping-up process. In both cases, the initial wave function is the ground eigenstate in the harmonic trap which is a slightly depleted BEC, $\rho_1(0) = 99.32\%$ and $\rho_2(0) = 0.68\%$, see Fig. 3 at $t = 0$. The evolution of $\rho_j(t)$ for the faster ramping-up process of $T_{\mathrm{ramp}} = 75$ looks like the "adiabatic" dynamics studied in the previous example but it is not such a dynamics. Indeed, prolonging the ramping-up time, e.g., to $T_{\mathrm{ramp}} = 500$, the time-dependent solution does not at all evolve towards the fragmented ground state, but rather to an intermediate state which, according to the occupation number analysis, remains condensed all the time. We have found such a behavior in many other numerical examples.

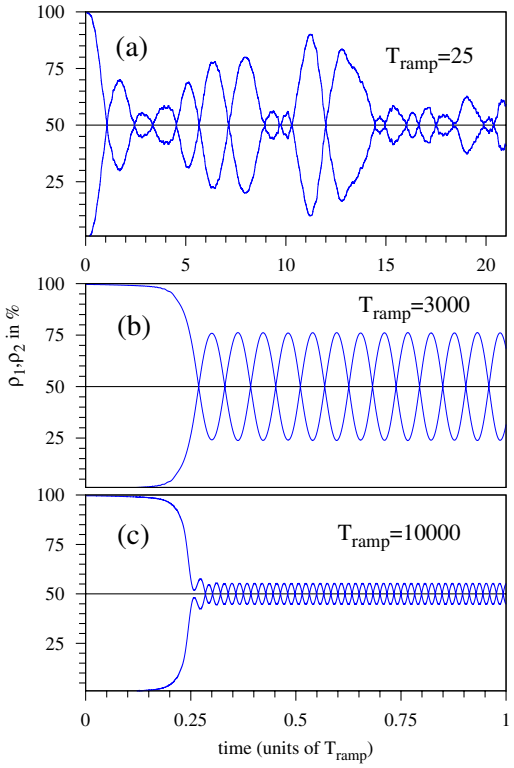

FIG. 2 (color online). Quantifying how difficult it is to (fully) fragment a condensate. Plotted are the natural occupation numbers $\rho_1(t)$ and $\rho_2(t)$ as a function of time for three ramping-up times T_{ramp}. The parameters used are the same as in Fig. 1. Increasing T_{ramp} the time-dependent many-body state approaches the ground state of the double-well potential which is a (fully) fragmented condensate. For $T_{\mathrm{ramp}} = 10\,000 = 13.7$ sec which is of the order of a condensate lifetime the amplitude of oscillations is still about 10%.

To investigate this "counterintuitive" regime, which we call *inverse* regime, we again compute the lowest eigenstates of the static double wells at different barrier heights. The relevant map of energy differences ΔE is plotted in Fig. 3(b) as a function of barrier height. This map has very interesting features—around some critical barrier height $V_{\mathrm{cr}} \approx 0.41V_{\max}$ the ground and lowest-excited states come very close to each other and interchange their order. Such a behavior signifying a very narrow avoided crossing (the width of which we cannot detect here) can appear only between states of very different physical origin. Indeed, at

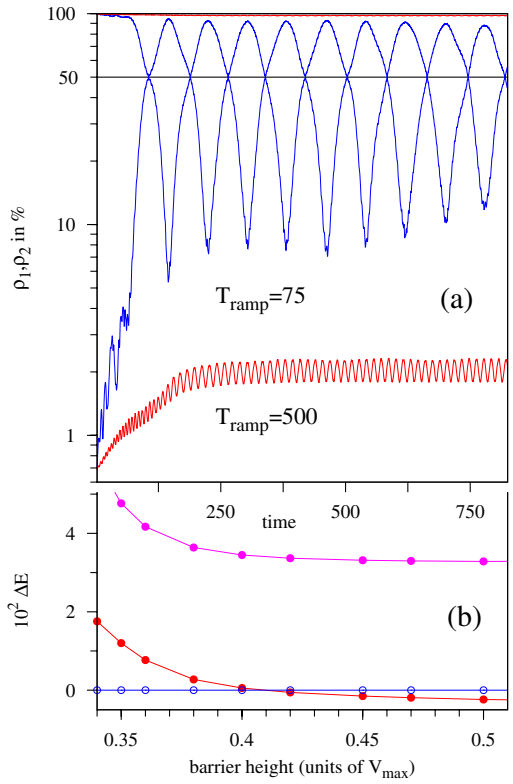

FIG. 3 (color online). Same as in Fig. 1 except for the stronger interaction strength $\lambda_0 = 0.3$. (a) Natural occupation numbers $\rho_1(t)$ and $\rho_2(t)$ as a function of time [initial conditions: $\rho_1(0) = 99.32\%$, $\rho_2(0) = 0.68\%$]. For $T_{\mathrm{ramp}} = 75$ the many-body wave function evolves from a condensed towards the twofold fragmented ground state. The "counterintuitive" regime is uncovered by employing a *longer* ramp-up time, e.g., $T_{\mathrm{ramp}} = 500$, in which the evolution of the condensate *is not* to the fragmented ground state, but to a low-lying coherent excited state. (b) Energy differences ΔE between the lowest-in-energy coherent state (○; taken as reference energy) and fragmented states (● curves) as a function of barrier height. Around $V_{\mathrm{cr}} \approx 0.41 V_{\mathrm{max}}$ the coherent ground state and lowest-excited fragmented state come very close to each other and interchange their order; see text for more details.

$V = 0.40 V_{\mathrm{max}}$, the ground state is a slightly depleted BEC, $\rho_1 = 98.14\%$, $\rho_2 = 1.86\%$, while the first excited is almost a totally twofold fragmented state: $\rho_1 = 51.0\%$, $\rho_2 = 49.0\%$. At $V = 0.42 V_{\mathrm{max}}$ the situation is inverse: the ground state is now twofold fragmented $\rho_1 = 50.32\%$, $\rho_2 = 49.68\%$, while the first excited state is condensed $\rho_1 = 98.12\%$, $\rho_2 = 1.88\%$.

The following picture of the splitting a BEC process emerges in the inverse regime. For a slow ramping-up process, only one quantum eigenstate is essentially populated although another state is crossing or very close by. Clearly, because of the very different physical nature of both states, the initially populated state cannot abruptly change its properties during the relevant time interval and the presence of the partner state essentially does not influence the dynamics. On the other hand, for a faster ramping-up process, more excited eigenstates are involved in the evolution and a coupling between these eigenstates allows the system to overcome the crossing point and evolve towards the lowest eigenstate which is a true twofold fragmented ground state.

Let us briefly summarize. We show that the dynamics of splitting of an ultracold bosonic cloud by ramping-up a barrier depends on the duration of the process and on the (effective) interaction strength between the bosons. There are (at least) two distinct regimes: (i) an *adiabatic* regime where the initial condensed ground state evolves towards the ground twofold fragmented eigenstate of the final double-well potential and asymptotically approaches it with increasing ramping-up time and (ii) an *inverse* regime where the initial condensed state evolves towards the ground twofold fragmented eigenstate only for short ramping-up times, while for slow ramping-up processes the time-dependent state stays condensed during all the evolution and thereby evolves to a *non*ground many-body eigenstate. The physical insight on these regimes follows from the analysis of the low-lying many-body excited states taken at different times. The above findings were made possible by developing MCTDHB capable of providing a quantitative description of the time evolution of the bosonic systems. MCTDHB opens up further possibilities to explore the challenging many-body dynamics of many-boson systems.

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