

Adiabaticity in nonlinear quantum dynamics: Bose-Einstein condensate in a time-varying box

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(Received 7 August 2001; published 7 February 2002; publisher error corrected 19 February 2002)

A simple model of an atomic Bose-Einstein condensate in a box whose size varies with time is studied to determine the nature of adiabaticity in the nonlinear dynamics obtained within the Gross-Pitaevskii equation (the nonlinear Schrödinger equation). Analytical and numerical methods are used to determine the nature of adiabaticity in this nonlinear quantum system. Criteria for validity of an adiabatic approximation are formulated.

DOI: 10.1103/PhysRevA.65.033607

PACS number(s): 03.75.Fi, 67.90.+z, 71.35.Lk

I. INTRODUCTION

The adiabatic theorem of quantum mechanics ensures that an eigenstate of a system whose Hamiltonian evolves sufficiently slowly in time (as determined by criteria for the applicability of the theorem) will remain in the same eigenstate, even though the eigenstate evolves in time [1–3]. Hence, a slowly evolving system that is initially in its ground state will remain in the ground state throughout the course of its evolution. The adiabatic theorem relies heavily on the superposition principle of quantum mechanics (although in classical mechanics similar theorems are valid for nonlinear systems [4]). It is of interest to determine to what extent adiabaticity carries over to *nonlinear* quantum systems, such as Bose-Einstein condensates (BECs) in the region where the mean-field description is appropriate. Well below the critical temperature, the mean-field description is based on the Gross-Pitaevskii equation (GPE),

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) + N_0 U_0 |\Psi|^2 \right] \Psi, \quad (1)$$

and this approximation often yields excellent results for the system dynamics, even when the external potential V varies with time. In Eq. (1), $U_0 = 4\pi a_0 \hbar^2/m$ is the atom-atom interaction strength that is proportional to the s -wave scattering length a_0 , and m is the atomic mass. The parameter N_0 in Eq. (1) is the total number of atoms, and the wave function Ψ is subject to the normalization $\int |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1$ (the normalization integral is a dynamical invariant of GPE). Adiabatic considerations regarding the GPE dynamics have been applied to cold Bosonic atoms trapped in optical lattices [5–8], and the formation of optical lattice gates for quantum computing from atomic BECs [9]. However, the applicability of the adiabaticity concept to BECs does not follow from the above-mentioned adiabatic theorem of quantum mechanics, since the nonlinearity does not allow applicability of the superposition principle to the GPE. On the other hand, adiabaticity of nonlinear wave equations, and in particular, of soliton solutions to such equations, have been extensively studied (for a review, see Ref. [10]). Nevertheless, BEC dynamical problems based on the GPE have their own specific features, so that this case can be different from that studied in

the framework of perturbed soliton solutions to the nonlinear Schrödinger equation (NLSE) in other contexts.

Here we develop a physically relevant one-dimensional BEC model that we study in detail by means of analytical and numerical methods to determine the nature of adiabaticity in nonlinear quantum systems within mean-field theory. There are several regimes in which adiabaticity can be experimentally and theoretically probed for nonlinear systems. The simplest regime is one for which the characteristic dynamical time scale (i.e., the time during which parameters of the Hamiltonian undergo an essential change), T , satisfies conditions

$$\tau_{AD} \ll T \ll \tau_{NL}. \quad (2)$$

Here, τ_{AD} is the quantum-mechanical linear adiabatic time scale determined in terms of the inverse of the difference of the energy eigenvalues at different values of time, $\tau_{AD} = \max\{\hbar/[\epsilon_1(t) - \epsilon_0(t)]\}$, where the maximum is taken with respect to a given time interval [2], while the nonlinear time scale is $\tau_{NL} = \max\{\hbar/\mu(t)\}$, with $\mu(t)$ being the instantaneous chemical potential [11]. In this case, the applicability of the adiabatic theorem of linear quantum mechanics [1–3] is ensured by the first inequality in Eq. (2), and nonlinearity cannot play a significant role in the dynamics due to the second inequality. Therefore, the dynamics must be adiabatic in this case. This regime applies to the NIST optical-lattice experiments wherein microsecond-duration light pulses are applied to a sodium BEC [12].

A more intriguing and more problematic regime is when the dynamical time scale is *large*, i.e., $\tau_{AD}, \tau_{NL} \ll T$. This case applies, e.g., to the BEC experiments reported in Refs. [6,7]. Here, the nonlinearity plays an essential role in the dynamics, and a relevant question is whether the dynamics can be adiabatic. Generally, the answer is no, since further time scales may appear in the multidimensional GPE, viz., a diffraction time, $\tau_{DF} = 2mL_0^2/\hbar$, where L_0 is the length of the system (see below), or a tunneling time scale, τ_{tun} (which itself may vary in the course of the system's evolution) [13]. If T is larger than *all* these time scales, clearly the dynamics will be adiabatic. In what follows, we show that the GPE does allow for adiabaticity when $\tau_{AD}, \tau_{DF}, \tau_{NL} \ll T$, and we give explicit criteria for the validity of adiabaticity in the

GPE for the specific problem considered here. We do so by means of an analytical estimate of corrections to (deviations from) the adiabatic approximation. We also present numerical results for the dynamics of this system when this condition does not apply.

II. THE DYNAMICAL MODEL

We consider a model based on the 1D GPE, in which the external potential $U(x)$ is an infinitely deep well,

$$U(x) = \begin{cases} 0, & 0 < x < L(t), \\ +\infty, & x < 0 \text{ or } x > L(t). \end{cases} \quad (3)$$

The size of the well $L(t)$ slowly varies with time, and we are interested in determining the behavior of the system in this case, to determine the applicability of adiabaticity. The 1D GPE takes the form

$$i\hbar \psi_t = -\frac{\hbar^2}{2m} \psi_{xx} + g|\psi|^2 \psi, \quad (4)$$

with the boundary conditions

$$\psi(0,t) = \psi(L(t),t) = 0, \quad (5)$$

and normalization of the wave function,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1. \quad (6)$$

The nonlinearity parameter g appearing in this 1D GPE is related to the nonlinearity parameter $N_0 U_0$ in its 3D counterpart, Eq. (1), and is determined so that $N_0 U_0 |\Psi_m|^2 = g |\psi_m|^2$, where Ψ_m and ψ_m are the maximum values of the 3D and 1D wave functions, respectively. This condition ensures that the time scales for the nonlinear interaction in the 3D and 1D cases are equal (see below and Ref. [11]).

This is the generalization of the particle in a box problem to the case where (a) the size of the box is varying with time, and (b) there are many bosonic particles in the box that are interacting via a mean field.

A typical situation in which the dynamics may be adiabatic is when the function $L(t)$ takes on constant values as $t \rightarrow \pm\infty$, and slowly varies in between on a long time scale T . We aim to find the final state $\psi(x, t = +\infty)$ into which an initial state $\psi(x, t = -\infty)$ will be transformed if T is sufficiently large, and to check whether the wave function $\psi(x, t)$ remains adiabatic during the course of the evolution, provided that the function $L(t)$ varies slowly enough (in practice, of course, the evolution time interval is large but finite). To determine what ‘‘sufficiently slow’’ means, we define the nonlinear time scale obtained directly from the GPE as [11]

$$t_{NL} = (g|\psi_m|^2/\hbar)^{-1} \approx \mu/\hbar, \quad (7)$$

where μ and $|\psi_m|$ are the chemical potential and maximum of the wave function in the initial configuration. The evolution is slow as compared to nonlinear time scale if $T \gg t_{NL}$. In many BEC systems, the nonlinear time scale is large com-

pared with the diffraction time scale $\tau_{DF} = 2mL_0^2/\hbar$, also obtained directly from the GPE [11], so we should have $T \gg t_{NL} \gg \tau_{DF}$.

It is convenient to transform the variables x , t , and ψ to new (dimensionless) variables τ , ξ , and u :

$$\xi \equiv x/L(t), \quad (8)$$

$$\tau \equiv \frac{\hbar}{2m} \int_0^t \frac{dt'}{L^2(t')}, \quad (9)$$

$$u \equiv \sqrt{2gm\hbar}^{-1} L(t) \psi. \quad (10)$$

Note that the problem is mapped onto a fixed spatial interval $\xi \in [0,1]$ of the dimensionless spatial variable ξ , and the boundary condition is therefore not time dependent when the problem is reformulated in terms of these variables. The 1D GPE (4) takes the following form in terms of the new variables:

$$iu_\tau + u_{\xi\xi} - |u|^2 u = i(L_\tau/L)(\xi u)_\xi, \quad (11)$$

where $L_\tau \equiv dL/d\tau$. Equation (11) is supplemented by boundary conditions following from Eq. (5),

$$u(\xi=0, \tau) = u(\xi=1, \tau) = 0. \quad (12)$$

The norm defined in terms of the transformed wave function u ,

$$N[u(\tau)] \equiv \int_0^1 |u(\xi, \tau)|^2 d\xi, \quad (13)$$

is *not* conserved in time, unlike the original norm, $\int_0^{L(t)} |\psi(x, t)|^2 dx = 1$. Indeed, as follows from the substitution of Eq. (10) for u into Eq. (13), the u norm is an explicit function of time,

$$N[u(\tau)] = \frac{2gm}{\hbar^2} L(\tau) \equiv n_0 \frac{L(\tau)}{L_0}, \quad (14)$$

where $L_0 \equiv L(t = -\infty)$ [alternatively, $L_0 \equiv L(t = t_0)$ if the initial moment in time is t_0]. The dimensionless nonlinear-strength parameter,

$$n_0 \equiv 2gmL_0/\hbar^2, \quad (15)$$

introduced in Eq. (14) will play an important role below.

When the system size $L(\tau)$ is a slowly varying function of time, the right-hand side (RHS) of Eq. (11) is small, being proportional to the logarithmic derivative of the slowly varying function. Therefore, Eq. (11) may be naturally considered as a perturbed self-defocusing NLSE, and the adiabatic methods for nonlinear wave equations reviewed in Ref. [10] might be applied. However, the perturbation term on the RHS of Eq. (11) need not allow straightforward application of the perturbation theory to the present problem since this term does *not* vanish at $\xi=0$ and $\xi=1$ when a general solution found in the zeroth-order approximation [the expression (18) below] is inserted into it. One can easily check that, as a

consequence of this, a perturbative expansion generated by the term on RHS of Eq. (11) is incompatible with the boundary conditions (12).

To resolve the problem, we transform the wave function once again, defining

$$u(\xi, \tau) \equiv v(\xi, \tau) \exp\left(\frac{i}{4} \frac{L_\tau}{L} \xi^2\right). \quad (16)$$

The transformation (16) generates a more convenient form of the perturbed NLS equation,

$$i v_\tau + v_{\xi\xi} - |v|^2 v = i \frac{L_\tau}{2L} v + \frac{LL_\tau - 2L_\tau^2}{4L^2} \xi^2 v, \quad (17)$$

which is subject to the same boundary conditions as in Eq. (12), $v(\xi=0, \tau) = v(\xi=1, \tau) = 0$. An obvious advantage of having the perturbed NLS equation in the form (17) is that now the perturbation vanishes at $\xi=0$ and $\xi=1$, once a solution found in the zeroth-order approximation vanishes at these points.

Note that the first term on the right-hand side of Eq. (17) is nonconservative. Accordingly, it is straightforward to see that this term leads to the exact relation (14) for the norm evolution. Another important fact is that the second term on the RHS of Eq. (17), unlike the first term, is *second-order small* with regard to derivatives of the slowly varying functions. In the perturbation-theory section that follows below, we will not consider effects produced by the second-order term, focusing solely on the most important first-order effects.

III. ADIABATIC PERTURBATION THEORY

A. Zeroth-order approximation

In zeroth-order approximation of the perturbation theory [neglecting the RHS of Eq. (17)], an exact stationary solution satisfying the zero boundary conditions at $\xi=0$ and $\xi=1$ is given by [14–16]

$$\begin{aligned} v(\xi, \tau) &= 2^{3/2} k K(k) \operatorname{sn}(2K(q)\xi, k) \exp(-i\mu\tau) \\ &\equiv V(\xi; k) \exp[i\phi(\tau)]. \end{aligned} \quad (18)$$

Here $\operatorname{sn}(\cdot, \cdot)$ is the doubly periodic Jacobi elliptic sine function, k is the corresponding elliptic modulus, $K(k)$ is the complete elliptic integral of the first kind, and the chemical potential μ is related to k as follows:

$$\mu = 4(1+k^2)K^2(k). \quad (19)$$

The modulus k , which takes values $0 \leq k \leq 1$, determines the strength of the nonlinearity: it is weak if $k \rightarrow 0$, and strong if $k \rightarrow 1$. In fact, k is related directly to the dimensionless nonlinearity-strength parameter n_0 defined in Eq. (15) as follows:

$$8K(k)[K(k) - E(k)] = n_0, \quad (20)$$

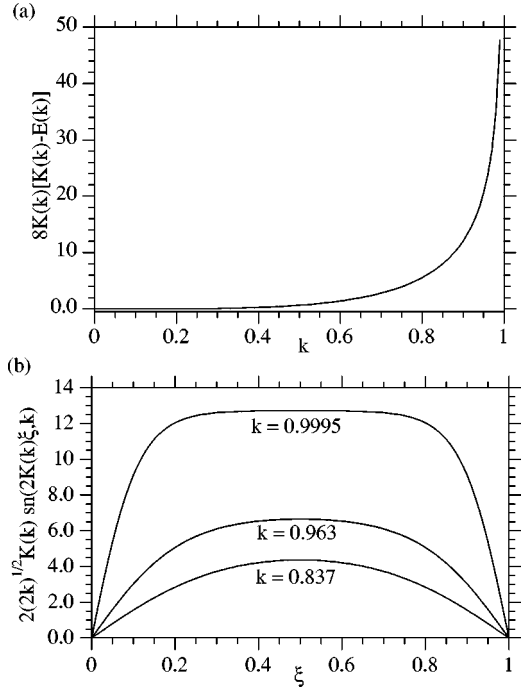


FIG. 1. (a) The expression $8K(k)[K(k) - E(k)]$ vs the elliptic modulus k . (b) The zeroth-order analytic solution $2^{3/2}kK(k)\operatorname{sn}(2K(q)\xi, k)$ for three different values of k . The normalization of these soliton solutions can be read off the curve in (a).

where $E(k)$ is the complete elliptic integral of the second kind. Thus, k completely determines the normalization of the initial wave function, and vice versa.

To illustrate the zeroth-order solution, plots of $8K(k)[K(k) - E(k)]$ vs k [see Eq. (20)], and $2^{3/2}kK(k)\operatorname{sn}(2K(q)\xi, k)$ vs ξ for three different values of k in the regime of strong nonlinearity, $k > 0.5$ [see Eq. (18)], are displayed in Figs. 1(a) and 1(b). We remark that an exact solution that can be expressed in terms of the Jacobi elliptic functions is frequently called a *cnoidal wave*, which stems from the notation *cn* for the Jacobi’s elliptic cosine, related to the elliptic sine.

B. The nonlinear adiabatic approximation

The first-order perturbation term on the RHS of Eq. (17) can be treated in terms of nonlinear adiabatic perturbation theory [10]. We stress that, unlike the perturbation term in the intermediate equation (11), which is “abnormal” in the sense that it is not compatible to the necessary boundary conditions, as it was explained above, the “normal” perturbation in Eq. (17) satisfies the boundary conditions. The applicability of simple perturbative techniques for this class of models can be proved using a rigorous expansion based on the inverse scattering transform for the unperturbed NLS equation (i.e., one can prove that the “simple techniques” yield, in the lowest-order nontrivial approximation, exactly the same results as the rigorous methods, see Ref. [10] and references therein).

The first standard step of the perturbative analysis is to apply the lowest-order adiabatic approximation. This ap-

proximation takes the unperturbed solution (18), that contains the parameter k , and makes it the first-order approximate solution to the perturbed equation, assuming that the modulus k is slowly varying with time, rather than remaining constant.

The slow dependence of the parameter(s) is introduced so as to cancel the secular divergence(s) in the perturbation theory. An important case is when the unperturbed solution contains a single nontrivial parameter (k , in the present case), and the perturbed equation gives rise to an exact relation replacing a conservation law existing in the unperturbed version of the equation [this exact relation is usually called a *balance equation* for the (former) conserved quantity]. This is the case in Eq. (14). Then, the time dependence of the parameter, i.e., $k(\tau)$, can be found in a very simple way by substitution of the zeroth-order approximation for the solution into the balance equation [10]. In the present case, this condition amounts to evaluation of the actual value of the norm (13), inserting the solution (18) into it, and then substituting the result into the exact relation (14). The final result is

$$8K(k)[K(k) - E(k)] = n_0 L(\tau)/L_0. \quad (21)$$

Equation (21) is a transcendental equation to determine $k(\tau)$ for a given function $L(\tau)$ and n_0 (recall that n_0 is a constant).

An essential ingredient of the adiabatic approximation is a consistent definition of the phase $\phi(\tau)$ for the first-order solution with variable $k(\tau)$. Indeed, substituting $k(\tau)$ back into the general expressions (18) and (19) for the wave function, it is easy to see that the consistently defined phase is

$$\phi(\tau) = - \int_{\tau_0}^{\tau} \mu(\tau') d\tau' \equiv -4 \int_{\tau_0}^{\tau} [1 + k^2(\tau')] K^2(k(\tau')) d\tau', \quad (22)$$

τ_0 being the initial time ($\tau_0 = -\infty$ in the usual formulation of the adiabatic approximation).

Thus, the full expression for the lowest-order perturbative solution obtained in the adiabatic approximation is

$$v(\xi, \tau) = V(\xi; k(\tau)) \exp[i\phi(\tau)], \quad (23)$$

where $V(\xi; k)$ and $\phi(\tau)$ are given by Eqs. (18) and (22), respectively. Note that expression (23) automatically satisfies the zero boundary conditions at the points $\xi=0$ and $\xi=1$.

Knowing a particular form of the slow temporal dependence $k(\tau)$ obtained from Eq. (21), one can find the temporal dependence of the solution's amplitude,

$$A(\tau) \equiv \max_{\xi} |v(\xi, \tau)| = 2^{2/3} k(\tau) K(k(\tau)). \quad (24)$$

The temporal dependence of state's width [which, for instance, can be defined as the full width at half-maximum of $|v(\xi, \tau)|^2$] can similarly be obtained in the adiabatic approximation from the above expressions. Using Eqs. (19) and (21), it is also possible to predict the evolution of the instantaneous value of the chemical potential $\mu(\tau)$.

C. Corrections to the lowest-order adiabatic approximation

Once the slow time dependence of $k(\tau)$ has been determined as described above, one can look for perturbation-induced corrections to the state's shape, which was not taken into account in the first-order adiabatic approximation. A solution to Eq. (17) including the corrections can be sought in the form of an expansion compatible with the zero boundary conditions, namely,

$$v(\xi, \tau) = \left[V(\xi; k) + \sum_{m=1}^{\infty} b_m(\tau) \sin(\pi m \xi) \right] \exp[i\phi(\tau)], \quad (25)$$

where the functions V and ϕ are those which were obtained in the preceding section.

The simplest way to derive evolution equations for the amplitudes $b_m(t)$ is to directly substitute the expansion (25) into Eq. (17), multiply the resulting equation by $\sin(\pi m \xi)$, and integrate from $\xi=0$ to $\xi=1$, carrying out this procedure for each integer m . The correction terms are neglected when substituting the expression (25) into the first perturbation term on the RHS of Eq. (17), as they would give rise to higher-order perturbations. Implementing this procedure, we use the classical Fourier expansion for the function sn,

$$\text{sn}(2K(k)\xi, k) = \frac{2\pi}{kK(k)} \sum_{p=1}^{\infty} \frac{Q^{p-1/2}}{1-Q^{2p-1}} \sin(\pi(2p-1)\xi), \quad (26)$$

$$Q(k) \equiv \exp\left[-\frac{\pi K(\sqrt{1-k^2})}{K(k)}\right]. \quad (27)$$

A complicated system of inhomogeneous linear evolution equations for $b_m(\tau)$ ensues. If m is odd, i.e., $m \equiv 2p-1$, we obtain

$$\begin{aligned} i \frac{db_{2p-1}}{d\tau} + R_{2p-1} b_{2p-1} - \sum_{n=1}^{\infty} M_{2p-1,n} (2b_n - b_n^*) \\ = \frac{iL_{\tau}}{L} \frac{\pi}{kK(k)} \frac{Q^{p-1/2}}{1-Q^{2p-1}}, \end{aligned} \quad (28)$$

and, if m is even, i.e., $m \equiv 2p$,

$$i \frac{db_{2p}}{d\tau} + R_{2p} b_{2p} - \sum_{n=1}^{\infty} M_{2p,n} (2b_n - b_n^*) = 0. \quad (29)$$

Here Q is the *Jacobi parameter* defined in Eq. (27), and the coefficients appearing on the left-hand sides of Eqs. (28) and (29) are

$$R_m \equiv 2(1+k^2)K^2(k) - \frac{1}{2}(\pi m)^2, \quad (30)$$

$$\begin{aligned} M_{mn} \equiv 4k^2 K^2(k) \int_0^1 \text{sn}^2(2K(k)\xi, k) [\cos\{\pi(m-n)\} \\ - \cos\{\pi(m+n)\}] d\xi. \end{aligned} \quad (31)$$

In fact, all the coefficients M_{mn} with m and n having opposite parities are zero, hence we may set $b_{2p} \equiv 0$, and we are left with the system of equations (28). Recall that one should substitute the time-dependent modulus $k(\tau)$ as found from Eqs. (21) into the above expressions.

This cumbersome system can be simplified if $k(\tau)$ does not take on values too close to unity. Then, sn remains close to the usual sine function [for instance, at $k^2 = 1/2$, the Jacobi parameter, which determines the anharmonicity of the expansion (26), is $Q = \exp(-\pi) \approx 0.043$, which may be regarded as a sufficiently small expansion factor]. Thus, to obtain a simple approximation for the coefficients M_{mn} defined in Eq. (31), one may simply set $\text{sn}(2K(k)\xi, k) \approx \sin(\pi\xi)$. Within this approximation the only nonzero components of the matrix (M_{mn}) are

$$\begin{aligned} M_{11} &= 3k^2 K^2(k), \quad M_{mm} = 2k^2 K^2(k) \quad (m > 1), \\ M_{m, m-2} &= M_{m-2, m} = -k^2 K^2(k). \end{aligned} \quad (32)$$

Furthermore, the RHS of Eq. (28) also greatly simplifies in the same approximation. It is different from zero solely for $m = 1$, being equal to $iL_\tau/(2L)$. Thus, the approximation that replaces the sn function by the usual sine leads to the following equations, instead of Eqs. (28) and (29):

$$\begin{aligned} i \frac{db_1}{d\tau} + \left[2(1-2k^2)K^2(k) - \frac{\pi^2}{2} \right] b_1 + 3k^2 K^2(k) b_1^* \\ + k^2 K^2(2b_3 - b_3^*) = \frac{iL_\tau}{2L}, \end{aligned} \quad (33)$$

$$\begin{aligned} i \frac{db_{2p-1}}{d\tau} + \left[2(1-k^2)K^2(k) - \frac{[\pi(2p-1)]^2}{2} \right] b_{2p-1} \\ + 2k^2 K^2(k) b_{2p-1}^* + k^2 K^2(2b_{2p-3} + 2b_{2p+1} - b_{2p-3}^* \\ - b_{2p+1}^*) = 0, \end{aligned} \quad (34)$$

where $p > 1$. Recall that all the amplitudes b_m with even values of m are zero.

Despite the fact that the approximate system consisting of Eqs. (33) and (34) is considerably simpler than the exact Eqs. (28), it can only be solved numerically by truncating the system of the linear equations at some finite integer. Nevertheless, some qualitative generic features of the solution can be determined. The general structure of the system is of the form

$$i \frac{dB}{d\tau} + \mathbf{A}(\tau)B = iC(\tau), \quad (35)$$

where B is a column vector of the variables b_{2p-1} , \mathbf{A} is a matrix of coefficients multiplying the variables b , and C is the vector column of free terms on the left-hand side, with the single nonzero entry $c_1 \equiv L_\tau/(2L)$. Both C and \mathbf{A} slowly depend upon time—the former directly, the latter via $k(\tau)$.

Solutions to the system (35) consist of terms of the type

$$\int_{\tau_0}^{\tau} \exp\left(-i \int_{\tau_0}^{\tau'} \omega(\tau'') d\tau''\right) f(\tau') d\tau', \quad (36)$$

where $\omega(\tau)$ is an eigenvalue of the matrix $\mathbf{A}(\tau)$, and $f(\tau)$ are slowly varying functions similar to the above-mentioned c_1 . Note that the time scales $2\pi/\omega$, determined by different eigenfrequencies ω , are, in fact, a mixture of the adiabatic and nonlinear time scales, τ_{AD} and τ_{NL} , defined in the Introduction.

The following conclusion can be made concerning the size of the *nonadiabatic* effects (shape corrections) considered above. If the function $L(\tau)$ slowly depends on τ with a characteristic time scale T (as defined in the Introduction), and if a characteristic value of ω is ω_0 (within the limits of its slow evolution on the time scale $\sim T$), the criterion for the applicability of the adiabatic approximation is

$$\omega_0 T / 2\pi \gg 1. \quad (37)$$

We stress that, as the characteristic times $2\pi/\omega_0$ taken for the different eigenfrequencies constitute a set including the adiabatic and nonlinear time scales τ_{AD} and τ_{NL} (see above), the inequality (37) is exactly the condition for the applicability of the adiabatic approximation conjectured in the Introduction.

The evolution equations (35) for the shape-correction amplitudes are to be solved for an initial state without shape corrections, i.e., $b_m(\tau = \tau_0) = 0 \quad \forall m$. If one takes the initial moment as $\tau_0 \rightarrow -\infty$ (as mentioned above, this is the standard assumption in the treatment of adiabatic processes [1,4]), one can determine eventual values of the shape-correction amplitudes as $b_m(\tau)$ at $\tau \rightarrow +\infty$. Classical estimates for integrals involving products of rapidly and slowly varying functions [1] show that the values of $b_m(\tau \rightarrow +\infty)$ are *exponentially small* when condition (37) is satisfied,

$$|b_m(\tau \rightarrow +\infty)| \sim \exp(-\text{const} \times \omega_0 T). \quad (38)$$

A particular value of the constant in this expression depends on the choice of the unperturbed state and on the form of the function $L(\tau)$. Hence, in analogy with the well-known theorems estimating nonadiabatic corrections to the adiabatic approximation in (nonlinear) classical mechanics [4], the $b_m(\tau \rightarrow +\infty)$ values are exponentially small.

IV. NUMERICAL RESULTS

We first present results for the amplitudes $b_m(\tau)$ in Eq. (25), obtained by numerically solving Eqs. (33) and (34). We take $k^2 = 0.3$, $L_0 = 1$, and

$$L(\tau) = L_0 \left[1 + \exp\left(-\frac{(\tau - T/2)^2}{2\sigma^2}\right) \right],$$

with $\sigma = T/10$. Figure 2 shows the computed excited-state probability

$$P_{\text{ex}}(\tau) \equiv \sum_{m=1}^{N_c} |b_m(\tau)|^2 \quad (39)$$

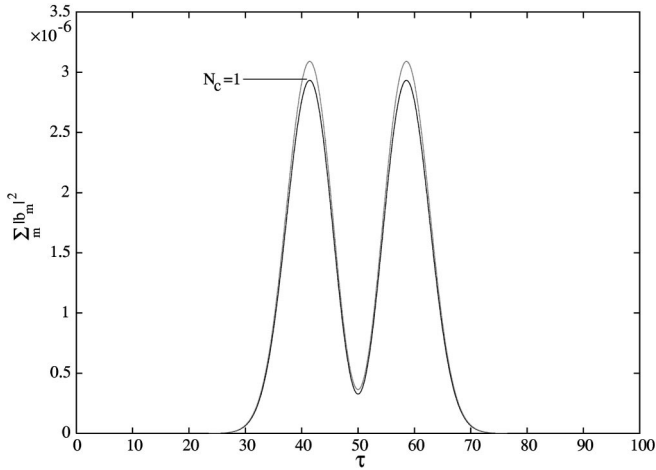


FIG. 2. The probability $\sum_{m=1}^{N_c} |b_m(\tau)|^2$ for the nonadiabatic correction to the state vs τ for $N_c = 1, 3, 5, 7, 9$ with $T = 100$. For $N_c \geq 3$ the curves lie on top of each other.

versus time τ , with the number of modes kept in the truncated calculation being $N_c = 1, 3, 5, 7$, and 9 , for $T = 100$. Except for $N_c = 1$, all the curves lie on top of each other, hence the results do converge very quickly as a function of the number of the modes. We see from Fig. 2 that the probability of finding excited states for all times is below 3.2×10^{-5} , and for $t = T$ the probability is exceedingly small, i.e., the process is almost completely adiabatic. A minimum of $P_{\text{ex}}(\tau = T/2)$ is expected from the general form of the perturbation equations since the derivative of $L(\tau)$ vanishes at $\tau = T/2$. For $T \lesssim 10$, the excited-state probability (39) begins to be large (> 0.2), and the adiabatic-theory results are no more reliable. For example, Fig. 3 shows the results for $T = 10$. Again the convergence as a function of the number of the modes is very fast, but the excited-state probability is not small. For times $\tau > T$, $P_{\text{ex}}(\tau)$ oscillates with time.

For stronger nonlinearity, $0.5 < k^2 \leq 1$, perturbative methods cannot be used (in particular, the approximation based on the replacement of the elliptic sine by the ordinary sine, as described in the above section, does not apply), so we directly solved Eq. (17) by using a split-step fast Fourier trans-

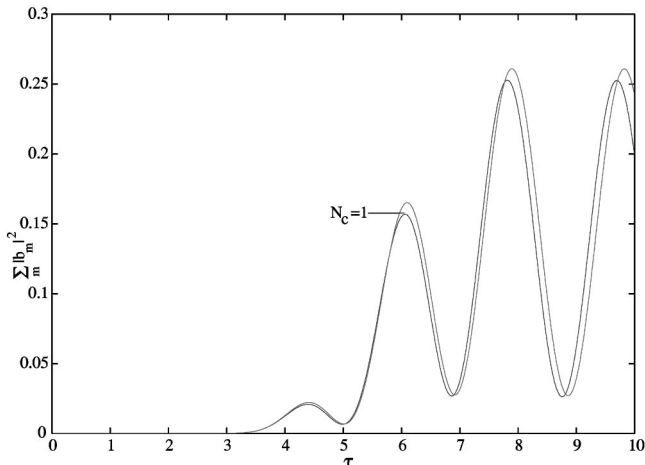


FIG. 3. Same as Fig. 2 except for $T = 10$.

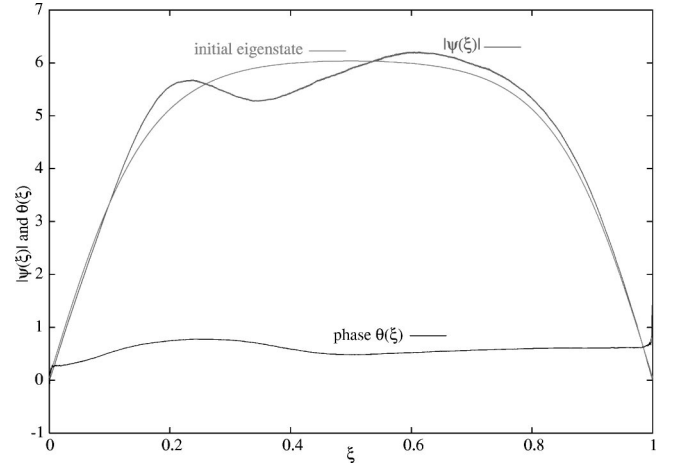


FIG. 4. The magnitude and phase of the wave function $\psi(\xi, \tau = T) = |\psi(\xi)|e^{i\theta(\xi)}$ vs the coordinate ξ in the box at the completion of the dynamical process, with $k = 0.963$ and $T = 1 \times 10^{-2}$. Also shown is the magnitude in the initial eigenstate.

form method, in order to check if adiabaticity still takes place in this regime. Figure 4 shows the results for the calculated wave function $\psi(\xi, \tau = T) = |\psi(\xi)|e^{i\theta(\xi)}$ vs ξ in the box at the completion of the dynamical process for small (nonadiabatic) time scale, $T = 0.01$, and for $k = 0.963$. Also shown for comparison is the initial eigenstate magnitude $|\psi(\xi, \tau = 0)|$. The magnitude of the wave function in the final state is not too different from that in the initial eigenstate, and the spatial variation of the phase is fairly flat. Figure 5 pertains to the same case, but with a larger time scale, $T = 1$. Now, the magnitudes of the wave function in the finite and initial state are barely distinguishable on the scale of the figure, and the spatial profile of the phase is almost flat. Thus, the process is largely adiabatic in the latter case.

V. CONCLUSION

We have presented a consistent derivation of the nonlinear dynamics for a simple model describing a BEC confined in a

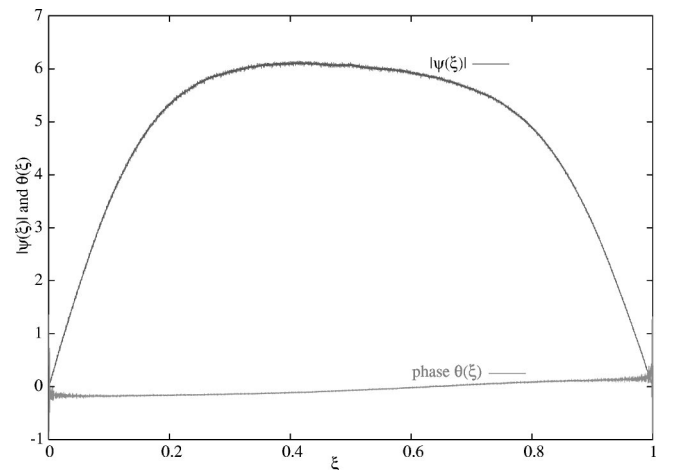


FIG. 5. The magnitude and phase of the wave function $\psi(\xi, \tau = T) = |\psi(\xi)|e^{i\theta(\xi)}$ vs the coordinate ξ in the box at the completion of the dynamical process, with $k = 0.963$ and $T = 1$.

box with a temporally varying size $L(\tau)$. The speed of the variation of $L(\tau)$ determines whether the dynamics is adiabatic. A “trivial” regime of adiabaticity is that for which $\tau_{AD} \ll T \ll \tau_{NL}$; in this paper, we have shown that adiabaticity can also be maintained when $\tau_{AD}, \tau_{DF}, \tau_{NL} \ll T$, where the various time scales have been defined in the Introduction. If other time scales appear, the condition $\tau_{AD}, \tau_{DF}, \tau_{NL} \ll T$ may not be sufficient to ensure adiabaticity. For example, if a barrier is present in the middle of the box, e.g., a repulsive δ function at $x=L_0/2$, then another time scale, corresponding to the time of tunneling under the barrier, τ_{tun} , is present in the problem. If this time scale is long compared with τ_{NL} , adiabaticity will not be maintained, and a nonvanishing spatially varying phase will develop across the condensate wave function [13]. Hence, the issue of adiabaticity in nonlinear problems must be investigated carefully; the perturbative techniques reviewed in Ref. [10] may be applicable, but additional considerations may play a role.

The particle in a box is a paradigm problem in one-body quantum mechanics. We have extended it to the many-body regime at least within a mean-field approach, and studied the adiabaticity for such a system when the size of the box varies with time. Specifically, we formulated the criteria for the validity of the adiabatic approximation for a BEC in a box whose size varies with time, developed the analytical and numerical tools for investigating adiabaticity in the dynamics within quantum mean-field theory, and presented results of calculations for this system.

ACKNOWLEDGMENTS

This work was supported in part by grants from the US-Israel Binational Science Foundation, the Israel Science Foundation, the James Franck Binational German-Israeli Program in Laser-Matter Interaction, and the Polish KBN 2/P03/B07819.

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- [1] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics* (Pergamon Press, New York, 1977).
- [2] A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1975), Vol. II, Chap. 17.
- [3] C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics* (Wiley, New York, 1977).
- [4] L.D. Landau and E.M. Lifshitz, *Mechanics* (Pergamon Press, New York, 1975).
- [5] D. Jaksch *et al.*, Phys. Rev. Lett. **82**, 1975 (1999).
- [6] B.P. Anderson and M.A. Kasevich, Science **282**, 1686 (1998).
- [7] C. Orzel *et al.*, Science **291**, 2386 (2001).
- [8] F.S. Cataliotti *et al.*, Science **293**, 843 (2001).
- [9] G.K. Brennen *et al.*, Phys. Rev. Lett. **82**, 1060 (1999).
- [10] Y.S. Kivshar and B.A. Malomed, Rev. Mod. Phys. **61**, 763 (1989).
- [11] M. Trippenbach, Y.B. Band, and P.S. Julienne, Phys. Rev. A **62**, 023608 (2000).
- [12] J. Denschlag, J. E. Simsarian, H. Haeffner, C. McKenzie, A. Browaeys, D. Cho, K. Helmerson, S. L. Rolston, and W. D. Phillips (unpublished).
- [13] Y.B. Band and M. Trippenbach, eprint cond-mat/0201123.
- [14] I.S. Gradshteyn and I.M. Ryzhik, *Tables of Integrals, Series, and Products* (Academic Press, New York, 1965).
- [15] An alternative notation for the Jacobi elliptic functions and the elliptic integrals is sometimes used. See, for example, *Handbook of Mathematical Functions*, Natl. Bur. Stand. Appl. Math. Ser., edited by M. Abramowitz and I.A. Stegun (U. S. GPO, Washington, DC, 1964), and Ref. [16]. In this alternative notation, $\widetilde{\text{sn}}[2\tilde{K}(m)\xi, m] \equiv \text{sn}[2K(q)\xi, k]$, where $m = k^2$ and $\tilde{K}(m) \equiv K(q)$. Also, $\tilde{E}(m) \equiv E(q)$.
- [16] L.D. Carr, C.W. Clark, and W.P. Reinhardt, Phys. Rev. A **62**, 063610 (2000).