

## Resonance solutions of the nonlinear Schrödinger equation: Tunneling lifetime and fragmentation of trapped condensates

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(Received 21 June 2004; revised manuscript received 21 March 2005; published 9 September 2005)

It is shown here how the lifetimes and energies of resonance states can be calculated by applying the complex scaling transformation to the nonlinear Schrödinger equation. It is essential to first apply the complex scaling transformation to the full Hamiltonian and to subsequently derive from the result the correct complex scaled nonlinear Schrödinger equation. The latter equation is physically relevant and amenable to numerical calculations. To analyze the results obtained by solving this equation, it is necessary to realize the close association of resonance phenomena with fragmentation of the system. As an illustrative example, we apply this theory to the Gross-Pitaevskii nonlinear equation to calculate the tunneling lifetime of a condensate inside an external (either optical or magnetic) trap. We show that by varying the scattering length, the external potential acts like a “selective membrane” which controls the direction of the flux of the cold atoms through the barriers and, thereby, controls the size of the stable condensate inside the trap.

DOI: [10.1103/PhysRevA.72.033605](https://doi.org/10.1103/PhysRevA.72.033605)

PACS number(s): 03.75.Lm, 03.65.Xp

### I. INTRODUCTION

The nonlinear Schrödinger equation (NLSE) appears in different fields of physics. In nuclear physics, the NLSE has usually been employed in relativistic mean-field and/or effective-field theory [1]. In nonlinear optics, the NLSE is associated with self-focusing and self-defocusing phenomena [2] and in atomic physics with the Gross-Pitaevskii (GP) equation for the dynamics of Bose-Einstein condensates (BECs), see for example [3–7]. In this work we focus on two subjects. The first one is on the calculations of resonance energies and lifetimes by applying the complex scaling transformations to the NLSE. This study is related to all fields in physics where the system has a finite lifetime and as time passes the system breaks up to subsystems which can be elementary particles, atoms, or photons.

The second subject we discuss in this paper is the fragmentation phenomenon which results from the bound-to-resonance transition. As an illustrative numerical example we study the resonance phenomena of a condensate in an external potential. The shape of the external potential is a quite general one. The potential parameters we have used are those that have been used before for studying new theories and computational methods for calculating resonance positions and widths, i.e., inverse lifetimes.

Tunneling of a BEC through a dynamical potential barrier has been demonstrated in the experiments of Phillips’ group [8] and of Raizen’s group [9]. The tunneling oscillations observed in Ref. [8] occurred by a two-state mechanism which is equivalent to the periodic transitions of particles from one potential well to a second one via a dynamical potential barrier. The experiments carried out by Raizen’s group show that transitions of cold atoms from one potential well to another can result from a three-state process [9]. Recently, it has been shown that the tunneling of cold atoms can be

controlled from full suppression to strong enhancement by varying slightly the experimental parameters [10]. Here, we address ourselves to the tunneling through a static potential barrier rather than a dynamical one. In principle, the underlying mechanisms should be closely related to those described in Refs. [8–10]. However, unlike the previous studies where the tunneling takes place between one bound state to another bound state, e.g., oscillatory transitions of the condensate from one potential well to another in Phillips’ experiment, we discuss here the tunneling of a BEC from a potential well to the continuum through a static potential barrier. In all BEC experiments, the condensates are trapped inside an open external potential well. Therefore, in the case of a positive scattering length, i.e., repulsive atom-atom interactions, a given external open potential well cannot trap a condensate with more than a critical number of atoms,  $N_c$ . The value of  $N_c$  can be determined on classical arguments like the overflow of the condensate out of the finite-sized open potential well. In magnetic traps the potential well is embedded in between potential barriers the size of which depend on the experimental parameters. Consequently, as the number of atoms  $N$  is increased, fractions of the condensate can tunnel through the potential barriers. What is the lifetime of the trapped condensate as  $N$  is increased? Can the condensate be stabilized inside the potential well as a fraction of it tunnels out through the potential barriers? Can we control the number of the atoms in the condensate by varying slightly the scattering length?

In order to answer these questions, we first have to find out how one can calculate resonance positions and lifetimes by solving the NLSE. This will be done here using the mathematically well-established method of complex rotation often also referred to as complex scaling [11–14]. As we will show in the next section, it is essential to apply the complex scaling transformation *before* the application of the mean-

field approximation that leads to the NLSE and not afterward. This is a crucial point in our application of complex scaling to the NLSE. Our theory is presented in Sec. II. As an illustrative numerical example, we apply in Sec. III the complex scaling method in the framework of the GP to a one-dimensional problem that describes a condensate captured in an optical and/or magnetic trap which consists of a well embedded in between two potential barriers.

We show in Sec. IV that by letting a fraction of the condensate tunnel through the potential barriers out of the trap, the residual reduced-in-size condensate is stabilized inside the external potential well “forever.” However, when the repulsive scattering length is appropriately chosen, it is possible to increase the number of the atoms in the condensate trapped in the well by letting cold atoms tunnel through the potential barriers from a reservoir of cold atoms located outside the trap into the potential well in the trap. In this sense, the external potential acts like a selective controlled “membrane.” In Sec. V, we conclude our findings.

## II. RESONANCE SOLUTIONS OF THE NONLINEAR SCHRÖDINGER EQUATION

### A. Resonance states of condensates

For a condensate with  $N$  cold atoms in an external trap,  $V_{ext}$ , the GP equation is given by [15]

$$\left(-\frac{\hbar^2}{2M}\nabla^2 + V_{ext}(\vec{r}) + U(N)\phi^2(\vec{r})\right)\phi(\vec{r}) = \mu(N)\phi(\vec{r}). \quad (1)$$

The nonlinear parameter,  $U(N)$ , is defined as

$$U(N) = U_0(N-1) = \frac{4\pi a_0 \hbar^2}{M}(N-1), \quad (2)$$

where  $a_0$  and  $M$  are the scattering length and the atomic mass, respectively. To simplify our discussion we assume, without loss of generality, that the solution  $\phi$  is a real function and, therefore, the nonlinear “potential” term is  $\phi^2(\vec{r})$  rather than  $|\phi(\vec{r})|^2$ .

The external trap is always an open trap. For example, a one-dimensional trap can be described roughly as a potential well embedded in between two potential barriers. Let us denote the threshold energy of the external potential by  $\mu_c$ .

By increasing the number of the atoms in the condensate which consists of  $N$  atoms with a positive scattering length,  $a_0 > 0$ , the nonlinear parameter  $U(N)$  acquires larger values and, thereby, the effective potential,  $V_{ext}(\vec{r}) + U(N)\phi^2(\vec{r})$ , becomes more shallow. Therefore, one might expect that as the number of atoms in the condensate is increased, the chemical potential  $\mu(N)$  increases as well. For a critical number of atoms in the condensate,  $N=N_c$ , the nonlinear parameter takes on a critical value  $U_c=U(N_c)$  and the chemical potential arrives at its threshold value  $\mu_c$ . If  $N$  is further increased,  $Q$  atoms tunnel through the potential barrier out of the potential well to stabilize the system. That is, only a fraction of  $XN$  atoms remains inside the potential well where  $(1-X) = Q/N$  is the fraction of atoms that have tunneled out through the potential barriers. The question we address here is how

the decay rate of the condensate can be calculated. The fragmentation phenomenon as described above is associated with the resonance phenomenon. This fragmentation occurs as a bound state of the condensate arrives at the threshold energy of the external potential. By increasing the value of the nonlinear parameter  $U(N)$ , this bound state of the condensate penetrates into the continuum and becomes a resonance state, i.e., a metastable state.

In conventional quantum mechanics the resonances are associated with wavepackets embedded in the continuum which are localized in the interaction region and cannot be associated with a *single* eigenstate of the system. However, the resonances are uniquely defined by imposing outgoing boundary conditions on the solutions of the time-independent Schrödinger equation [16]. A resonance state is associated with an eigenfunction of the Hamiltonian with an asymptote which has a zero amplitude for the incoming particles. That is,

$$\Psi_{res} \rightarrow \exp(+i\vec{k}_{res}\vec{r}). \quad (3)$$

Since the ratio of the amplitudes of the outgoing wave and the incoming wave defines the scattering matrix elements, the resonances are associated with the complex poles of the scattering matrix [17]. In the present case of a condensate, this implies that the chemical potential

$$\mu_{res}(N) = \frac{\hbar^2}{2M}k_{res}^2 \quad (4)$$

and the total energy associated with the resonance take on complex values. In this work we shall apply the complex scaling method to compute the resonances of a condensate. This method is briefly reviewed in Sec. II B.

Let us briefly discuss the physical meaning of the complex chemical potential  $\mu_{complex}(N)$  and the complex total energy  $\mathcal{E}$ . The complex chemical potential can be expressed as

$$\mu_{complex}(N) \equiv \mu(N) - \frac{i}{2}\gamma(N). \quad (5)$$

The real part of the chemical potential is the energy which is required to take an atom out of the well in the optical and/or magnetic trap. The energy of the external potential at infinite distance defines the threshold value of the chemical potential, which we denote as the threshold chemical potential,

$$\mu_c \equiv \mu_{threshold} = V_{ext}(r \rightarrow \infty). \quad (6)$$

At a fixed value of  $U_0$ , the chemical potential  $\mu(N)$  arrives at  $\mu_c$  when  $N$  arrives at the critical number  $N_c$  of bosons.  $N_c$  is the maximal number of atoms that can be trapped inside the potential well. We may, therefore, also call  $\mu_c = \mu(N_c)$  the critical value of the chemical potential. If  $N$  is increased beyond  $N_c$ , the chemical potential becomes complex. The imaginary part of the chemical divided by  $\hbar$

$$\frac{\gamma(N)}{\hbar} = \frac{-2 \text{Im } \mu_{complex}(N)}{\hbar} \quad (7)$$

is inversely proportional to the lifetime of a single boson in the condensate.

The complex energy per particle of the BEC reads

$$\frac{\mathcal{E}}{N} \equiv E(N) - \frac{i}{2}\Gamma(N). \quad (8)$$

In general,  $\mathcal{E}$  is determined as the complex eigenvalue of the full Hamiltonian. In the context of the NLSE, the energy is the expectation value of the Hamiltonian in the state  $\Psi = \phi(\vec{r}_1)\phi(\vec{r}_2)\dots\phi(\vec{r}_N)$ . The information on the energy of the condensate and its lifetime inside the potential well are respectively associated with the real and the imaginary parts of the complex energy  $\mathcal{E}(N)$ . The lifetime of the condensate in the potential well is given as usual by

$$\tau_{lifetime}(N) = \frac{\hbar}{\Gamma(N)}, \quad (9)$$

where  $\Gamma(N)$  is the *total* rate of decay per boson. The quantity  $\Gamma$  is a linear combination of partial widths,

$$\Gamma(N) = \sum_n \Gamma^{(n)}(N), \quad (10)$$

which describes the rate of decay of the condensate in the available open channels. The  $n$ th open channel is associated with  $n$  cold atoms that tunnel out of the well in the trap through the potential barriers. One may, therefore, expect that  $\Gamma(N) \geq \gamma(N)$ .

### B. Brief account of complex scaling

The complex scaling method is based on rigorous mathematical ground [11,12] and has been used before for calculating the lifetimes of metastable states in atomic, molecular, and nuclear physics [13,14]. Let us briefly describe the idea which stands behind this method.

As mentioned in Sec. II A, a resonance solution is associated with an eigenfunction of the Hamiltonian with an asymptote which is an outgoing wave with a complex momentum,  $\hbar\vec{k}_{res}$ . Without loss of generality, let us assume for the sake of simplicity that the resonance wave function has a spherical symmetric symmetry. In such a case,  $\Psi_{res}(r) \rightarrow \exp(ik_{res}r)$ , where  $k_{res} = |k_{res}|\exp(-i\alpha_{res})$ . Therefore, the resonance wave function diverges exponentially for  $0 < \alpha_{res} \leq \pi/2$ ,

$$\Psi_{res}(r) \rightarrow \exp[+i|k_{res}|\cos(\alpha_{res})r]\exp[+|k_{res}|\sin(\alpha_{res})r] \rightarrow \infty \quad (11)$$

and does not belong to the Hilbert space. In such cases the resonance wave function is not embedded in the Hermitian domain of the Hamiltonian and is associated with a complex eigenvalue. By carrying out the complex scaling transformation [13,14],

$$r \rightarrow re^{+i\theta}, \quad (12)$$

the resonance wave function becomes square integrable,

$$\begin{aligned} \Psi_{res}[r \exp(i\theta)] &\rightarrow \exp[+i|k_{res}|\cos(\theta - \alpha_{res})r] \\ &\times \exp[-|k_{res}|\sin(\theta - \alpha_{res})r] \rightarrow 0, \end{aligned} \quad (13)$$

for

$$\alpha_{res} \leq \theta \leq \frac{\pi}{4}. \quad (14)$$

The upper bound of  $\theta$  results from the effect of the complex transformation on the kinetic energy operator,

$$-\frac{\hbar^2}{2M}\hat{\nabla}_r^2 \rightarrow -e^{-2i\theta}\frac{\hbar^2}{2M}\hat{\nabla}_r^2. \quad (15)$$

A bound state is associated with an asymptote of an outgoing wave with purely imaginary momentum  $\hbar k_{bound} = i\hbar|k_{bound}|$ . It is clear that a bound state remains square integrable under the complex scaling transformation,

$$\begin{aligned} \Psi_{bound}[r \exp(i\theta)] &\rightarrow \exp[+i|k_{bound}|\cos(\theta)r] \\ &\times \exp[-|k_{bound}|\sin(\theta)r] \rightarrow 0, \end{aligned} \quad (16)$$

and is associated with the same real eigenvalue as obtained by solving the Schrödinger equation as usual when the Hamiltonian is Hermitian and the eigenfunctions are in the Hilbert space. For a more detailed discussion of the complex scaling transformation including its impact on the continuum, see Refs. [13,14].

In practice the transformation (12) leads to a complex scaled Hamiltonian,  $H(\theta)$ . The resonance states are uncovered in the lower half of the complex energy plane as the eigenvalues of  $H(\theta)$  as  $\theta$  is increased. The associated resonance eigenstates are square integrable.

Before closing the brief description of the complex scaling method, let us emphasize that while the density of states in the continuum of the Hermitian Hamiltonian is nonmonotonic and contains information about the resonance decay process, the continuum of the complex scaled Hamiltonian is a “white” continuum and varies monotonically with the energy. The entire information about the resonance decay process is in the resonance eigenfunctions that under the complex scaling transformation become square integrable.

### C. Direct application of complex scaling to the GP equation

By applying the complex scaling transformation (12) to the GP equation as defined in Eq. (1), we obtain the following nonlinear problem (which will be found later to be the *wrong* equation),

$$\begin{aligned} \left( -\frac{\hbar^2}{2M}e^{-2i\theta}\nabla^2 + V_{ext}(e^{i\theta}\vec{r}) + U_0(N-1)\phi_\theta^2 \right) \phi_\theta \\ = \mu_{complex}(N)\phi_\theta. \end{aligned} \quad (17)$$

In Eq. (17)  $\phi_\theta^2$  is a complex function due to the complex scaling transformation given in Eq. (12). Unlike the terms in the complex scaled Hamiltonian which are  $\theta$  dependent, any physical measurable quantity should be  $\theta$  independent once  $\theta$  fulfills the relation (14). However, as we shall see below

there is no way to get the resonance solutions by solving Eq. (17).

Why does the direct application of complex scaling to the GP equation fail? The answer to this question is embedded in the idea that the GP equation can be viewed as a linear Schrödinger equation with an effective potential,  $V_{eff} = V_{ext}(\vec{r}) + U\phi^2(\vec{r})$ , where  $\phi(\vec{r})$  is the resonance solution. As discussed in Sec. II B, the motivation behind the complex scaling of  $V_{eff}$  is the wish to change the asymptote of the resonance wave function from an exponentially diverging to an exponentially decaying behavior. The problem in this direct approach is that before applying the complex scaling transformation the resonance wave function is not square integrable as shown in Eq. (11). Therefore, the effective potential

$$V_{eff}(\vec{r}) = V_{ext}(\vec{r}) + U\phi_{res}^2(\vec{r}) \rightarrow \infty \quad (18)$$

diverges. In such a case,  $V_{eff}$  supports bound states only. We have here a paradox. If the solution of the GP equation is a resonance state which is associated with an outgoing asymptote, then  $V_{eff}$  should have a continuum spectrum as resonances are metastable states embedded in the continuum. However, if  $\phi$  is a resonance wave function which exponentially diverges, then  $V_{eff}$  supports bound states only. The solution to this problem is clear. It is impossible to derive the GP equation when the solution of the full problem is associated with a resonance wave function which diverges exponentially.

A few brief remarks are in order. Because of the above, it is plausible that one cannot find the numerically resonant solutions of Eq. (17). Indeed, our numerical studies using Eq. (17) failed. In a previous study, the use of a complex absorbing potential which has been added to the GP effective potential has been attempted rather than the complex scaling transformation [18].

It is well known that the complex scaling transformation is only rigorously applicable to potentials which are dilation analytic [11,12]. The analysis of nonlinear self-consistent equations has demonstrated that the underlying effective potentials are generally non dilation analytic because of the self-consistency involved [19]. This finding is a further indication that the complex scaling transformation cannot be applied directly to the GP equation. Since all bosons reside in a single orbital  $\phi(\vec{r})$ , which is computed self-consistently in the GP equation, it becomes clear that the dilation analyticity of the potential is more severely violated than in the Hartree-Fock equation for fermions, where each fermion resides in its own orbital and the impact of self-consistency is less dramatic. In Sec. II D, the problems addressed above are solved by first applying the complex scaling transformation to the full Hamiltonian from which, subsequently, the nonlinear GP equation is derived.

#### D. Derivation of NLSE from the complex scaled full Hamiltonian

Assuming a contact interaction between the  $N$  atoms in the condensate, the complex scaled full Hamiltonian is given by

$$\left( -\frac{\hbar^2}{2M} e^{-2i\theta} \sum_{j=1}^N \nabla_j^2 + \sum_{j=1}^N V_{ext}(e^{i\theta} \vec{r}_j) + U_0 \sum_{j=1}^N \sum_{j' \neq j} \delta_\theta(\vec{r}_j - \vec{r}_{j'}) \right) \Psi_\theta = \mathcal{E}(\text{complex}) \Psi_\theta, \quad (19)$$

where the  $\delta$  function is presented as a Gaussian with vanishing width and its complex scaled version takes on the following appearance

$$\delta_\theta(\vec{r}_j - \vec{r}_{j'}) = \lim_{\sigma \rightarrow 0} \left( \frac{1}{\sigma\pi} \right)^{D/2} \exp \left[ -\frac{\exp(i2\theta)(\vec{r}_j - \vec{r}_{j'})^2}{\sigma} \right]. \quad (20)$$

$D=1, 2, 3$  is the dimension of the BEC.

Note that in order to avoid the mathematical complications which result from the high singularity of a multidimensional  $\delta$  function, we will take the limit of  $\sigma \rightarrow 0$  only after the application of the Hartree approximation which leads to the GP nonlinear equation. The method described in this work can be applied to any potential and is used here for  $\delta$ -potentials for transparency only.

Eq. (20) can be rewritten to give

$$\delta_\theta(\vec{r}_j - \vec{r}_{j'}) = \exp(-i\theta D) \lim_{\tilde{\sigma} \rightarrow 0} \left( \frac{1}{\tilde{\sigma}\pi} \right)^{D/2} \exp \left[ -\frac{(\vec{r}_j - \vec{r}_{j'})^2}{\tilde{\sigma}} \right], \quad (21)$$

where

$$\tilde{\sigma} = \exp(-i2\theta)\sigma, \quad (22)$$

and

$$0 \leq \theta < \frac{\pi}{4}. \quad (23)$$

The latter relation leads to

$$\text{Re } \tilde{\sigma} > 0. \quad (24)$$

Here we proved that under the constrains given in (23) the complex scaled  $\delta_\theta$  function is equal to

$$\delta_\theta(\vec{r}_j - \vec{r}_{j'}) = \exp(-i\theta D) \delta(\vec{r}_j - \vec{r}_{j'}). \quad (25)$$

The usual GP nonlinear equation, Eq. (1), is obtained from the full Hamiltonian of the system by assuming that all atoms occupy the same orbital [15]. By analogy, we derive a NLSE starting from the complex scaled full Hamiltonian in Eq. (19) by assuming that the variational solution is given by

$$\Psi_\theta(\dots \vec{r}_j, \dots, \vec{r}_N) = \prod_{j=1}^N \phi_\theta(\vec{r}_j). \quad (26)$$

Using our above results for the complex scaled  $\delta_\theta$  function we arrive at the *correct* expression for the complex scaled GP nonlinear equation

$$\left(-\frac{\hbar^2}{2M}e^{-2i\theta}\nabla^2 + V_{\text{ext}}(e^{i\theta}\vec{r}) + U(N)e^{-i\theta D}\phi_\theta^2\right)\phi_\theta = \mu_{\text{complex}}(N)\phi_\theta, \quad (27)$$

which clearly differs from the one in Eq. (17) obtained by applying the complex scaling transformation directly to the usual GP equation. The complex energy of the BEC,  $\mathcal{E}$ , as defined in Eq. (8), is the expectation value,  $\mathcal{E} = \langle \Psi_\theta^* | H_\theta | \Psi_\theta \rangle$ . Here we use the  $c$ -product rather the conventional scalar product since  $\Psi_\theta$  is a complex function only due to the rotation of the internal coordinates of the Hamiltonian into the complex coordinate plane [20,21].  $\mathcal{E}$  is associated with the complex chemical potential as follows:

$$\frac{\mathcal{E}}{N} \equiv E(N) - i/2\Gamma(N) = \mu_{\text{complex}}(N) - \frac{U(N)}{2}e^{-i\theta D} \int \phi_\theta^4 d\vec{r}. \quad (28)$$

The complex chemical potential is defined by Eq. (27); see also Eq. (5). The quantity  $\mathcal{E}$  in Eq. (28) provides the GP complex mean-field energy of the condensate. Of course, this quantity is only an approximation to the exact energy in Eq. (19) which is associated with a complex eigenvalue of the full Hamiltonian (i.e., beyond the GP approximation).

### III. ILLUSTRATIVE EXAMPLE FOR CALCULATING RESONANCES BY SOLVING THE COMPLEX GP EQUATION

The complex version of the GP equation derived in Sec. II is applied here to a simple one-dimensional potential which qualitatively describes an external trap. We chose a model potential that has been used before in test-case studies of new theories and methods for calculating resonance lifetimes and energies [14,20,22–24]. The model potential is given by  $V_{\text{ext}}(x) = (x^2/2 - 0.8)\exp(-0.1x^2)$  and is shown in the inset of Fig. 1. Assuming that the atoms in the diluted BEC do not interact with one another, the atoms can be found either trapped inside the central potential well in the ground bound state or in one of the metastable states. The lifetime of a metastable state is equal to  $\hbar/\Gamma$  where  $\Gamma$  is the resonance width (one resonance state and the only bound state are indicated in the inset of Fig. 1). When the system is prepared in a metastable state then the survival probability  $S(t) = |\langle \Psi(t=0) | \Psi(t) \rangle|^2$  decays exponentially in time,  $S(t) = \exp(-\Gamma t/\hbar)$ , where  $\Psi(t)$  is the solution of the time-dependent Schrödinger equation. The bound and resonance states shown in Fig. 1 were first calculated for noninteracting cold atoms using the complex scaling method. The real eigenvalue associated with the bound state and the complex eigenvalue associated with the resonance state were found to be unaffected in more than eight significant figures when the complex scaling parameter  $\theta$  (called the rotational angle) is varied between 0.1 to 0.75 rad underlying the stability of the numerical procedure involved.

Unlike the failure to find the stable complex solutions of Eq. (17) (see also discussion in Sec. II C), the complex solutions of the newly derived NLSE, Eq. (27), were extremely

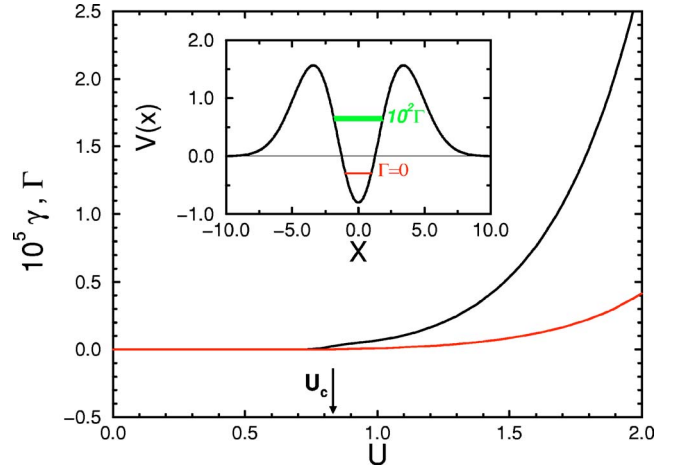


FIG. 1. (Color online) The rate of decay  $\gamma$  of a single atom (associated with the imaginary part of the chemical potential) and the rate of decay per atom  $\Gamma$  (associated with the imaginary part of the complex energy of the condensate) as a function of the nonlinear parameter  $U$ . The inset shows the external potential,  $V_{\text{ext}}(x) = (x^2/2 - 0.8)\exp(-0.1x^2)$  and its bound and resonance energy levels when it is assumed that the cold atoms in the condensate do not interact with one another.

stable with respect to small variations of the complex scaling parameter  $\theta$ . The bound and the resonance chemical potentials as well as the energies obtained in our calculations are  $\theta$  independent for  $\theta \geq 0$  and  $\theta \geq 0.3$  rad in the case of the bound state and resonance state, respectively. We used 400 particle-in-a-box basis functions as a basis set with a box size of  $L=50$  a.u. In each step of the calculations, we carried out iterative calculations to arrive at self-consistent converged results in eight digits of significant figures where the scaling angle  $\theta$  has been varied from 0.3 rad to 0.7 rad. By solving Eq. (27), we calculated the complex chemical potential  $\mu - i/2\gamma$ , and by solving Eq. (28), we calculated the complex energy per particle  $\mathcal{E}/N = E - i/2\Gamma$ . In Fig. 2, we present the results obtained from the calculations of the complex chemical potential as a function of the rotational angle  $\theta$ . As one can see from the results presented in Fig. 2, very stable converged values for the position and width of the chemical potential were found and similar stable results were obtained for the complex energy of the condensate by applying the complex scaling transformation to the GP equation as introduced above in Sec. II D.

In Fig. 1, we present our numerical results for  $\gamma(N)$  and  $\Gamma(N)$  as function of  $U(N) = U_0(N-1)$ . We mark by an arrow the critical value  $U_c = 0.8279$  for which the bound-to-resonance transition occurs. That is, for  $U(N) \leq U_c$ , one has  $\gamma=0$  and both  $\gamma(N)$  and  $\Gamma(N)$  acquire positive values when  $U(N) > U_c$ . From Fig. 1, one can see that  $\Gamma(N)$  increases more rapidly than  $\gamma(N)$  as the nonlinear coupling term  $U(N)$  is increased. In Fig. 3, we present the chemical potential  $\mu(N)$  and the energy  $E(N)$  as functions of  $U(N)$ . As one can see at the critical value of  $U_c$  where the resonances are “born,” the chemical potential is equal to zero,  $\mu_c = \mu(U_c) = 0$ . This is an expected result. The chemical potential is calculated by solving the NLSE, which determines the

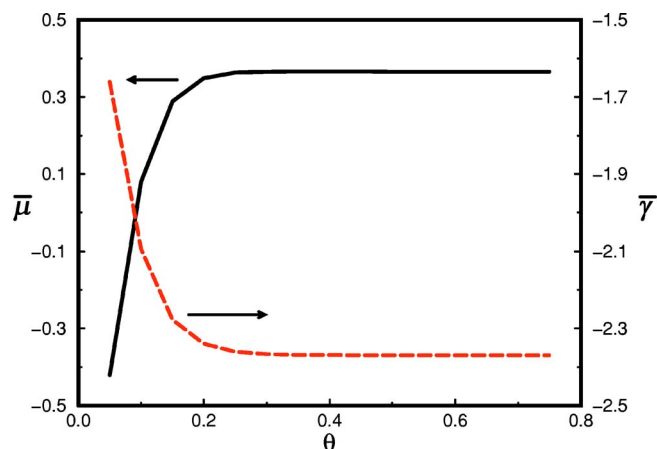


FIG. 2. (Color online) The real and the imaginary parts of the complex chemical potential as functions of the complex scaling parameter. The solid (black) line shows  $\bar{\mu} = (\mu - 0.36045)10^5$  and the dashed (red) line shows  $\bar{\gamma} = -(1 + 5 \times 10^4 \gamma)$ .  $\mu$  and  $\gamma$  are associated with the complex chemical potential:  $\mu = \text{Re } \mu_{\text{complex}}$  and  $\gamma = -2 \text{Im } \mu_{\text{complex}}$ . The nonlinear parameter is  $U(N) = 2$ .

atomic orbital  $\phi$ , and this equation is an effective one-atom equation.

From the shape of the external potential presented in Fig. 1, we see that the threshold energy of the external potential is equal to 0. We may interpret  $\mu$  as the energy needed to take an atom of the condensate out of the potential well, and  $\gamma(N)$  as the corresponding rate of decay. The total rate of decay per particle of the condensate from the external potential well through the potential barriers into the continuum is  $\Gamma(N)$ . The threshold energy of the BEC, which consists  $N$  atoms, i.e., the energy per particle at which the bound-to-resonance transition occurs, is about  $E_c \sim -0.249$  a.u. For  $U(N)$  below the critical value  $U_c = 0.8279$ , the BEC is trapped “forever” inside the well of the external potential trap. When  $U(N)$  exceeds this critical value, the condensate

is found in a metastable state (i.e., resonance state) and the condensate tunnels out of the trap through the barriers of the external potential. Why does the bound-to-resonance transition occur at a negative energy  $E_c$ ? The physical explanation lies in the many-body character of the problem. When a fraction of the  $N$ -particle repulsive BEC consisting of  $(1-X)N$  atoms tunnels out of the potential well into the continuum, a stabilization of the  $XN$  atoms, which remain inside the trap, takes place. The energy  $E_c$  is the energy per particle of the  $XN$  atoms, which remain in the trap.

The GP equation is an effective one-atom equation and describes only a single open channel of decay. In reality, the number of open channels is equal to the number of atoms that can tunnel through the potential barriers. This number depends on the energy of the condensate. However, within the framework of the GP mean-field approximation, the nonlinear parameter is  $U(N) \sim a_0 N$  and, therefore, one cannot distinguish between the number of atoms  $N$  in the condensate and the  $s$ -wave scattering length  $a_0$ , and, in particular, one cannot tell at a given value of  $U$ , which fraction of  $N$  will tunnel. As shown in Sec. IV, we can clarify this problem by taking into consideration the idea that the best mean field for condensates is not always obtained when all identical bosons of the condensate reside in a single one-particle function (a so-called orbital) [25–27].

#### IV. FRAGMENTATION AND STABILIZATION OF THE CONDENSATE WHEN THE EXTERNAL POTENTIAL ACTS AS A SELECTIVE “MEMBRANE”

Let us assume that the mean-field description of the interacting system (BEC with positive  $s$ -wave scattering length) is given by the ground state wave function  $\Psi$ , which is a product of two types of spatial orbitals  $\phi$  and  $\chi$ . There are  $n_1$  atoms which occupy the  $\phi$  orbital, whereas  $n_2 = N - n_1$  atoms which occupy the  $\chi$  orbital. Since the bosons are identical, the product should be symmetrized such that [25,26]

$$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = S \phi(\vec{r}_1) \phi(\vec{r}_2) \dots \phi(\vec{r}_{n_1}) \chi(\vec{r}_{n_1+1}) \chi(\vec{r}_{n_1+2}) \dots \chi(\vec{r}_N). \quad (29)$$

We associate the  $n_1$  atoms in the orbital  $\phi$  with the fraction of the condensate  $X = n_1/N$ , which is located in the well, and the  $n_2$  atoms in the orbital  $\chi$  with the fraction  $(1-X) = n_2/N$ , which has tunneled through the barriers into the continuum. Consequently,  $\phi$  is located in the trap and  $\chi$  well outside the trap where  $V_{\text{ext}} = 0$ , and we may consider these two orbitals to not overlap. Let  $E_\phi(X, U)$  be the energy per atom in the trap. Analogously, the energy per atom in the continuum is given by  $E_\chi[(1-X), U]$ . The resulting energy per atom of the whole system at a given  $U$  and  $X$  is thus

$$E_{\text{BEC}}(X, U) = X E_\phi(X, U) + (1-X) E_\chi[(1-X), U]. \quad (30)$$

We notice that  $E_\phi(X, U)$  is nothing but  $E(XU)$ , which is the energy per particle which we obtain by solving the GP equation, where the nonlinear parameter  $U = U_0(N-1) \sim U_0 N$  is replaced by the value  $XU = n_1 U_0$ . Because our condensate is repulsive, the energy  $E_\chi$  is known to be equal to zero [15] and we obtain the final result,

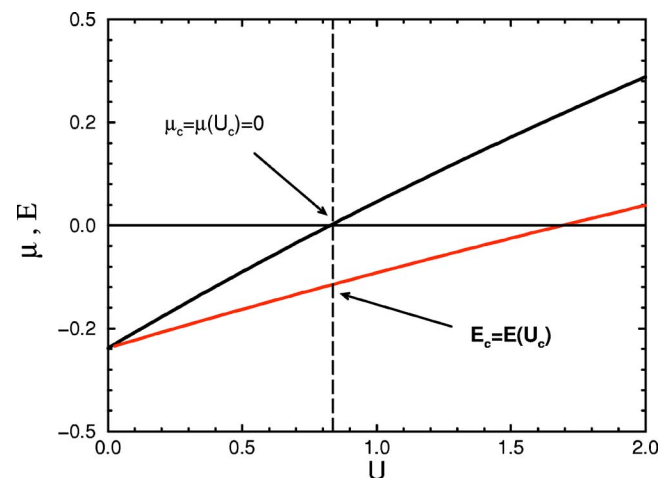


FIG. 3. (Color online) The chemical potential,  $\mu = \text{Re } \mu_{\text{complex}}$  and the energy of the BEC,  $E = \text{Re } \mathcal{E}$ , as function of  $U = U_0(N-1)$ . The critical value  $U_c$  is indicated by a broken vertical line. For  $U > U_c$ , the quantities  $\mu_{\text{complex}}$  and  $\mathcal{E}$  take on complex values (see Fig. 1).

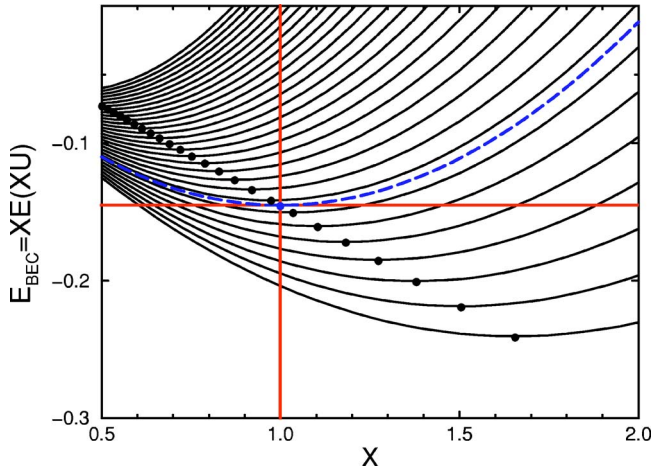


FIG. 4. (Color online) The energy per atom of the BEC assuming two sets of orbitals [Eqs. (29)–(31)]. Shown is the energy  $E_{BEC}$  as function of  $X=n_1/N$ , which is the fraction of the condensate that remains trapped inside the well of the external potential as a fraction  $(1-X)$  of the condensate has tunneled to the continuum through the potential barriers shown in Fig. 1. Each curve is associated with a different value  $U=0.5+0.05(j-1)\sim a_0N$  of the nonlinear parameter,  $j=1,2,3,\dots$  counting  $j$  from the bottom. The vertical line at  $X=1$  passes through the minimum of the energy curve for which  $U=U_c=0.8279$  shown as a dashed (blue) line.

$$E_{BEC}(X,U) = XE(XU), \quad (31)$$

which makes clear that  $E_{BEC}(X,U)$  can be derived from the curve  $E(U)$  in Fig. 3. In complete analogy, the rate of decay into the continuum per atom corresponding to  $E_{BEC}(X,U)$  is given by  $X\Gamma(XU)$  and can thus also be deduced from the curve  $\Gamma(U)$  in Fig. 1.

While for a given value of  $U$ , the Gross-Pitaevskii energy  $E(U)$  is just a number and does not provide us with the knowledge of how many atoms have tunneled,  $E_{BEC}(X,U)$  is the key to this information. In Fig. 4, we show the energy per atom of the condensate as a function of  $X$  for different values of  $U$ . The curves at the bottom of the figure are for small values of  $U$ , those at the top are for larger values of  $U$ . Each of the curves exhibits a minimum at  $X_c(U)$  and these minima play a central role in the understanding of the tunneling process. These minima are marked by solid dots. Let us consider a single curve in Fig. 4 for which  $X_c$  is smaller than 1 (the value  $X=1$  is marked in the figure by a vertical line).  $X=1$  implies that we have put  $N$  atoms in the condensate and, thus, is our starting point. Because of the variational principle, the condensate will minimize its energy by letting a fraction  $1-X_c$  of its atoms tunnel into the continuum and keep the fraction  $X_c$  in the well at which  $E_{BEC}$  takes on its minimum. Particles tunnel inside the condensate for small repulsive interactions due to the fact that a particle has less energy inside the well than in the continuum. The larger  $U$  is, the stronger is the interaction and with it the curvature of the energy curve in Fig. 4 around its minimum.

How does this appealing picture relate to the decay rate  $X\Gamma(XU)$ ? We know already from the scaled mean-field approach that  $\Gamma(U)$  changes from being zero to nonzero at the

bound-to-resonance transition point  $U_c$ . Therefore, for a given value of  $U$ , we find a particular value of  $X$  such that  $XU=U_c$ , and this  $X$  tells us at which fraction of the condensate the system is just still bound. If this is the case, there should be an intimate relation between this particular value of  $X$  and  $X_c$  at which  $E_{BEC}$  has its minimum. Indeed, we find that both values of  $X$  are *identical*, i.e.,  $X_c=U_c/U$ . Using the value  $U_c=0.8279$  found above, one readily reproduces the values of  $X$  at which any curve  $E_{BEC}(X,U)$  takes on its minimum for a given  $U$ . In particular,  $E_{BEC}(X,U_c)$ —which is the blue curve in Fig. 4—exhibits its minimum at  $X_c=1$ . This value implies that for  $U_c$  the condensate with  $N$  atoms is bound, while for  $U>U_c$  the fraction  $1-X_c$  tunnels to make the remaining fraction  $X_c<1$  bound.

It is essential to note that the critical values  $X_c$  and  $U_c$  can be determined from the above analysis without using the complex scaled mean-field results. The curves  $E_{BEC}(X,U)$  shown in Fig. 4 can be computed via Eq. (31) for all values of  $U$  from  $X=0$  up to  $X_c$  using *bound state* calculations only. This is a success of the two-orbital picture [25,26] used above to derive Eq. (31).

Once  $U\geq U_c$ , increasing the  $s$ -wave scattering length  $a_0$ , for instance, by applying an external magnetic field to adjust the relative energy of different internal states of the atoms [28], leads to an increase of  $U$  and hence to a reduction of the number of atoms inside the potential well (see Fig. 4). On the other hand, if we decrease the scattering length  $a_0$ , the trap can accommodate more atoms. Consequently, if there is a reservoir of cold atoms outside the trap, *some of them can tunnel through the barriers into the trap* thus increasing the number of atoms inside the trap. Note that in Fig. 4 the minima of  $E_{BEC}$  for  $U<U_c$  are at  $X_c>1$ , i.e., the condensate inside the trap is further stabilized if atoms are added. In this way, the size of the trapped condensate can be controlled and the trap acts as a “controllable membrane” by varying the  $s$ -wave scattering length (or by varying the depth of the trap potential). We hope that these fascinating results will stimulate new experiments.

## V. CONCLUDING REMARKS

In this work the complex scaling method has been applied to NLSEs with particular emphasis on the GP equation, which is very popular in the field of condensates. We have shown that a very ill-behaved equation results if the complex scaling method is applied directly to the GP operator. The correct complex scaled NLSE is obtained by first applying the complex scaling method to the full Hamiltonian of the system. From this complex scaled full Hamiltonian, it is then possible to determine the correct complex scaled NLSE in the same way as the GP equation is usually determined from the regular full Hamiltonian.

We discuss explicitly the tunneling of a condensate using an illustrative numerical example. The lifetime of the condensate is computed and the results are analyzed in terms of fragmentation of the condensate. It is shown that one can control the tunneling and even the direction of the flux of cold atoms by varying the scattering length or the parameters of the trap potential.

As indicated here, the resonance phenomenon results from the fragmentation of the BEC. Note, however, that fragmentation might happen also in bound systems as already indicated in the literature [25–27]. The fragmentation at open optical and/or magnetic traps occurs as the nonlinear parameter  $U(N)$  takes on a critical value at which the bound-to-resonance state transition takes place. As we show here, the conditions for fragmentation and thus for the bound-to-

resonance transition can be obtained using bound state calculations only.

#### ACKNOWLEDGMENTS

This work was supported in part by the Israel Science Foundation (Grant No. 1152/04), the Fund of Promotion of Research at the Technion, and by the DIP.

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