Tunneling lifetime of trapped condensates

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Abstract

Using the complex scaling transformation we calculate the tunneling lifetime of a condensate inside a magnetic/optical 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.
Tunneling of Bose-Einstein condensates (BEC) through a dynamical potential barrier has been demonstrated in the experiments of Phillips’ group [1]. 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 [2]. In contrast to the previous studies where the tunneling is through a dynamical potential barrier, we discuss here the tunneling of the 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 which is embedded in between potential barriers. Therefore, in the case of a positive scattering length (repulsive atom-atom interactions) a given external open potential well cannot trap a condensate with more than a finite critical number of atoms. As the number of the atoms in the condensate, $N$, is increased, fractions of the condensate can tunnel through the potential barriers.

What is the lifetime of a trapped condensate as $N$ is increased? Can we control the number of atoms in the condensate by varying slightly the scattering length? Using the complex scaling transformation which is based on rigorous mathematical ground [3,4] and has been used before for calculating the lifetimes of metastable states in atomic, molecular and nuclear physics [5,6] we show that the lifetime of the condensates can be calculated and the answer to the other question is positive as well.

For the sake of clarity and without loss of generality let us represent a simple one-dimensional external potential, $V_{\text{ext}}(x) = (x^2/2 - 0.8) \exp(-0.1x^2)$. For a single atom this external potential supports only a single bound state. Consequently, in the absence of interaction between the atoms of the BEC, the condensate can be found permanently trapped inside the potential well or be in one of the metastable states (so called resonances) where the atoms can tunnel out of the trap (see inset in Fig. 1). We shall see that in the presence of repulsive interaction between the atoms the situation changes. Whether the condensate can be in a bound state at all depends on the interaction strength and on the number of atoms.

Before discussing our results we discuss in the following metastable states and how they
are determined by complex scaling in the case of condensates. In hermitian quantum mechanics metastable states are associated with propagation of wavepackets escaping the potential well. However, in quantum scattering theory it is possible to associate metastable states with the solutions of the time-independent Schrödinger equation. The metastable states, as are the bound states, are associated with outgoing boundary conditions. In the case of BEC the metastable states are embedded in the continuum part of the external potential. It is known from scattering theory that outgoing solutions which are embedded in the continuum are obtained only when the wave vector, \( k \), gets complex values \( k = |k| \exp(-i\alpha) \), and hence the eigenvalues of the Hamiltonian, \( \{\mathcal{E}\} \), also become complex quantities [9]. Complex eigenvalues are obtained since the corresponding eigenfunctions diverge exponentially, i.e., \( \Psi_{res} \rightarrow \exp(\pm i|k| \cos(\alpha)x) \exp(\pm |k| \sin(\alpha)x) \rightarrow +\infty \) as \( x \rightarrow \pm \infty \), and are not embedded in the hermitian domain of the Hamiltonian. \( \{\text{Re}\mathcal{E}\} \) are associated with the energies of the metastable system and \( \{-2\text{Im}\mathcal{E}\} \), are associated with the rates of the decay (inverse lifetimes). By complex scaling of the internal coordinates in the Hamiltonian (in our case \( x \rightarrow x \exp(i\theta) \) where \( \theta \geq \alpha \)) the metastable states are taken back into the Hilbert space and become square integrable (like the bound states). This approach enabled developing the quantum theory for non-hermitian Hamiltonians (see the Reviews in Ref. [5]) and Ref. [6].

How to compute the resonances of BEC? The BEC consists of \( N \) atoms that are assumed to have contact potential interactions, \( U_0 \delta(\vec{r}_j - \vec{r}_{j'}) \), where \( U_0 = 4\pi a_0 \hbar^2 / M \) and \( a_0 \) is the s-wave scattering length [7]. To calculate the bound and the resonance (metastable) states, as explained above, we carry out the following similarity transformation [6], \( \mathcal{H}_{BEC} = \hat{S} \hat{H}_{BEC} \hat{S}^{-1} \), where \( \hat{S} \) is the complex scaling operator. The result of the complex scaling transformation is, \( \mathcal{H}_{BEC}(\theta) = -\hbar^2 / 2M \sum_j \left( \exp(-2i\theta) \nabla_j^2 + V_{\text{ext}}(\exp(i\theta)\vec{r}_j) \right) + U_0 \exp(-i\theta) \sum_{j,j' > j} \delta(\vec{r}_j - \vec{r}_{j'}) \). The bound and the resonance states are obtained by solving the complex eigenvalue problem, \( \mathcal{H}_{BEC}(\theta) \Psi(\theta) = \mathcal{E} \Psi(\theta) \), where \( \Psi(\theta) \) are square-integrable functions and \( \mathcal{E} \) are \( \theta \)-independent eigenvalues. The bound states (i.e., \( \text{Im}\mathcal{E} = 0 \)) are obtained in our case for any value of \( 0 \leq \theta < \pi/4 \). The resonance energies and widths per
atom, $\mathcal{E}/N \equiv E - i/2\Gamma$, are obtained when $\pi/4 > \theta > \theta_c$. The value of the critical scaling angle is given by $2\theta_c = \arctan 2E/\Gamma$ [5,6]. Let us return to the statement that $\Psi(\theta)$ are square-integrable functions. As we will see later this is an important point in the derivation of the non-linear Schrödinger equation for complex scaled Hamiltonians. Square integrability implies that the corresponding functions decay exponentially to zero. But this is not enough. We need to define the inner product. In hermitian quantum mechanics where $\hat{H}^\dagger = \hat{H}$ we use the common scalar product. In the case of complex scaled Hamiltonians $\hat{H}^\dagger \neq \hat{H}$. In our case (as in most studied physical cases for complex scaled Hamiltonians [6]), $\mathcal{H}_{BEC}^\dagger(\theta) = \mathcal{H}_{BEC}^*(\theta)$, and therefore the c-product rather than the scalar product should be used [6] such that, $(\Psi_j^*(\theta)|\Psi_j(\theta)) \equiv \langle \Psi_j^*(\theta)|\Psi_j(\theta) \rangle = \delta_{j',j}$, where $\Psi_j^*(\theta)$ and $\Psi_j(\theta)$ are any bound or resonance eigenfunctions of $\mathcal{H}_{BEC}(\theta)$ as defined above. Note that here we assume that for $\theta = 0$ (i.e., hermitian quantum mechanics) the eigenfunctions of $\hat{H}$ are real.

The non-linear Schrödinger equation, also known as the Gross-Pitvavesky equation, is commonly applied to condensates [7]. It is a mean field approximation to the full many-body Hamiltonian of the problem as the Hartree-Fock approximation is for fermions. All atoms are assumed to occupy the same orbital and the total wavefunction is a product of these orbitals [7]. Therefore, $\mathcal{E} = \langle \Psi^*(\theta)|\mathcal{H}_{BEC}|\Psi(\theta) \rangle$, where $\Psi(\theta) = \prod_{j=1}^{N} \phi(\vec{r}_j)$. Minimizing $\mathcal{E}$ with respect to the orbital, keeping in mind the definition of the inner product, leads to the complex scaled version of the non-linear Schrödinger equation:

$$\left( \hat{H}_0(\theta) + U \exp(-i\theta)\phi_\theta^2 \right) \phi_\theta = (\mu - \frac{i}{2} \gamma)\phi_\theta, \quad (1)$$

where, $\hat{H}_0(\theta) \equiv -\hbar^2 \exp(-2i\theta)/2M\nabla^2 + V_{\text{ext}}(\exp(i\theta)\vec{r})$ and $U = U_0(N-1) = (4\pi a_0 \hbar^2)(N-1)/2M$ is the relevant non-linear parameter. The complex chemical potential of the metastable state, $\mu - \frac{i}{2} \gamma$ ($\gamma = 0$ for bound states), is associated with the complex energy of the BEC per atom, $\mathcal{E}/N = E - i/2\Gamma$, as given by,

$$E - \frac{i}{2} \Gamma = \mu - \frac{i}{2} \gamma + \frac{U}{2} \exp(-i\theta) \int_{\text{all-space}} \phi_\theta^4 d\vec{r}. \quad (2)$$

Within the framework of the Gross-Pitvavesky approximation resonances can only be
calculated when the complex scaling transformation is applied to the BEC N-body Hamiltonian before applying the mean field approximation. To see why one cannot apply first the mean-field approximation and only later the complex scaling transformation, we start from the usual Gross-Pitaevsky Hamiltonian and scale it. The result is given by,

\[ H_{GP}(\theta) = \hat{S} \hat{H}_{GP} \hat{S}^{-1} = -\exp(-2i\theta)\hbar^2/2M\nabla^2 + V_{ext}(\exp(-i\theta)r) + U[\hat{S}\phi_{res}^*][\hat{S}\phi_{res}]. \]

The resonance solution of Eq. 1 is square integrable. It is, however, associated with the exponentially diverging unscaled resonance solution, \( \phi_{res} \), such that, \( \phi_{\theta} = \hat{S}\phi_{res} \rightarrow \exp(+i|k|\exp(+i(\theta - \alpha))r) \) where \( \theta > \alpha \). Therefore, \( [\hat{S}\phi_{res}^*][\hat{S}\phi_{res}] = \exp(-i2|k|\sin(\theta)\sin(\alpha)r) \exp(+2|k|\cos(\theta)\sin(\alpha)r) \rightarrow +\infty \) as \( r \rightarrow \infty \). Namely, the complex scaled non-linear potential term \( U[\hat{S}\phi_{res}^*][\hat{S}\phi_{res}] \) appearing in \( H_{GP}(\theta) \) diverges as \( r \rightarrow \infty \) (although \( \phi_{\theta} \) decays exponentially to zero) and its meaning is unclear. For \( U > 0 \) all states become bound and for \( U < 0 \) the potential is unbound from below. Therefore, it is impossible by this approach to get an eigenfunction which is associated with the complex scaled resonance eigenfunction. Note that this difficulty has been avoided in a previous study of bound-resonance state transitions using the Gross-Pitaevsky equation by inserting complex absorbing potentials in the regions where it has been assumed that the atoms do not interact with one another [8]. However, here we do not use this approximation and the atoms can interact everywhere and not only inside the external potential well.

We solved Eq. 1 for the 1D potential defined above, by increasing adiabatically the non-linear parameter \( U \). We used 400 particle-in-a-box basis functions as a basis set with the box size of \( L = 50 \, a.u. \). In each step of the calculations we carried out self-consistent field iterative calculations to get converged results in 8 significant figures where the scaling angle \( \theta \) has been varied from 0.3rad to 0.7rad. By solving Eq. 1 we calculated the complex chemical-potential, \( \mu - i/2\gamma \) and by solving Eq. 2 we computated the complex-energy per atom \( E/N = E - i/2\Gamma \).

In Fig. 1 we show \( \Gamma \) and \( \gamma \) as functions of \( U \). We mark by arrow the critical value \( U_c = 0.8279 \) for which the bound-resonance transition occurs. For \( U < U_c \) the system is bound, i.e. trapped forever in the well, and for \( U > U_c \) it is metastable and tunneling.
through the barriers occurs. The trap potential is depicted in the inset of the figure. The corresponding real parts $\mu(U)$ of the chemical potential and $E(U)$ of the energy are shown in Fig. 2 as functions of $U$. As one can see, at the critical value $U_c$ where the resonances are "born" the chemical potential vanishes, $\mu_c = \mu(U_c) = 0$. This is an expected result. We may interpret $\mu$ as the energy needed to take a single atom of the condensate out of the potential well. $\gamma$ is the corresponding rate of decay, i.e. $1/\gamma$ is the tunneling time of a single atom with a chemical potential $\mu$. The lifetime of the BEC resonance state is $1/(N\Gamma)$, which can be short if the condensate possesses many atoms. In a condensate all atoms are equivalent and each of them can tunnel with the same probability. Interestingly, $\Gamma > \gamma$ for all values of the non-linear coupling $U > U_c$ as can be seen in Fig. 1. The reason is presumably that $1/\Gamma$ is the lifetime per particle, and each of the BEC’s particles can tunnel through the barrier in different ways, as a single particle or together with several other equivalent particles. As mentioned above, $1/\gamma$, on the other hand, is associated with the tunneling of a single atom only.

How to visualize the decay of a many-body system like a BEC? Once the BEC is in a metastable state, a fraction of the atoms consisting of $(1-X)N$ atoms tunnels out of the potential well into the continuum. This leads to a stabilization of the system where $XN$ atoms remain in the trap. Since all the atoms in the trap repel each other, the energy of the $XN$ atoms is lower than that of the $N$ atoms. Tunneling proceeds until the fraction of atoms which remains in the trap forms a bound state. The number of atoms which will tunnel clearly depends on the energy of the condensate. However, within the framework of the Gross-Pitaevski mean-field approximation the non-linear parameter is $U = U_0(N - 1)$ where $N$ is the total number of atoms, and one cannot tell at a given value of $U$ which fraction of $N$ will tunnel. As we will show below we can enlighten this problem by taking into consideration the idea that not always the best mean-field for condensates is obtained for the case where all identical bosons of a condensate reside in a single orbital [10].

We consider here the scenario where the ground state $\Psi$ is a product of two types of spatial orbitals. There are $n_1$ atoms which occupy the $\phi$ orbital and $n_2 = N - n_1$ atoms occupy the
χ orbital. We associate the $n_1$ atoms in the orbital $\phi$ with the fraction of the condensate $X = n_1/N$ which are 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. Since $U = U_0(N - 1) \sim U_0 N$, the energy per atom in the trap $E_\phi(X, U)$ is nothing but $E(XU)$ which is reported in Fig. 2. 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 $E_{\text{BEC}}(X, U) =XE(XU) + (1 - X)E_\chi((1 - X), U)$. Because our condensate is repulsive, the energy $E_\chi$ is known to be equal to zero \cite{7} and we obtain the final result,

\begin{equation}
E_{\text{BEC}}(X, U) = XE(XU), \tag{3}
\end{equation}

which makes clear that $E_{\text{BEC}}(X, U)$ can be derived from the curve $E(U)$ in Fig 2. In complete analogy the rate of decay into the continuum per atom corresponding to $E_{\text{BEC}}(X, U)$ is given by $X\Gamma(XU)$ and is also already computed, see Fig. 1.

While for a given value of $U$ the Gross-Pitaevsky energy $E(U)$ is just a number and does not provide us with the knowledge on how many atoms have tunneled, $E_{\text{BEC}}(X, U)$ is the key to this information. In Fig. 3 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 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. 3 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 is thus 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 $E_{\text{BEC}}$ takes on 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 non-zero at the bound-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. 3- 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. 3 can be computed via Eq.3 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 [10] used above to derive Eq. 3.

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 [11], leads to an increase of \( U \) and hence to a reduction of the number of atoms inside the potential well (see Fig. 3). 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. 3 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.
REFERENCES

[1] W. K. Hensinger et al., Nature (London) 412, 52 (2001).

[2] V. Averbukh et al., Phys. Rev. Lett. 89, 253201 (2002).

[3] E. Balslev, J. M. Combes, Commun. Math. Phys. 22, 280 (1971).

[4] B. Simon, Commun. Math. Phys. 27, 1 (1992); Ann. Math. 97, 247 (1973).

[5] W. P. Reinhardt, Annu. Rev. Phys. Chem. 33, 223 (1982).

[6] N. Moiseyev, Physics Reports, 302, 211 (1998).

[7] F. Dalfovo et al., Rev. Mod. Phys., 71, 463 (1999).

[8] N. Moiseyev et al., J. Phys. B 37, L193 (2004).

[9] J.R. Taylor, “Scattering Theory: The Quantum Theory of Non-relativistic Collisions”, John Wiley & Sons, Inc. (1972).

[10] L. S. Cederbaum and A. I Streltsov, Phys. Lett. A 318, 564 (2003).

[11] C. A. Regal et al, Phys. Rev. Lett. 92, 040403 (2004).
FIG. 1. The rate of decay $\gamma$ of a single atom and the total rate of decay per atom $\Gamma$ as a function of the non-linear parameter $U$ (see Eq. 1 and text). The inset shows the external trap potential used.

FIG. 2. The chemical potential $\mu$ (the real part of the complex eigenvalue in Eq. 1) and the mean-field energy of the BEC per atom $E$ (the real part of the complex energy $\mathcal{E}/N$, see Eq. 2 in the text) as a function of the non-linear parameter $U$. 
FIG. 3. The energy per atom $E_{BEC}(X,U)$ as a function of the fraction of atoms $X$ which remains in the trap while a fraction $1-X$ of the condensate has tunneled through the barriers into the continuum. Each curve shown is for a different value of the non-linear parameter $U$. From bottom to top the $j$-th curve in black is associated with $U=0.5 + 0.05(j-1)$. The blue curve is for $U = U_c$. The minima of the $E_{BEC}$ curves are at $X=X_c$ (solid dots) and play a central role in understanding the tunneling (see text).