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LETTER TO THE EDITOR

Transition from resonances to bound states in nonlinear systems: application to Bose–Einstein condensates

Nimrod Moiseyev[1,5], L D Carr[2,6], Boris A Malomed[3] and Y B Band[4]

[1] Institute of Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 01238, USA
[2] Laboratoire Kastler Brossel, Departement de physique, Ecole normale supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France
[3] Department of Interdisciplinary Studies, Faculty of Engineering, Tel Aviv University, Tel Aviv 69978, Israel
[4] Departments of Chemistry and Electro-Optics, Ben-Gurion University of the Negev, Beer-Sheva, 84105, Israel

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Abstract

It is shown using the Gross–Pitaevskii equation that resonance states of Bose–Einstein condensates with attractive interactions can be stabilized into true bound states. A semiclassical variational approximation and an independent quantum variational numerical method are used to calculate the energies (chemical potentials) and linewidths of resonances of the time-independent Gross–Pitaevskii equation; both methods produce similar results. Borders between the regimes of resonances, bound states and, in two and three dimensions, collapse are identified.

Resonances are metastable quantum states which have finite lifetimes; they play a key role in different types of scattering phenomena [1]. Simon *et al* [2] provided conditions for sharp transitions from a resonance to a true bound state as a parameter in the system's Hamiltonian is varied. These quantum phase transitions have been studied theoretically and experimentally in the context of the linear Schrödinger equation [3]. Our objective here is to search for similar transitions in nonlinear systems, such as Bose–Einstein condensates (BECs) [4]. In particular, we address the question of whether resonance states of a BEC with attractive binary atomic interactions can be stabilized into bound states by making the effective nonlinearity increasingly negative (through increase of the number of atoms, or tuning the s-wave scattering length a_s near a Feshbach resonance to be more negative). As the existence and stability of eigenfunctions of nonlinear wave equations is also a central issue in other fields, and nonlinear Schrödinger-type equations apply to many of them, including nonlinear optics, spin waves in

[5] Permanent address: Department of Chemistry and Minerva Center for Nonlinear Physics of Complex Systems, Technion—Israel Institute of Technology Haifa 32000, Israel.
[6] Present address: JILA, National Institute of Standards and Technology and Physics Department, University of Colorado, Boulder, CO 80309-0440, USA.

magnetic films, Langmuir waves in hot plasmas and gravity surface waves in fluids, the study of the effect of nonlinearity on resonances is of general physical interest.

We develop two independent complementary approaches to this problem. The first utilizes a variational Gaussian ansatz for the quasi-stationary state and the WKB approximation to calculate the tunnelling rate. The second utilizes a fully quantum variational method with an absorbing potential, which, in the case of the linear Schrödinger equation, may be shown formally [5] to be equivalent to the exterior scaling transformation [6]. We note parenthetically that complex scaling has been previously used to predict resonances for nonlinear Hartree–Fock models arising in electronic structure calculations of atoms and molecules [7]. In both approaches, we seek to determine the energies and linewidths of resonance states of the Gross–Pitaevskii equation (GPE), which is a nonlinear Schrödinger equation (NLS), derived in the mean-field approximation. In the context of the BEC, the 'energy' may be interpreted as the chemical potential which is the real part of the eigenvalue associated with a resonance state, i.e., $\mathrm{Re}(\mu)$. The 'linewidth' γ may be interpreted as the coefficient in the rate equation, $\mathrm{d}N/\mathrm{d}t = -\gamma(N)N$, where N is the number of trapped atoms in the BEC and $\gamma(N) = -2\,(\mathrm{Im}(\mu))\,/\hbar$ is the decay rate. We emphasize that $\mathrm{Im}(\mu)$ is a function of N: thus the tunnelling problem associated with the decay of the resonance is a nonlinear one, and the lifetime of a resonance can be obtained by integrating $\mathrm{d}N/[-\gamma(N)N]$. In the BEC, such nonlinear tunnelling problems have been studied theoretically for bright solitons [8] and experimentally in the context of the relaxation of condensate spin domains [9].

The two general methods are applied to the specific case of an external potential in the form of a harmonic well multiplied by a Gaussian envelope. This choice of the potential is motivated by studies of optically trapped BECs [10], where the waist of the trapping laser beam creates a broad Gaussian envelope. The central harmonic well may be created by a second, more narrowly focused laser beam, or by a higher Hermite–Gauss mode of the laser, as used in creating BEC waveguides [11], or by a laser beam with embedded vorticity induced by passing the beam through a phase mask [12]. The lifetime given by tunnelling of a quasi-bound resonant state can be reduced by other loss processes, such as three-body recombination and interactions with the background gas in the vacuum, as in the case for any trapped BEC. However, as these loss processes are the same for both resonant and bound states, tunnelling of the mean field can cause a measurable reduction in lifetime. An external potential in the GPE is similar to the waveguiding profile created by a transverse modulation of the refractive index that appears in the generalized NLS used for modelling propagation of spatial beams in optical media in effectively 1D (planar waveguide) and 2D (bulk) geometries [13]. The potential that we introduce below corresponds to the waveguiding profile that can be easily engineered in optical media.

The time-independent isotropic GPE with such an external potential can be written in terms of dimensionless variables scaled to the harmonic oscillator frequency ω and length $\ell_{\mathrm{ho}} \equiv \sqrt{\hbar/m\omega}$ as

$$-[\Psi'' + (D-1)\Psi'/r]/2 + V(r)\Psi + U_0|\Psi^2|\Psi = \mu\Psi, \tag{1}$$

$$V(r) = (V_0 + r^2/2)\exp(-\alpha r^2), \tag{2}$$

$$\beta_D \int_0^\infty \mathrm{d}r\, r^{D-1}|\Psi|^2 = 1. \tag{3}$$

Here $\Psi(r)$ is the normalized wavefunction, μ is the above-mentioned complex eigenvalue, $\beta_{1,2,3} = 2, 2\pi, 4\pi$ for the spatial dimension $D = 1, 2, 3$, and $U_0 \propto a_s N$ is the appropriately scaled nonlinearity coefficient in dimension D [20], with a_s the s-wave scattering length. The prime stands for $\mathrm{d}/\mathrm{d}r$, and $\alpha \equiv (\ell_{\mathrm{ho}}/\ell_{\mathrm{Gauss}})^2$ is a parameter which characterizes the structure

of the potential. For a broad Gaussian envelope, which pertains to the experimentally available optical trap described above, $\alpha \ll 1$.

Variational WKB approach. Approximate solutions to equation (1) with potential (2) can be obtained via variational methods. We adopt a Gaussian ansatz, $\Psi_{\rm an}(r) = A\exp[-r^2/(2\rho^2)]$, where the width ρ and amplitude A are variational parameters. Substituting the ansatz into the normalization condition (3) and the Lagrangian of the GPE (for the time being, $\mathrm{Im}(\mu)$ is disregarded) and minimizing it with respect to ρ and A, one obtains $A^2 = 2/[\beta_D \rho^D \Gamma(D/2)]$, and

$$\mathrm{Re}(\mu) = \{(-4+D)/\rho^2 + (1+\alpha\rho^2)^{-2-D/2}[4V_0 + (4+D)\rho^2 - \alpha(D+4V_0\alpha)\rho^4]\}/4, \tag{4}$$

$$|U_0| = \Gamma(D/2)2^{-2+D/2}\beta\rho^{-2+D}(1+\alpha\rho^2)^{-2-D/2} \times \{-2(1+\alpha\rho^2)^{2+D/2} + \rho^4[2 - 4V_0\alpha - \alpha(D+4V_0\alpha)\rho^2]\}, \tag{5}$$

where $\Gamma(D/2)$ is a Gamma function. The solution is stable in the framework of the time-dependent GPE if $\mathrm{dRe}(\mu)/\mathrm{d}|U_0| \leqslant 0$, which is known as the Vakhitov–Kolokolov criterion [14].

One can now apply the WKB approximation to find $\mathrm{Im}(\mu)$ [15]. In the 1D case, it is given by the standard expressions

$$\gamma = \exp\left(-2\left|\int_{r_1}^{r_2} \mathrm{d}r\, p(r)\right|\right) \Big/ T, \tag{6}$$

$$p = \sqrt{2[\mu - V_{\rm eff}(r)]}, \qquad T = 4\left|\int_0^{r_1} \mathrm{d}r/p(r)\right|, \tag{7}$$

where $V_{\rm eff}(r) \equiv [V(r) + U_0|\Psi(r)|^2]$, and the endpoints $r = r_1$ and $r = r_2$ are found from $p(r) = 0$. In the 2D and 3D cases, it is necessary to transform the GPE into a 1D form via $\Psi = \phi/\sqrt{r}$ and $\Psi = \phi/r$, respectively (for the spherical wave). In the former case, this yields $V_{\rm eff}(r) = V(r) - (1/8)r^{-2} + U_0 r^{-1}|\phi^2|$, whereas in the latter, $V_{\rm eff}(r) = V(r) + U_0 r^{-2}|\phi^2|$. Note that $\mathrm{Im}(\mu) = -\gamma/2$ in these units; also, γ must be multiplied by 2 in the 1D case to account for tunnelling from both sides of the well. Results for the 1D, 2D and 3D cases are illustrated in the figures below.

Exterior complex scaling of the GPE. In the linear Schrödinger equation ($U_0 = 0$), resonances are associated with complex eigenvalues of the Hamiltonian which are obtained by imposing outgoing-wave boundary conditions on Ψ. Such eigenvectors are sometimes called Siegert states. They are not in the Hilbert space, hence the Hamiltonian is a *non-Hermitian* operator over the class of functions including the Siegert states. In order to calculate resonances, it is convenient to carry out a similarity transformation which 'brings back' the resonances to the Hilbert space. A well-known transformation of this kind is complex scaling, wherein the coordinates are rotated into the complex plane by a fixed angle θ [16, 17]. When θ is sufficiently large, the resonance eigenfunctions become square-integrable. Although the complex eigenvalues are θ-independent, provided $\tan(2\theta) > \gamma/[2\mathrm{Re}(\mu)]$, the corresponding resonance eigenfunctions do depend on θ: therefore the nonlinearity prevents direct application of complex scaling to the GPE. However, with the use of exterior [6] or smooth exterior scaling [18, 19], the potential $V(r)$ remains unscaled except at large r, and the small distortion of the effective nonlinear potential, $U_0|\Psi|^2$, may be neglected.

It has been shown for the linear Schrödinger equation that smooth exterior scaling transformations are equivalent to adding a reflection-free complex absorbing potential (CAP)

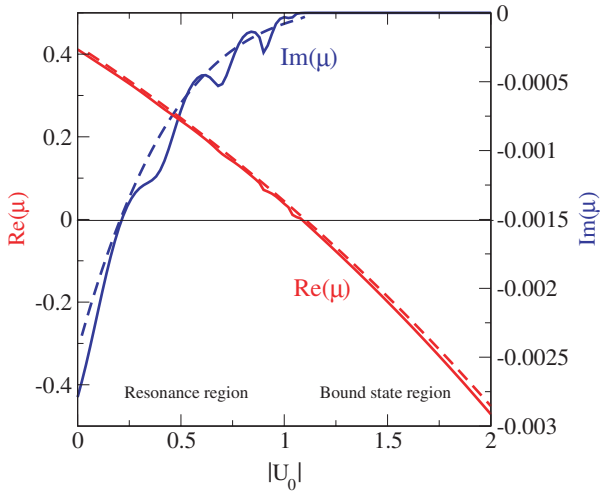

Figure 1. *One dimension.* Shown is the Re(μ) and Im(μ) versus $|U_0|$ for the potential in the form of a harmonic well times the Gaussian envelope (see equation (2)), with $\alpha \equiv (\ell_{\rm ho}/\ell_{\rm Gauss})^2 = 0.2$. Solid curves: results of the numerical method utilizing a complex scaling method. Dashed curves: the variational WKB approximation. The critical point for the conversion of the resonance into a bound state is $\left|U_0^{\rm crit}\right| = 1.09$.

to the Hamiltonian [19], which is often approximated by a local negative imaginary potential. We chose $V_{\rm CAP}(r) = -{\rm i}\lambda(r - r_0)^4$, if $r > r_0$, and $V_{\rm CAP}(r) = 0$, if $r \leqslant r_0$, where r_0 is a point near the edge of the grid, and λ is a variational parameter (unrelated to the above variational approximation). This CAP is the most common one used in calculations of resonances in atoms, molecules and nuclei. The value of λ is found numerically from the variational condition ${\rm d}\mu/{\rm d}\lambda = 0$, where μ is generally complex, and stationary solutions with respect to small variation of λ are obtained; note that stationary solutions in the λ-variational space requires optimization of another parameter, such as the box size in physical space, L (see the 'cusp' condition in [16]). The value of r_0 is chosen so that the wavefunction is exponentially small for $r > r_0$; this ensures that the smooth exterior scaling transformation does not distort the effective potential $V_{\rm eff}(r)$ (for a detailed discussion of this point, see [5, 19] and references therein).

In our calculations, sinusoidal functions were used as a basis set in the 1D and 3D cases, and Bessel functions in 2D. Starting from zero, the nonlinear strength parameter U_0 was decreased in steps of $\delta U_0 < 0$, so that the overlap between the solutions for U_0 and $U_0 + \delta U_0$ was close to unity, to ensure that the evolution of a single resonance was followed. Thus, resonances could be identified by the CAP method, at each step of the iteration, in the same manner as in linear quantum mechanics.

GPE resonances and bound states. Consider first the case of one dimension and no offset, i.e., $D = 1$ and $V_0 = 0$. No bound states and a single resonance exist in this potential for the linear Schrödinger ($U_0 = 0$); the latter has Re(μ) = 0.411 34 and Im(μ) = −0.002 7894. Beginning with this known result, the Re(μ) and Im(μ) were calculated numerically as a function of the nonlinear parameter U_0 by adiabatically decreasing the nonlinear parameter from zero. These numerical results, and those obtained via the above analytical methods, are displayed in figure 1. The transition from the resonance to a true bound state occurs at $U_0^{\rm crit} = -1.09$. It is noteworthy that, despite the well-known fact that any 1D symmetric

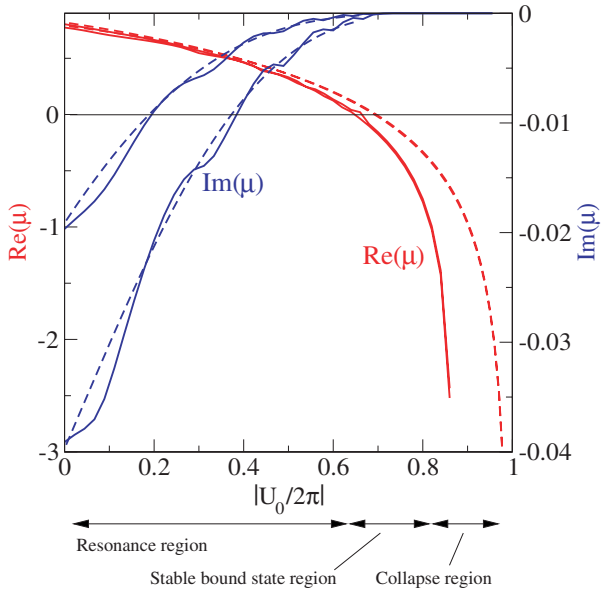

Figure 2. *Two dimensions.* Same as in figure 1 for two different values of the potential-shape parameter, $\alpha = 0.16$ and $\alpha = 0.18$ (the upper and lower curves, respectively; the analytical curves for $\mathrm{Re}(\mu)$ at both values of α completely overlap). Regions of the resonance, bound state and collapse are indicated.

potential with minimum below the asymptotic value of the potential gives rise to at least one bound state in linear quantum mechanics, the *nonlinear* 1D GPE creates a bound state only if $-U_0 \geqslant \left|U_0^{\mathrm{crit}}\right|$ (i.e., if $U_0 \leqslant U_0^{\mathrm{crit}}$).

In the 2D case with $V_0 = 0$, the numerical solution of equations (4) and (5) shows that a resonance or bound state can exist for $\alpha < \alpha_c = 0.192\,45$, where the tunnelling rate diverges as $\alpha_c - \alpha \to +0$. For $\alpha \geqslant \alpha_c$, the potential walls are too thin to retain the condensate. The cases of $\alpha = 0.18$ and $\alpha = 0.16$ are shown in figure 2. The numerical study demonstrates that collapse occurs at the point $U_0^{\mathrm{coll}}/(2\pi) = -0.86$, while the variational approximation gives a result 13% larger (because the above ansatz is a poor approximation near the collapse, see [8] and references therein). The transition from the resonance to a bound state takes place at the point $U_0^{\mathrm{crit}}/(2\pi) = -0.66$. These values vary slightly with α.

In the 3D case, we again start by considering $V_0 = 0$. Varying α, we found that resonances never turn into bound states as the nonlinearity coefficient U_0 is made more negative. Instead, the condensate collapses[7], as shown in figure 3; the variational approximation produces exactly the same result (details are not displayed here). It is not surprising that collapse sets in after the stabilization of the bound state in the 2D case (figure 2), while this does not happen in 3D: as is well known, the cubic nonlinearity gives rise to weak and strong collapse in 2D and 3D, respectively (the nonlinear term of the effective potential in 2D and 3D is $U_0 r^{-1}|\phi|^2$ and $U_0 r^{-2}|\phi|^2$, respectively).

The above result for the 3D case may be understood as follows: the variational approximation with the Gaussian ansatz shows that the chemical potential at the collapse point in the isotropic 3D harmonic well *without* a Gaussian envelope is $\mu^{\mathrm{coll}} = 0.224$. Since this value is greater than zero, and the full potential has $V(\infty) = 0$, it is not possible to

[7] What actually happens in the case of collapse cannot be determined within the mean-field description. We do not address this issue here.

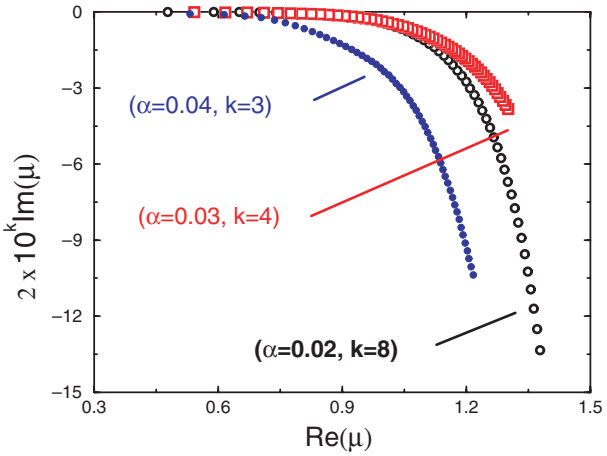

Figure 3. *Three dimensions.* The width of the resonance states versus energy for three different wells with $V(0) = V(\infty)$ (i.e., $V_0 = 0$): $\alpha \equiv (\ell_{\rm ho}/\ell_{\rm Gauss})^2 = 0.02, 0.03$ and 0.04. For the definition of k, see the label attached to the vertical axis. In each case, the collapse point is reached before the resonance can be stabilized into a bound state. The variational WKB approximation produces similar results (not shown here).

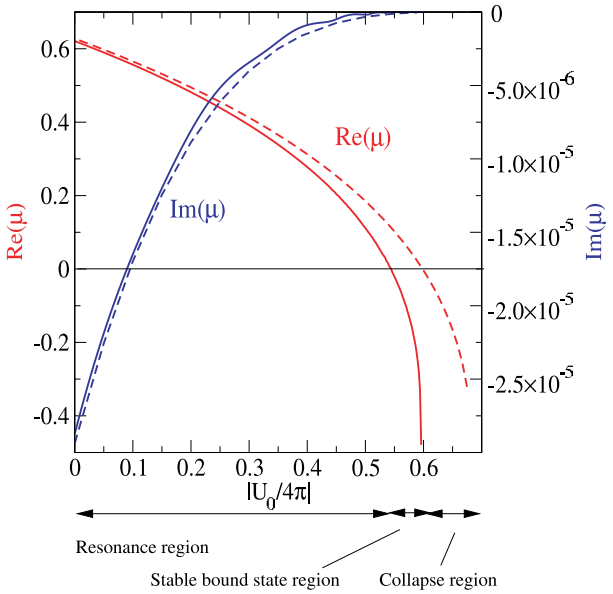

Figure 4. *Three dimensions.* Same as in figure 1 for the potential (2) with $\alpha = 0.02$ and $V_0 = -0.8$ (so that $V(0) = V(\infty) - 0.8$). The offset $V_0 < 0$ allows for the stabilization of the resonance into a bound state, unlike the case shown in figure 3.

transform a resonance into a bound state. However, lowering $V(0) \equiv V_0$ (see equation (2)) with respect to $V(\infty)$ makes such a transition possible. To illustrate this, the case of $V_0 = -0.8$ and $\alpha = 0.02$ is shown in figure 4. The corresponding potential (2) has a single resonance and no bound states in the linear limit ($U_0 = 0$). The figure shows that, as $|U_0|$ increases, the width and energy of the resonance decrease, and indeed the resonance is stabilized into

a bound state at the point $U_0^{\rm crit}/(4\pi) = -0.552$. As in the 1D and 2D cases, the variational WKB approximation provides for reasonable accuracy, as compared to the numerical results.

Clearly, our two independent methods may also be used to address the question of whether BECs with *repulsive* nonlinearity have a critical point beyond which bound states trapped in a potential well destabilize into resonances as the nonlinearity is increased.

In conclusion, we have demonstrated within a mean-field approximation that resonances in a BEC can be transformed into true bound states, as the strength of the attractive nonlinearity increases beyond a critical value $\left|U_0^{\rm crit}\right|$. Borders between three different dynamical regimes, namely resonances, bound states and collapse, have been delineated. In 1D, resonances can always be stabilized into bound states, as collapse is not possible. In 2D, we find that the transition of the resonance into a bound state can be readily achieved before collapse occurs, as the collapse is weak in this case. However, in 3D, where collapse is strong, the critical value for the transition, $\left|U_0^{\rm crit}\right|$, can be made smaller than the collapse threshold, $\left|U_0^{\rm coll}\right|$, only if $V(0) < V(\infty)$, i.e., the floor of the potential well is lower than at infinity. In optically trapped BECs, this can be achieved by means of depression of the effective potential well with a red-detuned laser.

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