Trapping, tunneling & fragmentation of condensates in optical traps

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N. Moiseyev, L. D. Carr, B. A. Malomed, and Y. B. Band,
Transition from resonances to bound states in nonlinear systems: Application to Bose-Einstein condensates.
Journal of Physics B, (2004), 37(9), L193-L200.

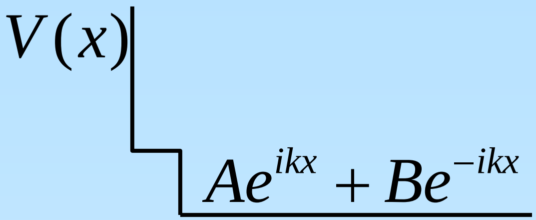
L.S. Cederbaum and N. Moiseyev,
On the collapse and restoration of condensates in n dimensions in the mean-field approximation.
Israel Journal of Chemistry (2003), 43(3-4), 267-277.

N. Moiseyev and L. S. Cederbaum,
Tunneling lifetime of trapped condensates.
Los Alamos National Laboratory, Preprint Archive, Condensed Matter (2004), 1-11, arXiv:cond-mat/0406189.

Resonances

- **Are localized metastable states with finite lifetime.**
- **In Hermitian Quantum Mechanics resonances cannot be represented by a single state of the Hamiltonian.**
- **The resonance is depicted by a large density of states around the resonance energy.**
- **Resonances are associated with the complex poles of the scattering matrix.**

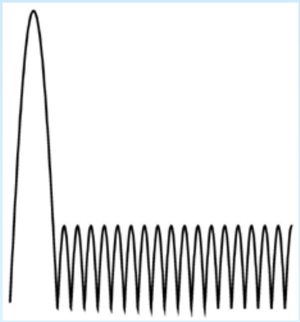
Hermitian QM



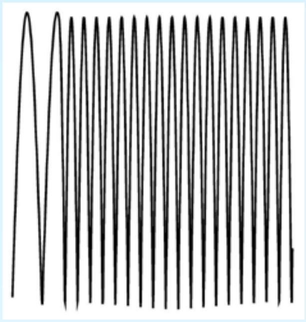
$$E = \frac{(\hbar k)^2}{2m} \qquad E > 0$$

continuous spectrum

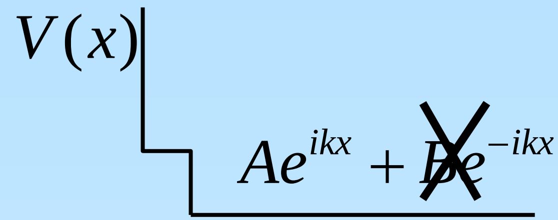
$$E = \varepsilon_1^{res} \pm \Gamma$$



E-between resonances



Non Hermitian QM

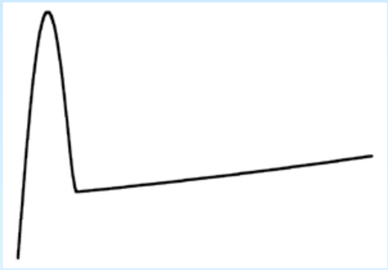


$$E = \varepsilon_n - \frac{i}{2}\Gamma_n$$

discrete spectrum
resonances

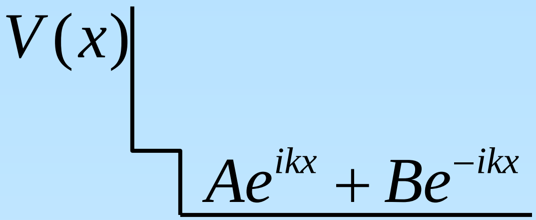
$$E = \varepsilon_1 - \frac{i}{2}\Gamma_1$$

$$k = |k| e^{-i\varphi}$$



Hermitian QM	Non Hermitian QM

Hermitian QM



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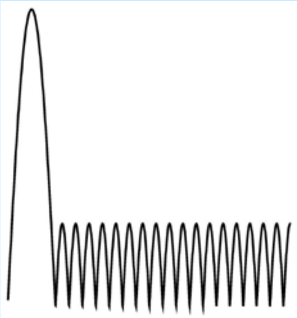
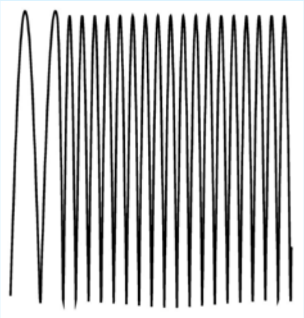
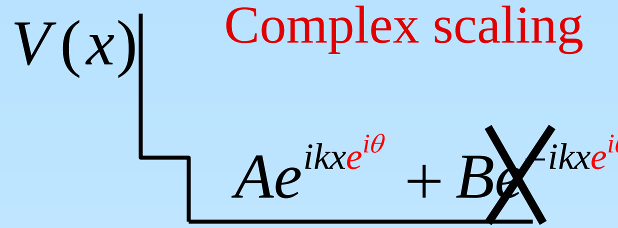


E-between resonances



Non Hermitian QM

Complex scaling



$$E = \varepsilon_n - \frac{i}{2}\Gamma_n$$

discrete spectrum resonances

$$E = \varepsilon_1 - \frac{i}{2}\Gamma_1$$

$$k = |k| e^{-i\varphi}$$

$$k = |k| e^{-i\varphi} e^{i\theta}$$

continuum: $Ae^{ikxe^{i\theta}} + Be^{-ikxe^{i\theta}}$

to avoid divergence-

$$k = |k| e^{-i\theta} \quad \Rightarrow \quad E = |E| e^{-2i\theta}$$

Complex Scaling

In order to avoid the divergence of the resonance wavefunction it is convenient to scale the coordinate such that : $x \rightarrow xe^{i\theta}$

This can be done by the following scaling operators:

$\hat{S} \longrightarrow e^{i\theta x \frac{\partial}{\partial x}}$ **Such that** $\hat{S}\psi_{res} \rightarrow 0$ **as** $x \longrightarrow \infty$

The Schrodinger equation takes the form:

$$(\hat{S}\hat{H}\hat{S}^{-1})(\hat{S}\psi) = E(\hat{S}\psi) \quad \Rightarrow \quad \tilde{H}_\theta \tilde{\psi}_\theta = E_\theta \tilde{\psi}_\theta$$

Complex scaling: Reviews

W. P. Reinhardt, Annu. Rev. Phys. Chem. **33**, 223 (1982)

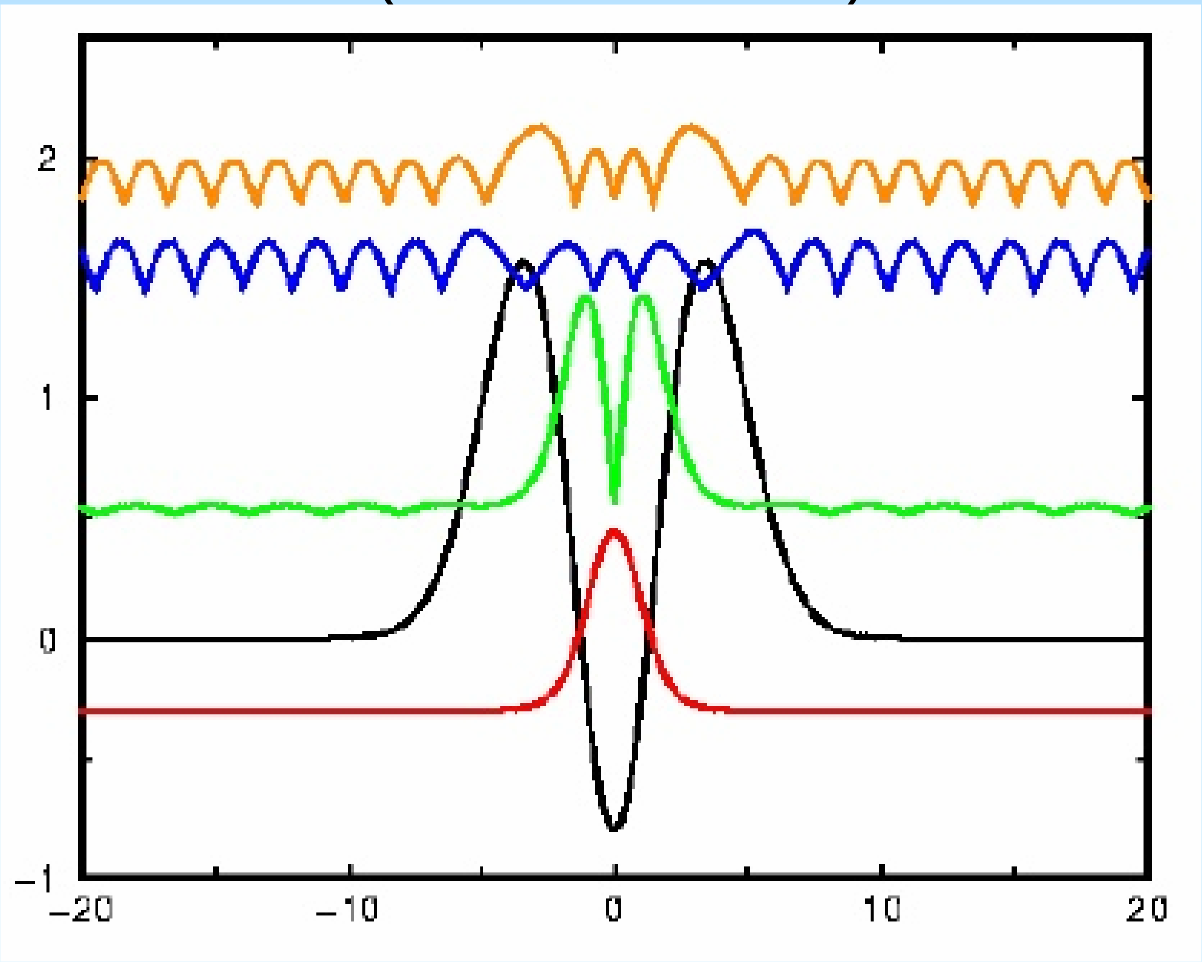
N. Moiseyev. Phys. Rep. **302**, 211 (1998)

Reflection free CAPs by the Smooth-Exterior-Scaling transformation

N. Moiseyev, J. Phys. B, **31**, 1431, (1998)

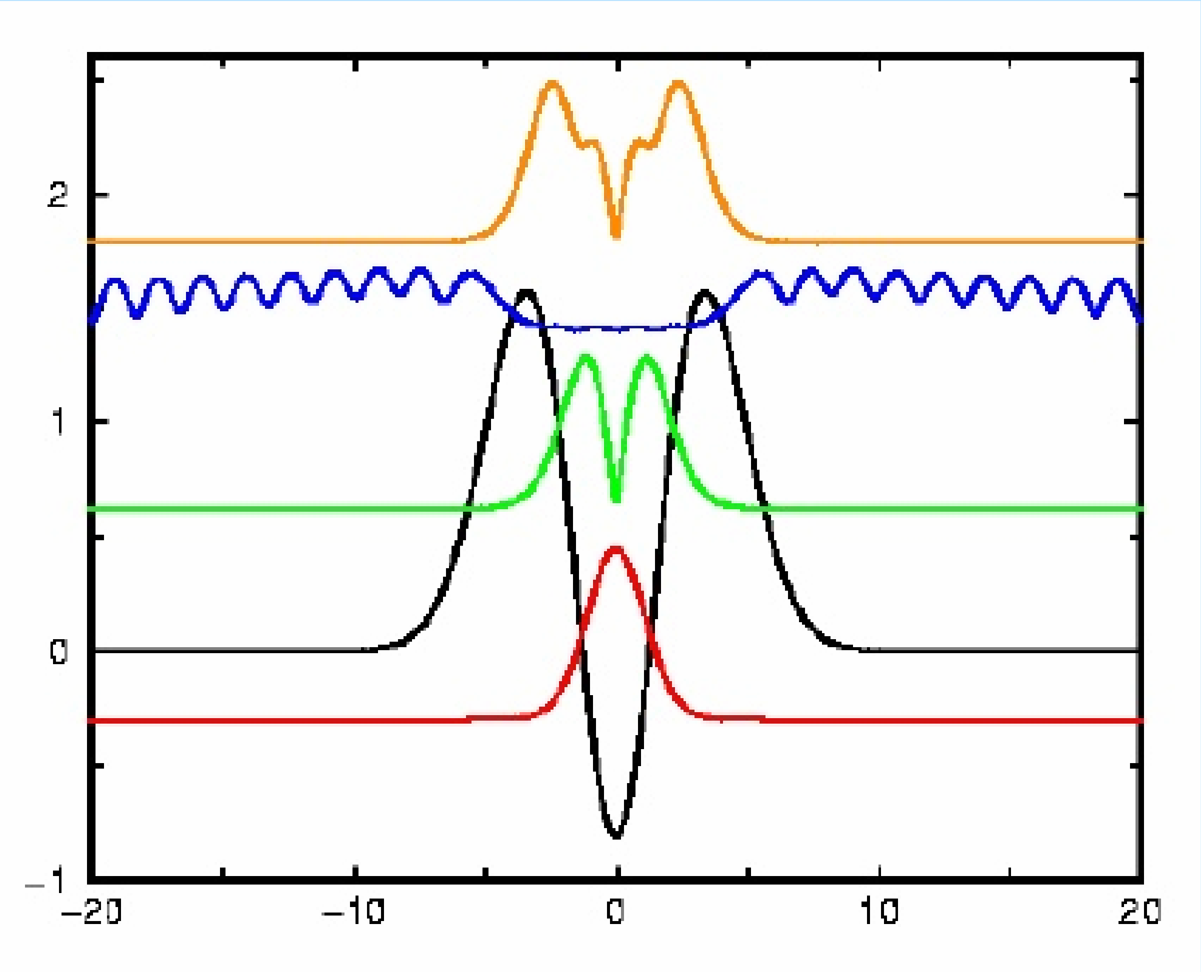
Hermitian (conventional) QM variational calculations

(numerical exact)

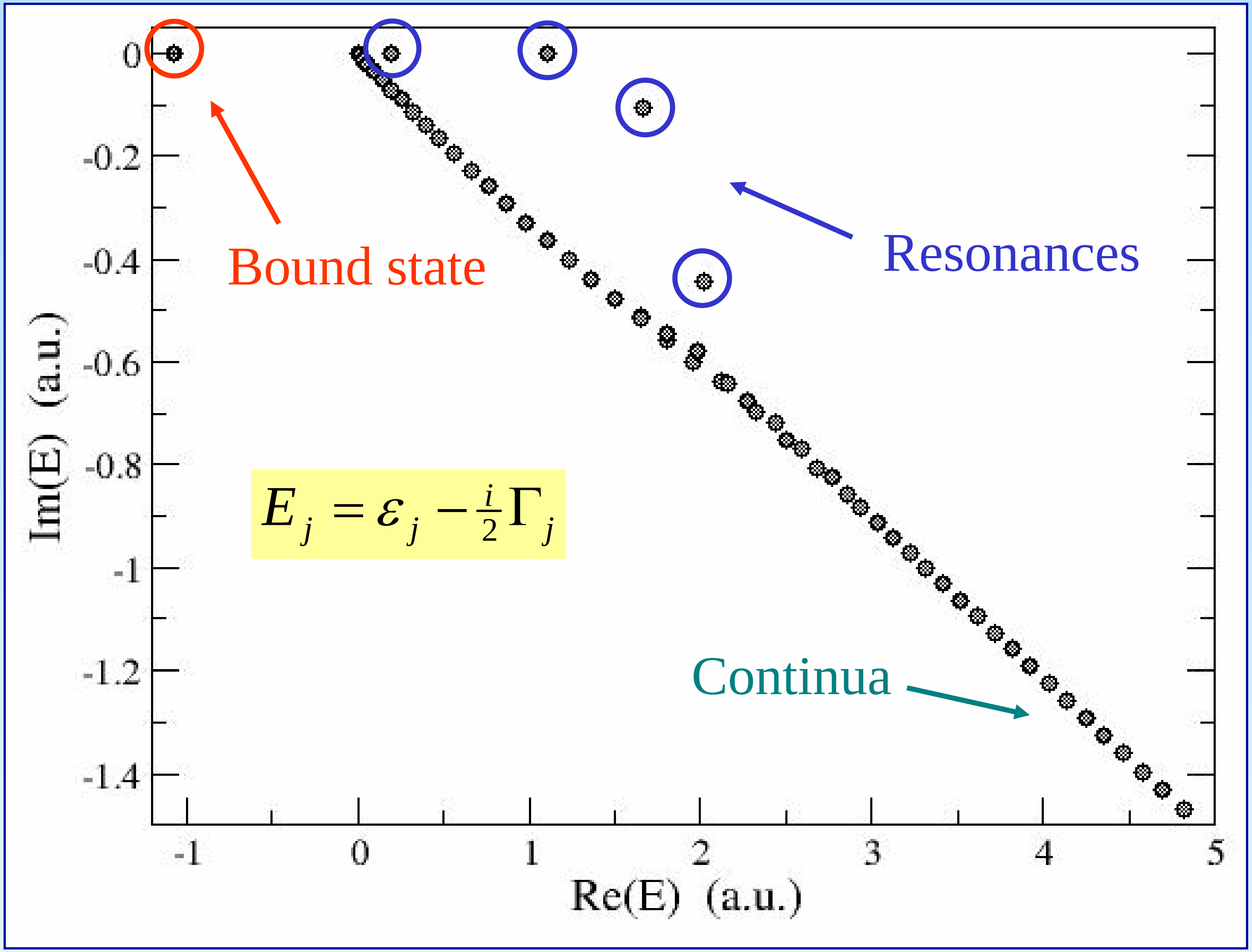


Bound, resonance, continuum states for 1-atom in 1D trap

Non-hermitian QM variational calculations



Bound, tunneling resonance, continuum and above-barrier resonance states



Non-interacting atoms in 1D optical trap

(odd-parity resonances obtained in 3D spherical symmetric potential)

BEC-model Hamiltonian

$$\left(T + \sum V(\vec{r}_j) + \frac{a_0}{2} \sum_{j=1}^{N} \sum_{j' \neq j}^{N} \delta(\vec{r}_j - \vec{r}_{j'}) \right) \psi = \varepsilon \psi$$

GP: $\psi = \phi(\vec{r}_1) \ldots . \phi(\vec{r}_N)$ $\qquad U = a_0 (N-1)$

$$\left(T + V(\vec{r}) + \frac{U}{2} |\phi(\vec{r})|^2 \right) \phi = \mu \phi \qquad E = \frac{\varepsilon}{N} = \mu - \frac{U}{2} \int |\phi(\vec{r})|^4 \, d\vec{r}$$

$$if \quad N > N_c \quad (GP: \; U > U_c)$$

$a_0 > 0$ Bound to resonance state transition

$a_0 < 0$ Resonance to bound state transition

OPEN QUESTIONS

- How resonances can be calculated for the NLSE (GP)?
- In 3D , negative scattering length BEC: are the resonance/bound-state transitions take place before the collapse of the BEC ?
- How the fraction of the atoms that are tunneled through the external potential barriers can be extracted from the GP calculations ?

How resonances can be calculated for the NLSE (GP)?

A: Complex scaling:

$$\vec{q}_j = \vec{r}_j e^{+i\theta} \quad T_\theta = e^{-2i\theta}\sum_j T_{\vec{r}_j} \quad V_\theta = \sum_j V(\vec{r}_j e^{+i\theta}) \quad \delta(\vec{q}_{j'} - \vec{q}_j) = e^{-i\theta n}\delta(\vec{r}_{j'} - \vec{r}_j)$$

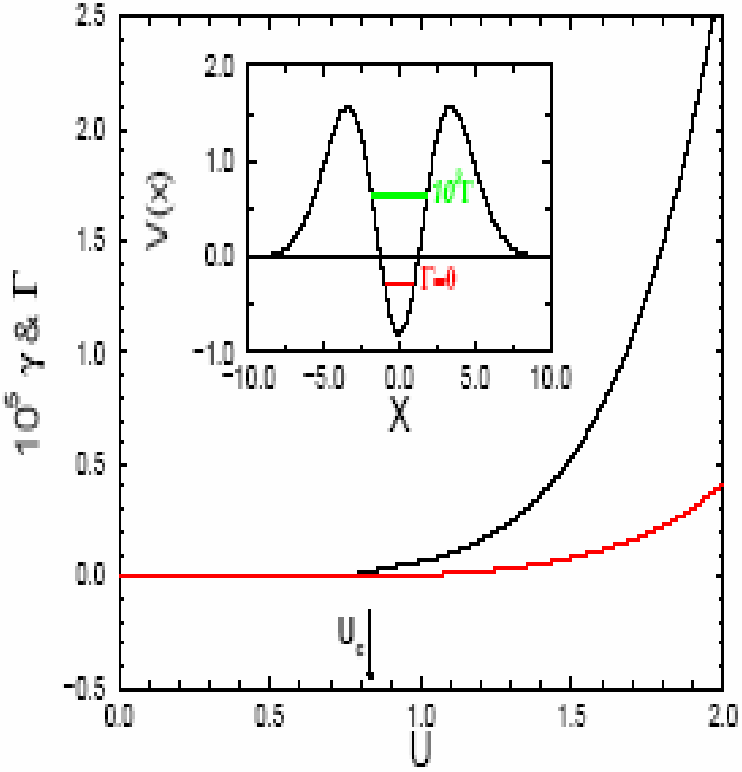
NLSE (GP): $H_\theta^\dagger = H_\theta^* \quad \Rightarrow \quad \left|\phi_\theta\right\rangle = \phi_\theta(r) \quad \left\langle\phi_\theta\right| = \phi_\theta(r)$

$$\left(e^{-2i\theta}T_{\vec{r}} + V(\vec{r}e^{+i\theta}) + \frac{U}{2}e^{-i\theta}\phi_\theta^2(\vec{r})\right)\phi_\theta(\vec{r}) = \mu(complex)\phi_\theta(\vec{r})$$

$$U = a_0(N-1)$$

$$\gamma(N) = -2\,\mathrm{Im}\,\gamma/\hbar = -\frac{1}{N}\frac{dN}{dt}$$

Resonances for BEC with a positive scattering length

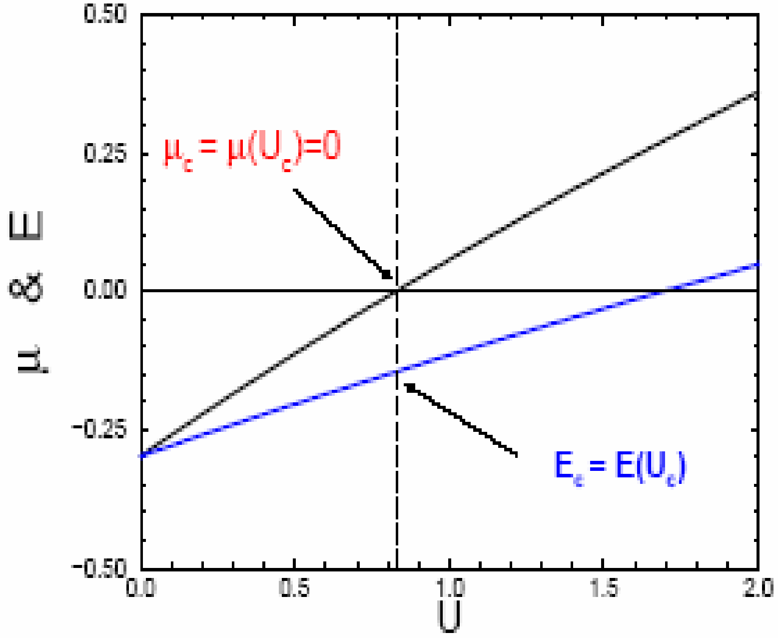


$$E = \frac{\varepsilon}{N} = \mu - \frac{U}{2} \int \phi(\vec{r})^4 \, d\vec{r}$$

$$\gamma = -2 \,\mathrm{Im}\, \mu \qquad \Gamma = -2 \,\mathrm{Im}\, E$$

FIG. 1. The rate of decay γ of a single atom and the total rate of decay per atom Γ as a function of the non-linear parameter U (see Eq. 1 and text). The inset shows the external trap potential used.

Energy and Chemical potential



Transition from bound (U<Uc) to resonance (U>Uc)

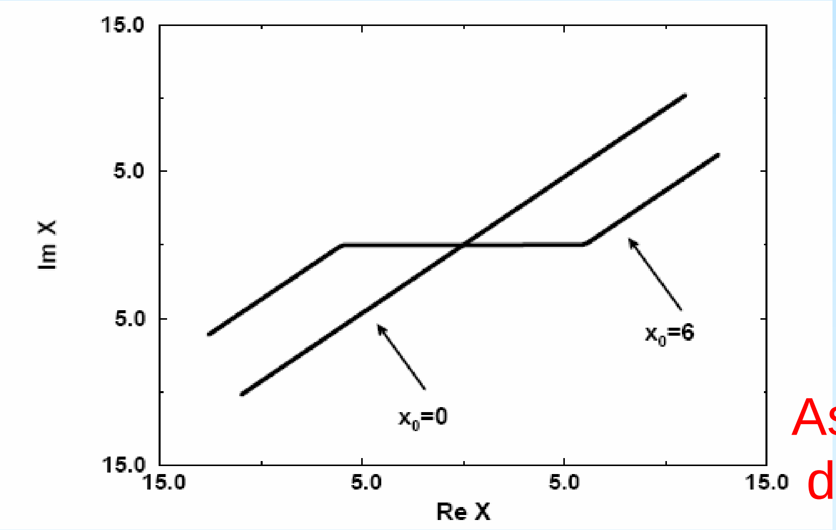
FIG. 2. The chemical potential μ(the real part of the complex eigenvalue in Eq. 1) and the mean-field energy of the BEC per atom E (the real part of the complex energy $\mathcal{E}/N$, see Eq. 2 in the text) as a function of the non-linear parameter U.

Q: Why Ec< 0 ? A(?): The threshold for 1-atom (chemical pot) is 0 . The threshold of E <0 is due to fraction of N atoms that tunnel through the potential barriers

How resonances can be calculated for the NLSE (GP)?

B: Smooth-Exterior Complex Scaling (SES):

$$\vec{q}_j = F_\theta(\vec{r}_j) \qquad T_\theta = T_{\vec{r}_j} + V_{SES-CAP} \qquad V(\vec{r}_j) = V(F_\theta(\vec{r}_j)) \qquad \delta(\vec{q}_{j'} - \vec{q}_j) = \delta(F_\theta(\vec{r}_{j'}) - F_\theta(\vec{r}_j))$$



$$V_{SES-CAP} = V_0^\theta(x) + V_1^\theta(x)\frac{d}{dx} + V_2^\theta(x)\frac{d^2}{dx^2}$$

NLSE（GP）:

Assumption: the atoms tunneling outside do not interact.

$$\delta(\vec{q}_{j'} - \vec{q}_j) = \delta(\vec{r}_{j'} - \vec{r}_j)$$

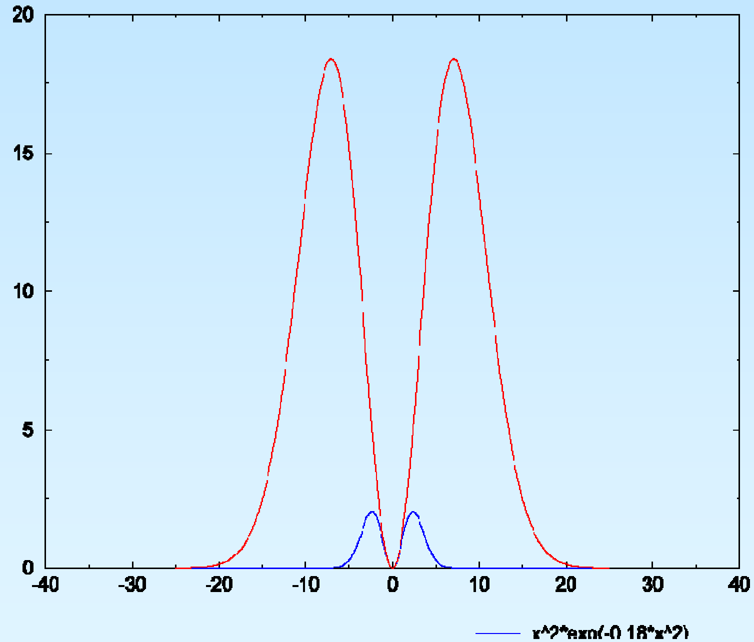
$$\left(T_{\vec{r}} + V(\vec{r}) + U\phi_{SES}^2(\vec{r}) + V_{SES-CAP}\right)\phi_{SES}(\vec{r}) = \mu(complex)\phi_{SES}(\vec{r})$$

$$\phi_{SES}^2(\vec{r}) \to |\phi_{SES}(\vec{r})|^2$$

(out going flux in GP Eq.)

Resonance to bound-state transitions for BEC
with negative scattering length

(SES-CAP approximated by a local CAP)



1D BEC

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+V(x)+\frac{U}{2}|\phi_{CAP}(x)|^2+V_{CAP}\right)\phi_{CAP}(x)=\mu(complex)\phi_{CAP}(x)$$

$$U_0 \equiv U = a_0(N-1) < 0$$

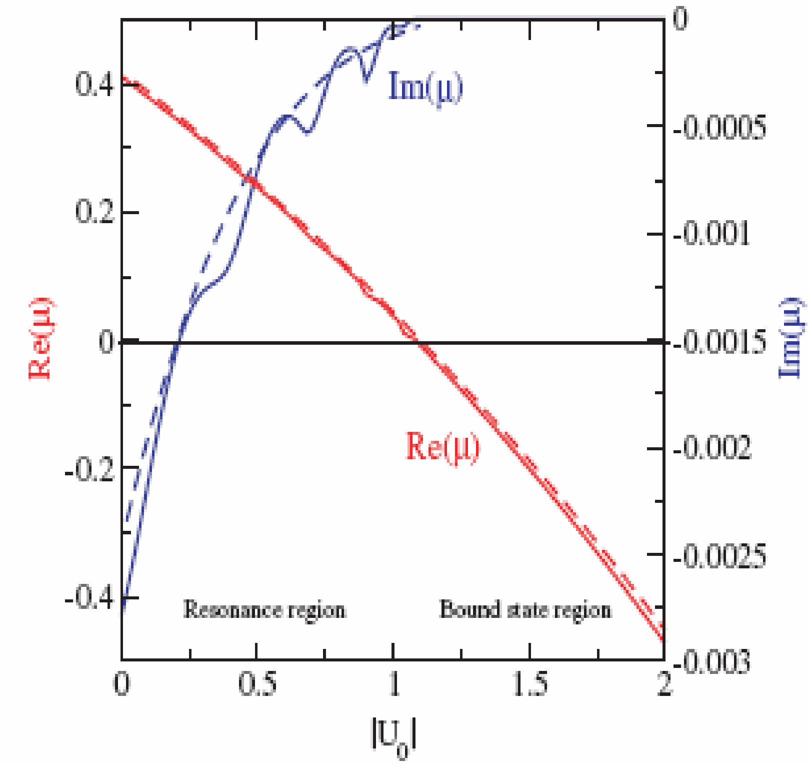


Figure 1. *One dimension.* Shown is the Re(μ) and Im(μ) versus $|U_0|$ for the potential in the form of a harmonic well times the Gaussian envelope (see equation (2)), with $\alpha \equiv (\ell_{ho}/\ell_{Gauss})^2 = 0.2$. Solid curves: results of the numerical method utilizing a complex scaling method.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

2D BEC

$$\left(T_\rho + V(\rho) + \frac{U}{4\pi\rho}|\phi_{CAP}(\rho)|^2 + V_{CAP}(\rho)\right)\phi_{CAP}(\rho) = \mu\phi_{CAP}(\rho) \quad ; \quad U_0 \equiv U = a_0(N-1)$$

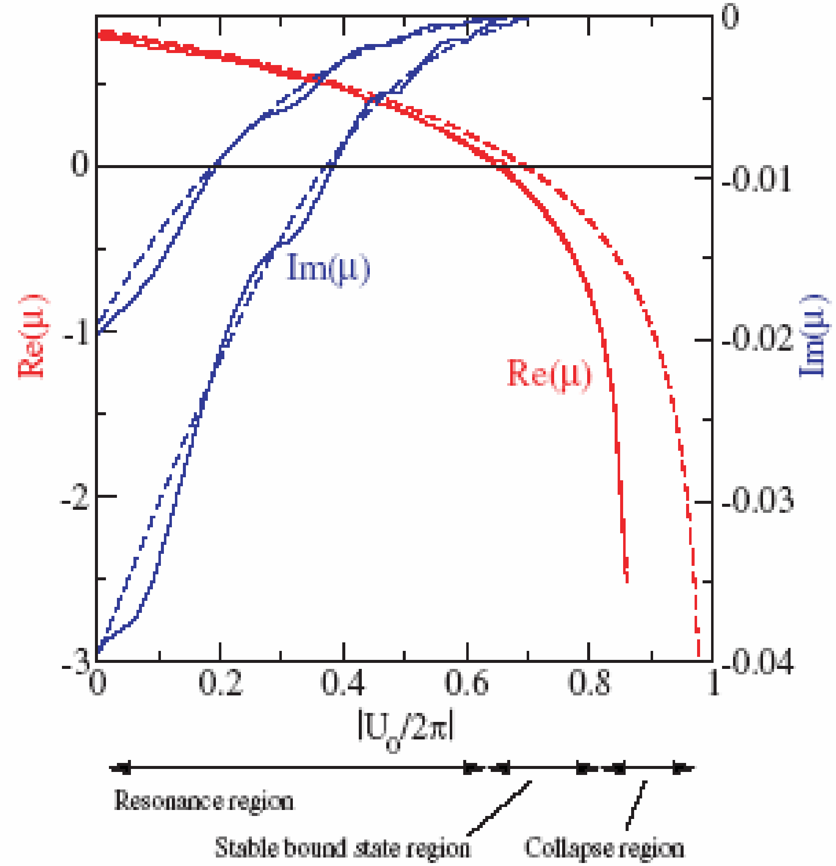
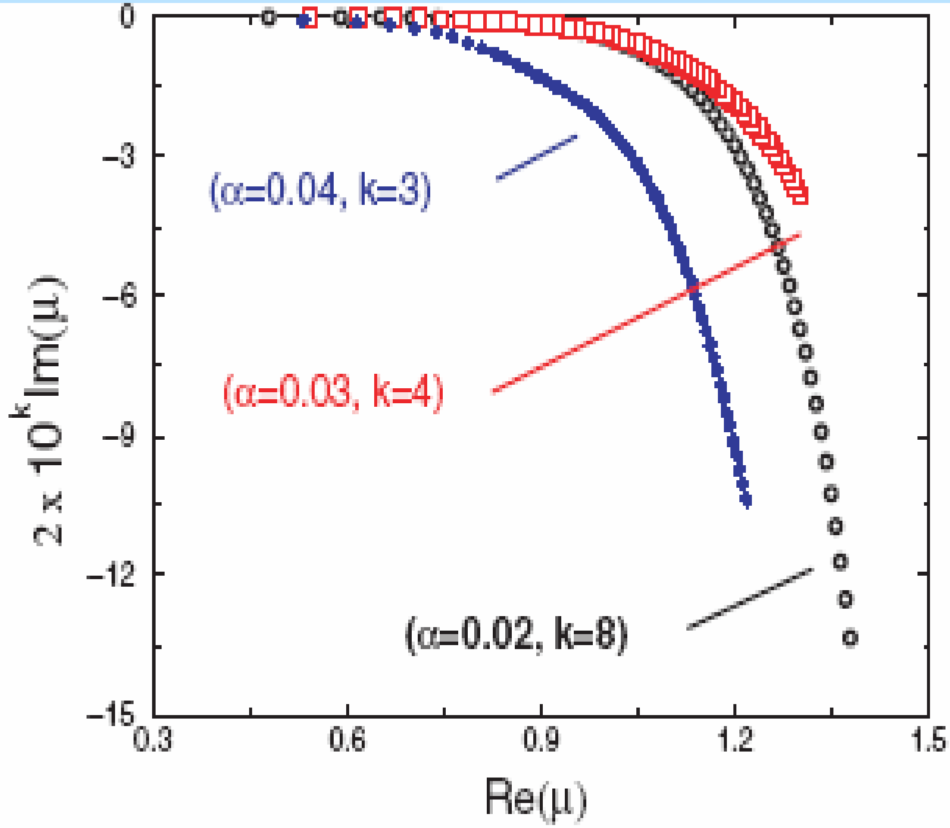


Figure 2. *Two dimensions.* Same as in figure 1 for two different values of the potential-shape parameter, $\alpha = 0.16$ and $\alpha = 0.18$ (the upper and lower curves, respectively; the analytical curves for Re(μ) at both values of α completely overlap). Regions of the resonance, bound state and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

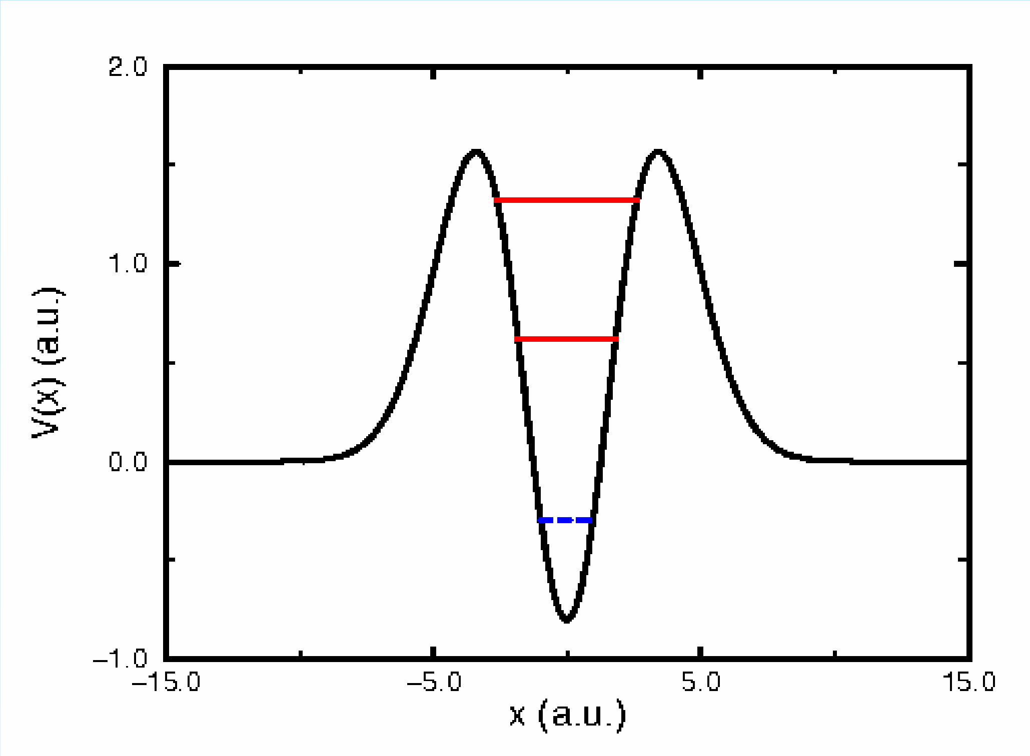
3D BEC

$$\left(T_r + V(r) + \frac{U}{8\pi r^2}|\phi_{CAP}(r)|^2 + V_{CAP}(r)\right)\phi_{CAP}(r) = \mu\phi_{CAP}(r) \quad ; \quad U_0 \equiv U = a_0(N-1) < 0$$



Collapse before resonance/bound Transitions !

Figure 3. *Three dimensions.* The width of the resonance states versus energy for three different wells with $V(0) = V(\infty)$ (i.e., $V_0 = 0$): $\alpha \equiv (\ell_{ho}/\ell_{Gauss})^2 = 0.02, 0.03$ 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).



In 3D only the odd states survive

In 3D NO BOUND STATE

In 3D Only ONE resonance tunneling state survives

3D optical trap
Resonance to bound-state transition BEFORE collapse of BEC

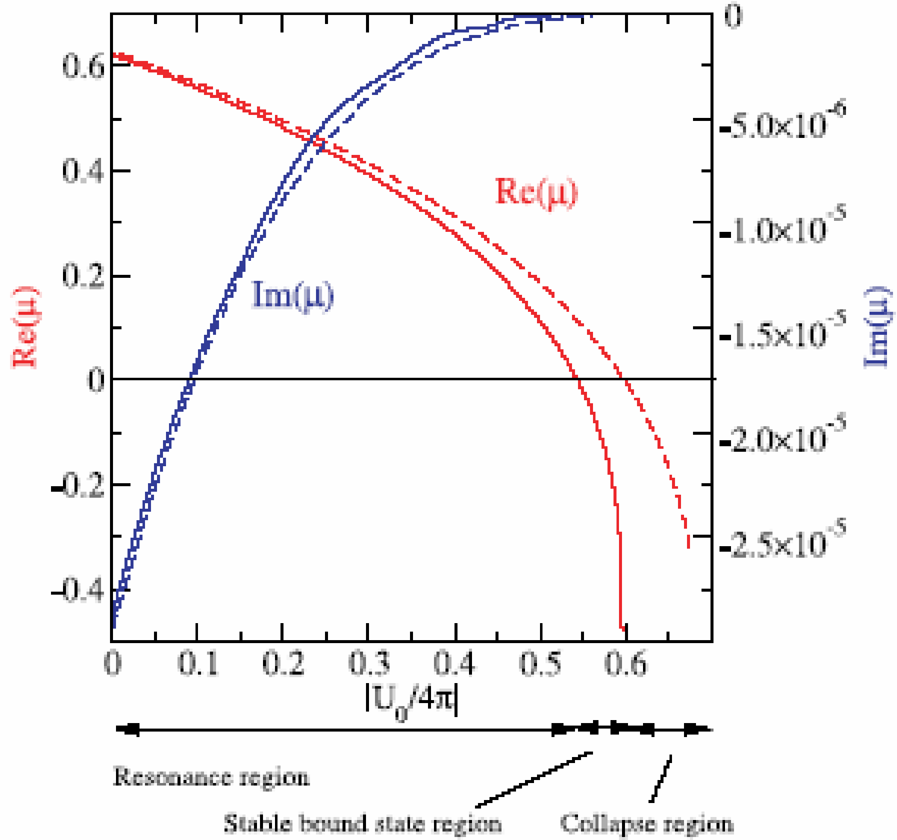


Figure 4. *Three dimensions.* Same as in figure 1 for the potential (2) with $\alpha = 0.02$ and $V_0 = -0.8$ (so that $V(0) = V(\infty) - 0.8$). The offset $V_0 < 0$ allows for the stabilization of the resonance into a bound state, unlike the case shown in figure 3.

Q: Can we avoid the collapse in 3D BEC ?

in spherical symmetric optical trap

The key point is to associate the collapse phenomena with the unbounded spectrum from below due to the -|U|/r^2 term which acts like a “black hole”

Therefore, V(r) should be LESS singular than 1/r^2 at the origion

The excluded volume idea: $V(r)=\infty \quad when \quad r<r_0$

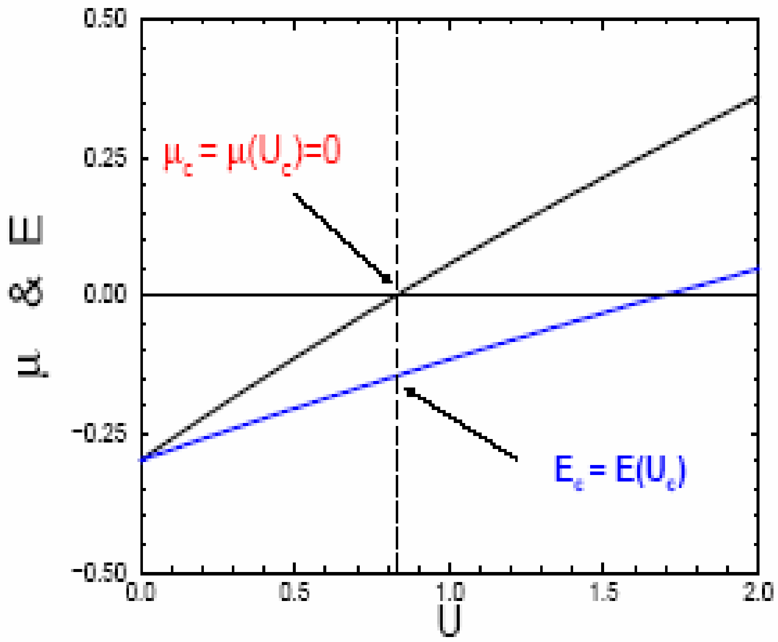
With Cederbaum we proved for Harmonic potential:

$$-\frac{|U|}{2r^2}\int |\phi_{HO}(r)|^4 dr = -\frac{|U|}{2r_0^2} J_3(r_0)\int |\phi_{HO}(r)|^4 dr \quad where \quad 0\le J_3(r_0)\le 1$$

NO COLLAPSE

AS WE HAVE SHOWN BEFORE

Energy and Chemical potential



Transition from bound (U<Uc) to resonance (U>Uc)

FIG. 2. The chemical potential μ(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.

Q: Why Ec< 0 ? A(?): The threshold for 1-atom (chemical pot) is 0 . The threshold of E <0 is due to fraction of N atoms that tunnel through the potential barriers

Q: Why Ec<0 ?

A: due to fragmentation

$$\mu_c = \mu(U_c) = 0 \quad E_c = E(U_c) < 0$$

$$n_1 - atoms \quad in \quad the \quad potential \quad well \quad occupy \quad the \quad \phi \quad orbital$$

$$n_2 - atoms\ tunnel\ through\ the\ potential \quad barriers \quad occupy \quad the\ \chi\ orbital$$

Fraction remains inside the trap

$$X = \frac{n_1}{N} \qquad 1 - X = \frac{n_2}{N}$$

$$U = \frac{a_0}{2}(N-1) \approx \frac{a_0}{2} N \qquad E_{BEC}(X,U) = XE(XU) + (1-X)E_\chi[(1-X)U]$$

$$Pitaevskii \quad (\mathrm{Re}v.Mod.Phys. \quad 1999) \quad E_\chi = 0$$

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

Transition from bound to a resonance state (positive scattering length) occurs at: Uc=0.8279

Fraction of atoms inside the potential well X

Bound/resonance transition Xc(U)=Uc/U

The bound/resonance transition should happen at the minimal energy where:

$$\left.\frac{\partial E_{BEC}}{\partial X}\right|_{X_c(U)} = 0$$

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$$\left.\frac{\partial E_{BEC}}{\partial X}\right|_{X_c(U)} = 0$$

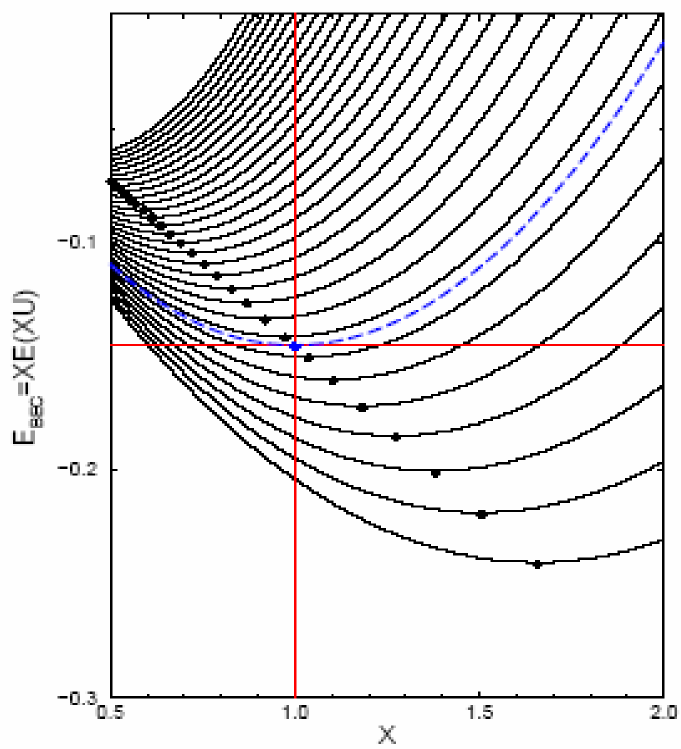

FIG. 3. The energy per atom $E_{BEC}(X, U)$ as a function of the fraction of atoms X which remains in the trap while a fraction 1-X of the condensate has tunneled through the barriers into the continuum. Each curve shown is for a different value of the non-linear parameter U. From bottom to top the j-th 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=Xc (solid dots) and play a central role in understanding the tunneling (see text).

- How resonances can be calculated for the NLSE (GP)?

A: By using complex scaling with inversed complex scaled scattering length, or by introducing the reflection-free CAPs derived from the smooth-exterior-scaling procedure.

- In 3D BEC (negative scattering length): are the resonance/bound-state transition take place before the collapse of the BEC ?

A: Construct an optical trap with a resonance state close to the threshold OR a spherically symmetric trap with excluded volume to prevent the atoms to approach the central point r=0.

- How the fraction of the atoms that are tunneled through the external potential barriers can be extracted from the GP calculations ?

A: Define E(X,U)=XE(X,U) where E the mean energy per atom obtained in GP calculations where,

X=(number of atoms remain inside the trap)/N

Resonance to bound state transitions occur at Xc,

$$\left.\frac{\partial E(X,U)}{\partial X}\right|_{Xc} = 0$$

$$\Gamma = -2\,\mathrm{Im}\,E \quad is \quad function \quad of \quad N$$

Rate of decay of N atoms in the well to n_1<N atoms where (N-n_1) tunnel through the poetntail barriers.

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N. Moiseyev and L. S. Cederbaum,
Tunneling lifetime of trapped condensates.
Los Alamos National Laboratory, Preprint Archive, Condensed Matter (2004), 1-11, arXiv:cond-mat/0406189.