Resonances for the non-linear Schroedinger equation by complex scaling transformations

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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.

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.

Complex scaling: Reviews

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

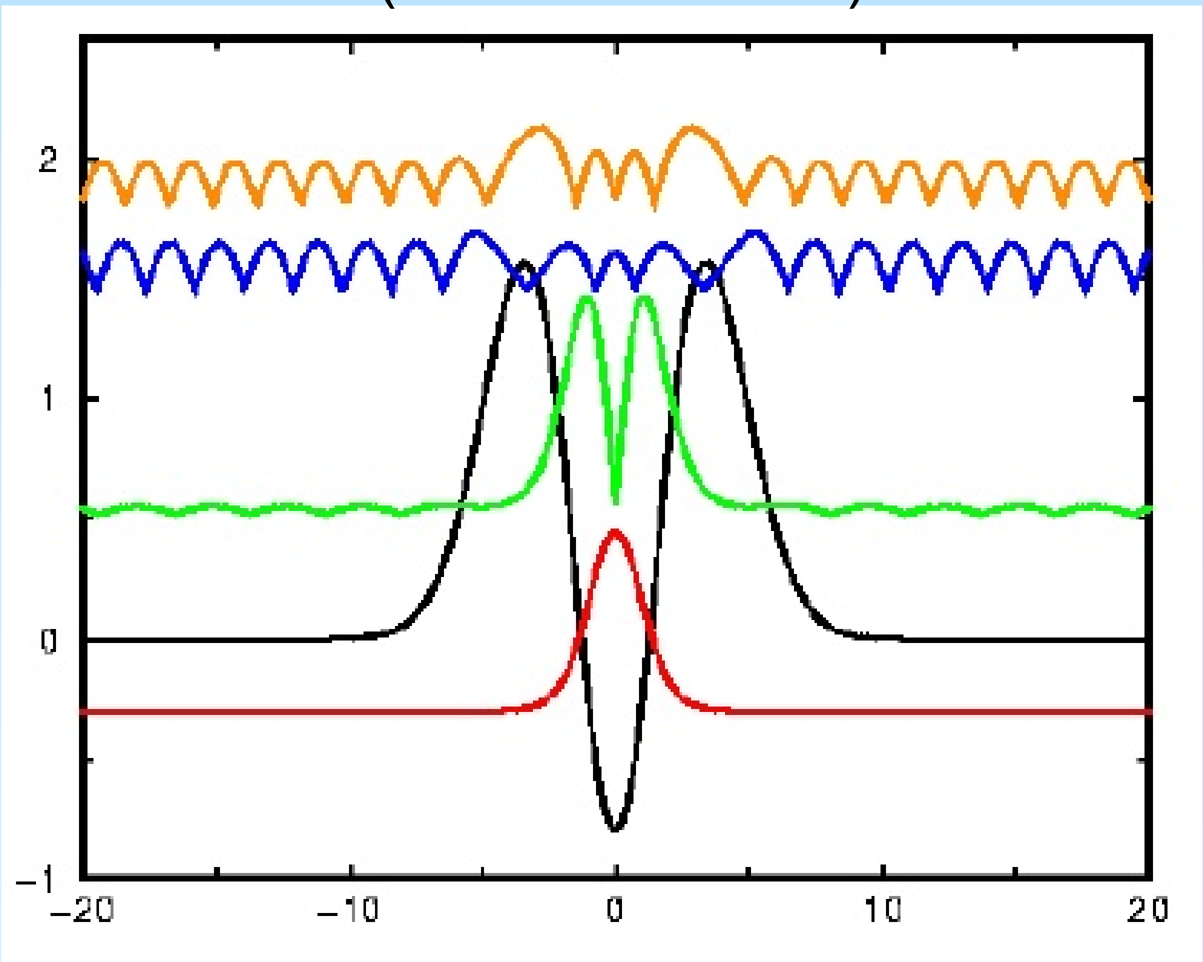
N. Moiseyev. Phys. Rep. **302**, 211 (1998)

Reflection free CAPs by the Smooth-Exterior-Scaling transformation

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

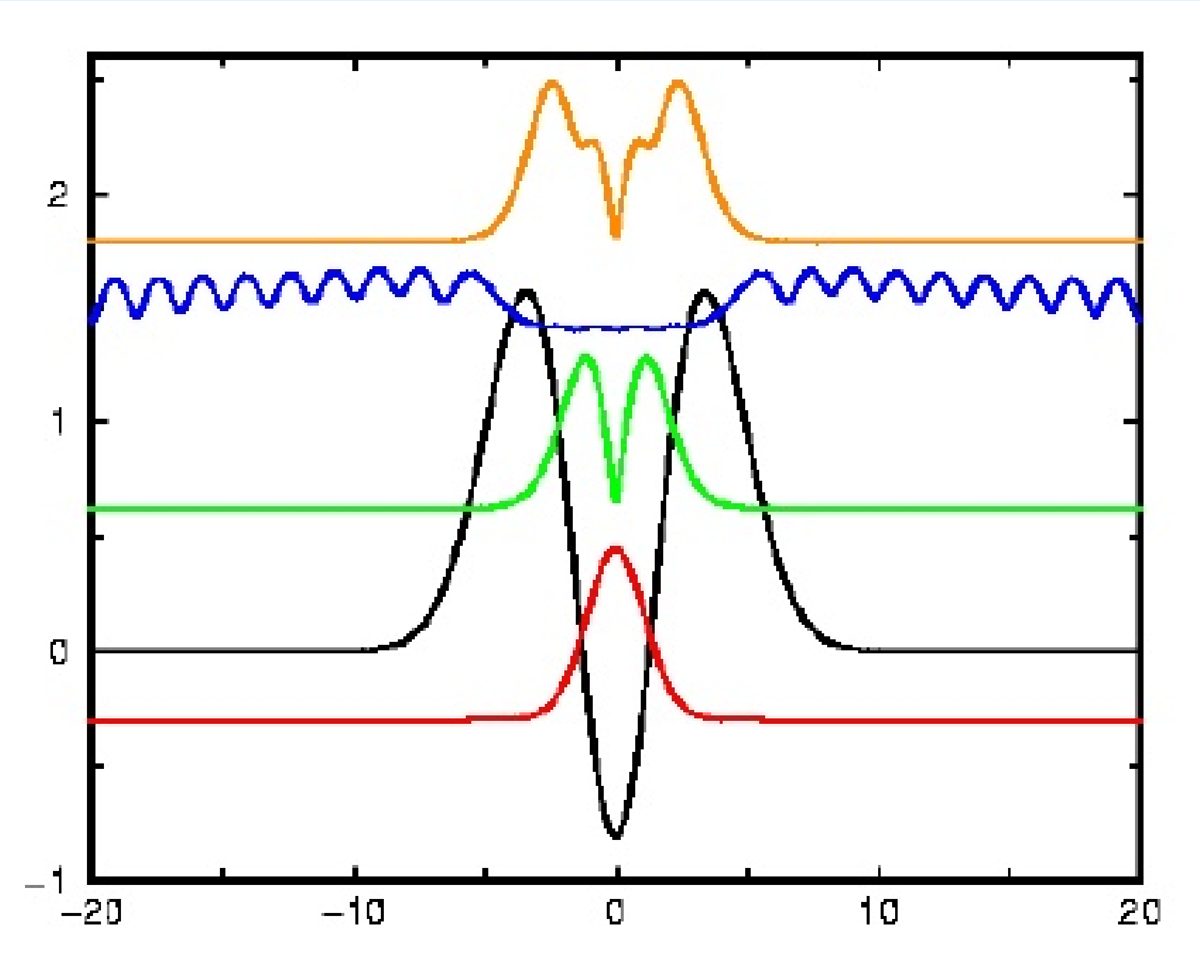
Hermitian (conventional) QM variational calculations

(numerical exact)

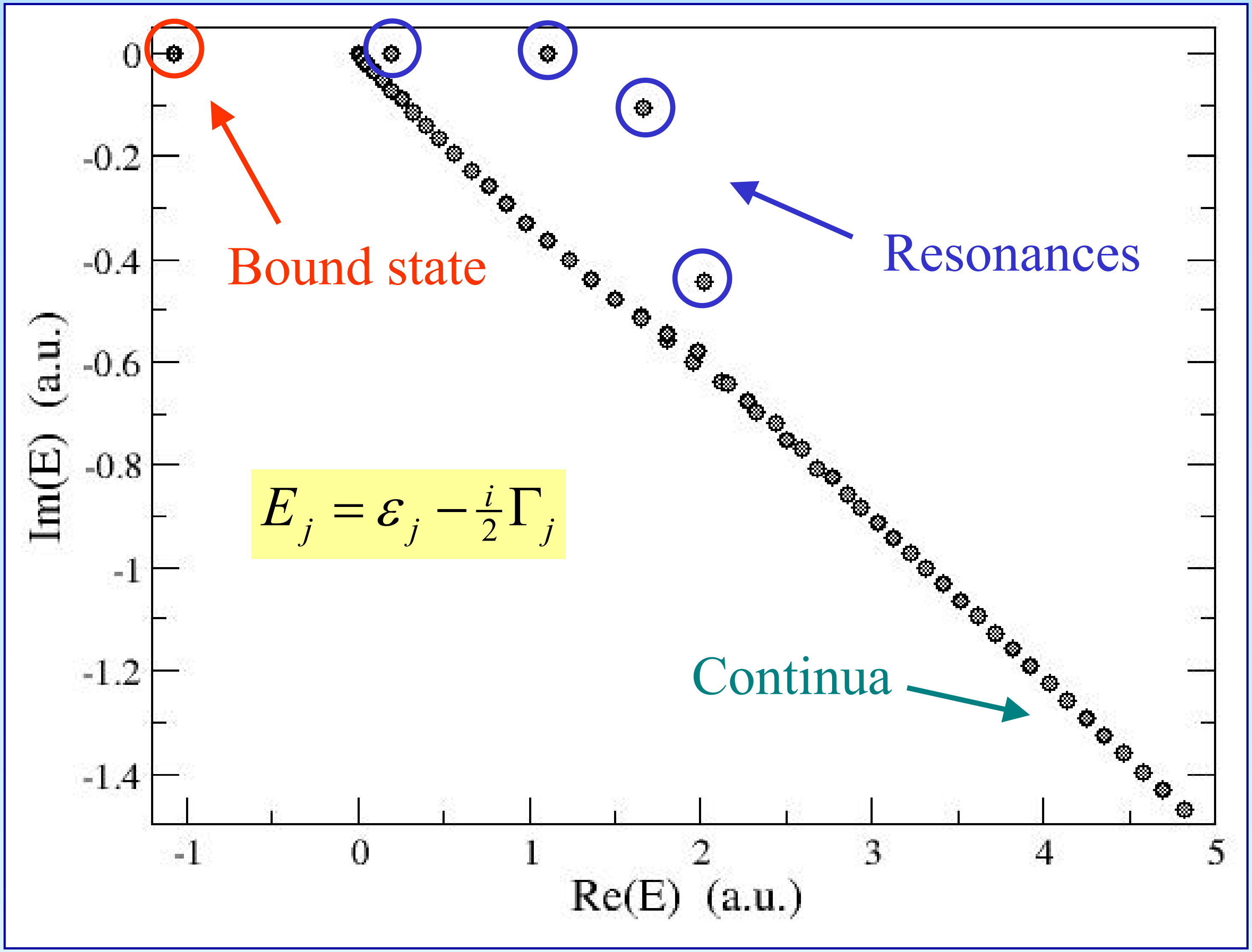


Bound, resonance, continuum states for 1-atom in 1D trap

Non-hermitian (complex scaling) QM variational calculations



Bound, tunneling resonance, continuum and above-barrier resonance states
(NOTE THAT RESONANCES ARE SQAURE INTEGRABLE FUNCTIONS)



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

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

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

$a_0>0$ Bound to resonance state transition

$a_0<0$ Resonance to bound state transition

OPEN QUESTION

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

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A: Complex scaling:

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

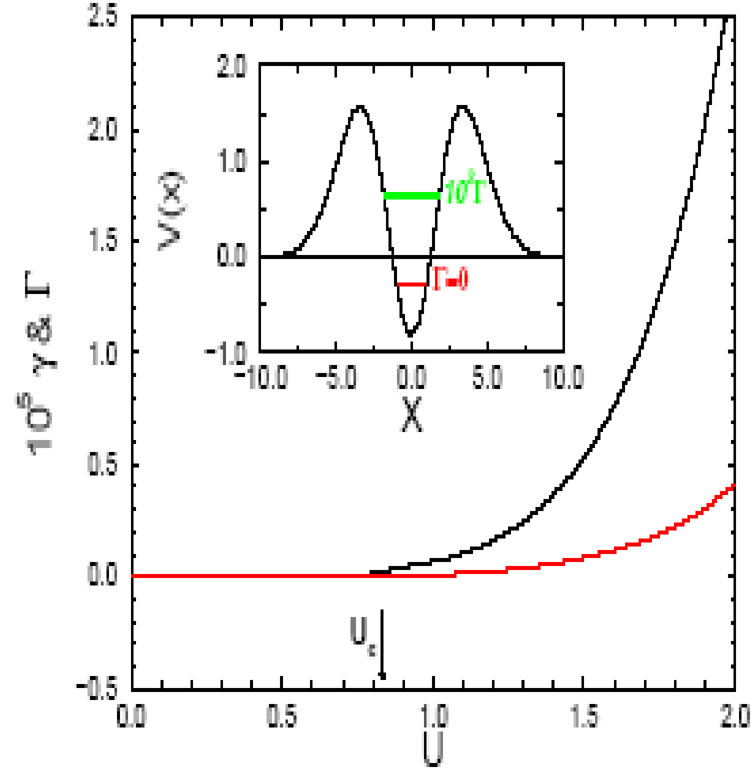
NLSE (GP): $H_\theta^\dagger = H_\theta^* \quad \Rightarrow \quad |\phi_\theta\rangle = \phi_\theta(r) \quad \langle\phi_\theta| = \phi_\theta(r)$

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

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

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

Resonances for BEC with a positive scattering length

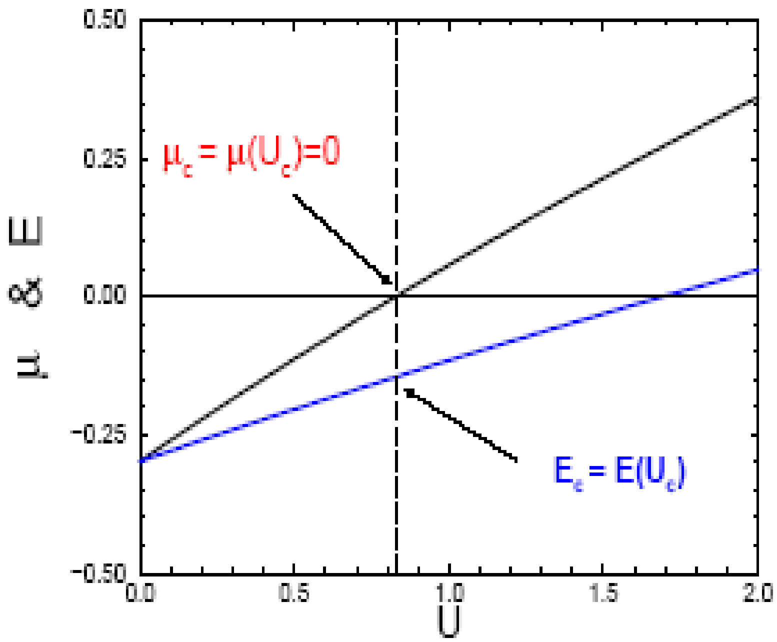


$$E = \frac{\varepsilon}{N} = \mu - \frac{U}{2}\int \phi(\vec{r})^4 d\vec{r}$$

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

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)

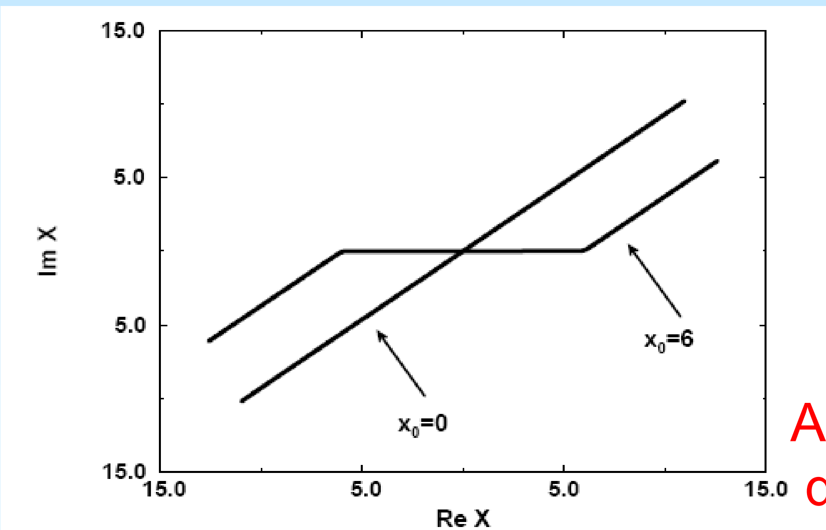
FIG. 2. The chemical potential μ(the real part of the complex eigenvalue in Eq. 1) and the mean-field energy of the BEC per atom E (the real part of the complex energy $\mathcal{E}/N$, see Eq. 2 in the text) as a function of the non-linear parameter U.

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.

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

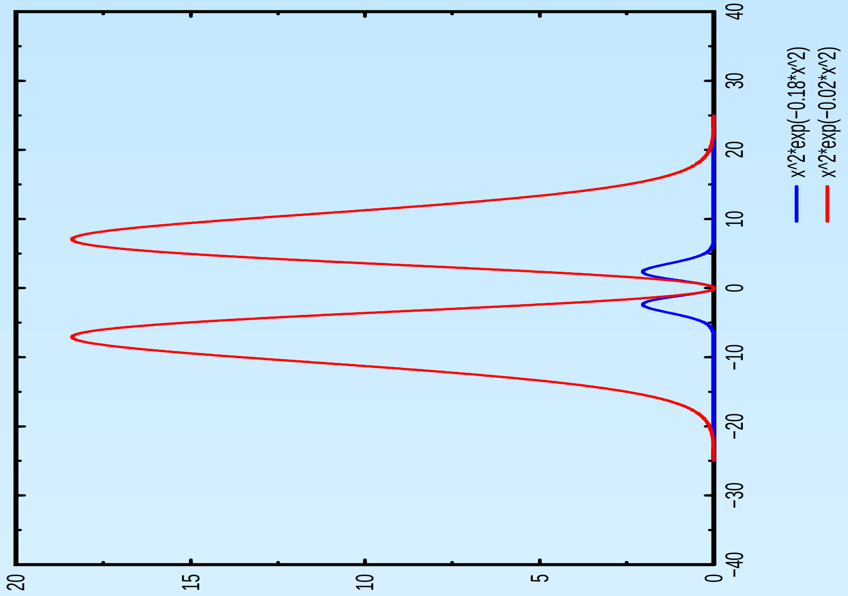
$$\left(T_{\vec{r}} + V(\vec{r}) + U\phi_{SES}^2(\vec{r}) + V_{SES-CAP}\right)\phi_{SES}(\vec{r}) = \mu(complex)\phi_{SES}(\vec{r})$$

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

(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

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

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

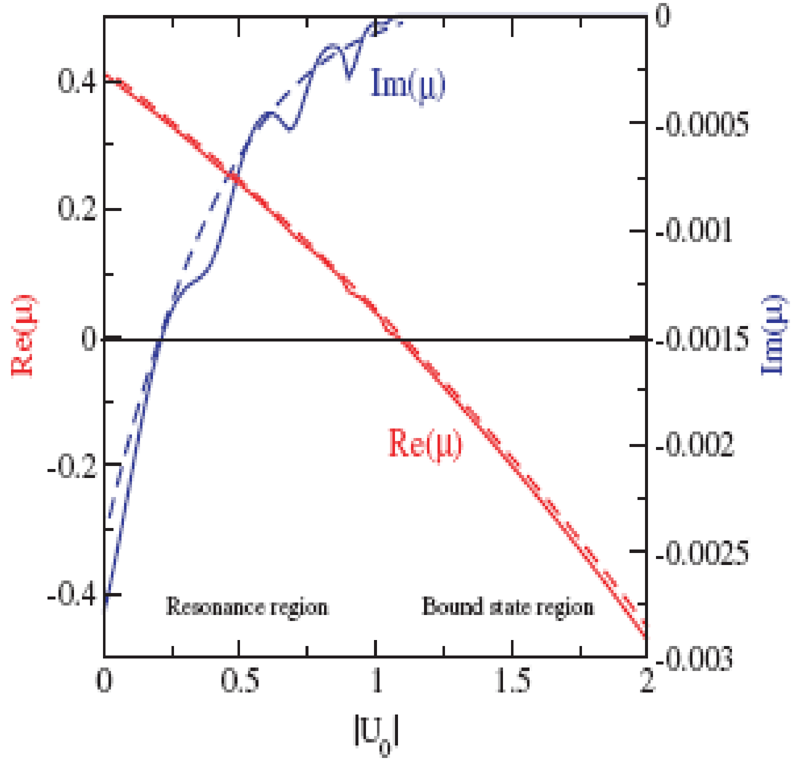


Figure 1. *One dimension.* Shown is the Re(μ) and Im(μ) versus $|U_0|$ for the potential in the form of a harmonic well times the Gaussian envelope (see equation (2)), with $\alpha \equiv (\ell_{ho}/\ell_{Gauss})^2 = 0.2$. Solid curves: results of the numerical method utilizing a complex scaling method.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

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

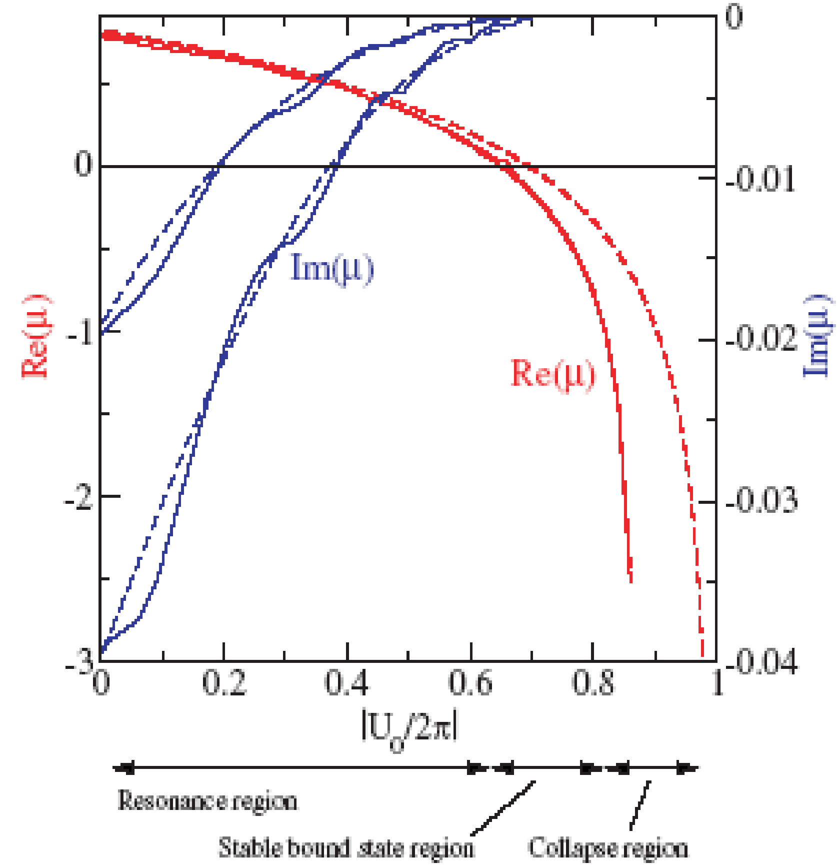
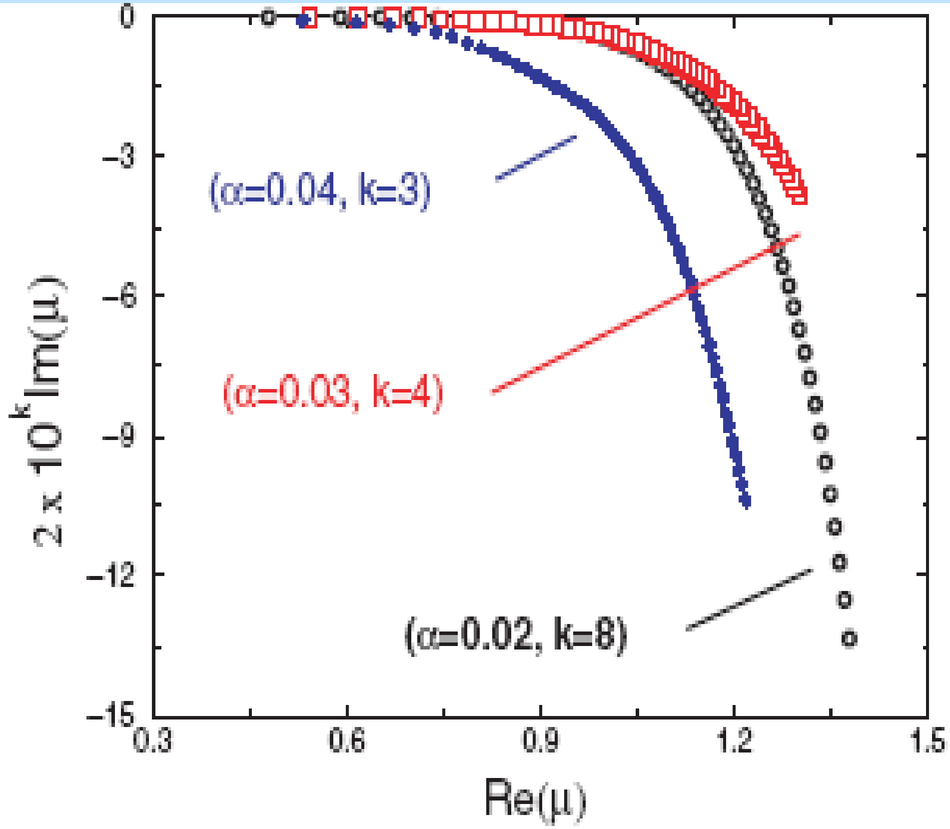


Figure 2. *Two dimensions.* Same as in figure 1 for two different values of the potential-shape parameter, $\alpha = 0.16$ and $\alpha = 0.18$ (the upper and lower curves, respectively; the analytical curves for Re(μ) at both values of α completely overlap). Regions of the resonance, bound state and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

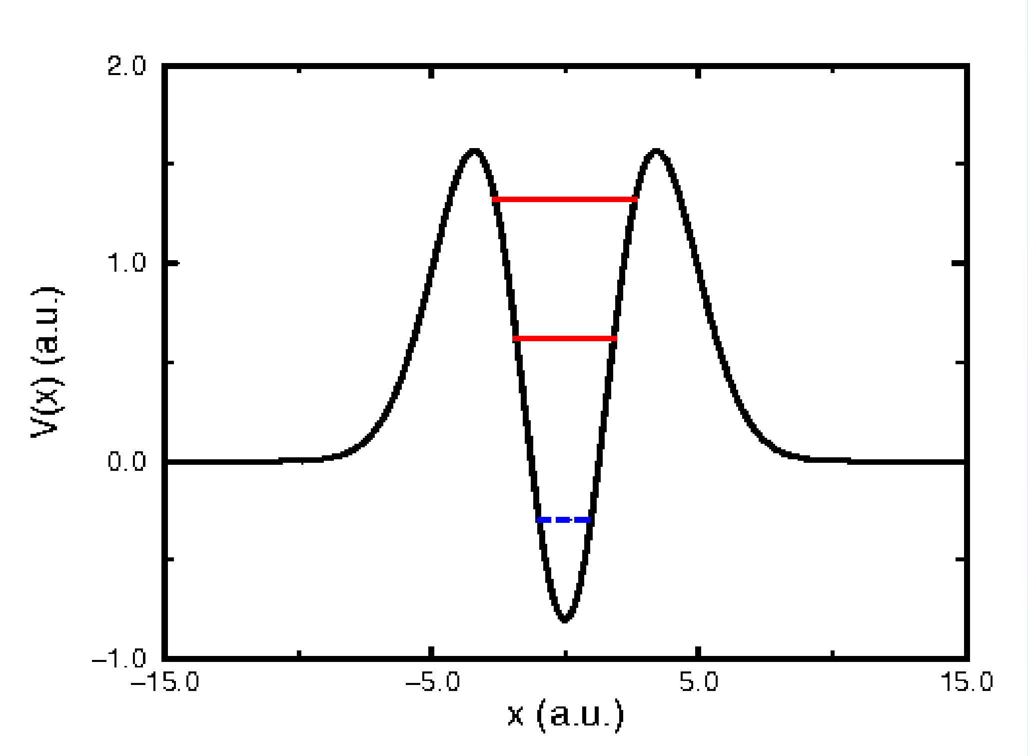
3D BEC

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



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

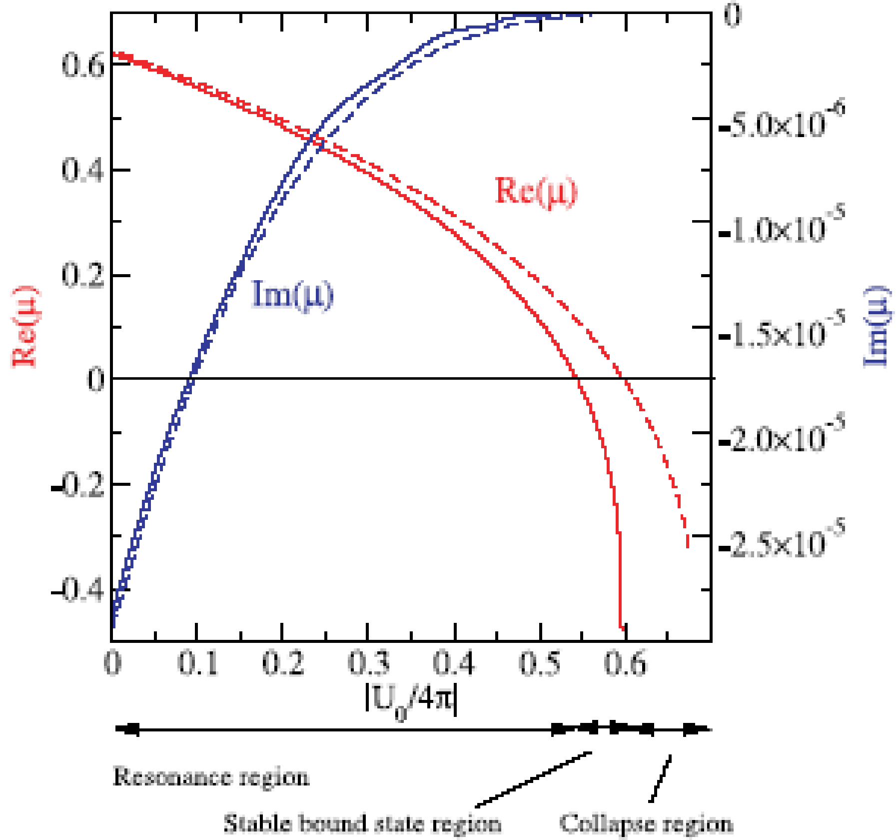


Figure 4. *Three dimensions.* Same as in figure 1 for the potential (2) with $\alpha = 0.02$ and $V_0 = -0.8$ (so that $V(0) = V(\infty) - 0.8$). The offset $V_0 < 0$ allows for the stabilization of the resonance into a bound state, unlike the case shown in figure 3.

- 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.