Bose-Einstein condensates in $\mathcal{PT}$-symmetric double wells

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Outline

1. $\mathcal{PT}$ symmetric quantum systems
   - Properties and appearance
   - A proposal for a Bose-Einstein condensate
2. Numerical approach to Bose-Einstein condensates in a $\mathcal{PT}$ symmetric double well
   - Gross-Pitaevskii equation
   - Two methods: Variational Gaussian and numerically exact
3. Numerical solutions
   - $\mathcal{PT}$ symmetric and $\mathcal{PT}$ broken states in one and three dimensions
   - Temporal evolution
4. Conclusion

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Non-Hermitian $\mathcal{PT}$ symmetric Hamiltonians

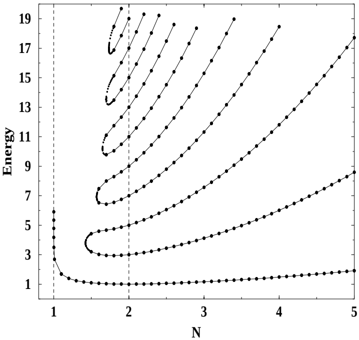


FIG. 1. Energy levels of the Hamiltonian $H = p^2 - (ix)^N$ as a function of the parameter N. There are three regions: When $N \geq 2$ the spectrum is real and positive. The lower bound of this region, $N = 2$, corresponds to the harmonic oscillator, whose energy levels are $E_n = 2n + 1$. When $1 < N < 2$, there are a finite number of real positive eigenvalues and an infinite number of complex conjugate pairs of eigenvalues. As N decreases from 2 to 1, the number of real eigenvalues decreases; when $N \leq 1.42207$, the only real eigenvalue is the ground-state energy. As N approaches 1^+, the ground-state energy diverges. For $N \leq 1$ there are no real eigenvalues.

Bender, Boettcher PRL 80, 5243 (1998)

$\mathcal{PT}$ symmetric quantum systems

Symmetry operators:

- Parity: spatial reflections $\mathcal{P} : x \to -x \;, \quad p \to -p$
- Time reversal $\mathcal{T} : x \to x \;, \quad p \to -p \;, \quad \mathrm{i} \to -\mathrm{i}$

$\mathcal{PT}$ symmetric Hamiltonians

$$[\mathcal{PT}, H] = 0$$

- Necessary condition:

$$\begin{aligned} [\mathcal{PT}, H] &= \mathcal{PT}\left(\frac{p^2}{2m} + V(x)\right) - \left(\frac{p^2}{2m} + V(x)\right)\mathcal{PT} \\ &= \left(V^*(-x) - V(x)\right)\mathcal{PT} \stackrel{!}{=} 0 \end{aligned}$$

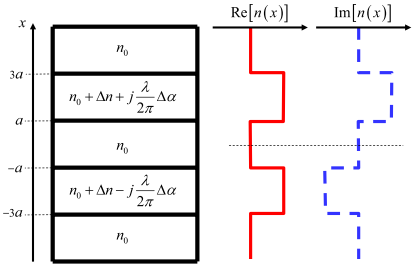
- Required form of the potential:

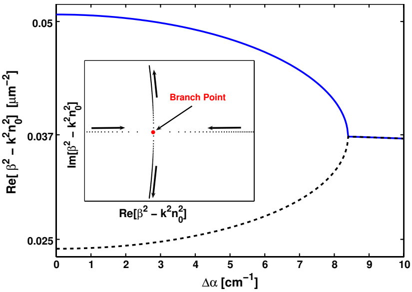
$$V^*(-x) = V(x)$$

Optical waveguides

Theoretical description and eigenvalues

- Optical waveguide with gain and loss terms represented by a complex potential.
- Description equivalent to a one-dimensional Schrödinger equation.
- Real eigenvalues are found below a critical value of the imaginary contribution.
- Beyond an exceptional point the modes become complex and complex conjugate.

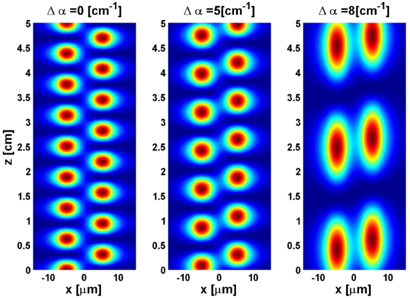




S. Klaiman et al., Phys. Rev. Lett. 101, 080402 (2008)

Optical waveguides

Temporal evolution and experimental verification

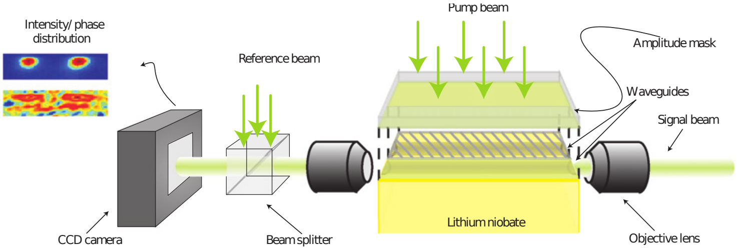


Left: Power distribution of a propagating mode (increasing imaginary contribution from left to right), theory

S. Klaiman et al., Phys. Rev. Lett. 101, 080402 (2008)

Bottom: Experimental setup

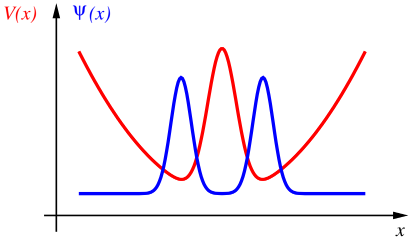
C. E. Rüter et al., Nature Physics 6, 192 (2010)



BEC in a $\mathcal{PT}$ symmetric double well

Proposal by Klaiman et al., PRL 101, 080402 (2008)

- Setup with matter waves: real quantum system.
- Bose-Einstein condensate in a double well.
- First well: particles are injected: gain term
- Second well: particles are removed: loss term



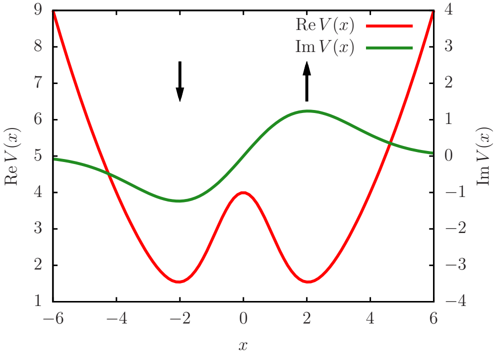
Outline

$\mathcal{PT}$ symmetric external potential

Form of the potential

$$V(\boldsymbol{x}) = \frac{m}{2}\omega_x^2 x^2 + \frac{m}{2}\omega_{y,z}^2(y^2+z^2) + v_0 e^{-\sigma x^2} + \mathrm{i}\Gamma x \mathrm{e}^{-\rho x^2}$$

$\mathcal{PT}$ symmetry in x direction:



Gain/loss term Γ:

- influences the probability amplitude of the whole condensate
- atoms are in-/outcoupled coherently

Gross-Pitaevskii equation

System of units:

- Length scale: $a_0 = \sqrt{\hbar/m\omega_{y,z}}$
- Unit of energy: $E_0 = \hbar^2/2ma_0^2$
- Dimensionless potential:
  $V(\boldsymbol{x}) = \omega_x^2 x^2 + y^2 + z^2 + v_0 e^{-\sigma x^2} + \mathrm{i}\Gamma x \mathrm{e}^{-\rho x^2}$

Time-dependent Gross-Pitaevskii equation

$$\mathrm{i}\dot{\psi}(\boldsymbol{x},t) = \left(-\Delta + V(\boldsymbol{x}) - g|\psi(\boldsymbol{x},t)|^2\right)\psi(\boldsymbol{x},t)$$

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Time-dependent Gross-Pitaevskii equation

$$\mathrm{i}\dot{\psi}(\boldsymbol{x},t) = \left(-\Delta + V(\boldsymbol{x}) - g|\psi(\boldsymbol{x},t)|^2\right)\psi(\boldsymbol{x},t)$$

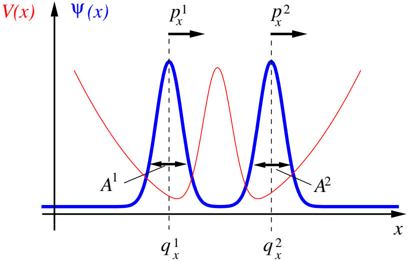
Is the GPE $\mathcal{PT}$ symmetric?

- Interaction term: $-g|\psi(\boldsymbol{x},t)|^2$
- The wave function $\psi(\boldsymbol{x},t)$ affects the symmetry of the Hamiltonian's real part.
- The Hamiltonian is only $\mathcal{PT}$ symmetric if the solution's square modulus $|\psi(\boldsymbol{x},t)|^2$ is a symmetric function of x!

Variational Gaussian procedure

Gaussian ansatz

$$\psi(\boldsymbol{z}, \boldsymbol{x}) = \sum_{k=1}^{2} \mathrm{e}^{-(A_x^k (x-q_x^k)^2 + A_{y,z}^k (y^2+z^2) - \mathrm{i} p_x^k (x-q_x^k) + \varphi^k)}$$



Variational parameters:

- widths: $A_x^1, A_x^2, A_{y,z}^1, A_{y,z}^2 \in \mathbb{C}$
- positions: $q_x^1, q_x^2 \in \mathbb{R}$
- momenta: $p_x^1, p_x^2 \in \mathbb{R}$
- amplitudes/phases: $\varphi^1, \varphi^2 \in \mathbb{C}$

In total: 16 real parameters
(12 in one dimension)

Dynamics: contained in the variational parameters

$$\boldsymbol{z}(t) = \left\{ A_x^k(t), A_{y,z}^k(t), q_x^k(t), p_x^k(t), \varphi^k \right\}$$

Equations of motion

McLachlan time-dependent variational principle

$$\delta I = \delta ||i\phi(t) - H\psi(t)||^2 \stackrel{!}{=} 0 \,, \qquad \dot{\psi} \equiv \phi$$

- Equations of motion:

$$\begin{aligned}
\dot{A}_x^k &= -4\mathrm{i}\left((A_x^k)^2 + (A_{y,z}^k)^2\right) + \mathrm{i}V_{2;x}^k \\
\dot{A}_{y,z}^k &= -4\mathrm{i}\left((A_x^k)^2 + (A_{y,z}^k)^2\right) + \mathrm{i}V_{2;y,z}^k \\
\dot{q}_x^k &= 2p_x^k + s_x^k \\
\dot{p}_x^k &= -\operatorname{Re} v_{1;x}^k - 2\operatorname{Im} A_x^k s_x^k - 2\operatorname{Re} V_{2;x}^k q_x^k \\
\dot{\varphi}^k &= \mathrm{i}v_0^k + 2\mathrm{i}(A_x^k + A_{y,z}^k) - \mathrm{i}(p_x^k)^2 - \mathrm{i}p_x^k s_x^k + \mathrm{i}q_x^k v_{1;x}^k + \mathrm{i}q_x^k V_{2;x}^k q_x^k
\end{aligned}$$

with $s_x^k = \frac{1}{2}(\operatorname{Re} A_x^k)^{-1}(\operatorname{Im} v_{1;x}^k + 2\operatorname{Im} V_{2;x}^k q_x^k)$

- Effective potential terms $\boldsymbol{v} = (v_0^1, \ldots, v_{1;x}^1, \ldots, V_{2;x}^1, \ldots)$: $\boldsymbol{K}\boldsymbol{v} = \boldsymbol{r}$
  matrix $\boldsymbol{K}$: (weighted) overlap integrals of the Gaussians
  vector $\boldsymbol{r}$: (weighted) Gaussian averages of all potential terms

Stationary states

Conditions

$$\dot{A}_x^k = \dot{A}_{y,z}^k = \dot{q}_x^k = \dot{p}_x^k = 0 \qquad \text{12 conditions}$$

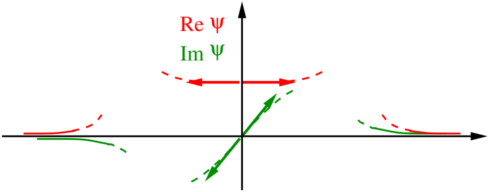
$$\dot{\varphi}^k = \mathrm{i}\mu \qquad \text{4 conditions}$$

$$||\psi|| = 1 \qquad \text{1 condition}$$

Numerical procedure:

- Arbitrary global phase $\rightarrow$ one Gaussian parameter is free: property of the Gross-Pitaevskii equation
- 15 Gaussian parameters can be varied together with $\mathrm{Re}\,\mu$ and $\mathrm{Im}\,\mu$ $\rightarrow$ 17 parameters
- Stationary states can be found with a 17-dimensional root search.
- In one dimension: 13 conditions and 13 parameters
- Only a small difference in the numerical effort.

In one dimension: numerically exact integration



Procedure:

- The arbitrary global phase is exploited: $\mathrm{Im}\,\psi(0) = 0$
- Five real initial values have to be chosen:

$$\mathrm{Re}\,\psi(0)\ , \quad \psi'(0) \in \mathbb{C}\ , \quad \mu \in \mathbb{C}$$

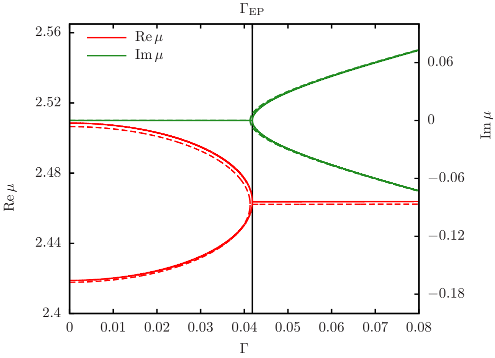
- Five conditions have to be fulfilled:

$$\psi(\infty) \to 0\ , \quad \psi(-\infty) \to 0\ , \quad ||\psi|| = 1$$

- Five-dimensional root search.

Outline

Spectrum without nonlinearity ($g = 0$)



Example

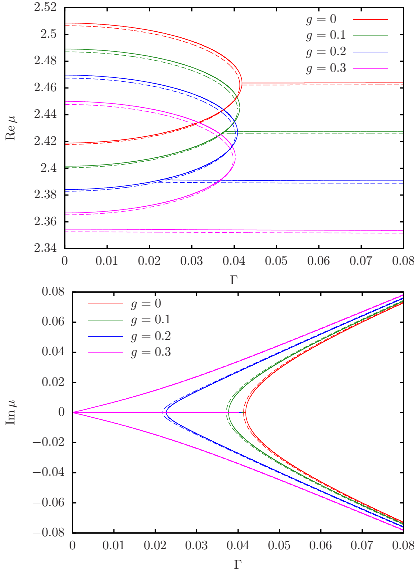
$0 < \Gamma < 0.08$, variational (solid) and numerically exact (dashed) eigenvalues:

- Two real solutions below Γ_{EP}.
- Appearance of an exceptional point.
- Two complex conjugate solutions for $\Gamma > \Gamma_{\mathrm{EP}}$.

Summary

The model reveals the known features of complex Hamiltonians with $\mathcal{PT}$ symmetry.

Spectrum with increasing nonlinearity ($g = 0 \ldots 0.3$)



Example

$0 < \Gamma < 0.08$, variational (solid) and numerically exact (dashed) eigenvalues

Observation

- Real eigenvalue branches merge and vanish at a value Γ_{EP}.
- Complex eigenvalues are born at a value $\Gamma_{\mathrm{c}} < \Gamma_{\mathrm{EP}}$.
- For sufficiently small nonlinearities there is a range in which only real eigenvalue solutions exist.

Eigenvalues of the three-dimensional problem

- Expectation: The one-dimensional calculation should contain already all important features.

Eigenvalues of the three-dimensional problem

- Expectation: The one-dimensional calculation should contain already all important features.
- Comparison of the eigenvalues of the full three-dimensional problem with those in one dimension.
  - An energy shift of $\Delta\mu = 2$ is expected: harmonic oscillator ground states for y and z directions.
  - The nonlinearity parameter g has to be rescaled: We require

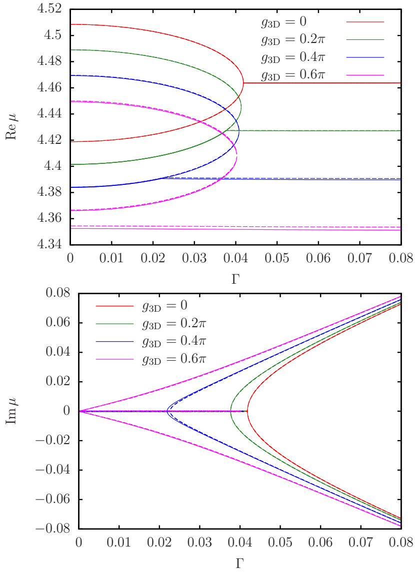
$$\int_{\mathbb{R}^3} dx\, dy\, dz\, g_{3\mathrm{D}} |\psi_{3\mathrm{D}}(\boldsymbol{x})|^4 \stackrel{!}{=} \int_{\mathbb{R}} dx\, g_{1\mathrm{D}} |\psi_{1\mathrm{D}}(x)|^4$$

and obtain

$$g_{1\mathrm{D}} = g_{3\mathrm{D}} \int_{\mathbb{R}^2} dydz |\psi_0(y)|^4 |\psi_0(z)|^4$$

$$g_{3\mathrm{D}} = 2\pi g_{1\mathrm{D}}.$$

Comparison of the energies in three and one dimension



Example

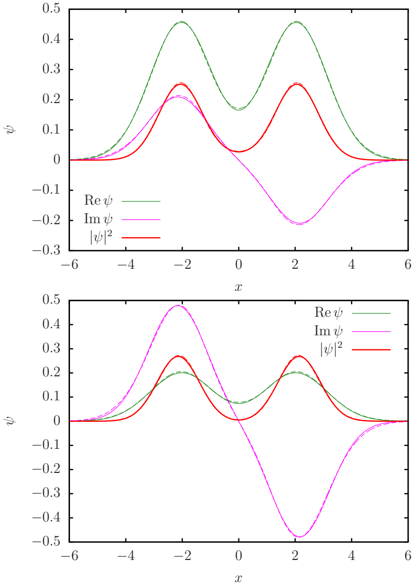
$g_{1D} = 0 \ldots 0.2$

- solid: three-dimensional calculation
- dashed: one-dimensional calculation shifted by $\Delta\mu = 2$

Finding

- Almost no difference.
- One-dimensional description is very good.
- One-dimensional calculations in the following parts.

Wave functions for real eigenvalues



Critical question

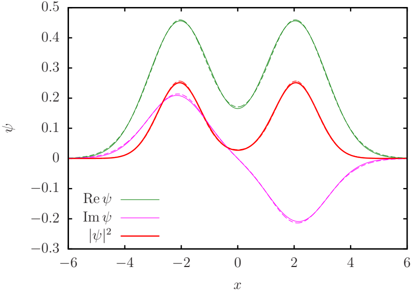
Does the nonlinearity $g|\psi(x)|^2$ destroy the $\mathcal{PT}$ symmetry of the Hamiltonian?

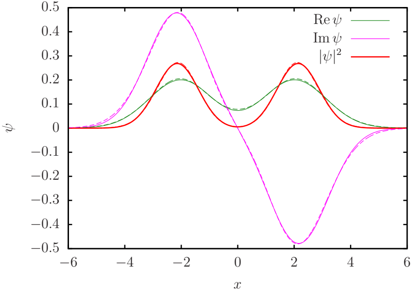
Example

$g = 0.2$, $\Gamma = 0.03$, ground (upper panel) and excited (lower panel) state:

- Square modulus: symmetric

Wave functions for real eigenvalues





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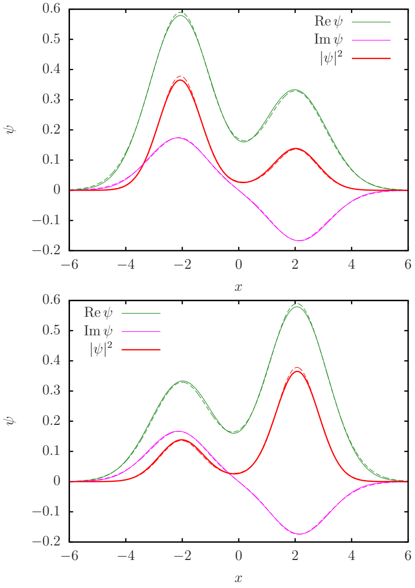
Example

$g = 0.2$, $\Gamma = 0.03$, ground (upper panel) and excited (lower panel) state:

- Square modulus: symmetric
- The nonlinear Hamiltonian picks as eigenstates wave functions which render itself $\mathcal{PT}$ symmetric!

Wave functions for complex eigenvalues



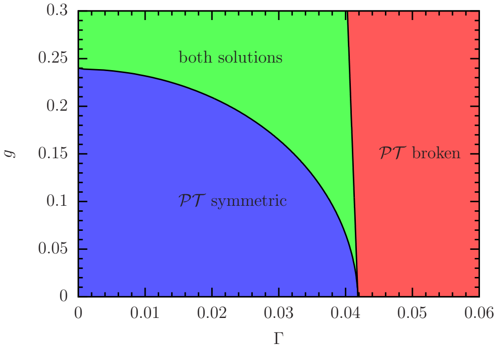
Example

$g = 0.2$, $\Gamma = 0.03$, states with
$\mathrm{Re}\,\mu < 0$ (upper panel)
$\mathrm{Im}\,\mu > 0$ (lower panel)

Important differences:

- Wave functions with broken $\mathcal{PT}$ symmetry!
- Also the Hamiltonian loses its $\mathcal{PT}$ symmetry!
- Solutions lose their physical relevance: decay or growth of the probability amplitude $\rightarrow$ nonlinear potential term $g|\psi|^2$ changes with time!

Phase diagram



Summary of the observations

- As soon as $g \neq 0$, in a range $\Gamma_c < \Gamma < \Gamma_{EP}$ $\mathcal{PT}$ symmetric and $\mathcal{PT}$ broken states coexist.
- The appearance of $\mathcal{PT}$ broken states depends on both the nonlinearity and the non-Hermiticity.

Question

Will the stationary $\mathcal{PT}$ symmetric states be observable? Are they stable with respect to quantum fluctuations?

- Ansatz for small perturbations:

$$\psi(x,t) = \psi_0(x,t) + \delta e^{-i\mu t}\left(u(x)e^{\lambda^* t} + v^*(x)e^{\lambda t}\right)$$

- Bogoliubov-de Gennes equations:

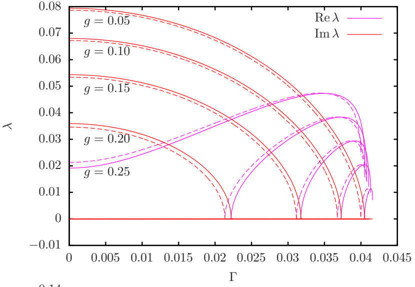
$$\frac{\partial^2}{\partial x^2}u(x) = \left(V(x) - \mu - i\lambda^* - 2g\left|\psi_0(x)\right|^2\right)u(x) - g\psi_0^2(x)v(x)$$
$$\frac{\partial^2}{\partial x^2}v(x) = \left(V^*(x) - \mu^* + i\lambda^* - 2g\left|\psi_0(x)\right|^2\right)v(x) - g\psi_0^{*2}(x)u(x)$$

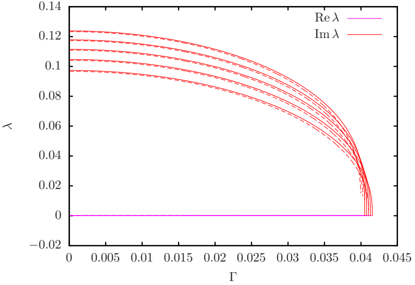
- Variational approach: Jacobian

$$\delta\dot{\tilde{\boldsymbol{z}}} = J\delta\tilde{\boldsymbol{z}}\ , \quad \text{with} \quad J = \frac{\partial\dot{\tilde{\boldsymbol{z}}}}{\partial\tilde{\boldsymbol{z}}}\ , \quad \delta\tilde{z}_i'(t) = \delta\tilde{z}_i'(0)e^{\lambda_i t}$$

Stability of the eigenstates

Stability eigenvalues of the $\mathcal{PT}$ symmetric states





Example

$0 < \Gamma < \Gamma_{\mathrm{EP}}$, ground (upper panel) and excited (lower panel) state

Influence of other states

- Imaginary eigenvalues: stable, real eigenvalues: unstable.
- Ground state: becomes unstable as soon as the $\mathcal{PT}$ broken branches emerge!
- Excited state: always stable.

Question

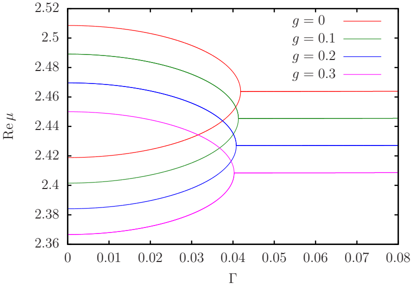
The real branches vanish at the branch point and the complex eigenvalues bifurcate only from the ground state. Can this be explained?

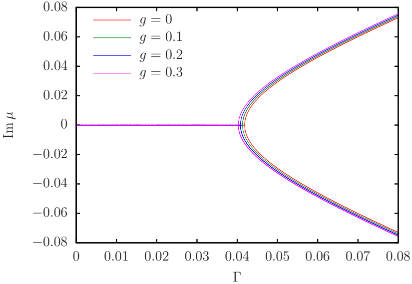
Analytic extension

- $g|\psi(x)|^2$ is non-analytic.
- Eigenstates with complex eigenvalues bifurcating from the branch point can be found by an appropriate analytic continuation.
- Idea: Below the branch point we have $\psi^*(x) = \psi(-x)$.
- The replacement $g|\psi(x)|^2 \to \psi(x)\psi(-x)$ will not change the $\mathcal{PT}$ symmetric states.

Analytic continuation

Calculation of the eigenvalues





Example

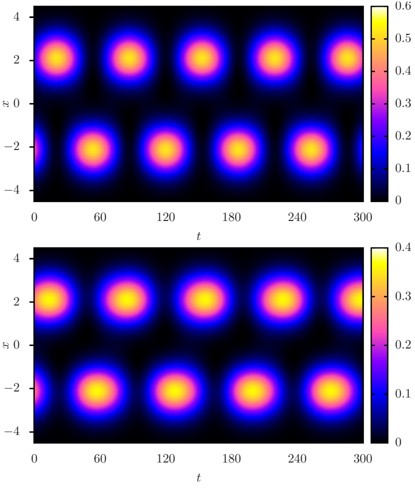
$0 < \Gamma < 0.08$

Different behaviour

- Two complex conjugate eigenvalues bifurcate from the branch point at which the real eigenvalues vanish.
- Structure known from exceptional points appears.
- Other analytic forms might resolve the extension of the $\mathcal{PT}$ broken states for $\Gamma < \Gamma_c$.

Temporal evolution for $\Gamma < \Gamma_{\mathrm{EP}}$

$$\psi(x, t = 0) = \frac{1}{\sqrt{2}} \left(\psi_{GS}(x) + \psi_{ES}(x)\right)$$



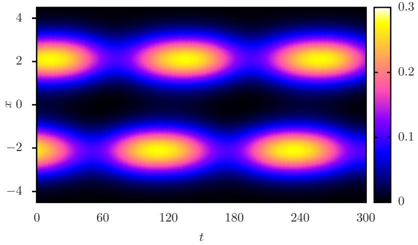
Example

$g = 0.2$, $\Gamma = 0$ (upper panel) and $\Gamma = 0.02$ (lower panel)

Observation

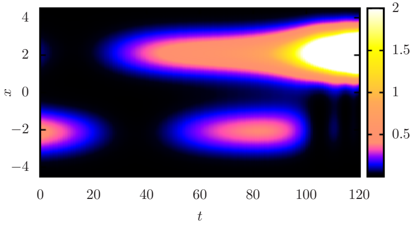
- The probability density oscillates between both wells.
- The beat frequency and the phase relation between both wells depend on Γ.

Temporal evolution for $\Gamma \geq \Gamma_{\mathrm{EP}}$



Example

- $g = 0.2$, $\Gamma = 0.04$
- Probability amplitude pulsates in both wells.



Example

- $g = 0.2$, $\Gamma = 0.03$
- $t = 0$: Only the well with loss is populated.
- The probability amplitude "explodes".

Outline

Summary

- $\mathcal{PT}$ symmetric Bose-Einstein condensates are stable up to a critical strength of the contact interaction and should be observable in an experiment.
- $\mathcal{PT}$ symmetric eigenfunctions exist in nonlinear quantum systems and render the Hamiltonian itself $\mathcal{PT}$ symmetric.
- Complex energy eigenvalues belong to eigenstates with broken $\mathcal{PT}$ symmetry destroying the Hamiltonian's symmetry. They influence the stability of the ground state.
- At a branch point two real eigenvalues vanish, however, a pair of complex conjugate eigenvalues emerging at the critical parameter value can only be exposed in an analytic extension of the model.

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references:
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D. Dast, D. Haag, H. Cartarius, G. Wunner, R. Eichler, J. Main, Fortschr. Phys., in press, DOI: 10.1002/prop.201200080 (2012)

Outlook

Next steps

- Better understanding of the nonlinearity's influence: matrix models, . . .
- More detailed investigation of the stability change of the ground state.
- Possible extension: additional long-range dipole-dipole interaction.
- Detailed microscopic treatment: improved understanding of the loss and gain processes.

Solutions with complex chemical potential

Question

Solutions with complex μ are no true stationary states of the time-dependent Gross-Pitaevskii equation. Are they meaningless?

- Comparison of the norm $N^2 = \int |\psi|^2 \, \mathrm{d}x$ for the correct temporal evolution with the expectation from $\exp(-2 \, \mathrm{Im} \, \mu t)$

Solutions with complex chemical potential

Question

Solutions with complex μ are no true stationary states of the time-dependent Gross-Pitaevskii equation. Are they meaningless?

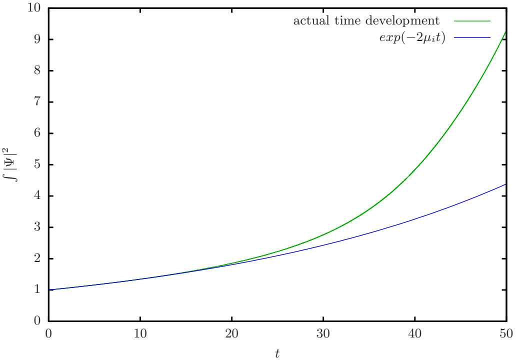
- Comparison of the norm $N^2 = \int |\psi|^2 \, \mathrm{d}x$ for the correct temporal evolution with the expectation from $\exp(-2 \, \mathrm{Im} \, \mu t)$
- Introduce the norm difference:

$$D = \sqrt{\int_{\text{right well}} |\psi|^2 \, \mathrm{d}x} - \sqrt{\int_{\text{left well}} |\psi|^2 \, \mathrm{d}x}$$

- Comparison of the norm difference D of the correct temporal evolution with that of stationary solutions with adapted effective g:

$$g \to g N^2$$

Short time behaviour

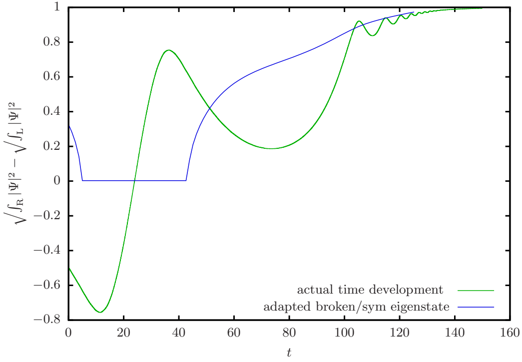


Initial "stationary" state with $\mathrm{Im}\,\mu > 0$

Onset of the norm growth is correctly described by the imaginary part of the energy eigenvalue.

Large time behaviour

Initial “stationary” state with $\mathrm{Im}\,\mu < 0$

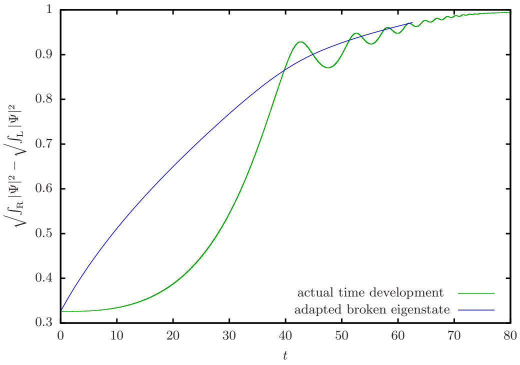


Initially decaying state

Growth for long times “along” the adapted “stationary” state with positive imaginary part.

Large time behaviour

Initial "stationary" state with $\operatorname{Im}\mu > 0$



Initially growing state

Time evolution follows the line of the adapted "stationary" state. Its influence does not vanish completely.

$\mathcal{PT}$ symmetry and nonlinear systems

Considerations of $\mathcal{PT}$ symmetric systems with nonlinearity include:

- $\mathcal{PT}$ symmetric Bose-Hubbard system
  E.M. Graefe, H. J. Korsch, and A. E. Niederle, Phys. Rev. Lett. 101, 150408 (2008)
  E. M. Graefe, U. Günther, H. J. Korsch, A. E. Niederle, J. Phys. A 41, 255206 (2008)
  E.M. Graefe, H. J. Korsch, and A. E. Niederle, Phys. Rev. A 82, 013629 (2010)

- Quantum mechanical model potentials
  Z. Musslimani, K.G. Makris, R. El-Ganainy, and D.N. Christodoulides, Phys. Rev. Lett. 100, 30402 (2008)
  Z.H. Musslimani, K.G. Makris, R. El-Ganainy, and D.N. Christodoulides, J. Phys. A 41, 244019 (2008)

- Optical systems with nonlinearity
  H. Ramezani, T. Kottos, R. El-Ganainy, and D.N. Christodoulides, Phys. Rev. A 82, 043803 (2010)

- Bose-Einstein condensate in an idealized double δ trap
  H. Cartarius and G. Wunner, Model of a PT symmetric Bose-Einstein condensate in a delta-functions double well, preprint arXiv:1203.1885, 2012