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

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PHHQP XI, Paris, 28 August 2012



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Outline

- 1 \mathcal{PT} symmetric quantum systems
 - \mathcal{PT} symmetric waveguides
 - 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

 $\bullet \ \mathcal{PT}$ symmetric and \mathcal{PT} broken states in one and three dimensions

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- Temporal evolution
- Analytical continuations and exceptional point behaviour

5 Conclusion

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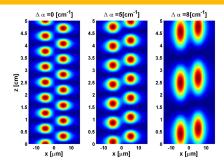
Temporal evolution

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Optical waveguides

Temporal evolution and experimental verification

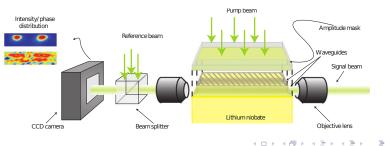


Left: Power distribution of a propagating mode (increasing imaginary contribution from left to right), theory

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

Experimental setup

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

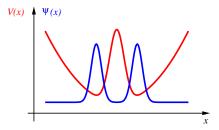


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BEC in a \mathcal{PT} symmetric double well

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



\mathcal{PT} symmetry and nonlinear systems

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

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, Phys. Rev. A 86, 013612 (2012) 2012

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Temporal evolution

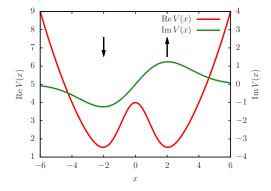
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Form of the potential

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

 \mathcal{PT} symmetry in x direction:



Gain/loss term Γ :

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

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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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Gross-Pitaevskii equation

System of units:

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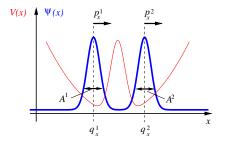
Is the GPE \mathcal{PT} symmetric?

- Interaction term: $-g|\psi({m x},t)|^2$
- 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

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



Variational parameters:

- \bullet widths: $A^1_x, A^2_x, A^1_{y,z}, A^2_{y,z} \in \mathbb{C}$
- 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:

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

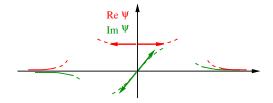
 Effective potential terms v = (v₀¹,..., v₁¹,x,..., V₂¹,x,...): Kv = r matrix K: (weighted) overlap integrals of the Gaussians vector r: (weighted) Gaussian averages of all potential terms

Conditions $\dot{A}_x^k = \dot{A}_{y,z}^k = \dot{q}_x^k = \dot{p}_x^k = 0$ 12 conditions $\dot{\varphi}^k = i\mu$ 4 conditions $||\psi|| = 1$ 1 condition

Numerical procedure:

- Arbitrary global phase → one Gaussian parameter is free: property of the Gross-Pitaevskii equation
- 15 Gaussian parameters can be varied together with ${\rm Re}\,\mu$ and ${\rm Im}\,\mu$ \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: ${\rm Im}\,\psi(0)=0$
- Five real initial values have to be chosen:

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

• Five conditions have to be fulfilled:

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

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• Five-dimensional root search.

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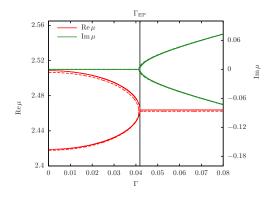
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Spectrum without nonlinearity (g = 0)



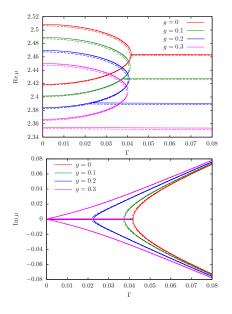
Example

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

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

Summary

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



Example

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

Observation

- Real eigenvalue branches merge and vanish at a value $\Gamma_{\rm EP}.$
- Complex eigenvalues are born at a value $\Gamma_{\rm c} < \Gamma_{\rm EP}.$
- 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.

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Eigenvalues of the three-dimensional problem

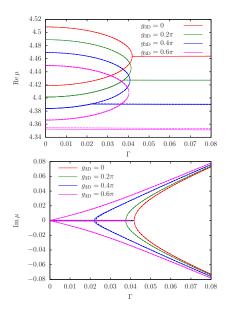
- Expectation: The one-dimensional calculation should contain already all important features.
- Comparison of the eigenvalues of the full three-dimensional problem with those in one dimension.
 - An energy shift of $\Delta\mu=2$ is expected: harmonic oscillator ground states for y and z directions.
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

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

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and obtain

$$g_{1D} = g_{3D} \int_{\mathbb{R}^2} dy dz |\psi_0(y)|^4 |\psi_0(z)|^4$$
$$g_{3D} = 2\pi g_{1D}.$$



Example

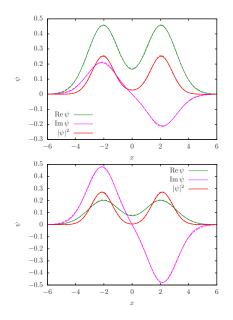
 $g_{1\mathrm{D}} = 0 \dots 0.2$

- 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

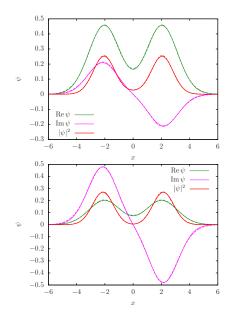
g = 0.2, $\Gamma = 0.03$, ground (upper panel) and excited (lower panel) state:

• Square modulus: symmetric

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Wave functions for real eigenvalues



Critical question

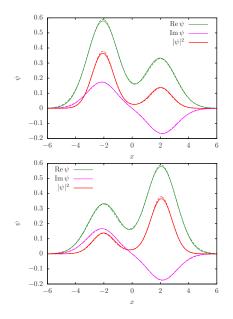
Does the nonlinearity $g|\psi(x)|^2$ destroy the \mathcal{PT} symmetry of the Hamiltonian?

Example

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

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

Wave functions for complex eigenvalues

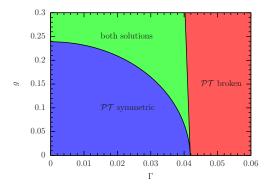


Example

g = 0.2, $\Gamma = 0.03$, states with Re $\mu < 0$ (upper panel) 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!



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.

Stability of the eigenstates

Stability analysis

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:

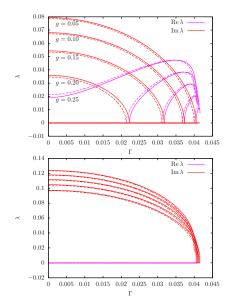
$$\frac{\partial^2}{\partial x^2} u(x) = \left(V(x) - \mu - i\lambda^* - 2g \left| \psi_0(x) \right|^2 \right) u(x) - g\psi_0^2(x)v(x)$$
$$\frac{\partial^2}{\partial x^2} v(x) = \left(V^*(x) - \mu^* + i\lambda^* - 2g \left| \psi_0(x) \right|^2 \right) v(x) - g\psi_0^{*2}(x)u(x)$$

• Variational approach: Jacobian

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

Stability of the eigenstates

Stability eigenvalues of the \mathcal{PT} symmetric states



Example

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

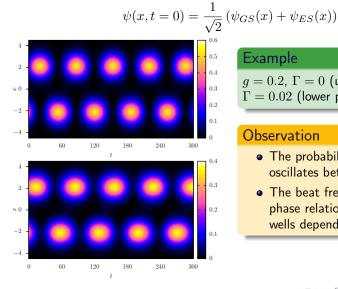
Influence of other states

- Imaginary eigenvalues: stable, real eigenvalues: unstable.
- Ground state: becomes unstable as soon as the *PT* broken branches emerge!
- Excited state: always stable.

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



Example

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

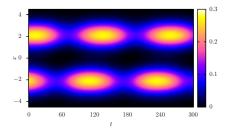
Observation

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

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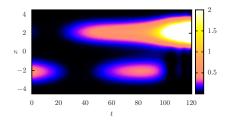
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Temporal evolution for $\Gamma \geq \Gamma_{\rm EP}$



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".

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Complete mathematical structure of an exceptional point

Question

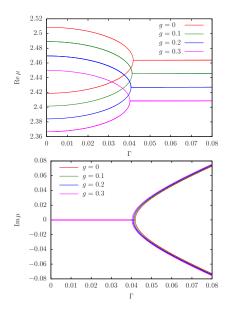
The real branches vanish at the branch point and the complex eigenvalues bifurcate only from the ground state. Can this be explained?

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 I

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 can resolve the extension of the \mathcal{PT} broken states for $\Gamma < \Gamma_{\rm c}.$

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analytical continuation II

decompose the wave function, $\psi=\psi_{\rm r}+{\rm i}\psi_{\rm i}$, the double well potential, $V=V_{\rm r}+{\rm i}V_{\rm i}$, the chemical potential, $\mu=\mu_{\rm r}+{\rm i}\mu_{\rm i}$, and the GPE into real and imaginary parts:

$$-\psi_{\rm r}'' + V_{\rm r}\psi_{\rm r} - V_{\rm i}\psi_{\rm i} - g(\psi_{\rm r}^2 + \psi_{\rm i}^2)\psi_{\rm r} = \mu_{\rm r}\psi_{\rm r} - \mu_{\rm i}\psi_{\rm i} -\psi_{\rm i}'' + V_{\rm r}\psi_{\rm i} + V_{\rm i}\psi_{\rm r} - g(\psi_{\rm r}^2 + \psi_{\rm i}^2)\psi_{\rm r} = \mu_{\rm r}\psi_{\rm i} + \mu_{\rm i}\psi_{\rm r}$$

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analytical continuation II

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analytical continuation: allow the real and imaginary parts of the wave function and the chemical potential to become complex quantities again:

$$\begin{split} \psi_{\mathrm{r}} &= \psi_{\mathrm{rr}} + \mathrm{i} \psi_{\mathrm{ri}} \,, \quad \psi_{\mathrm{i}} = \psi_{\mathrm{ir}} + \mathrm{i} \psi_{\mathrm{ii}} \\ \mu_{\mathrm{r}} &= \mu_{\mathrm{rr}} + \mathrm{i} \mu_{\mathrm{ri}} \,, \quad \mu_{\mathrm{i}} = \mu_{\mathrm{ir}} + \mathrm{i} \mu_{\mathrm{ii}} \end{split}$$

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analytical continuation II

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$$-\psi_{\mathbf{i}}'' + V_{\mathbf{r}}\psi_{\mathbf{i}} + V_{\mathbf{i}}\psi_{\mathbf{r}} - g(\psi_{\mathbf{r}}^2 + \psi_{\mathbf{i}}^2)\psi_{\mathbf{r}} = \mu_{\mathbf{r}}\psi_{\mathbf{i}} + \mu_{\mathbf{i}}\psi_{\mathbf{r}}$$

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you can either plot the 4 real quantities $\mu_{\rm rr}, \mu_{\rm ri}, \mu_{\rm ir}, \mu_{\rm ii}$ separately, or split

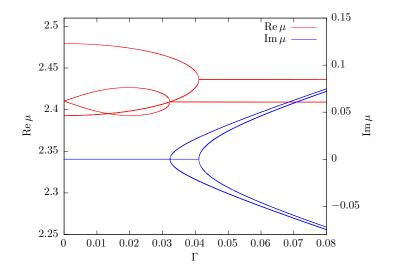
$$\mu = \mu_{\rm rr} + i\mu_{\rm ri} + i(\mu_{\rm ir} + i\mu_{\rm ii})$$

into real and imaginary part again

$$\mu = (\mu_{\rm rr} - \mu_{\rm ii}) + i(\mu_{\rm ri} + \mu_{\rm ir})$$

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analytical continuation II, spectrum for g = 0.15



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• At the branch point, the three eigenfunctions are identical. Can we find evidence for EP 3 behaviour?

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- Encircling the branch point by extending one parameter, the strength of the loss and gain term Γ , into the complex plane, is not enough.

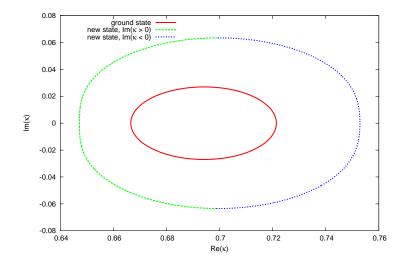
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- At the branch point, the three eigenfunctions are identical. Can we find evidence for EP 3 behaviour?
- Encircling the branch point by extending one parameter, the strength of the loss and gain term Γ , into the complex plane, is not enough.

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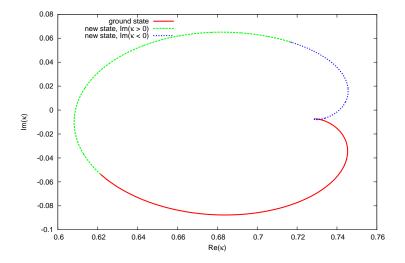
• Introduce a small asymmetry into the double well potential, e.g., $V_{\rm asym} = Ax {\rm e}^{-\varrho x^2}$, and encircle the branch point around A = 0 in the complex extended A plane.

exceptional point behaviour: encircling with complex Γ



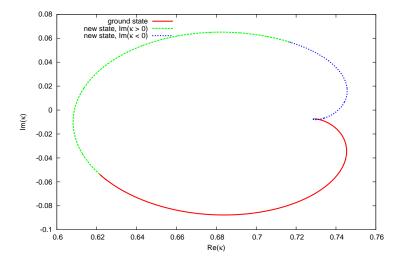
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exceptional point behaviour: encircling with complex A



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exceptional point behaviour: encircling with complex A



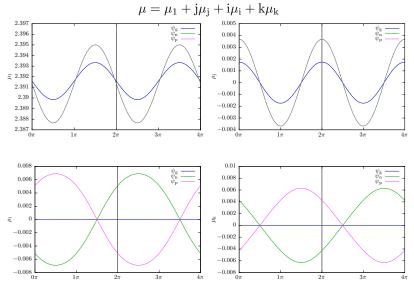
in agreement with findings of Demange and Graefe (J. Phys. A 45, 025303 (2012)) in a simple matrix model for three coalescing eigenvectors

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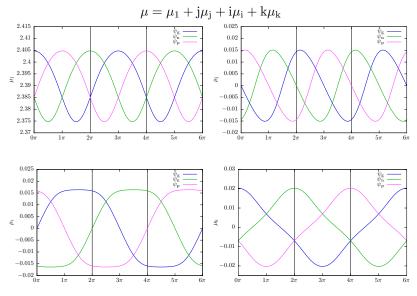
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encircling in the complex extended nonlinearity plane



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encircling in the complex extended asymmetry plane



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Outline

- $\bigcirc \mathcal{PT}$ symmetric quantum systems
 - *PT* symmetric waveguides
 - 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

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- Temporal evolution
- 4 Analytical continuations and exceptional point behaviour

5 Conclusion

- \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.
- In analytical extensions, the model mathematically exhibits rich structure of branching and exceptional-points (EP 3-type) behaviour, which should be explored in more detail in the future.

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.

references:

H. Cartarius, G. Wunner, Phys. Rev. 86, 013612 (2012)
D. Dast, D. Haag, H. Cartarius, G. Wunner, R. Eichler, J. Main, Fortschr. Phys., in press, DOI: 10.1002/prop.201200080 (2012)

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 $\exp(-2\,\mathrm{Im}\,\mu t)$

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Question

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

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

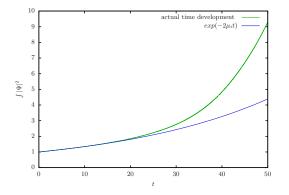
$$D = \sqrt{\int_{\text{right well}} |\psi|^2 \, \mathrm{d}x} - \sqrt{\int_{\text{left well}} |\psi|^2 \, \mathrm{d}x}$$

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

$$g \rightarrow g N^2$$

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Short time behaviour

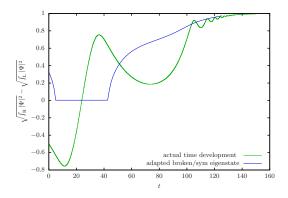


Initial "stationary" state with $\operatorname{Im} \mu > 0$

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

Large time behaviour

Initial "stationary" state with ${\rm Im}\,\mu<0$



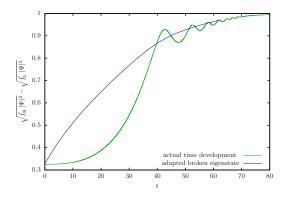
Initially decaying state

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

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Large time behaviour

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



Initially growing state

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

Non-Hermitian \mathcal{PT} symmetric Hamiltonians

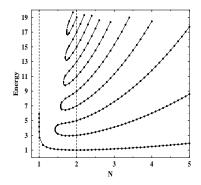


FIG. 1. Energy levels of the Hamiltonian $H = p^2 - (ix)^N$ as a function of the parameter N. There are three regions: When $N \ge 2$ the spectrum is real and positive. The lower bound of this region, N = 2, corresponds to the harmonic oscillator, whose energy levels are $E_n = 2n + 1$. When 1 < N < 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) ヘロト ヘロト ヘモト ヘモト

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\mathcal{PT} symmetric quantum systems

Symmetry operators:

- Parity: spatial reflections $\mathcal{P}: x \to -x$, $p \to -p$

 \mathcal{PT} symmetric Hamiltonians

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

• Necessary condition:

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

• Required form of the potential:

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

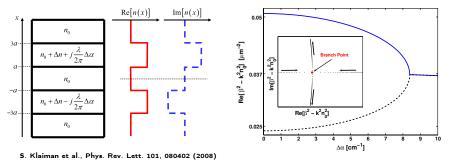
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Optical waveguides

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.



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