# Bifurcations, order, and chaos in Bose-Einstein condensates with long-range interactions


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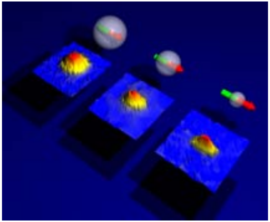
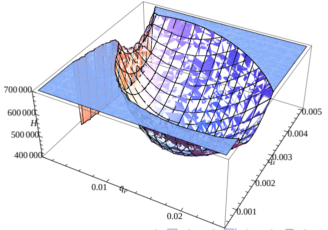




# 1. Introduction

- Bose-Einstein condensation: neutral atoms are caught in a trap and cooled down to $\approx$ zero temperature, where a macroscopic quantum state forms in which all bosons occupy the same ground state
- Gross-Piatevksii equation for Bose-Einstein condensates (BEC)
- BEC with long-range interactions

# ground state of interacting neutral atoms at $T = 0$

system of $N$ identical bosons in an external potential $U(\vec{r})$, interacting via a two-body interaction potential $V(\vec{r}, \vec{r}\,')$

- many-body Hamiltonian

$$H = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_i U(\vec{r}_i) + \sum_{i<j} V(\vec{r}_i, \vec{r}_j)$$

- Zero-temperature bosonic ground state: $\Psi = \prod_{i=1}^{N} \psi(i)$

## Hartree equation for single-particle orbital $\psi$

$$\left\{ \frac{\vec{p}^{\,2}}{2m} + U(\vec{r}) + (N-1) \int V(\vec{r}, \vec{r}\,') |\psi(\vec{r}\,')|^2 d^3\vec{r}\,' \right\} \psi(\vec{r}) = i\hbar \frac{\partial \psi(\vec{r})}{\partial t}$$

- nonlinear Schrödinger equation
- superposition principle no longer applicable

# Bose-Einstein condensation of "ordinary" neutral atoms ($^7$Li, $^{85}$Rb, ...): potentials

- external trapping potential to confine the condensate

$$U(\vec{r}) = \frac{m}{2}\left(\omega_x^2\, x^2 + \omega_y^2\, y^2 + \omega_z^2\, z^2\right)$$

$\omega_x,\ \omega_y,\ \omega_z$: trapping frequencies

- dilute condensate, weakly interacting atoms $\Longrightarrow$ only the short-range contact two-body interaction ($s$-wave scattering interaction) active

$$V_s(\vec{r},\vec{r}') = \frac{4\pi a \hbar^2}{m}\ \delta(\vec{r}-\vec{r}')$$

$a$: $s$-wave scattering length

# Bose-Einstein condensation of "ordinary" neutral atoms ($^7$Li, $^{85}$Rb, ...): Hartree and Gross-Pitaevskii equation

**Hartree equation for single-particle orbital $\psi$**

$$\left\{ \frac{\vec{p}^{\,2}}{2m} + \frac{m}{2} (\vec{\omega} \cdot \vec{r})^2 + (N-1) \frac{4\pi a \hbar^2}{m} |\psi(\vec{r})|^2 \right\} \psi(\vec{r}) = i\hbar \frac{\partial \psi(\vec{r})}{\partial t}$$

- for $N \gg 1$: $(N-1) \approx N$,

  define macroscopic wave function $\Psi(\vec{r}) := \sqrt{N}\psi(\vec{r})$, i.e. $||\Psi||^2 = N$

**Gross-Pitaevskii equation for $\Psi$**

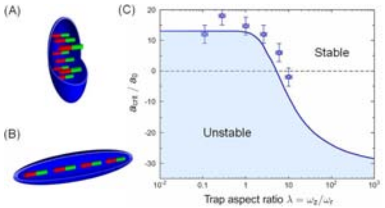
$$\left\{ \frac{\vec{p}^{\,2}}{2m} + \frac{m}{2} (\vec{\omega} \cdot \vec{r})^2 + \frac{4\pi a \hbar^2}{m} |\Psi(\vec{r})|^2 \right\} \Psi(\vec{r}) = i\hbar \frac{\partial \Psi(\vec{r})}{\partial t}$$

# BEC of neutral atoms with additional long-range interaction: dipolar atoms (experiments by Pfau et al., PRL **94**, 160401 (2005))

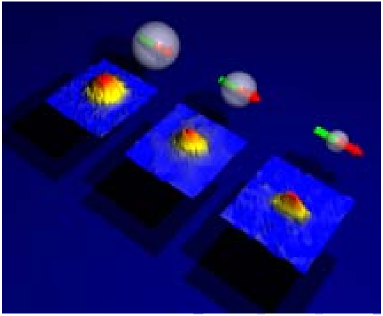
chromium ($^{52}$Cr): large magnetic moment, $\mu = 6\mu_{\rm B}$, i.e. also a long-range dipole-dipole interaction is active

$$V_{\rm dd}(\mathbf{r}, \mathbf{r}') = \frac{\mu_0 \mu^2}{4\pi} \frac{1 - 3\cos^2\theta'}{|\mathbf{r} - \mathbf{r}'|^3}$$

- new aspect: relative strength of the long-range and short-range interactions can be tuned by Feshbach resonances (change of the scattering length $a$)



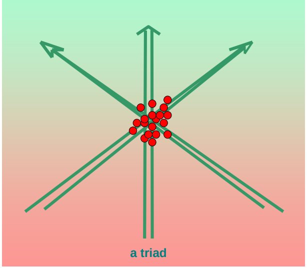

www.pi5.uni-stuttgart.de/forschung/chromium1/chromium1.html



# BEC of neutral atoms with alternative long-range interaction: gravity-like 1/r interaction

Motivation: proposal by D.O. O'Dell, S. Giovanazzi, G. Kurizki, V.M. Akulin, PRL 84, 5697 (2000)

6 "triads" of intense off-resonant laser beams average out $1/r^3$ interactions in the near-zone limit of the retarded dipole-dipole interaction of neutral atoms in the presence of radiation $I$, while retaining the weaker $1/r$ interaction




resulting atom–atom potential in the near-zone:

$$U(\vec{r},\vec{r}\,') = -\frac{11}{4\pi}\,\frac{Ik^2\alpha^2}{c\varepsilon_0^2}\,\frac{1}{|\vec{r}-\vec{r}\,'|}$$

- gravity-like interaction: $V_u(\vec{r},\vec{r}\,') = -\dfrac{u}{|\vec{r}-\vec{r}\,'|}$, "monopolar atoms"
- novel physical feature: *self-trapping* of the condensate, without external trap,
- theoretical advantage: for self-trapping analytical variational calculations are feasible

# purpose of this talk

to study the classical and the quantum nonlinear effects of the Gross-Pitaevskii equations for cold

- monopolar quantum gases ($1/r$ interaction) and
- dipolar quantum gases (dipole-dipole interaction)

# outline of the talk

- 1. Introduction
- 2. Scaling properties of the Gross-Pitaevskii equations with long-range interactions
- 3. Quantum results: solutions of the *stationary* Gross-Pitaevskii equations
- 4. Nonlinear dynamics of Bose-Einstein condensates with atomic long-range interactions

# 2.1 Gross-Pitaevskii equation for atoms with gravity-like interaction in an isotropic trap

### Gross-Piatevskii equation for orbital $\psi$

$$\left\{\frac{\vec{p}^{\,2}}{2m}+\frac{m\omega_0^2}{2}r^2+N\left[\frac{4\pi a\hbar^2}{m}|\psi(\vec{r})|^2-u\int\frac{|\psi(\vec{r}')|^2}{|\vec{r}-\vec{r}'|}d^3\vec{r}'\right]\right\}\psi(\vec{r})=\varepsilon\psi(\vec{r})$$

- natural units: trap energy $\hbar\omega_0$, oscillator length $a_0$
  self-trapping: $\hbar\omega_0\to 0$, $a_0=\sqrt{\hbar/m\omega_0}\to\infty$, bad units
- more adequate: "atomic units"
  analogy $u\Leftrightarrow e^2/4\pi\varepsilon_0$: "fine-structure constant" $\alpha_u:=u/\hbar c$
- "Bohr radius" $a_u=\lambda_{\mathrm{C}}/\alpha_u=\hbar/mu$
- "Rydberg energy" $E_u=\alpha_u^2 mc^2/2=\hbar^2/2ma_u^2$

# Gross-Piatevskii equation for monopolar gases

**in "atomic units"**

$$\underbrace{\left\{-\Delta + \gamma^2 r^2 + N 8\pi \frac{a}{a_u} |\psi(\vec{r})|^2 - 2N \int\int \frac{|\psi(\vec{r}\,')|^2}{|\vec{r} - \vec{r}\,'|} d^3\vec{r}\,'\right\}}_{\text{mean-field Hamiltonian} H_{\mathrm{mf}}} \psi(\vec{r}) = \varepsilon \psi(\vec{r})$$

- three physical parameters:

  $\gamma = \hbar\omega_0 / E_{\mathrm{u}}$: trap frequency

  $N$ : particle number,

  $a/a_u$: relative strength of scattering and gravity-like potential
- estimate: $a \sim 10^{-9}$ m, $a_u \sim 2.5 \times 10^{-4}$ m, thus
  $a/a_u \sim 10^{-6} - 10^{-5}$

**scaling property of $H_{\mathrm{mf}} \Rightarrow$ only <u>two</u> relevant parameters: $\gamma/N^2, N^2\, a/a_u$**

mean field energy: $E(N, N^2 a/a_u, \gamma/N^2)\,/N^3 \;=\; E(N = 1, a/a_u, \gamma)$

# 2.2 Gross-Pitaevskii equation for atoms with dipolar interaction in an axisymmetric trap

## Gross-Pitaevskii equation for orbital $\psi$

$$\left(\hat{h} + N\left\{\frac{4\pi a\hbar^2}{m}\left|\psi\left(\mathbf{r}\right)\right|^2 + \frac{\mu_0\mu^2}{4\pi}\int d^3r'\frac{1-3\cos^2\vartheta'}{\left|\mathbf{r}-\mathbf{r}'\right|^3}\left|\psi\left(\mathbf{r}'\right)\right|^2\right\}\right)\psi\left(\mathbf{r}\right) = \varepsilon\psi\left(\mathbf{r}\right)$$

with

$$\hat{h} = -\frac{\hbar^2}{2m}\Delta_{\mathbf{r}} + V_{\text{trap}}\left(\mathbf{r}\right)$$

and

$$V_{\text{trap}} = m(\omega_\rho^2 r^2 + \omega_z^2 z^2)/2$$

- units of length: $a_{\rm d}$ energy: $E_{\rm d}$ frequency $\omega_{\rm d}$

$$a_{\rm d} = \frac{\mu_0\mu^2 m}{2\pi\hbar^2} \qquad E_{\rm d} = \hbar^2/(2ma_{\rm d}^2) \qquad \omega_{\rm d} = E_{\rm d}/\hbar,$$

# Gross-Pitaevskii equation for dipolar gases

**in dimensionless form:**

$$\Big[ \; -\Delta + \gamma_\rho^2 \rho^2 + \gamma_z^2 z^2 + N 8\pi \frac{a}{a_d} |\psi(\mathbf{r})|^2$$

$$+ \quad N \int |\psi(\mathbf{r}\,')|^2 \frac{(1 - 3\cos^2\vartheta')}{|\mathbf{r} - \mathbf{r}\,'|^3} d^3\mathbf{r}\,' \Big] \, \psi(\mathbf{r}) = \varepsilon \, \psi(\mathbf{r})$$

with

$$\gamma_{\rho,z} = \omega_{\rho,z}/(2\omega_{\rm d})$$

- 4 physical parameters: $N, a/a_d, \gamma_\rho, \gamma_z$, $(\bar\gamma = \gamma_\rho^{2/3}\gamma_z^{1/3}$, $\lambda = \gamma_z/\gamma_\rho$ )

**scaling property of $H_{\rm mf}$ $\Rightarrow$ only <u>three</u> relevant parameters: $N^2\bar\gamma, \;\lambda, \; a/a_{\rm d}$**

mean field energy: $E(N, a/a_{\rm d}, N^2\bar\gamma, \lambda) \, = \, E(N=1, a/a_{\rm d}, \bar\gamma, \lambda)\,/N^2$

# 3. Quantum results: solutions of the *stationary* Gross-Pitaevskii equations

$1/r$ interaction (monopolar quantum gases):

- variational with an isotropic Gaussian type orbital:

  $\psi = A \exp(-k^2 r^2/2)$

- numerically accurate by outward integration of the extended Gross-Pitaevskii equation

dipole-dipole interaction (dipolar quantum gases):

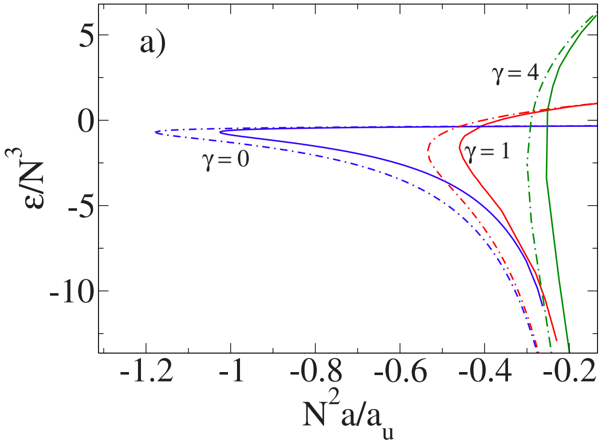
- variational with an axisymmetric Gaussian type orbital:

  $\psi = A \exp(-k_\rho^2 \rho^2/2 - k_z^2 z^2/2)$

  coupled system of nonlinear equations resulting from $\frac{\partial E}{\partial k_\rho} = 0, \frac{\partial E}{\partial k_z} = 0$ is solved numerically for given trap parameters and scattering length

# $1/r$ interaction: chemical potential

for different trap frequencies

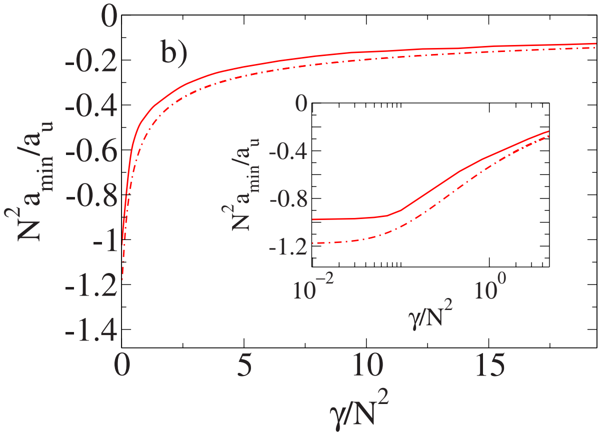



solid: accurate numerical calculation

dashed: variational

two stationary solutions are born at the critical point in a tangent bifurcation, below the critical point no stationary solutions exist

# $1/r$ interaction: bifurcation point as a function of trapping frequency

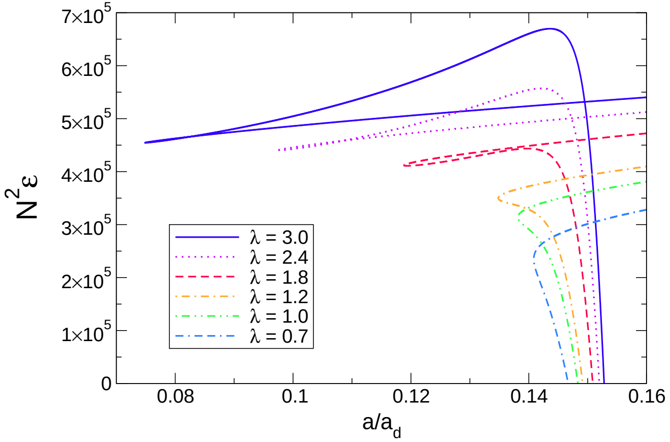



solid: accurate numerical calculation

dashed: variational

# dipole-dipole interaction: chemical potential

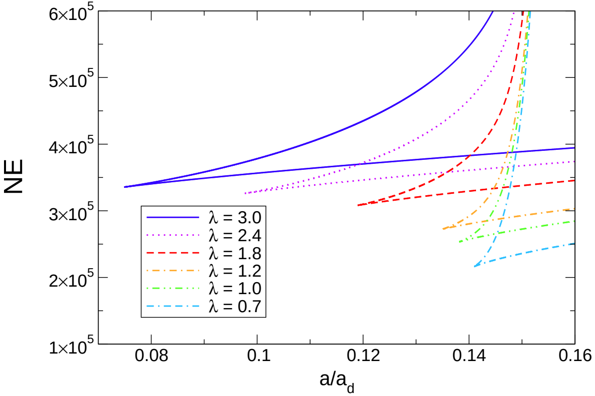
for $N^2\bar{\gamma} = 3.4 \times 10^4$ and different trap aspect ratios



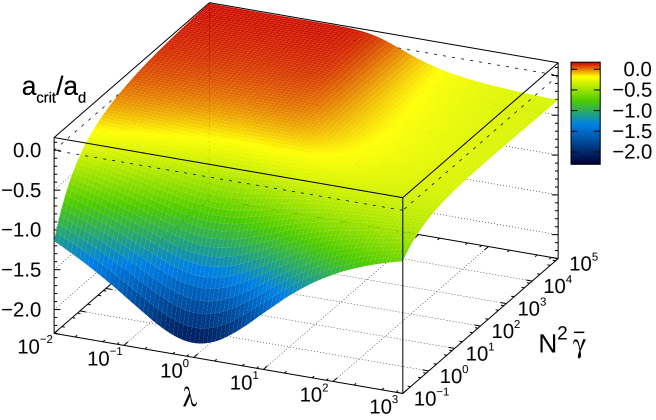

two stationary solutions are born at the critical scattering length in a tangent bifurcation, below the critical scattering length no stationary solutions exist

# dipole-dipole interaction: bifurcation of the mean-field energy

for $N^2\bar{\gamma} = 3.4 \times 10^4$ and different trap aspect ratios



# dipole-dipole interaction: universal dependence of the critical scattering length $a_{\text{crit}}/a_{\text{d}}$ on the trap geometry:



# Bose-Einstein condensates with long-range interactions: tangent bifurcations and exceptional points

## résumé so far

- Stationary solutions appear only in certain regions of the parameter space.
- Two solutions appear in a tangent bifurcation at the critical value in parameter space.
- At the tangent bifurcation the chemical potential, the mean field energy, and the wave functions are identical.
- This behaviour is typical of exceptional points.
- The bifurcation points indeed turn out to be exceptional points.

# 4. Nonlinear dynamics of Bose-Einstein condensates with atomic long-range interactions

starting point:

- time-dependent Gross-Piatevskii equation for accurate numerical calculations

$$\left[-\frac{\hbar^2}{2m}\Delta + V_{\text{ext}}(\mathbf{r}) + N\left(\frac{4\pi a\hbar^2}{m}|\psi(\mathbf{r})|^2 + V_{\text{int}}(\mathbf{r})\right)\right]\psi(\mathbf{r}) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r})$$

  - $V_{\text{int}}$ = electromagnetically induced attractive $1/r$ interaction
  - $V_{\text{int}}$ = dipole-dipole interaction

- time-dependent variational principle for variational calculations

$$||i\phi(t) - H\psi(t)||^2 \overset{!}{=} \min \text{ with respect to } \phi \quad (\phi \equiv \dot{\psi}).$$

  Using a complex parametrization of the trial wave function $\psi(t) = \chi(\boldsymbol{\lambda}(t))$, the variation leads to the equations of motion for the parameters $\boldsymbol{\lambda}(t)$:

$$\left\langle \frac{\partial\psi}{\partial\boldsymbol{\lambda}} \middle| i\dot{\psi} - H\psi \right\rangle = 0 \leftrightarrow K\dot{\boldsymbol{\lambda}} = -i\mathbf{h} \text{ with } K = \left\langle \frac{\partial\psi}{\partial\boldsymbol{\lambda}} \middle| \frac{\partial\psi}{\partial\boldsymbol{\lambda}} \right\rangle, \mathbf{h} = \left\langle \frac{\partial\psi}{\partial\boldsymbol{\lambda}} \middle| H \middle| \psi \right\rangle$$

# 4.1 BEC with $1/r$ interaction, self-trapping, variational

Gaussian trial wave function $\psi(r,t) = \exp\{\mathrm{i}[A(t)r^2 + \gamma(t)]\}$,

$A, \gamma$ complex functions, equations of motion for $A = A_r + iA_i$:

$$\dot{A}_r = -2(A_r^2 - A_i^2) + \frac{4}{\sqrt{\pi}} A_i^{3/2} \left( aA_i - \frac{1}{6} \right) , \; \dot{A}_i = -4A_r A_i$$

replace the variational width parameters $A = A_r + iA_i$ with two other dynamical quantities

$$q = \frac{1}{2}\sqrt{\frac{3}{A_i}} = \sqrt{\langle r^2 \rangle} , \quad p = A_r \sqrt{\frac{3}{A_i}} ,$$

# equations of motion in Hamiltonian form

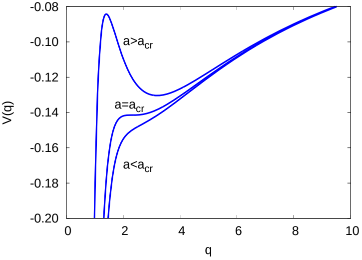
mean-field energy:

$$E = H(q,p) = T + V = p^2 + \frac{9}{4q^2} + \frac{3\sqrt{3}a}{2\sqrt{\pi}q^3} - \frac{\sqrt{3}}{\sqrt{\pi}q}$$

converts the Gross-Pitaevskii equation into a one-dimensional classical autonomous Hamiltonian system with potential $V(q)$:

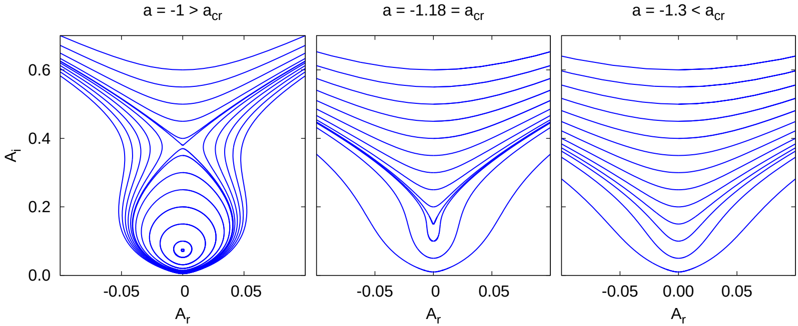
$$\dot{q} = \frac{\partial H}{\partial p} = 2p$$

$$\dot{p} = -\frac{\partial H}{\partial q} = \frac{9}{2q^3} + \sqrt{\frac{3}{\pi}}\frac{9a}{2q^4} - \sqrt{\frac{3}{\pi}}\frac{1}{q^2} .$$



# BEC with $1/r$ interaction, self-trapping, variational

phase portraits for different scattering lengths $a \equiv N^2 a/a_{\mathrm{u}}$




fixed points: $\hat{A}_r = 0,\ \hat{A}_i = \frac{1}{6a} + \frac{\pi}{8a^2}\left(1 \pm \sqrt{1 + 8a/3\pi}\right)$ clear indication of a *stable* and *unstable* stationary state.

## 4.2 Linear stability analysis of variational and exact quantum solutions for monpolar gases

# linear stability analysis of the variational solutions

Linearization of the equations of motion around the stable $(+)$ and unstable $(-)$ stationary states with the ansatz $A_{r,i}^{(\mathrm{lin})}(t) = A_{r,i}^{(0)} e^{\lambda t}$ yields the eigenvalues

$$\lambda_+ = \pm \frac{8\mathrm{i}}{9\pi} \frac{\sqrt[4]{1+\frac{8a}{3\pi}}}{\left(\sqrt{1+\frac{8a}{3\pi}}+1\right)^2}\,, \quad \lambda_- = \pm \frac{8}{9\pi} \frac{\sqrt[4]{1+\frac{8a}{3\pi}}}{\left(\sqrt{1+\frac{8a}{3\pi}}-1\right)^2}$$

- The eigenvalues $\lambda_+ = \pm \mathrm{i}\omega$ are always imaginary for $a > -3\pi/8$.
  Time evolution: $A_{r,i}^{(\mathrm{lin})}(t) = A_{r,i}^{(0)} e^{\mathrm{i}\omega t} \hat{=}$ elliptic fixed point, condensate oscillates periodically
- The eigenvalues $\lambda_-$ are positive and negative real for $a > -3\pi/8$.
  Time evolution: $A_{r,i}^{(\mathrm{lin})}(t) = A_{r,i}^{(0)} e^{\lambda_- t} \hat{=}$ hyperbolic fixed point, condensate collapses

# linear stability analysis of the exact quantum solutions

Linearization of the time-dependent Gross-Pitevskii equation around the stationary solutions $\hat{\psi}(\boldsymbol{r}, t)$ with the Fréchet derivative (using real and imaginary parts of the wave function) leads to:

$$\frac{\partial}{\partial t}\delta\psi^R(\boldsymbol{r},t) = \left(-\Delta - \varepsilon + 8\pi a\hat{\psi}(\boldsymbol{r})^2 - 2\int \mathrm{d}\boldsymbol{r}'\,\frac{\hat{\psi}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\right)\delta\psi^I(\boldsymbol{r},t)$$

$$\frac{\partial}{\partial t}\delta\psi^I(\boldsymbol{r},t) = \left(-\Delta - \varepsilon + 24\pi a\hat{\psi}(\boldsymbol{r})^2 - 2\int \mathrm{d}^3\boldsymbol{r}'\,\frac{\hat{\psi}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\right)\delta\psi^R(\boldsymbol{r},t)$$

$$+ 4\hat{\psi}(\boldsymbol{r})\int \mathrm{d}^3\boldsymbol{r}'\,\frac{\hat{\psi}(\boldsymbol{r}')\,\delta\psi^R(\boldsymbol{r}',t)}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

- Note: $\delta\psi^R(\boldsymbol{r})$ and $\delta\psi^I(\boldsymbol{r})$ can be complex wave functions.
- Only radially symmetric solutions are searched.

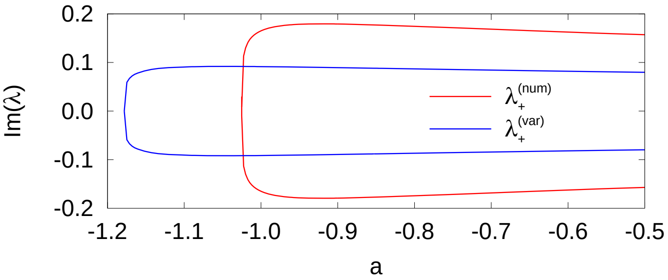
# linearized integro-differential equations

- Using the ansatz for the eigenmodes

$$\delta\psi^R(\boldsymbol{r},t) = \delta\psi_0^R(\boldsymbol{r})\mathrm{e}^{\lambda t}\,,\ \delta\psi^I(\boldsymbol{r},t) = \delta\psi_0^I(\boldsymbol{r})\mathrm{e}^{\lambda t}$$

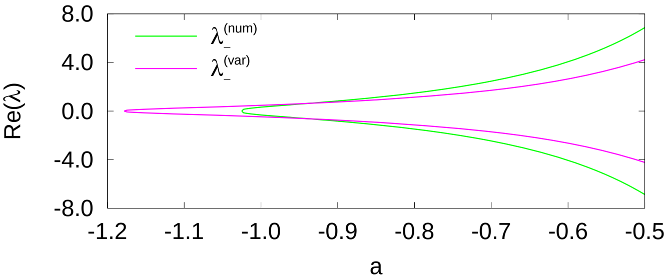
  the two coupled integro-differential equations are transformed to ordinary differential equations with boundary conditions.
- Including the stationary wave function, the potential, and the linearized potential a total set of 18 real-valued first order differential equations must be solved.
- 6 real parameters must be varied to fulfill the boundary conditions.
- Because of a symmetry of the differential equations the stability eigenvalues occur in pairs: $\lambda_1 = -\lambda_2$

# stability eigenvalues for the ground state: numerical vs. variational results




- There is a pair $\lambda_1 = -\lambda_2$ of purely imaginary eigenvalues which agree qualitatively very good with the variational calculation.
- Further purely imaginary eigenvalues can be found for "higher" states of the linearized system.

# stability eigenvalues for the collectively excited stationary state: numerical vs. variational results

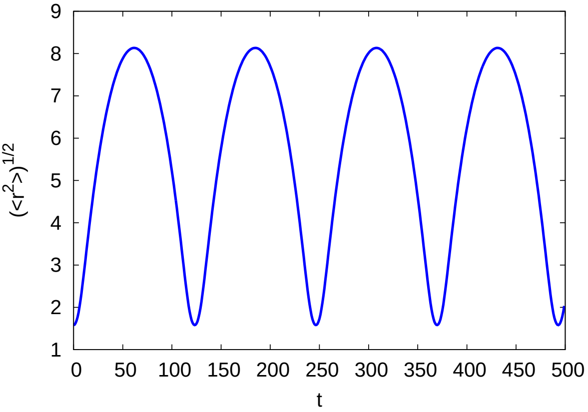



- There is a pair $\lambda_1 = -\lambda_2$ of purely real eigenvalues which agree qualitatively very good with the variational calculation.
- Further purely imaginary eigenvalues were found for "higher" states of the linearized system.

# 4.3 Time evolution of condensates of monopolar gases

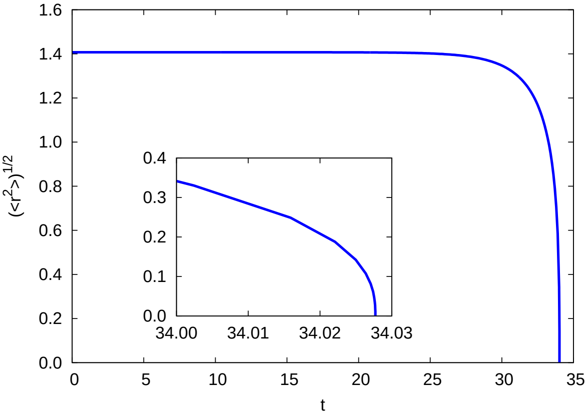
# time evolution of the condensate: variational

above bifurcation point, stable region, $a = -1 > a_{\rm cr}$, $A_i(0) = 0.3$



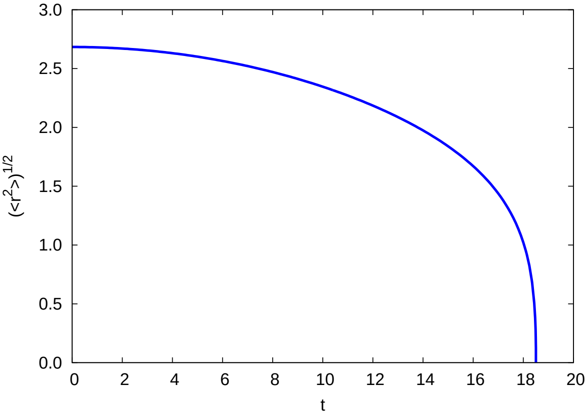
# time evolution of the condensate: variational

above bifurcation point, beyond separatrix, $a = -1 > a_{\rm cr}$, $A_i(0) = 0.38$



# time evolution of the condensate: variational

below bifurcation point, $a = -1.3 < a_{\rm cr}$, $A_i(0) = 0.1$



# exact time-dependent quantum mechanical calculations

numerically exact propagation of perturbed stationary states $\psi_{\pm}(r)$

$$\psi(r) = f \cdot \psi_{\pm}(r \cdot f^{2/3})$$

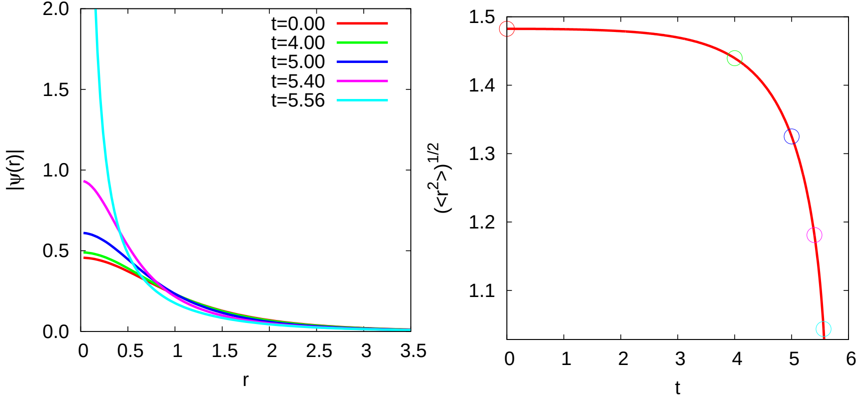
$\psi_+$ : stable stationary state
$\psi_-$ : unstable stationary state

exact computations performed by the split operator method using the splitting $H = T + V$

$$e^{-i\tau(T+V)} = e^{-i(\tau/2)T} e^{-i\tau V} e^{-i(\tau/2)T} + O(\tau^3)$$

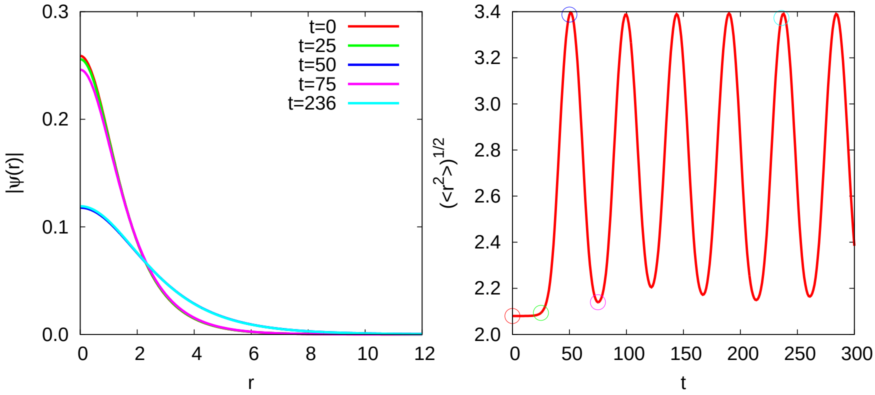
# exact BEC dynamics, in the vicinity of $\psi_-$

Scaled scattering length $a = -0.85$ and $f = 1.001$



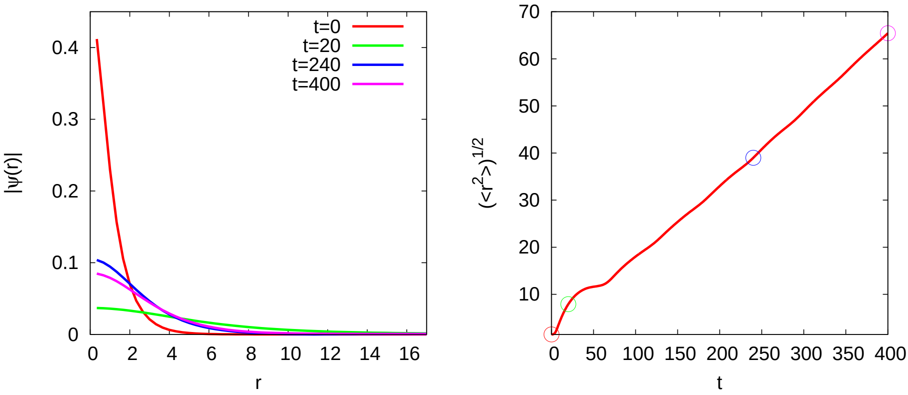
# exact BEC dynamics, in the vicinity of $\psi_-$

Scaled scattering length $a = -1.0$ and $f = 1.00$



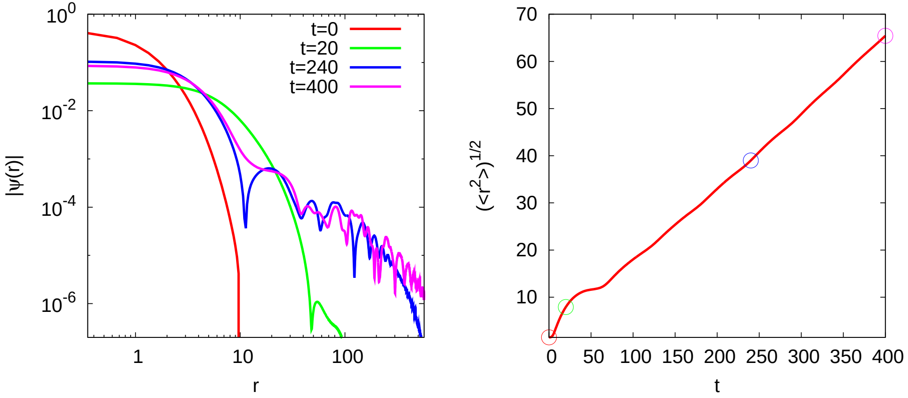
# exact BEC dynamics, in the vicinity of $\psi_-$

Scaled scattering length $a = -0.85$ and $f = 0.99$



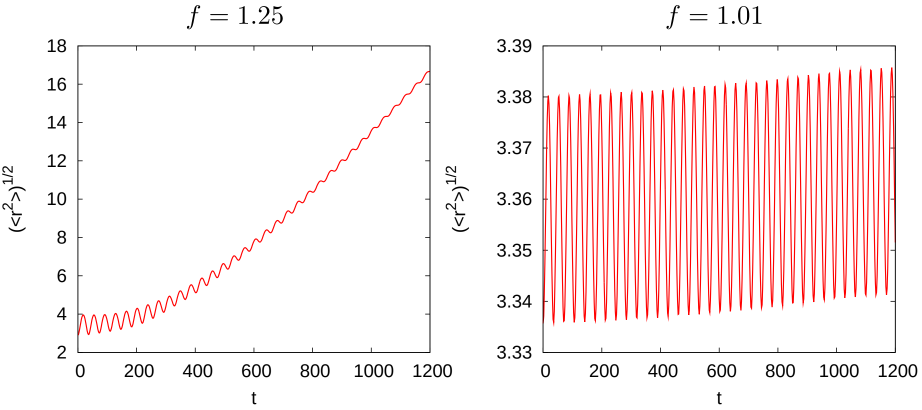
# exact BEC dynamics, in the vicinity of $\psi_-$

Scaled scattering length $a = -0.85$ and $f = 0.99$



# exact BEC dynamics, in the vicinity of $\psi_+$

Scaled scattering length $a = -0.85$



# 4.4 Dynamics of BEC with dipole-dipole interaction, variational

axisymmetric Gaussian trial function

$$\psi(r,z,t) = e^{i(A_\rho \rho^2 + A_z z^2 + \gamma)}; \quad A_\rho = A_\rho(t),\ A_z = A_z(t),\ \gamma = \gamma(t)$$

Equations of motion follow from the time dependent variational principle

$$\begin{aligned}
\dot{A}_\rho^r &= -4((A_\rho^r)^2 - (A_\rho^i)^2) + f_\rho(A_\rho^i, A_z^i, \gamma^i) \\
\dot{A}_\rho^i &= -8A_\rho^r A_\rho^i \\
\dot{A}_z^r &= -4((A_z^r)^2 - (A_z^i)^2) + f_z(A_\rho^i, A_z^i, \gamma^i) \\
\dot{A}_z^i &= -8A_z^r A_z^i \\
\dot{\gamma}^r &= -4A_\rho^i - 2A_z^i + f_\gamma(A_\rho^i, A_z^i, \gamma^i) \\
\dot{\gamma}^i &= 4A_\rho^r + 2A_z^r
\end{aligned}$$

solved with the initial values $A_\rho^r = 0,\ A_\rho^i > 0, A_z^r = 0, A_z^i > 0$ and

$$\gamma^i = \frac{1}{2}\ln\frac{\pi^{3/2}}{2\sqrt{2}A_\rho^i\sqrt{A_z^i}},$$

Four remaining coupled ODEs for $\dot{A}_\rho^r, \dot{A}_\rho^i, \dot{A}_z^r, \dot{A}_z^i$ !

# equations of motion in Hamiltonian form

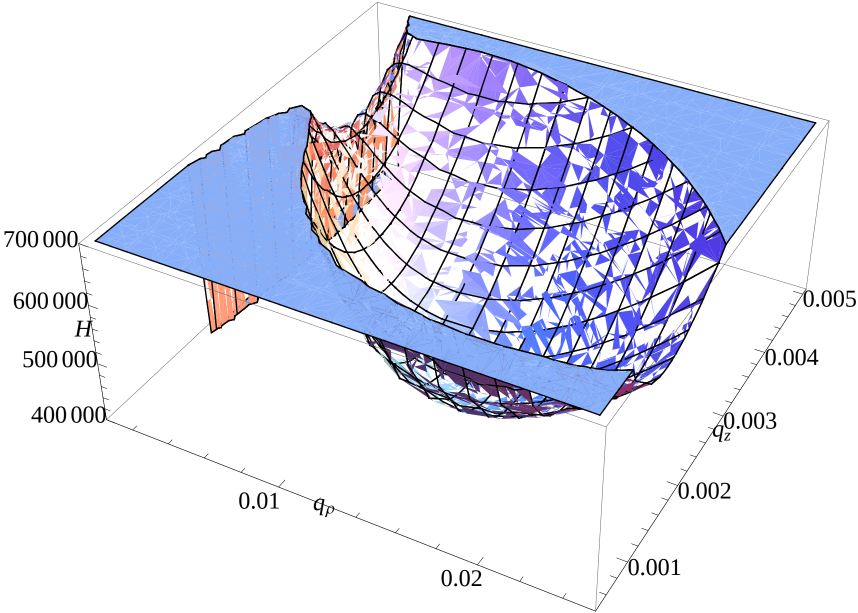
introduction of new variables $q_\rho, q_z, p_\rho, p_z$:

$\mathrm{Re}\, A_\rho = \frac{p_\rho}{4q_\rho}$, $\mathrm{Im}\, A_\rho = \frac{1}{4q_\rho^2}$, $\mathrm{Re}\, A_z = \frac{p_z}{4q_z}$, $\mathrm{Im}\, A_z = \frac{1}{8q_z^2}$

equations of motion for $q_\rho, q_z, p_\rho, p_z$ follow from the Hamiltonian:

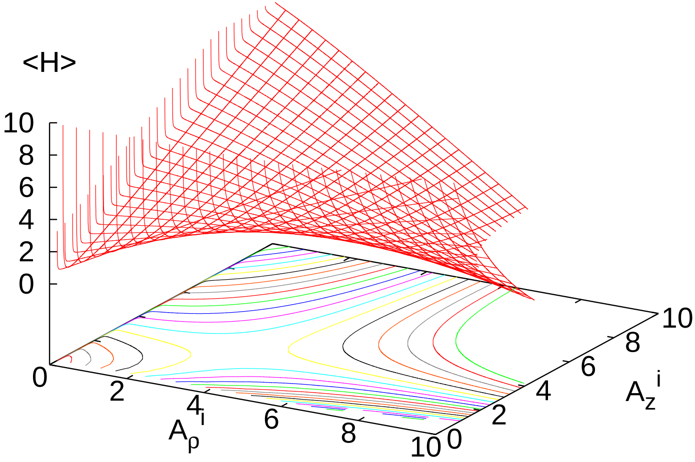
$$H = T + V = \frac{p_\rho^2}{2} + \frac{p_z^2}{2} + \frac{1}{2q_\rho^2} + 2\gamma_\rho^2 q_\rho^2 + \frac{a\sqrt{\frac{1}{q_z^2}}}{2\sqrt{2\pi}q_\rho^2} + \frac{1}{8q_z^2} + 2\gamma_z^2 q_z^2$$
$$+ \frac{\sqrt{\frac{1}{q_z^2}}\left(1 + \frac{q_\rho^2}{q_z^2} - \frac{3q_\rho^2 \arctan[\sqrt{\frac{q_\rho^2}{2q_z^2} - 1}]}{q_z^2\sqrt{\frac{2q_\rho^2}{q_z^2} - 4}}\right)}{6\sqrt{2\pi}q_\rho^4(\frac{1}{q_z^2} - \frac{2}{q_\rho^2})}$$

# 2d nonintegrable Hamiltonian system, potential $V(q_\rho, q_z)$



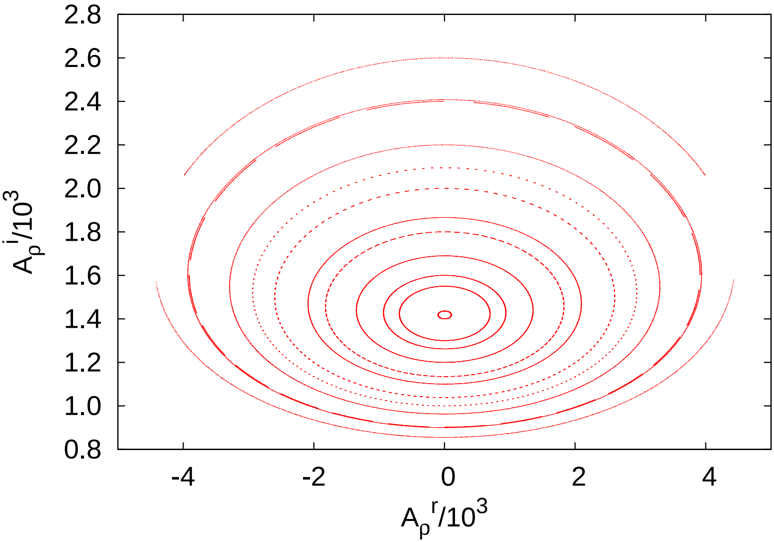
# mean field energy as a functions of the width parameters $A_\rho^i$, $A_z^i$

$$A_\rho^r = 0,\ A_z^r = 0$$



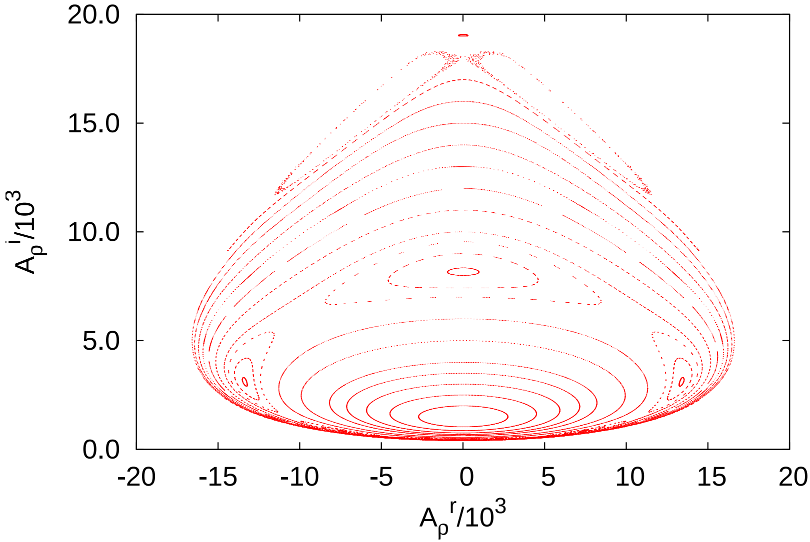
# Poincaré surface of section

$$\langle H \rangle = 450000, \quad \sqrt[3]{\gamma_z \gamma_\rho^2} = 3.4 \times 10^4, \quad \gamma_z/\gamma_\rho = 6, \quad a = 0.1$$



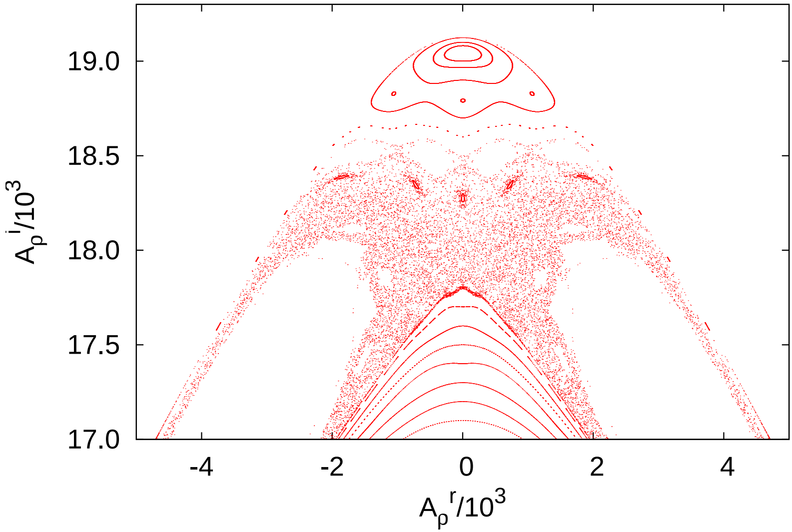
# Poincaré surface of section

$$\langle H \rangle = 624000, \quad \sqrt[3]{\gamma_z \gamma_\rho^2} = 3.4 \times 10^4, \quad \gamma_z/\gamma_\rho = 6, \quad a = 0.1$$



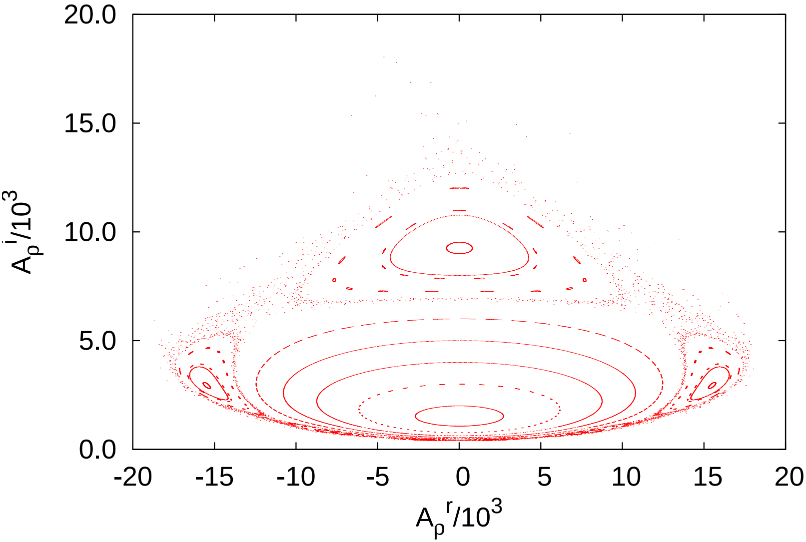
# Poincaré surface of section

$$\langle H \rangle = 624000, \quad \sqrt[3]{\gamma_z \gamma_\rho^2} = 3.4 \times 10^4, \quad \gamma_z/\gamma_\rho = 6, \quad a = 0.1$$



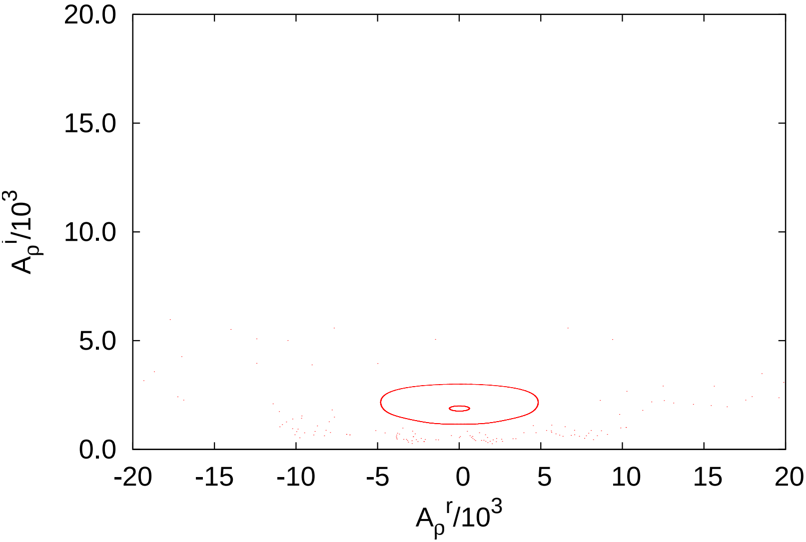
# Poincaré surface of section

$$\langle H \rangle = 900000, \quad \sqrt[3]{\gamma_z \gamma_\rho^2} = 3.4 \times 10^4, \quad \gamma_z/\gamma_\rho = 6, \quad a = 0.1$$



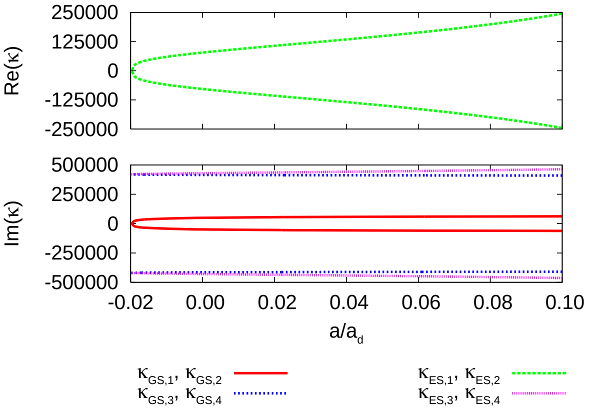
# Poincaré surface of section

$$\langle H \rangle = 6000000, \quad \sqrt[3]{\gamma_z \gamma_\rho^2} = 3.4 \times 10^4, \quad \gamma_z/\gamma_\rho = 6, \quad a = 0.1$$



# 4.5 Linear stability analysis of the variational solutions

linearization of the equations of motion for the real and imaginary parts of $A_r$ and $A_z$ around the stable and unstable stationary state yields four eigensolutions $\psi_{\rm lin} \propto e^{\kappa t}$ with eigenvalues $\kappa$ for each state




$$N^2\bar{\gamma} = 3.4 \times 10^4,\ \lambda = 6$$

exact dynamic calculations for dipolar quantum gases: under way

# Summary and conclusions

Motto: "Let's face BEC through nonlinear dynamics"

- variational forms of the BEC wave functions (of a given symmetry class) convert BECs via the Gross-Pitaevskii equation into Hamiltonian systems that can be studied using the methods of nonlinear daynamics
- the results serve as a useful guide to look for nonlinear dynamic effects in numerically exact quantum calculations of BECs
- existence of stable islands as well as chaotic regions for excited states of dipolar BECs could be checked experimentally

# Related articles


- H. Cartarius, J. Main, G. Wunner; Phys. Rev. Lett. **99**, 173003 (2007)
- I. Papadopoulos, P. Wagner, G. Wunner, J. Main; Phys. Rev. A **76**, 053604 (2008)
- H. Cartarius, J. Main, G. Wunner; Phys. Rev. A **77**, 013618 (2008)
- H. Cartarius, T. Fabčič, J. Main, G. Wunner; Phys. Rev. A **77**, 013615 (2008)
- P. Wagner, H. Cartarius, T. Fabčič, J. Main, G. Wunner; Preprint arXiv:0802.4055 (2008)

# Bonus material: exceptional points in linear quantum systems

## Definition and properties

Exceptional points are the coalescence of two (or even more) eigenstates at a certain parameter value of a system.

$$\boldsymbol{M}(\lambda)\vec{x}(\lambda) = e(\lambda)\vec{x}(\lambda)$$

- Two complex eigenvalues are identical (degeneracy).
- At the exceptional point a branch point singularity appears.
- The corresponding space of eigenvectors is one-dimensional.

## Appearance in quantum systems

- Exceptional points can appear as degeneracies of complex energy eigenvalues of non-Hermitian Hamiltonians which describe resonances.
- Example for a real physical system: Hydrogen atom in crossed electric and magnetic fields

# A simple example

## $2 \times 2$ matrix with an exceptional point

$$\boldsymbol{M}(\lambda) = \begin{pmatrix} 1 & \lambda \\ \lambda & -1 \end{pmatrix}$$

- Eigenvalues: $e_1 = \sqrt{1+\lambda^2}, \qquad e_2 = -\sqrt{1+\lambda^2}$
- Eigenvectors:

$$\vec{x}_1(\lambda) = \begin{pmatrix} -\lambda \\ 1-\sqrt{1+\lambda^2} \end{pmatrix} \qquad \vec{x}_2(\lambda) = \begin{pmatrix} -\lambda \\ 1+\sqrt{1+\lambda^2} \end{pmatrix}$$

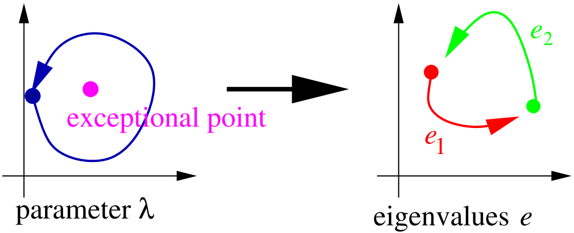
## There are two exceptional points for $\lambda = \pm\mathrm{i}$

$$\boldsymbol{M}(\pm\mathrm{i}) = \begin{pmatrix} 1 & \pm\mathrm{i} \\ \pm\mathrm{i} & -1 \end{pmatrix}, \qquad e_{1,2}(\pm\mathrm{i}) = 0, \qquad \vec{x}(\pm\mathrm{i}) = \begin{pmatrix} \mp\mathrm{i} \\ 1 \end{pmatrix}$$

# Circle around an exceptional point in the parameter space

## A further property of exceptional points

The two eigenvalues which degenerate at the exceptional point are permuted if a closed loop around the exceptional point is traversed in parameter space.




- The end point of the path of the first eigenvalue is the starting point of the second and vice versa.
- The combined paths of both eigenvalues lead to a closed loop.

# Self trapped condensate with attractive $1/r$-interaction

- Scaled extended Gross-Pitaevskii equation in "atomic units":

$$\varepsilon\psi(\vec{r}) = \left[-\Delta_{\vec{r}} + \left(8\pi a\,|\psi(\vec{r})|^2 - 2\int \mathrm{d}^3\vec{r}\,' \frac{|\psi(\vec{r}\,')|^2}{|\vec{r}-\vec{r}\,'|}\right)\right]\psi(\vec{r})$$

- Trial wave function for a variational solution:

$$\psi(\vec{r}) = A\exp\left(\frac{-k^2\vec{r}^2}{2}\right), \quad k_\pm = \frac{1}{2}\sqrt{\frac{\pi}{2}}\frac{1}{a}\left(\pm\sqrt{1+\frac{8}{3\pi}a} - 1\right)$$

## Degeneracy: *analytical* results

$$a = -\frac{3\pi}{8} \qquad \rightarrow \qquad k_+ = k_-, \quad E_+ = E_- \quad \varepsilon_+ = \varepsilon_-,$$

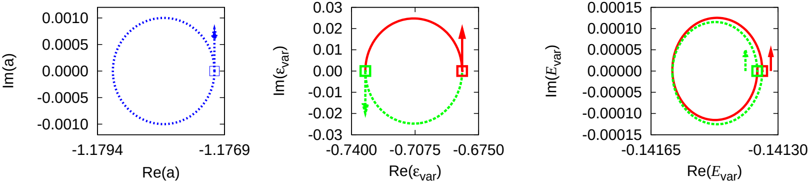
- Energies are identical
- Wave functions $\psi_{k_+}$ and $\psi_{k_-}$ are identical

# $1/r$: Circle around the degeneracy

## Exceptional point?

- A two-dimensional parameter space is required: extension to complex numbers: $a \in \mathbb{C}$
- A clear proof is the permutation of two eigenvalues if a circle around the critical parameter value is traversed:

$$a = -\frac{3\pi}{8} + re^{i\varphi}, \qquad \varphi = 0 \ldots 2\pi$$




We have confirmed our results with numerically exact calculations.

# $1/r$: Mean field energy and chemical potential for $r \ll 1$

## Fractional power series expansion of the mean field energy

$$\tilde{E}_\pm(\varphi) = -\frac{4}{9\pi} + 0 \cdot \sqrt{r} e^{i\varphi/2} + \frac{32}{27\pi^2} \cdot \sqrt{r}^2 e^{i\varphi} \pm \left(\frac{4}{9\pi} - \frac{32}{9\pi^2}\right) \cdot \sqrt{r}^3 e^{(3/2)i\varphi} + O\left(\sqrt{r}^4\right)$$

- The first order term with the phase factor $e^{i\varphi/2}$ vanishes.
- Responsible for the permutation: third order term

## Fractional power series expansion of the chemical potential

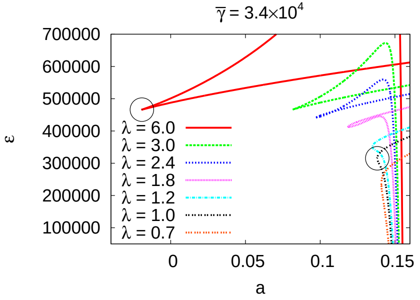
$$\tilde{E}_\pm(\varphi) = -\frac{20}{9\pi} \pm \frac{8}{3\pi} \cdot \sqrt{r} e^{i\varphi/2} - \left(\frac{4}{3\pi} + \frac{128}{27\pi^2}\right) \cdot \sqrt{r}^2 e^{i\varphi} \pm \left(\frac{8}{9\pi} - \frac{64}{9\pi^2}\right) \cdot \sqrt{r}^3 e^{(3/2)i\varphi} + O\left(\sqrt{r}^4\right)$$

- The first order term with the phase factor $e^{i\varphi/2}$ does not vanish.

# Dipolar condensate

## Scaled extended Gross-Pitaevskii equation

$$\varepsilon\psi(\vec{r}) = \Big[ -\Delta + \gamma_r^2 r^2 + \gamma_z^2 z^2 + 8\pi a\,|\psi(\vec{r})|^2 + \int \mathrm{d}^3\vec{r}'\,|\psi(\vec{r})|^2\,\frac{1-3\cos^2\theta'}{|\vec{r}-\vec{r}'|^3}\Big]\psi(\vec{r})$$

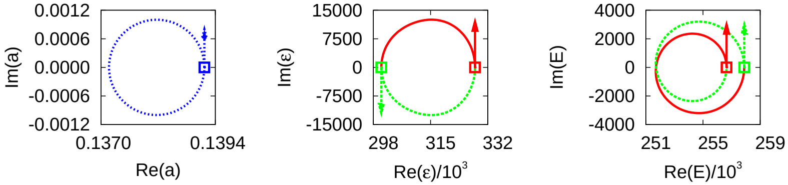



- Three-dimensional real parameter space:
  - $\bar{\gamma} = \gamma_r^{2/3}\gamma_z^{1/3}$
  - $\lambda = \gamma_z/\gamma_r$
  - $a$
- Complex extension is possible: $a \in \mathbb{C}$

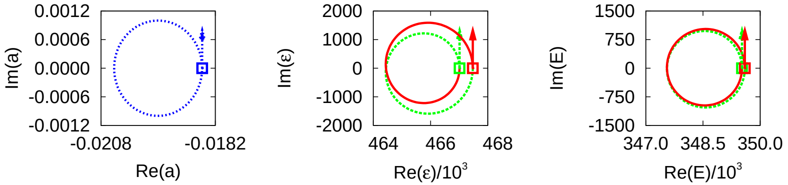
# Dipolar condensate: Circle around the degeneracy

$$a = a_{\text{crit}} + re^{i\varphi}, \qquad \varphi = 0 \ldots 2\pi$$

- $\lambda = 1$: attractive dipole-dipole interaction




- $\lambda = 6$: repulsive dipole-dipole interaction



# discovery of exceptional points in stationary solutions of the Gross-Pitaevskii equation

- Exceptional points are branch point singularities, which are known from open quantum systems.
- A "nonlinear version" of an exceptional point appears in the bifurcating solutions of the (extended) Gross-Pitaevskii equation:
    - BEC in a harmonic trap
    - BEC with attractive $1/r$ interaction
    - BEC with dipole-dipole interaction
- The identification of the exceptional points is possible with a complex extension of the scattering length.
- BECs near the collapse point are experimental realizations of a real physical system close to exceptional points.