Mathematical Models & Numerical Simulation for Bose-Einstein Condensation

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BEC@JILA, 95’

Vortex@ENS
Outline

Bose-Einstein condensation (BEC)
- Theoretical prediction & Experimental realization
- Mathematical Models (GPE / NLSE)

Ground states
- Existence, uniqueness & non-existence
- Numerical methods & results

Dynamics
- Well-posedness & dynamical laws
- Numerical methods & collapse of a BEC in 3D

Extension to rotation, nonlocal interaction & spin-orbit

Conclusions

BEC@ETH, 98'

BEC@MIT, 00'
Theoretical predication of BEC

**S.N. Bose:** Z. Phys. 26 (1924)

- Study black body radiation: object very hot
- Two photons be counted up as either identical or different
- Bose statistics or Bose-Einstein statistics


- Apply the rules to atoms in cold temperatures
- Obtain Bose-Einstein distribution in a cold gas

\[
n_i = \frac{1}{e^{(\varepsilon_i - \mu)/k_B T} - 1} := f(\varepsilon_j), \quad j = 0, 1, 2, \ldots, \quad \mu < \varepsilon_0 < \varepsilon_1 < \ldots
\]
Einstein’s prediction on BEC: At zero or ‘low’ temperatures, most particles behavior in the same way (at quantum mechanical ground state — minimum energy state)! —gregarious behavior----- quantum phase transition happens at extremely low temperatures --- degenerate quantum gas -- `super atom’ --- fifth matter of state.
FIG. 2. Criterion for Bose-Einstein condensation. At high temperatures, a weakly interacting gas can be treated as a system of “billiard balls.” In a simplified quantum description, the atoms can be regarded as wave packets with an extension of their de Broglie wavelength $\lambda_{dB}$. At the BEC transition temperature, $\lambda_{dB}$ becomes comparable to the distance between atoms, and a Bose condensate forms. As the temperature approaches zero, the thermal cloud disappears, leaving a pure Bose condensate.
Experimental results


- Li (Lithium)

A New Form of Matter Unveiled

Physicists create the long-sought Bose-Einstein condensate, allowing easier exploration of quantum mechanics, while other researchers celebrate a new planet, a gene for eyes, brain images, and more

Back in 1924, Albert Einstein predicted the existence of a new phase of matter, an exotic state in which atoms defied the laws of classical physics and followed only the dictums of quantum mechanics. In 1995, by chilling wisps of gas to ultracold temperatures, physicists finally got their first good look at this state, named the Bose-Einstein condensate after Einstein and Indian physicist Satyendra Bose. This year's work ends an arduous quest and ushers in a new age of exploration in atomic and condensed-matter physics.

We salute the condensate as Molecule of the Year for 1995, but this peculiar form of matter is not a molecule. Indeed, this year's magnificent achievement was to elude the everyday forces that bind atoms together into molecules and so unmask the more subtle powers of quantum mechanics. While atoms in an ordinary gas dart about in all directions, the atoms in the condensate move in lock step, at identical speed and direction. They have relinquished their individual identities to become a single, collective entity, and their organized condition is expected to give rise to bizarre properties.

The condensate's unusual nature makes it an ideal workshop for exploring the counterintuitive realm of quantum mechanics. So 6 months after the first dramatic report, experimentalists are rushing to create and explore this new phase, while theorists calculate its properties. Physicists are already angling to apply the new knowledge, hoping to capitalize on the condensate's unique aspects to create a laser that shoots beams of atoms instead of light. Understanding the laws that govern matter in this cold, coherent state may help physicists understand the mysteries of superconductivity and perhaps even the early universe.

Physicists have glimpsed Bose-Einstein condensation before, but never in a system where they could study all its properties. For example, pairs of electrons and electron holes, known as excitons, have been observed to form condensates in semiconductors, but these last only a few millionths of a second. In ultracold liquid helium, up to 10% of the atoms are thought to be Bose-condensed, and this is intimately linked to startling properties such as superfluidity, which allows this fluid to creep up the sides of a beaker. But in liquid helium, the condensate is modified by the classical forces between atoms, so the quantum-mechanical signature is muddied.

To create a pure condensate, physicists need supercold atoms, where no heat veils the quantum forces. Yet the atoms must be kept in a gaseous phase and prevented from collapsing into a solid or liquid. In July, by cooling atoms of rubidium to within a whisper of absolute zero, researchers at a lab run jointly by the National Institute of Standards and Technology and the University of Colorado managed this feat. In an ultracold cloud of gas, they saw their boldest dreams come true, as a textbook example of Bose-Einstein condensation took shape. When they graphed the distribution of the atoms' velocities, they saw a now-classic portrait, with a dramatic peak close to zero.
Experimental difficulties

- Low temperatures, almost absolutely zero (nK)
- Low density in a gas

FIG. 1. Generic phase diagram common to all atoms: dotted line, the boundary between non-BEC and BEC; solid line, the boundary between allowed and forbidden regions of the temperature-density space. Note that at low and intermediate densities, BEC exists only in the thermodynamically forbidden regime.
Experimental techniques

- Laser cooling
- Magnetic trapping
- Evaporative Cooling

($100k—300k)$
Experimental results

Experimental implementation
- JILA (95'): First experimental realization of BEC in a gas
- NIST (98'): Improved experiments
- MIT, ENS, Rice,
- ETH, Oxford,
- Peking U., NUS, ...

2001 Nobel prize in physics:
- C. Wiemann: U. Colorado
- E. Cornell: NIST
- W. Ketterle: MIT

ETH (02’, Rb, 300,000)
## Properties of BEC in experiments

<table>
<thead>
<tr>
<th>Kinds of atom</th>
<th>$^{87}\text{Rb}, \ ^7\text{Li}, \ ^{23}\text{Na}, \ ^{52}\text{Cr}, \ ^{4}\text{He}, \ldots$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperatures</td>
<td>$50\text{nK} -- - 2\text{μK}$</td>
</tr>
<tr>
<td>Density</td>
<td>$10^{11} -- - 10^{15} \text{cm}^{-3}$</td>
</tr>
<tr>
<td># of atoms</td>
<td>$100(\ ^7\text{Li}) -- - 10^6(\ ^{23}\text{Na}) -- - 10^9(\ ^{4}\text{He})$</td>
</tr>
<tr>
<td>Spatial size</td>
<td>Sphere at diameter 10--15μm</td>
</tr>
<tr>
<td></td>
<td>cigar-shaped at length 300μm &amp; diameter 15μm</td>
</tr>
<tr>
<td>Life span</td>
<td>A few seconds to several minutes</td>
</tr>
</tbody>
</table>
Brief BEC research history in physics

Milestones

– 1924 ----- Prediction of BEC by A. Einstein

– 1938-----London & Tisza linked BEC & superfluidity in liquid helium 4

– 1995 --- Experiments of BEC in ultracold gas of alkali atoms

– Since then--- BEC begins a new era in atomic, molecular & optical (AMO) physics & quantum optics; attracts interests of computational, applied & pure mathematicians.

Some famous physicists in BEC research


Mathematical models

N-body problem
- (3N+1)-dim linear Schroedinger equation

Mean field theory -- zero or `extremely' low temperatures
- Gross-Pitaevskii equation (GPE): \( T < T_c = O(nK) \)
- (3+1)-dim nonlinear Schroedinger equation (NLSE)

Quantum kinetic theory -- high temperatures
- High temperature: QBME (3+3+1)-dim
- Around critical temperature: QBME+GPE
- Below critical temperature: GPE
Model for a BEC at zero temperature
– with \( N \) identical bosons

**N-body problem** – \( 3N+1 \) dim. (linear) Schrödinger equation

\[
\frac{i\hbar}{\partial t} \Psi_N(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, t) = H_N \Psi_N(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, t), \quad \text{with}
\]

\[
H_N = \sum_{j=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_j^2 + V(\mathbf{x}_j) \right) + \sum_{1 \leq j < k \leq N} V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k)
\]

**Hartree ansatz** \( \Psi_N(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, t) \approx \prod_{j=1}^{N} \psi(\mathbf{x}_j, t), \mathbf{x}_j \in \mathbb{R}^3 \)

**Fermi interaction** \( V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k) = g\delta(\mathbf{x}_j - \mathbf{x}_k) \) with \( g = \frac{4\pi\hbar^2 a_s}{m} \)

**Dilute quantum gas** -- two-body elastic interaction

\[
E_N(\Psi_N) := \int_{\mathbb{R}^{3N}} \overline{\Psi}_N H_N \Psi_N \, d\mathbf{x}_1 \cdots d\mathbf{x}_N \approx NE(\psi) \quad \text{--energy per particle}
\]
Model for a BEC – with \( N \) identical bosons

Energy per particle – mean field approximation \((\text{Lieb et al, 00'})\)

\[
E(\psi) = \int_{\mathbb{R}^3} \left[ \frac{\hbar^2}{2m} \left| \nabla \psi \right|^2 + V(\bar{x}) |\psi|^2 + \frac{Ng}{2} |\psi|^4 \right] d\bar{x} \quad \text{with} \quad \psi := \psi(\bar{x}, t)
\]


\[
\frac{i\hbar}{\partial_t} \psi(\bar{x}, t) = \frac{\delta E(\psi)}{\delta \bar{\psi}} = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\bar{x}) + Ng |\psi|^2 \right] \psi, \quad \bar{x} \in \mathbb{R}^3
\]

Proper non-dimensionalization & dimension reduction— \( \text{GPE/NLSE} \)

\[
i \frac{\partial}{\partial_t} \psi(\bar{x}, t) = -\frac{1}{2} \nabla^2 \psi + V(\bar{x}) \psi + \beta |\psi|^2 \psi, \quad \bar{x} \in \mathbb{R}^d \quad \text{with} \quad \beta = \frac{4\pi Na_s}{x_s}
\]
**Other applications of GPE/NLSE**

\[ i \partial_t \psi(\bar{x}, t) = -\frac{1}{2} \nabla^2 \psi + V(\bar{x}) \psi + \beta |\psi|^2 \psi \]

- **For laser beam propagation**
- **In plasma physics:** wave interaction between electrons and ions
  - Zakharov system---NLSE + wave equation, …..
- **In quantum chemistry:** chemical interaction based on the first principle
  - Schrödinger-Poisson system
- **In materials science:**
  - First principle computation, DFT, …
  - Semiconductor industry
- **In nonlinear (quantum) optics**
- **In biology** – protein folding
- **In superfluids** – flow without friction, liquid \(^4\)He
The Gross-Pitaevskii equation (GPE/NLSE)

\[ i \frac{\partial}{\partial t} \psi(\vec{x}, t) = -\frac{1}{2} \nabla^2 \psi + V(\vec{x}) \psi + \beta |\psi|^2 \psi \]

- \( t \): time
- \( \vec{x} \): spatial coordinate \((d=1,2,3)\)
- \( \psi(\vec{x}, t) \): complex-valued wave function
- \( V(\vec{x}) \): real-valued external potential
- \( \beta \): dimensionless interaction constant
  - \( =0 \): linear; \( >0 (<0) \): repulsive (attractive) interaction
- \( \beta = 0 \): Schrödinger equation (E. Schrödinger 1925’)
- \( \beta \neq 0 \): GPE (E.P. Gross 1961’; L.P. Pitaevskii 1961’)

E. Schrödinger
Conservation laws

\[ i \partial_t \psi(\vec{x}, t) = -\frac{1}{2} \nabla^2 \psi + V(\vec{x}) \psi + \beta |\psi|^2 \psi \]

- **Dispersive**
- **Time symmetric:** \( t \rightarrow -t \) \& take conjugate \( \Rightarrow \) unchanged!!
- **Time transverse (gauge) invariant**

\[ V(\vec{x}) \rightarrow V(\vec{x}) + \alpha \Rightarrow \psi \rightarrow \psi e^{-i\alpha t} \Rightarrow \rho = |\psi|^2 \quad --\text{unchanged}!! \]

- **Mass conservation**

\[ N(t) := N(\psi(\bullet, t)) = \int_{\mathbb{R}^d} |\psi(\vec{x}, t)|^2 d\vec{x} \equiv \int_{\mathbb{R}^d} |\psi(\vec{x}, 0)|^2 d\vec{x} = 1, \quad t \geq 0 \]

- **Energy conservation**

\[ E(t) := E(\psi(\bullet, t)) = \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla \psi|^2 + V(x)|\psi|^2 + \frac{\beta}{2} |\psi|^4 \right] d\vec{x} \equiv E(0), \quad t \geq 0 \]
Stationary states

Stationary states (ground & excited states)

\[ \psi(\bar{x}, t) = \phi(\bar{x}) e^{-it\mu} \]

Nonlinear eigenvalue problems: Find \((\mu, \phi)\) s.t.

\[ \mu \phi(\bar{x}) = -\frac{1}{2} \nabla^2 \phi(\bar{x}) + V(\bar{x})\phi(\bar{x}) + \beta |\phi(\bar{x})|^2 \phi(\bar{x}), \quad \bar{x} \in \mathbb{R}^d \]

with \[ \|\phi\|^2 := \int_{\mathbb{R}^d} |\phi(\bar{x})|^2 d\bar{x} = 1 \]

Time-independent NLSE or GPE:

Eigenfunctions are

- Orthogonal in linear case & Superposition is valid for dynamics!!
- Not orthogonal in nonlinear case !!!! No superposition for dynamics!!!
Ground states

The eigenvalue is also called as chemical potential

$$\mu := \mu(\phi) = E(\phi) + \frac{\beta}{2} \int_{\mathbb{R}^d} |\phi(\vec{x})|^4 \, d\vec{x}$$

- With energy

$$E(\phi) = \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla \phi(\vec{x})|^2 + V(\vec{x})|\phi(\vec{x})|^2 + \frac{\beta}{2} |\phi(\vec{x})|^4 \right] d\vec{x}$$

Ground states -- nonconvex minimization problem

$$E(\phi_g) = \min_{\phi \in S} E(\phi) \quad S = \left\{ \phi \mid \|\phi\| = 1, \quad E(\phi) < \infty \right\}$$

- Euler-Lagrange equation $\Rightarrow$ nonlinear eigenvalue problem
Existence & uniqueness

\[ C_b = \inf_{0 \neq f \in H^1(\mathbb{R}^2)} \frac{\|\nabla f\|_{L^2(\mathbb{R}^2)}^2}{\|f\|_{L^4(\mathbb{R}^2)}^4} \]

\textbf{Theorem} (Lieb, etc, PRA, 02'; Bao & Cai, KRM, 13') If potential is confining

\[ V(\bar{x}) \geq 0 \quad \text{for} \quad \bar{x} \in \mathbb{R}^d \quad \& \quad \lim_{|\bar{x}| \to \infty} V(\bar{x}) = \infty \]

- There exists a ground state if one of the following holds
  
  (i) \( d = 3 \) & \( \beta \geq 0 \);  
  (ii) \( d = 2 \) & \( \beta > -C_b \);  
  (iii) \( d = 1 \) & \( \beta \in \mathbb{R} \)

- The ground state can be chosen as nonnegative \( |\phi_g|, \text{i.e.} \phi_g = |\phi_g|e^{i\theta_0} \)
- Nonnegative ground state is unique if \( \beta \geq 0 \)
- The nonnegative ground state is strictly positive if \( V(\bar{x}) \in L^2_{\text{loc}} \)
- There is no ground stats if one of the following holds
  
  (i)' \( d = 3 \) & \( \beta < 0 \);  
  (ii)' \( d = 2 \) & \( \beta \leq -C_b \)
Key Techniques in Proof

- **Positivity & semi-lower continuous**
  \[ E(\phi) \geq E(|\phi|) = E(\sqrt{\rho}), \quad \forall \phi \in S \quad \text{with} \quad \rho = |\phi|^2 \]

- The energy \( \tilde{E}(\rho) := E(\sqrt{\rho}) \) is **bounded below** if conditions (i) or (ii) or (iii) and strictly **convex** if \( \beta \geq 0 \)

- **Confinement** potential implies decay at far field

- The set \( S = \left\{ \rho \mid \int_{\mathbb{R}^d} \rho(\tilde{x}) \, d\tilde{x} = 1 \quad \& \quad \tilde{E}(\rho) < \infty \right\} \) is **convex** in \( \rho \)

- Using convex minimization theorem

- **Non-existence** result
  \[ E(\phi_\varepsilon) \xrightarrow{\varepsilon \to 0} -\infty \]

- \( \phi_\varepsilon(\tilde{x}) = \frac{1}{(2\pi\varepsilon)^{d/4}} \exp\left(-\frac{|\tilde{x}|^2}{2\varepsilon}\right), \quad \tilde{x} \in \mathbb{R}^d \quad \text{with} \quad \varepsilon \to 0 \)
Computing ground states

Idea: Steepest decent method + Projection

\[ \partial_t \varphi(x, t) = -\frac{1}{2} \frac{\delta E(\varphi)}{\delta \varphi} = \frac{1}{2} \nabla^2 \varphi - V(x) \varphi - \beta |\varphi|^2 \varphi, \quad t_n \leq t < t_{n+1} \]

\[ \varphi(x, t_{n+1}) = \frac{\varphi(x, t_{n+1})}{\| \varphi(x, t_{n+1}) \|}, \quad n = 0, 1, 2, \cdots \]

\[ \varphi(x, 0) = \varphi_0(x) \quad \text{with} \quad \| \varphi_0(x) \| = 1. \]

- The first equation can be viewed as choosing \( t = i \tau \) in NLSE
- For linear case: (Bao & Q. Du, SIAM Sci. Comput., 03')
  \[ E_0(\varphi(., t_{n+1})) \leq E_0(\varphi(., t_n)) \leq \cdots \leq E_0(\varphi(., 0)) \]
- For nonlinear case with small time step, CNGF
Normalized gradient glow

Idea: letting time step go to 0 \( (\text{Bao & Q. Du, SIAM Sci. Comput., 03}') \)

\[ \partial_t \phi(\bar{x}, t) = \frac{1}{2} \nabla^2 \phi - V(\bar{x}) \phi - \beta |\phi|^2 \phi + \frac{\mu(\phi(., t))}{\| \phi(., t) \|^2} \phi, \quad t \geq 0, \]

\[ \phi(\bar{x}, 0) = \phi_0(\bar{x}) \quad \text{with} \quad \| \phi_0(\bar{x}) \| = 1. \]

- **Mass conservation & energy diminishing**

  \[ \| \varphi(., t) \| = \| \varphi_0 \| = 1, \quad \frac{d}{dt} E(\varphi(., t)) \leq 0, \quad t \geq 0 \]

- **Numerical discretizations**
  
  - **BEFD**: Energy diminishing & monotone \( (\text{Bao & Q. Du, SIAM Sci. Comput., 03}') \)
  
  - **TSSP**: Spectral accurate with splitting error \( (\text{Bao & Q. Du, SIAM Sci. Comput., 03}') \)
  
  - **BESP**: Spectral accuracy in space & stable \( (\text{Bao, I. Chern & F. Lim, JCP, 06}') \)
Ground states in 1D & 3D
Dynamics

Time-dependent NLSE / GPE

\[ i \frac{\partial}{\partial t} \psi(\vec{x}, t) = -\frac{1}{2} \nabla^2 \psi + V(\vec{x})\psi + \beta |\psi|^2 \psi, \quad \vec{x} \in \mathbb{R}^d, \quad t > 0 \]

\[ \psi(\vec{x}, 0) = \psi_0(\vec{x}) \]

Well-posedness & dynamical laws

- Well-posedness & finite time blow-up
- Dynamical laws
  - Soliton solutions
  - Center-of-mass
  - An exact solution under special initial data
- Numerical methods and applications
Well-posedness

**Theorem** (T. Cazenave, 03'; C. Sulem & P.L. Sulem, 99'')

**Assumptions**

(i) \( V(\bar{x}) \in C^\infty(\mathbb{R}^d) \), \( V(\bar{x}) \geq 0 \), \( \forall \bar{x} \in \mathbb{R}^d \) & \( D^\alpha V(\bar{x}) \in L^\infty(\mathbb{R}^d) \) \( |\alpha| \geq 2 \)

(ii) \( \psi_0 \in X = \left\{ u \in H^1(\mathbb{R}^d) \mid \|u\|^2_X = \|u\|^2_{L^2} + \|\nabla u\|^2_{L^2} + \int_{\mathbb{R}^d} V(\bar{x}) u(\bar{x}) \, d\bar{x} < \infty \right\} \)

- **Local** existence, i.e.
  \( \exists T_{\text{max}} \in (0, \infty] \), s. t. the problem has a unique solution \( \psi \in C([0,T_{\text{max}}), X) \)

- **Global** existence, i.e. \( T_{\text{max}} = +\infty \) if
  \( d = 1 \) or \( d = 2 \) with \( \beta \geq -C_b / \|\psi_0\|^2_{L^2(\mathbb{R}^d)} \) or \( d = 3 \) & \( \beta \geq 0 \)
Finite time blowup

**Theorem** (T. Cazenave, 03’; C. Sulem & P.L. Sulem, 99’) **Assumptions**

\[ \beta < 0 \quad \& \quad V(\bar{x})d + \bar{x} \cdot \nabla V(\bar{x}) \geq 0, \quad \forall \bar{x} \in \mathbb{R}^d \quad \text{with} \quad d = 2,3 \]

\[ \psi_0 \in X \quad \text{with finite variance} \quad \delta_V(0) := \int |\bar{x}|^2 \psi_0(\bar{x})d\bar{x} < \infty \]

- There exists finite time blowup, i.e. \( T_{\text{max}} < +\infty \) if one of the following holds
  (i) \( E(\psi_0) < 0 \)
  (ii) \( E(\psi_0) = 0 \) \& \( \text{Im} \int \overline{\psi}_0(x) (\bar{x} \cdot \nabla \psi_0(\bar{x})) d\bar{x} < 0 \)
  (iii) \( E(\psi_0) > 0 \) \& \( \text{Im} \int \overline{\psi}_0(x) (\bar{x} \cdot \nabla \psi_0(\bar{x})) d\bar{x} < -\sqrt{E(\psi_0)}d \|\bar{x}\psi_0\|_{L^2} \)

- **Proof:**
  \[ \delta_V(t) := \int |\bar{x}|^2 |\psi(\bar{x},t)|^2 d\bar{x} \Rightarrow \delta_V(t) \leq 2d E(\psi_0), \quad t \geq 0, \quad d = 2,3 \]
  - (i) **Variance identity:**
    \[ \Rightarrow \delta_V(t) \leq d E(\psi_0)t^2 + \delta_V(0)t + \delta_V(0) \Rightarrow \exists 0 < t^* < \infty \& \delta_V(t^*) = 0!! \]
  - (ii) **Uncertainty principle:**
    \[ 1 = \|\psi\|^2_{L^2} \leq \|\bar{x}\psi\|^2_{L^2} \|\nabla \psi\|^2_{L^2} = \sqrt{\delta_V(t)} \|\nabla \psi\|^2_{L^2} \]
Time-splitting spectral method (TSSP)

For $[t_n, t_{n+1}]$, apply time-splitting technique (Bao, Jaksch & Markowich, JCP, 03')

- Step 1: Discretize by spectral method & integrate in phase space exactly

$$i \partial_t \psi(\tilde{x}, t) = -\frac{1}{2} \nabla^2 \psi + V(\tilde{x})\psi + \beta |\psi|^2 \psi$$

- Step 2: solve the nonlinear ODE analytically

$$i \partial_t \psi(\tilde{x}, t) = V(\tilde{x})\psi(\tilde{x}, t) + \beta |\psi(\tilde{x}, t)|^2 \psi(\tilde{x}, t)$$

$$\downarrow \partial_t (|\psi(\tilde{x}, t)|^2) = 0 \implies |\psi(\tilde{x}, t)| = |\psi(\tilde{x}, t_n)|$$

$$i \partial_t \psi(\tilde{x}, t) = V(\tilde{x})\psi(\tilde{x}, t) + \beta |\psi(\tilde{x}, t_n)|^2 \psi(\tilde{x}, t)$$

$$\implies \psi(\tilde{x}, t) = e^{-i(t-t_n)[V(\tilde{x})+\beta|\psi(\tilde{x}, t_n)|^2]} \psi(\tilde{x}, t_n)$$

Use $2^{nd}$ order Strang splitting (or $4^{th}$ order time-splitting)
Properties of TSSP

- **Explicit** & computational cost per time step: $O(M \ln M)$
- Time symmetric: yes
- Time transverse invariant: yes
- Mass conservation: yes
- Stability: yes
- Dispersion relation without potential: yes
- **Accuracy**
  - Spatial: spectral order; Temporal: 2\textsuperscript{nd} or 4\textsuperscript{th} order
- Best resolution in strong interaction regime: $\beta \gg 1$
3D collapse & explosion of BEC

\[ i \frac{\partial}{\partial t} \psi(\vec{x}, t) = -\frac{1}{2} \nabla^2 \psi + V(\vec{x})\psi + \beta |\psi|^2 \psi \]

Experiment (Donley et., Nature, 01’)
- Start with a stable condensate \((a_s>0)\)
- At \(t=0\), change \(a_s\) from (+) to (-)
- Three body recombination loss

Mathematical model (Duine & Stoof, PRL, 01’)
\[ i \frac{\partial}{\partial t} \psi(\vec{x}, t) = -\frac{1}{2} \nabla^2 \psi + V(\vec{x})\psi + \beta |\psi|^2 \psi - i\delta_0 \beta^2 |\psi|^4 \psi \]
\[ \beta = \frac{4\pi N a_s}{x_s} \]
Numerical results (Bao et., J Phys. B, 04)

Jet formation
3D Collapse and explosion in BEC

$$\beta = \frac{4\pi N a_s}{x_s}$$
3D Collapse and explosion in BEC
Rotating BEC

**GPE / NLSE** with an angular momentum rotation

\[
i \frac{\partial}{\partial t} \psi(\vec{x}, t) = \left[ -\frac{1}{2} \nabla^2 + V(\vec{x}) - \Omega L_z + \beta |\psi|^2 \right] \psi, \quad \vec{x} \in \mathbb{R}^d, \quad t > 0
\]

\[
L_z := xp_y - yp_x = -i(x\partial_y - y\partial_x) \equiv -i\partial_\theta, \quad L = \vec{x} \times \vec{P}, \quad \vec{P} = -i\nabla
\]

**Mass** conservation

\[
N(t) = \int_{\mathbb{R}^d} |\psi(\vec{x}, t)|^2 d\vec{x}
\]

**Energy** conservation

\[
E_\Omega(\psi) := \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla \psi|^2 + V(x)|\psi|^2 - \Omega \psi L_z \psi + \frac{\beta}{2} |\psi|^4 \right] d\vec{x}
\]

Vortex @MIT
Ground states

Ground states – Seiringer, CMP, 02'; Bao, Wang & Markowich, CMS, 05'; ....

\[ \min_{\phi \in S} E_{\Omega}(\phi) \]

Existence & uniqueness

- Exists a ground state when \( \beta \geq 0 \) & \( |\Omega| \leq \min \{\gamma_x, \gamma_y\} \)
- Uniqueness when \( |\Omega| < \Omega_c(\beta) \)
- Quantized vortices appear when \( |\Omega| \geq \Omega_c(\beta) \)
- Phase transition & bifurcation in energy diagram

Numerical methods --- GFDN & BEFD or BEFP
Ground states with different $\Omega$
Ground states of rapid rotation

BEC@MIT
Dynamics – Bao, Du & Zhang, SIAP, 05’; Bao & Cai, KRM, 13’; …

Numerical methods

A new formulation

\[ \tilde{x} = A(t)^{-1} x \quad \& \]

\[ \phi(\tilde{x}, t) := \psi(\tilde{x}, t) = \psi(A(t)\tilde{x}, t) \]

- A rotating Lagrange coordinate:

\[ A(t) = \begin{bmatrix} \cos(\Omega t) & \sin(\Omega t) \\ -\sin(\Omega t) & \cos(\Omega t) \end{bmatrix} \quad \text{for } d = 2; \quad A(t) = \begin{bmatrix} \cos(\Omega t) & \sin(\Omega t) & 0 \\ -\sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{for } d = 3 \]

- GPE in rotating Lagrange coordinates

\[ i \partial_t \phi(\tilde{x}, t) = \left[ -\frac{1}{2} \nabla^2 + V(A(t)\tilde{x}) + \beta |\phi|^2 \right] \phi, \quad \tilde{x} \in \mathbb{R}^d, \quad t > 0 \]

- Analysis & numerical methods -- Bao & Wang, JCP6’; Bao, Li & Shen, SISC, 09’; Bao, Marahrens, Tang & Zhang, 13’, ……
Dynamics of a vortex lattice
Dipolar BEC (or quantum gas)

**GPE with long-range anisotropic DDI**

$$i \partial_t \psi(\vec{x}, t) = \left[ -\frac{1}{2} \nabla^2 + V(\vec{x}) - \Omega L_z + \beta |\psi|^2 + \lambda \left( U_{\text{dip}} \ast |\psi|^2 \right) \right] \psi$$

- **Trap potential**
  $$V(\vec{x}) = \frac{1}{2} (\gamma_x x^2 + \gamma_y y^2 + \gamma_z z^2)$$

- **Interaction constants**
  $$\beta = \frac{4\pi N a_s}{x_s} \quad (\text{short-range}), \quad \lambda = \frac{mN \mu_0 \mu_{\text{dip}}^2}{3\hbar^2 x_s} \quad (\text{long-range})$$

- **Long-range dipole-dipole interaction kernel**
  $$U_{\text{dip}}(\vec{x}) = \frac{3}{4\pi} \frac{1 - 3(\vec{n} \cdot \vec{x})^2 / |\vec{x}|^2}{|\vec{x}|^3} \quad = \quad \frac{3}{4\pi} \frac{1 - 3 \cos^2(\theta)}{|\vec{x}|^3}$$

**References:**

- S. Yi & L. You, PRA 61 (2001), 041604(R);
- D. H. J. O’Dell, PRL 92 (2004), 250401
A New Formulation

Using the identity (O’Dell et al., PRL 92 (2004), 250401, Parker et al., PRA 79 (2009), 013617)

\[
U_{\text{dip}}(\vec{x}) = \frac{3}{4\pi r^3} \left(1 - \frac{3(\vec{n} \cdot \vec{x})^2}{r^2}\right) = -\delta(\vec{x}) - 3\partial_{\vec{n}\vec{n}} \left(\frac{1}{4\pi r}\right)
\]

\[
U_{\text{dip}}(\xi) = -1 + \frac{3(\vec{n} \cdot \xi)^2}{|\xi|^2}
\]

Dipole-dipole interaction becomes

\[
U_{\text{dip}}\psi^* |\psi|^2 = - |\psi|^2 - 3\partial_{\vec{n}\vec{n}} \varphi
\]

\[
\varphi = \frac{1}{4\pi r} |\psi|^2 \Leftrightarrow -\nabla^2 \varphi = |\psi|^2
\]

Figure 1. The Rosensweig instability [32] of a ferrofluid (a colloidal dispersion in a carrier liquid of subdomain ferromagnetic particles, with typical dimensions of 10 nm) in a magnetic field perpendicular to its surface is a fascinating example of the novel physical phenomena appearing in classical physics due to long range, anisotropic interactions. Figure reprinted with permission from [34]. Copyright 2007 by the American Physical Society.
A New Formulation

Gross-Pitaevskii-Poisson type equations (Bao, Cai & Wang, JCP, 10')

\[
i \partial_t \psi(\vec{x}, t) = \left[ -\frac{1}{2} \nabla^2 + V(\vec{x}) - \Omega \nabla_z + (\beta - \lambda) |\psi|^2 - 3\lambda \partial_{\vec{n}} \varphi \right] \psi
\]

\[- \nabla^2 \varphi(\vec{x}, t) = |\psi(\vec{x}, t)|^2, \quad \vec{x} \in \mathbb{R}^3, \quad \lim_{|\vec{x}| \to \infty} \varphi(\vec{x}, t) = 0\]

- Energy

\[E(\psi(\cdot, t)) := \int_{\mathbb{R}^3} \left[ \frac{1}{2} |\nabla \psi|^2 + V(\vec{x}) |\psi|^2 - \Omega |\nabla_z \psi|^2 + \frac{\beta - \lambda}{2} |\psi|^4 + \frac{3\lambda}{2} |\partial_{\vec{n}} \nabla \varphi|^2 \right] d \vec{x}\]

- Model in 2D

\[\rightarrow_{2D} \left( -\Delta_{\perp} \right)^{1/2} \varphi(\vec{x}, t) = |\psi(\vec{x}, t)|^2, \quad \vec{x} \in \mathbb{R}^2, \quad \lim_{|\vec{x}| \to \infty} \varphi(\vec{x}, t) = 0\]

Ground state – Carles, Markowich & Sparber, 08'; Bao, Cai & Wang, JCP, 10'; Bao, Ben Abdallah & Cai, SIMA, 12'

Dynamics – Carles, Markowich & Sparber, 08'; Bao, Cai & Wang, JCP, 10'; Bao & Cai, KRM, 13'; via nonuniform FFT (NUFFT)

Dimension reduction – Carles, Markowich & Sparber, 08'; Cai, Rosenkranz, Lei & Bao, PRA, 10'; Bao & Cai, KRM, 13'
Ground State Results

**Theorem** (Existence, uniqueness & nonexistence) (Carles, Markowich & Sparber, 08'; Bao, Cai & Wang, JCP, 10')

- **Assumptions**
  
  $V_{\text{ext}}(\vec{x}) \geq 0, \quad \forall \vec{x} \in \mathbb{R}^3$ \quad \& \quad \lim_{|\vec{x}| \to \infty} V_{\text{ext}}(\vec{x}) = +\infty \quad \text{(confinement potential)}$

- **Results**

  - There exists a ground state $\phi_g \in S$ if $\beta \geq 0$ \quad \& \quad $-\frac{\beta}{2} \leq \lambda \leq \beta$

  - Positive ground state is unique $\quad \phi_g = e^{i\theta_0} |\phi_g| \quad \text{with} \quad \theta_0 \in \mathbb{R}$

  - Nonexistence of ground state, i.e. $\lim_{\phi \in S} E(\phi) = -\infty$
    
    - Case I: $\beta < 0$
    
    - Case II: $\beta \geq 0 \quad \& \quad \lambda > \beta$ or $\lambda < -\frac{\beta}{2}$
Dynamics of a vortex lattice
Spin-orbit coupled BEC

Coupled GPE with a spin-orbit coupling & internal Josephson junction

\[ i \frac{\partial}{\partial t} \psi_1 = \left[ -\frac{1}{2} \nabla^2 + V(\vec{x}) + ik_0 \partial_x + \delta + (\beta_{11} |\psi_1|^2 + \beta_{12} |\psi_2|^2) \right] \psi_1 + \Omega \psi_{-1} \]

\[ i \frac{\partial}{\partial t} \psi_{-1} = \left[ -\frac{1}{2} \nabla^2 + V(\vec{x}) - ik_0 \partial_x + \delta + (\beta_{21} |\psi_1|^2 + \beta_{22} |\psi_2|^2) \right] \psi_{-1} + \Omega \psi_1 \]


Applications ---- Topological insulator

Analysis & numerical methods:
– For ground state & dynamics (Bao & Cai, SIAP, 15')
Fig. 3.1. Ground states $\tilde{\Phi}_3 = (\tilde{\phi}_1^3, \tilde{\phi}_2^3)^T$ for a SO-coupled BEC in 2D with $\Omega = 50$, $\delta = 0$, $\beta_{11} = 10$, $\beta_{12} = \beta_{21} = \beta_{22} = 9$ for: (a) $k_0 = 0$, (b) $k_0 = 1$, (c) $k_0 = 5$, (d) $k_0 = 10$, (e) $k_0 = 50$, and (f) $k_0 = 100$. In each subplot, top panel shows densities and bottom panel shows phases of the ground state $\tilde{\phi}_1^3$ (left column) and $\tilde{\phi}_2^3$ (right column).
Fig. 3.2. Ground states $\Phi_g = (\phi_1^g, \phi_2^g)^T$ for a SO-coupled BEC in 2D with $k_0 = 10$, $\delta = 0$, $\beta_{11} = 10$, $\beta_{12} = \beta_{21} = \beta_{22} = 9$ for: (a) $\Omega = 1$, (b) $\Omega = 10$, (c) $\Omega = 50$, (d) $\Omega = 200$, (e) $\Omega = 300$, and (f) $\Omega = 500$. In each subplot, top panel shows densities and bottom panel shows phases of the ground state $\phi_1^g$ (left column) and $\phi_2^g$ (right column).
Conclusions & Future Challenges

Conclusions:

– BEC and its model at zero temperature--- GPE/NLSE
– Ground states
  • Existence, uniqueness, non-existence
  • Numerical methods -- BEFD
– Dynamics
  • Well-posedness & dynamical laws
  • Numerical methods -- TSSP

Future Challenges

– Spinor BEC; random potential; nonlocal interaction, interaction with impurities
– BEC at finite temperature: GPE+QBE; Bogoloboliv excitation; ....
– Fermion condensation; Rydberg gas--- nonlocal interaction in high dimension, ....
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