Impurities immersed in Bose-Einstein condensates

February 4th 2013
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Short overview

- Intro
  - Experiments and motivation
  - GPS equations

- Static impurities
  - Static self-trapping
  - Induced interactions

- Impurity dynamics
  - Breathing oscillations
  - Dynamical self-trapping

- Three-body recombination
Some People Involved

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Stephen R. Clark
Oxford, Singapore (CQT)

Tomi Johnson
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Weizhu Bao
Singapore (Uni)

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Madison (Uni of Wisconsin)
Defects in Bose-Einstein condensates

Impurities

Vortices

Solitons

Nonlinearity of the GP-equation is important.
Current experiments

- Single impurities in BECs
- Control impurity-BEC interactions
- Control trapping potentials
- Control number of impurities

A. Widera (Kaiserslautern)

M. Inguscio (Florence)

M. Köhl (Cambridge)
M. Oberthaler (Heidelberg)
D. Schneble (New York)

Why impurities?

- Impurity dynamics tells about environment
  - Fluctuation-dissipation theorem
  - Linear vs non-linear

- Learn about interactions
  - Controlled three-body loss

- Quantum simulation (any dimension)
  - Mimick electron transport
  - General field theories

- Historically He$^3$ in superfluid He$^4$
General model – GPS equations

- Single impurity $\chi(r)$ interacting with BEC $\psi(r)$
  \[
  i\hbar \partial_t \psi = -\frac{\hbar^2}{2m_b} \nabla^2 \psi + g|\psi|^2 \psi
  \]
  GP equation ($g > 0$)
  \[
  i\hbar \partial_t \chi = -\frac{\hbar^2}{2m_a} \nabla^2 \chi
  \]
  Schrödinger equation

- Density–density interaction with coupling $\kappa = \eta g$
- Coupling can be attractive or repulsive

- Normalization for $\psi(r)$ and $\chi(r)$
  \[
  \int \text{d}r |\psi(r)|^2 = N \quad \text{and} \quad \int \text{d}r |\chi(r)|^2 = 1
  \]

- Problem different from two-component BECs (bulk terms dominate)
General model – GPS equations

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  GP equation ($g > 0$)  
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- Problem different from two-component BECs (bulk terms dominate)
Static Impurities
Self-trapping effect

- \( \chi(r) \) and \( \psi(r) \) are in large box and vanish at boundary
- Coupling \( \kappa \) can lead to localisation of \( \chi(r) \)

Weak interactions
- \( \chi(r) \) delocalized
- \( \psi(r) \) constant

Large repulsive interaction
- \( \chi(r) \) localized
- \( \psi(r) \) vortex-like

Large attractive interaction
- \( \chi(r) \) localized
- \( \psi(r) \) peaked

localization length
Time-independent model

- Dimensionless equations for stationary system

\[ \psi = -\frac{1}{2} \nabla^2 \psi + \beta \gamma^D |\chi|^2 \psi + |\psi|^2 \psi \]
\[ \varepsilon \chi = -\frac{\alpha}{2} \nabla^2 \chi + \beta |\psi|^2 \chi \]

- Energy of the system

\[ E_{\text{bec}} = \gamma^{-D} \int d\mathbf{r} \left( \frac{1}{2} |\nabla \psi|^2 - |\psi|^2 + \frac{1}{2} |\psi|^4 \right) \]
\[ E_{\text{int}} = \beta \int d\mathbf{r} |\chi|^2 |\psi|^2 \]
\[ E_{\text{kin}} = \frac{\alpha}{2} \int d\mathbf{r} |\nabla \chi|^2 \]

Healing length \( \xi = \hbar / \sqrt{gn_0 m_b} \)

Energy scale \( gn_0 \)

\( \alpha = m_b / m_a \)
\( \beta = \kappa / g \)
\( \gamma = d / \xi \)

\( \alpha, \gamma \) are of order 1 for “natural” parameters
Weak interactions: Self-trapping threshold

- Consider small deformations $\delta \psi = \psi - 1$ of BEC (expand in $\beta$)

\[
\left( -\frac{1}{2} \nabla^2 + 2 \right) \delta \psi = -\beta \gamma^D |\chi|^2 \\
\left( -\frac{\alpha}{2} \nabla^2 + 2\beta \delta \psi \right) \chi = (\varepsilon - \beta) \chi
\]

- Obtain non-local non-linear Schrödinger equation

\[
\left( -\frac{1}{2} \nabla^2 - 2\zeta \int \mathrm{d}r' G(r - r') |\chi(r')|^2 \right) \chi = \varepsilon' \chi \\
\left( -\frac{1}{2} \nabla^2 + 2 \right) G(r) = \delta(r) \quad \text{Helmholtz equation}
\]

- $\chi(r)$ depends on single parameter $\zeta = \beta^2 \gamma^D / \alpha$

- Approximation is valid for $|\beta| \gamma^D / \ell_{\text{local}}^D \ll 1$

Weak interactions: Self-trapping threshold

- Energy functional $F[\chi]$ for non-local NLSE

$$F[\chi] = \frac{\alpha}{2} \int \text{d}r |\nabla \chi|^{2} - \beta^{2}\gamma^{D} \int \text{d}r \text{d}r' |\chi(r)|^{2}G(r-r')|\chi(r')|^{2}$$

- Use Gaussian trial function of width $\sigma$

1d localized for arbitrarily small interaction

$\sigma \sim 1/\zeta$ for $\sigma \gg 1$

2d localization for $\zeta > 2\pi$

3d localization for $\zeta > 31.7…$

$$\beta\gamma^{D}/\sigma^{D} \ll 1$$

Strong interactions: Asymmetry

- For $|\beta| >> 1$ impurity is highly localized $|\chi(r)|^2 \approx \delta(r)$
- Equation for $\psi(x)$ in presence of $\delta$-impurity in 1D

$$\left[ -\frac{1}{2} \partial_{xx} - 1 + |\psi(x)|^2 + \beta \gamma \delta(x - x_0) \right] \psi(x) = 0$$

$$\psi(x) = \coth(|x| + c) \quad \text{attractive}$$
$$\psi(x) = \tanh(|x| + c) \quad \text{repulsive}$$

Difference not captured by perturbative approach

$$\psi(x_0) = -\frac{\beta \gamma}{2} + \sqrt{1 + \left(\frac{\beta \gamma}{2}\right)^2}$$
Energy scaling and collapse

- Trial function for impurity and BEC
  \[ \chi_\sigma(x) = (\pi \sigma^2)^{-d/4} \prod_{j=1}^{d} \exp\left(-\frac{x_j^2}{2\sigma^2}\right) \]  
  \[ \psi_\sigma(x) = 1 + \frac{a}{\sigma^{\delta/2}} \prod_{j=1}^{d} \exp\left(-\frac{x_j^2}{b\sigma^2}\right) \]  
  Gaussian deformation

- Deformation finite in the limit \( \sigma \to 0 \)

- Scaling of energy in the limit \( \sigma \to 0 \)
  \[ E_{\text{int}} \sim \beta \sigma^{-\delta} \quad E_{\text{kin}} \sim \sigma^{-2} \quad E_{\text{bec}} \sim c_0 \sigma^{d-\delta-2} + \sum_{j=1}^{4} c_j \sigma^{d-j\delta/2} \]

- No ground state for attractive impurities in 3d
1D numerical results

- Set $\alpha = 1$, $\gamma = 0.5$ and vary $\beta$ over wide range

> Linearization accurate for small $\beta$

> Strong BEC deformation
2D numerical results

- Set $\alpha = 1$, $\gamma = 0.5$ and vary $\beta$

> Linearization accurate for small $\beta$
> Correct threshold for critical $\beta$
> Critical attractive coupling
3D numerical results

- Set $\alpha = 1$, $\gamma = 0.5$ and change $\beta$

- Linearization fails completely
- Sharp jump to localized state
- No ground state for attractive impurities
BEC induced interactions

- Interaction caused by BEC deformation

\[ F[\chi] = \frac{\alpha}{2} \int \text{d}r |\nabla \chi|^2 - \beta^2 \gamma^D \int \text{d}r \text{ d}r' |\chi(r)|^2 G(r-r') |\chi(r')|^2 \]

interaction energy

Short range repulsion
+ Induced attraction

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Cluster formation

BEC induced interactions

- Dynamics of impurity cluster


Cheerios effect
Dynamic Impurities
Experiment by Inguscio Group

- Bose gas in one-dimensional tubes
- Impurity in a tight dipole potential
- Tune interactions between Bose gas and impurity

Experimental procedure

- Sequence of trapping potentials and interactions

1. Impurity is **tightly trapped**
2. Impurity-Bose gas **interactions** are switched on
3. Tight impurity **trap switched off** at time $t = 0$
4. Breathing **oscillations** in shallow potential $t > 0$
Experimental observations

- Properties of breathing oscillations

![Graphs showing Axial width (µm) over time (ms) for different values of η.](Image)

Amplitude depends on interaction η

![Graphs showing Normalized width σ_ω over -η and η for attractive and repulsive interactions.](Image)
Experimental observations

- Properties of breathing oscillations

We want to understand...
- Frequency and amplitude of the oscillations
- Damping of the oscillations
- Suppression of amplitude by interactions

Amplitude depends on interaction $\eta$
Model for experiment at zero temperature

\[ i\hbar \frac{\partial \chi}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m_a} + \frac{m_a}{2} \Omega_a^2 r^2 + \eta g |\varphi|^2 \right) \chi \]

\[ i\hbar \frac{\partial \varphi}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m_b} + v_b + \eta g |\chi|^2 + g |\varphi|^2 \right) \varphi \]

**Step 1: Solve equations numerically (code from W. Bao)**
- Ground state => normalized gradient flow method
- Evolution => time-splitting sine-spectral method

**Step 2: Find analytical solutions**

- Weak K-Rb interactions
- Excitation of the Bose gas => damped oscillations

- Impurity density
- Bose gas density
Dynamic self-trapping

- Strong K-Rb interactions
- Strong interactions $\Rightarrow$ self-trapping $\Rightarrow$ small amplitudes

- Impurity density
- Bose gas density

attractive impurities
$\Rightarrow$ density bulge
Oscillations in the TF-regime

- Coupled GPS equations

\[
i\hbar \frac{\partial \chi}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m_a} + \frac{m_a}{2} \Omega_a^2 r^2 + \eta g |\varphi|^2 \right) \chi
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\]

- Thomas-Fermi approximation for Bose gas (no damping)

- Self-focusing non-linear Schrödinger equation

\[
i\hbar \frac{\partial \chi}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m_a} + \eta gn_0 - \eta^2 g |\chi|^2 + \frac{m_a}{2} \Omega_a^2 r^2 \right) \chi
\]

- Inhomogeneity => linear term $\eta$

- Self-trapping => quadratic term $\eta^2$
Oscillations in the TF-regime

- Coupled GPS equations

\[ i\hbar \frac{\partial \chi}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m_a} + \frac{m_a}{2} \Omega_a^2 r^2 + \eta g|\varphi|^2 \right) \chi \]

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\[ i\hbar \frac{\partial \chi}{\partial t} = \left( -\frac{\hbar^2 \nabla^2}{2m_a} + \eta \rho_0 - \eta^2 g|\chi|^2 + \frac{m_a}{2} \Omega_a^2 r^2 \right) \chi \]

- Inhomogeneity => linear term $\eta$

- Self-trapping => quadratic term $\eta^2$
Evolution of impurity width

- Gaussian ansatz for impurity wave function

\[ \chi(r, \sigma, \gamma) = \left( \frac{\pi \sigma^2}{d} \right)^{-d/4} \exp \left( -r^2 / 2\sigma^2 - i\gamma r^2 \right) \]

- Newton-like e.o.m. for spread \( \sigma \) with potential \( V(\sigma) \)

\[
m_a \ddot{\sigma} = -\frac{\partial V(\sigma)}{\partial \sigma} \quad \quad \gamma = -\frac{m_a \dot{\sigma}}{2\hbar \sigma}
\]

1. \( V_0(\sigma) = \frac{\hbar^2}{2m_a \sigma^2} + \frac{m_a}{2} \Omega^2 \sigma^2 \) --- “free” oscillation of Gaussian

2. \( V_{st}(\sigma) = -\frac{\eta^2 \sigma^2}{d(2\pi)^{d/2} \sigma^d} \) --- self-trapping potential \( \sim \eta^2 \)

3. \( V_{inh}(\sigma) = \eta \mu_b \left[ \frac{2}{d} \tilde{\Gamma} \left( \frac{d}{2}, \frac{R^2}{\sigma^2} \right) - \frac{\sigma^2}{R^2} \tilde{\Gamma} \left( 1 + \frac{d}{2}, \frac{R^2}{\sigma^2} \right) \right] \) --- inhomogeneous background \( \sim \eta \)
Homogeneous Bose gas

Potential

\[ V = \frac{\hbar \Omega_2}{|\eta|} \]

\(|\eta| = 0, 1, 2, 3\)

Amplitude

\[ \frac{\sigma}{w_0} \]

Initial spread of impurity

Frequency

\[ \omega, \Omega_2 \]

Strong interaction \( \eta \) results in

- deeper effective potential \( V(\sigma) \)
- significantly smaller amplitudes
- higher oscillation frequency
Homogeneous Bose gas

Strong interaction $\eta$ results in
- deeper effective potential $V(\sigma)$
- significantly smaller amplitudes
- higher oscillation frequency
Damping by phonons

- Include Bogoliubov-phonons of the Bose gas

\[ \hat{H}_b = E_0 + \sum_{q} \hbar \omega_q \hat{b}^\dagger_q \hat{b}_q \]

- Impurity acts as classical driving force

\[ \hat{H}_{ab} = \eta g n_0 + \eta g \sum_{q \neq 0} (\hat{b}^\dagger_q + \hat{b}_q) f_q \]

\[ f_q = \sqrt{\frac{n_0 \epsilon_q}{V \hbar \omega_q}} \int dr |\chi(r)|^2 e^{i q \cdot r} \]

- Coherent-state ansatz for ground state and evolution

\[ |\Psi\rangle = |\sigma, \gamma\rangle \otimes |\{\alpha_q\}\rangle \]

\[ |\{\alpha_q\}\rangle = \otimes_q e^{-|\alpha_q|^2/2} e^{\alpha_q \hat{b}^\dagger_q} |0\rangle \]

\[ L = \langle \Psi | (i\hbar \partial_t - \hat{H}) |\Psi\rangle \]

\[ S = \int dt \; L \]

coherent states of phonon modes
Energy loss of impurities

- Energy loss of impurity with linear phonon spectrum

\[
\frac{dE(t)}{dt} = \frac{K\eta^2 g^2 n_0}{m_b c} \left\{ -\frac{ct e^{-c^2 t^2/\Sigma^2(t,0)}}{\Sigma^3(t,0)} + c \int_0^t dt' \frac{[\Sigma^2(t, t') - 2c^2(t-t')^2]}{\Sigma^5(t, t')} e^{-c^2(t-t')^2/\Sigma^2(t,t')} \right\}
\]

\[
\Sigma(t, t') = [\sigma^2(t) + \sigma^2(t')]^{1/2}
\]

- Non-Markovian effects decaying on time scale \(\sigma/c\)

- Strong damping if impurity is highly localized

\[
\frac{dE}{dt} \sim \eta^2 \cdot \frac{g n_0}{\hbar} \cdot \frac{g}{\xi} \cdot \left(\frac{\xi}{\ell}\right)^2
\]

healing length

size of impurity
Energy loss of impurities

- Solve equation for $\sigma(t)$ including loss

- Analytic results

- Numerical solution of coupled GPS equation

Very different from “standard” damping
- Non-Markovian
- Partly reversible exchange of energy

Impurity absorbs energy from Bose gas
Energy loss of impurities

- Solve equation for $\sigma(t)$ including loss

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- Numerical solution of coupled GPS equation

Impurity absorbs energy from Bose gas
Energy loss of impurities

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Impurity absorbs energy from Bose gas
Three-body recombination
Realistic BEC suffers from three-body recombination

\[ \frac{dN}{dt} = -K_3 \int d\mathbf{r} n^3(\mathbf{r}, t) \]

\[ -i\hbar \frac{K_3}{2} |\psi|^4 \psi \]

add damping to GP equation

TBR might remove divergence of density in 2D and 3D

TBR caused by impurities can be observed (Rb-Rb-Cs)

Bloch Group, Phys. Rev. Lett. 102, 030408 (2009)
Three-body recombination

- Solve time-dependent system by using TSSP method

\[
i\hbar \partial_t \psi = -\frac{\hbar^2}{2m_b} \nabla^2 \psi + \kappa |\chi|^2 \psi + g|\psi|^2 \psi - i\hbar \frac{K_3}{2} |\psi|^4 \psi
\]

\[
i\hbar \partial_t \chi = -\frac{\hbar^2}{2m_a} \nabla^2 \chi + \kappa |\psi|^2 \chi
\]

- Find non-equilibrium steady-state for attractive interactions \( \kappa < 0 \)

- Compare loss depending on interaction \( \kappa \) with experimental results

Three-body recombination

- Solution for 1D BEC in a box

\[ i\hbar \partial_t \psi = -\frac{\hbar^2}{2m_b} \nabla^2 \psi + \kappa |\chi|^2 \psi + g |\psi|^2 \psi - i\hbar \frac{K_3}{2} |\psi|^4 \psi \]

Standard solution \( \tanh(x) \)

Particle loss \( K_3 > 0 \)
Coupled GPS equations describe

- Static and dynamic self-trapping
- Dissipation of energy into the BEC
- Induced impurity-impurity interaction

Variational ansatz yields conceptual understanding of exact numerical results.
Coupled GPS equations describe

- Static and dynamic self-trapping
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Variational ansatz yields conceptual understanding of exact numerical results.

Impurities are the new vortices!
References

Dynamics of Single Neutral Impurity Atoms Immersed in an Ultracold Gas
N. Spethmann, F. Kindermann, S. John, C. Weber, D. Meschede and A. Widera

Quantum dynamics of impurities in a one-dimensional Bose gas

Polarons and Bose recondensation: A self-trapping approach

Strong-Coupling Polarons in Dilute Gas Bose-Einstein Condensates

Self-trapping of impurities in Bose-Einstein condensates: Strong attractive and repulsive coupling

Dynamics, dephasing and clustering of impurity atoms in Bose–Einstein condensates

Transport of strong-coupling polarons in optical lattices

Induced interaction and crystallization of self-localized impurity fields in a BEC

Breathing oscillations of a trapped impurity in a Bose gas

An Explicit Unconditionally Stable Numerical Method for Solving Damped Nonlinear Schrödinger Equations with a Focusing Nonlinearity
Classical Theory of Boson Wave Fields

E. P. Gross

This is to be studied as a Hamiltonian governing the motion of two coupled classical fields \( \psi(x, t), \Phi(q, t) \). We are to find solutions of the equations of motion

\[
\begin{align*}
    i\hbar \dot{\Phi}(q, t) &= -\frac{\hbar^2}{2m} \nabla^2 \Phi + \Phi \int U(|q - x|) \psi^+(x, t) \psi(x, t) \, d^3x, \\
    i\hbar \dot{\psi} &= -\frac{\hbar^2}{2M} \nabla^2 \psi + \psi \int V(x - y) \psi^+(y) \psi(y) \, d^3y
\end{align*}
\]

subject to \( \int \psi^+ \psi \, d^3x = N \), \( \int \Phi^* \Phi \, d^3q = 1 \).