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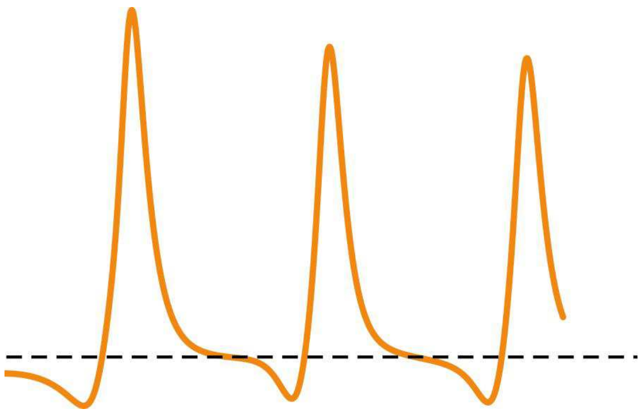
Impurities immersed in Bose-Einstein condensates

February 4th 2013
Martin Bruderer



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

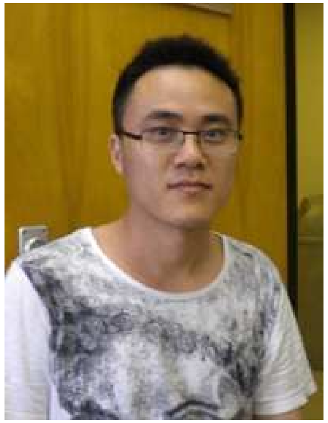
Some People Involved

Dieter Jaksch
Oxford, Singapore (CQT)

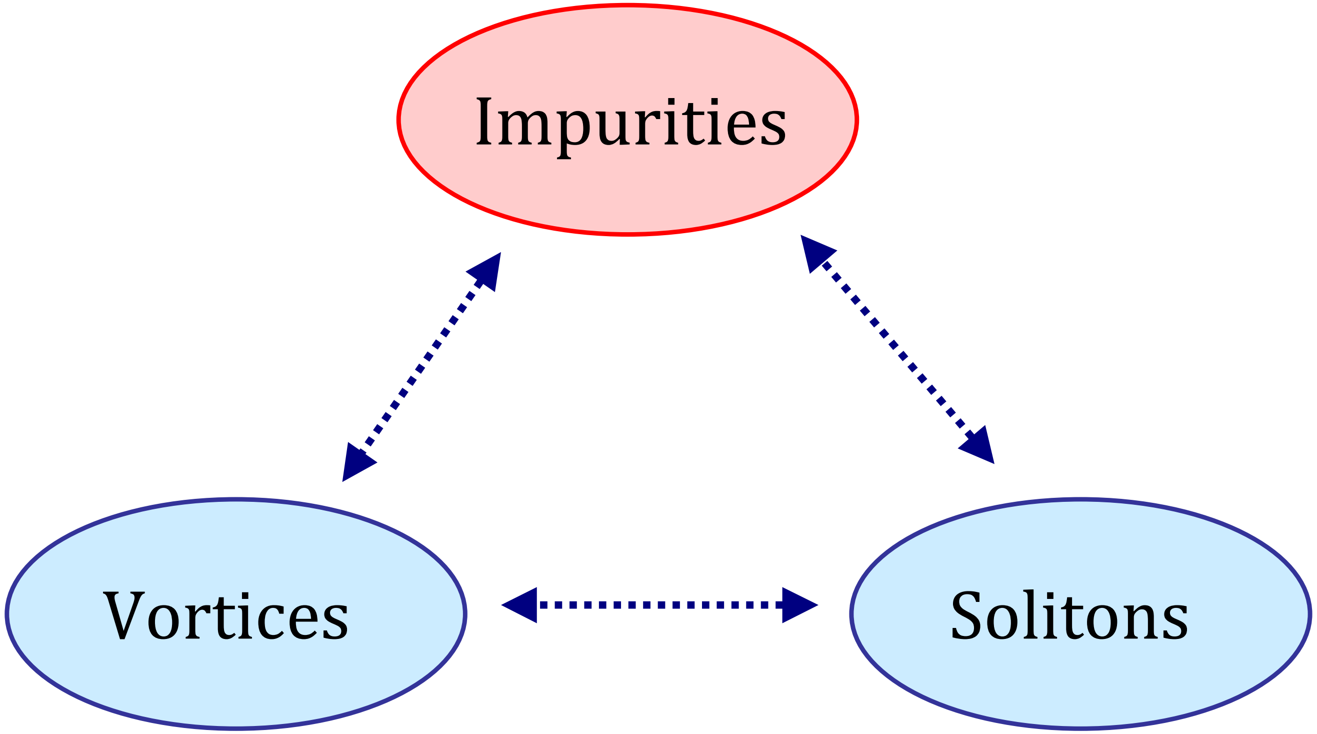
Stephen R. Clark
Oxford, Singapore (CQT)

Tomi Johnson
Oxford

Weizhu Bao
Singapore (Uni)



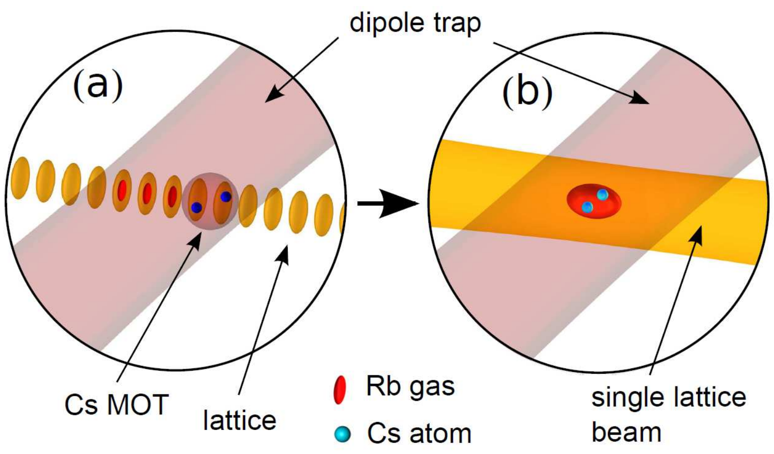
Yongyong Cai
Madison (Uni of Wisconsin)



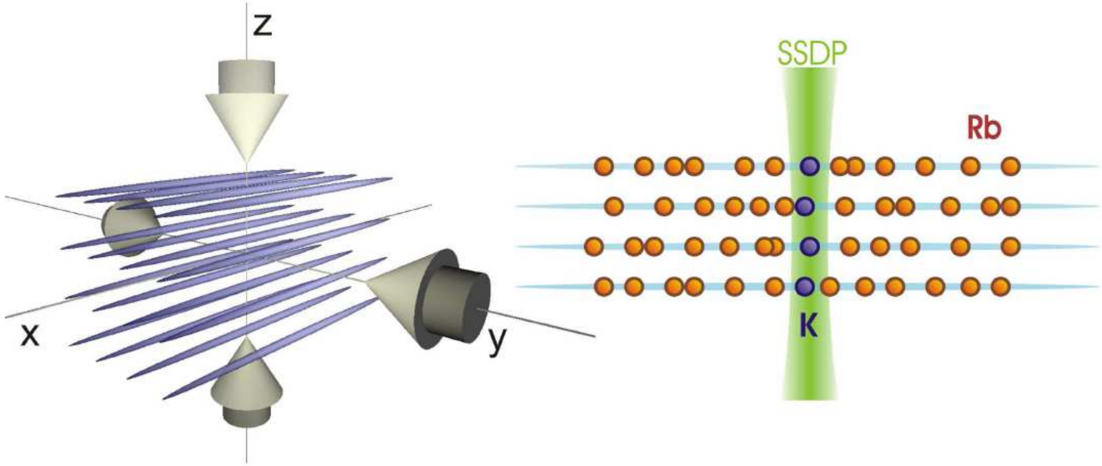
Nonlinearity of the GP-equation is important.

Current experiments

A. Widera (Kaiserslautern)



M. Inguscio (Florence)



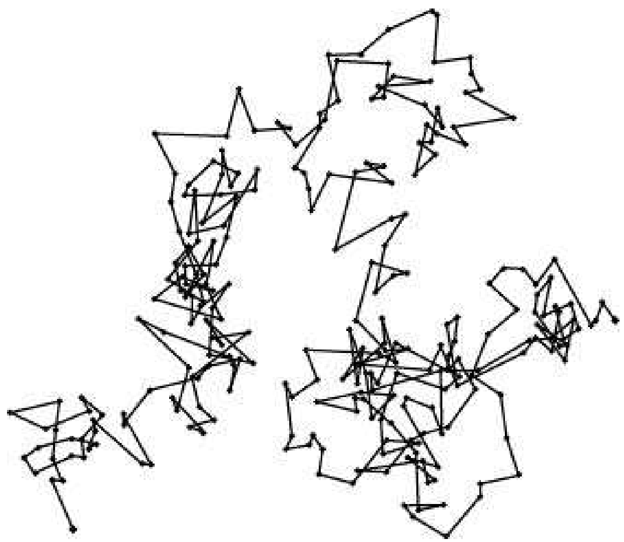
- Single impurities in BECs
- Control impurity-BEC interactions
- Control trapping potentials
- Control number of impurities

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

Widera Group, Phys. Rev. Lett. **109**, 235301 (2012)
Inguscio Group, Phys. Rev. A **85**, 023623 (2012)

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



Brownian motion

General model – GPS equations

- Single impurity $\chi(r)$ interacting with BEC $\psi(r)$

$$
\begin{aligned}
i\hbar\partial_t\psi &= -\frac{\hbar^2}{2m_b}\nabla^2\psi + g|\psi|^2\psi \\
i\hbar\partial_t\chi &= -\frac{\hbar^2}{2m_a}\nabla^2\chi
\end{aligned}
$$

GP equation ($g > 0$)

Schrödinger equation

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

- Normalization for $\psi(r)$ and $\chi(r)$

$$
\int d\mathbf{r}|\psi(\mathbf{r})|^2 = N \quad \text{and} \quad \int d\mathbf{r}|\chi(\mathbf{r})|^2 = 1
$$

- Problem different from two-component BECs (bulk terms dominate)

General model – GPS equations

- Single impurity $\chi(r)$ interacting with BEC $\psi(r)$

$$
\begin{aligned}
i\hbar\partial_t\psi &= -\frac{\hbar^2}{2m_b}\nabla^2\psi + \kappa|\chi|^2\psi + g|\psi|^2\psi \\
i\hbar\partial_t\chi &= -\frac{\hbar^2}{2m_a}\nabla^2\chi + \kappa|\psi|^2\chi
\end{aligned}
$$

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- Problem different from two-component BECs (bulk terms dominate)

Static Impurities

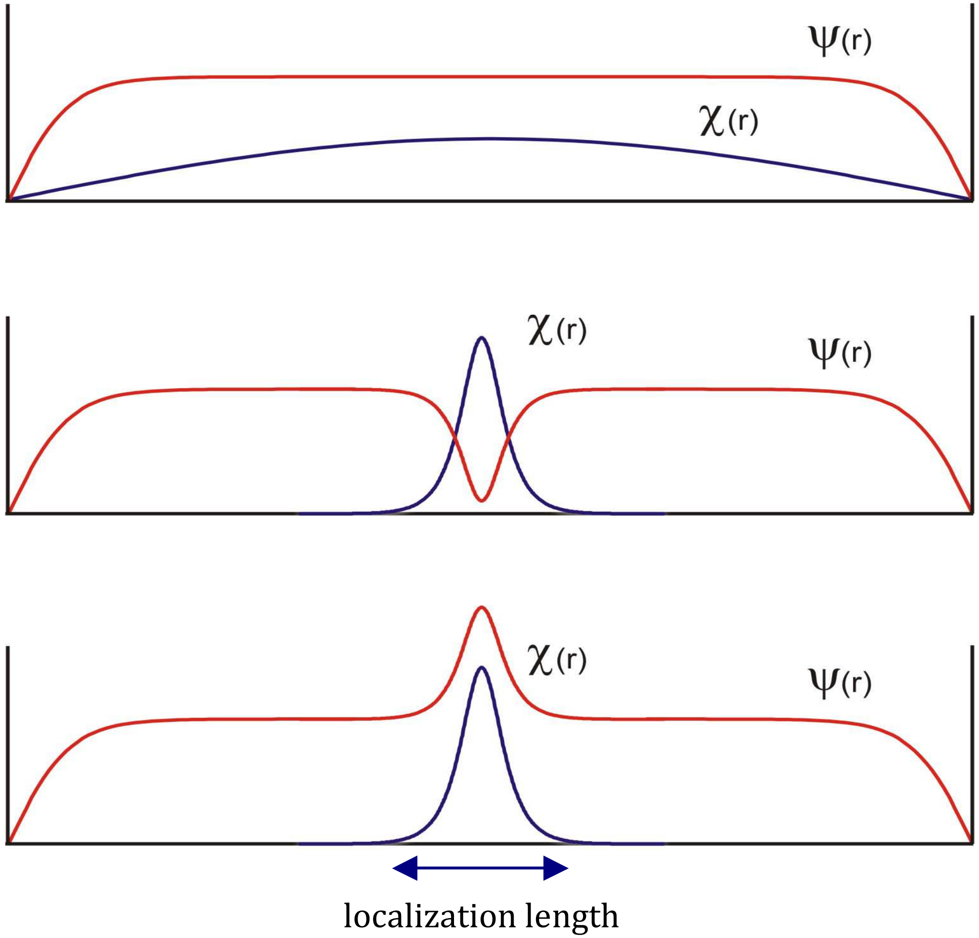
Self-trapping effect

- $\chi(r)$ and $\psi(r)$ are in large box and vanish at boundary
- Coupling κ 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



Time-independent model

- Dimensionless equations for stationary system

$$
\begin{aligned}
\psi &= -\frac{1}{2}\nabla^2\psi + \beta\gamma^D|\chi|^2\psi + |\psi|^2\psi \\
\varepsilon\chi &= -\frac{\alpha}{2}\nabla^2\chi + \beta|\psi|^2\chi
\end{aligned}
$$

$$
\begin{aligned}
\alpha &= m_b/m_a \\
\beta &= \kappa/g \\
\gamma &= d/\xi
\end{aligned}
$$

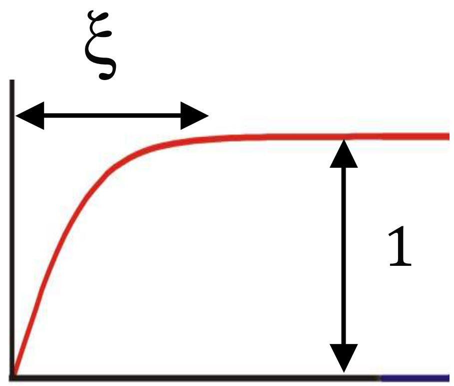
- Energy of the system

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

α, γ are of order 1 for "natural" parameters

Healing length $\xi = \hbar/\sqrt{g n_0 m_b}$

Energy scale $g n_0$



Weak interactions: Self-trapping threshold

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

$$
\begin{aligned}
\Big(-\frac{1}{2}\nabla^2 + 2\Big)\delta\psi &= -\beta\gamma^D|\chi|^2 \\
\Big(-\frac{\alpha}{2}\nabla^2 + 2\beta\,\delta\psi\Big)\chi &= (\varepsilon - \beta)\chi
\end{aligned}
$$

- Obtain non-local non-linear Schrödinger equation

$$
\Big(-\frac{1}{2}\nabla^2 - 2\zeta\int d\mathbf{r}' G(\mathbf{r}-\mathbf{r}')|\chi(\mathbf{r}')|^2\Big)\chi = \varepsilon'\chi
$$

$$
\Big(-\frac{1}{2}\nabla^2 + 2\Big)G(\mathbf{r}) = \delta(\mathbf{r})
$$

Helmholtz equation

  - χ(r) depends on single parameter $\zeta = \beta^2\gamma^D/\alpha$
  - Approximation is valid for $|\beta|\gamma^D/\ell_{\rm loc}^D \ll 1$

Lee D. K. K. and Gunn J. M. F., Phys. Rev. B **46,** 301(1992)

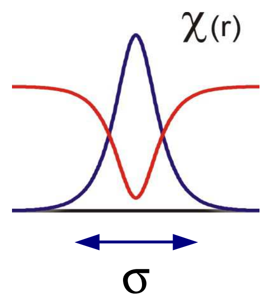
Cucchietti F. M. and Timmermans E., Phys. Rev. Lett.**96,** 210401 (2006)

Weak interactions: Self-trapping threshold

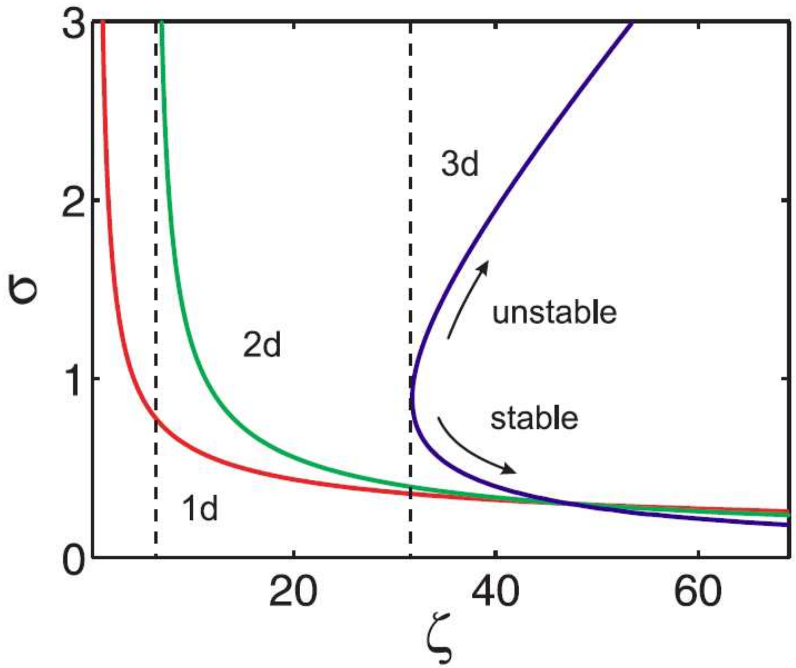
- Energy functional F[χ] for non-local NLSE

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

interaction energy



- Use Gaussian trial function of width σ



1d localized for arbitrarily small interaction

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

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

3d localization for $\zeta > 31.7...$

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

MB, W. Bao and D. Jaksch, EPL **82**, 30004 (2008)

Strong interactions: Asymmetry

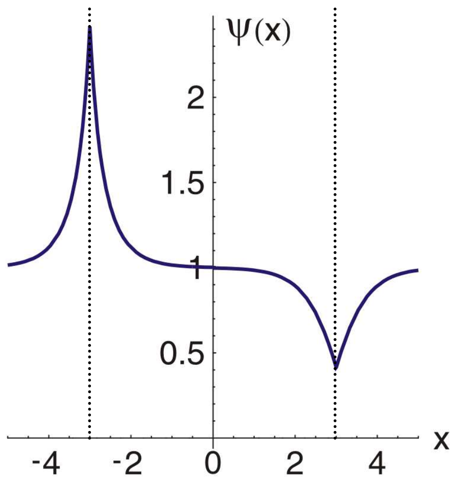
- For |β| >> 1 impurity is highly localized $|\chi(r)|^2 \approx \delta(r)$
- Equation for ψ(x) in presence of δ-impurity in 1D

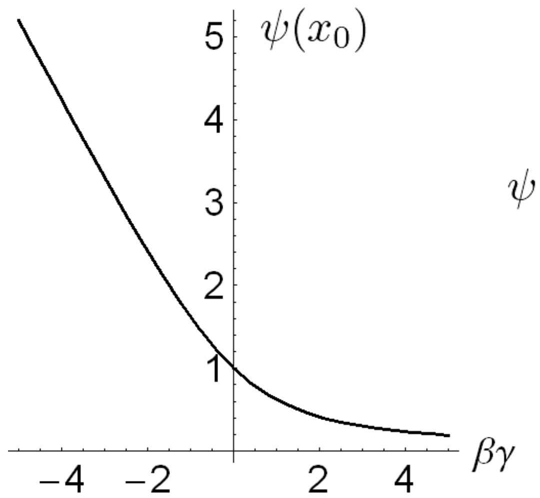
$$\left[-\frac{1}{2}\partial_{xx} - 1 + |\psi(x)|^2 + \beta\gamma\,\delta(x-x_0)\right]\psi(x) = 0$$

$$\psi(x) = \coth(|x|+c) \qquad \text{attractive}$$

$$\psi(x) = \tanh(|x|+c) \qquad \text{repulsive}$$

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

$$\chi_\sigma(\mathbf{x}) = (\pi\sigma^2)^{-d/4} \prod_{j=1}^{d} \exp(-x_j^2/2\sigma^2)$$ Gaussian

$$\psi_\sigma(\mathbf{x}) = 1 + \frac{a}{\sigma^{\delta/2}} \prod_{j=1}^{d} \exp(-x_j^2/b\sigma^2)$$ Gaussian deformation

$$\int \mathrm{d}\mathbf{x} |\delta\psi(\mathbf{x})|^2 \sim \sigma^{d-\delta} \qquad \delta \leqslant d$$ Deformation finite in the limit $\sigma \to 0$

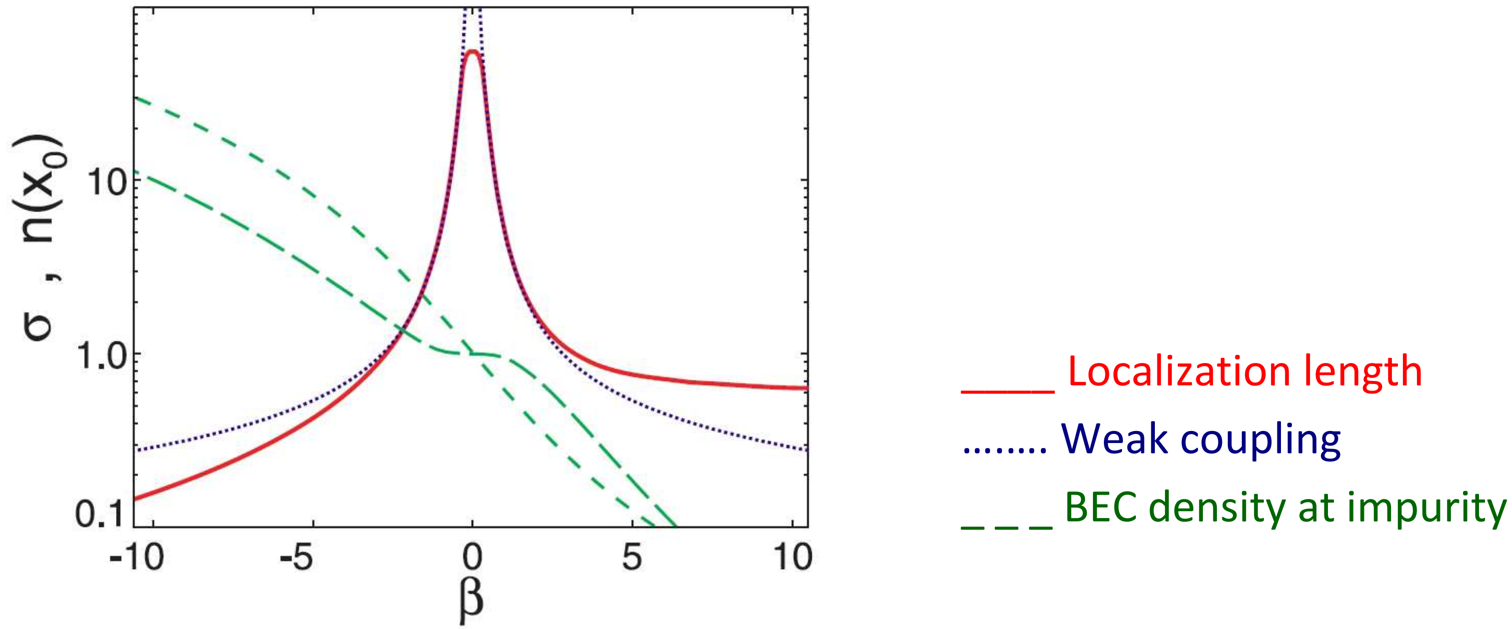
- Scaling of energy in the limit $\sigma \to 0$

$$E_{\mathrm{int}} \sim \beta\sigma^{-\delta} \qquad E_{\mathrm{kin}} \sim \sigma^{-2} \qquad E_{\mathrm{bec}} \sim c_0\sigma^{d-\delta-2} + \sum_{j=1}^{4} c_j\, \sigma^{d-j\delta/2}$$

- No ground state for attractive impurities in 3d

1D numerical results

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



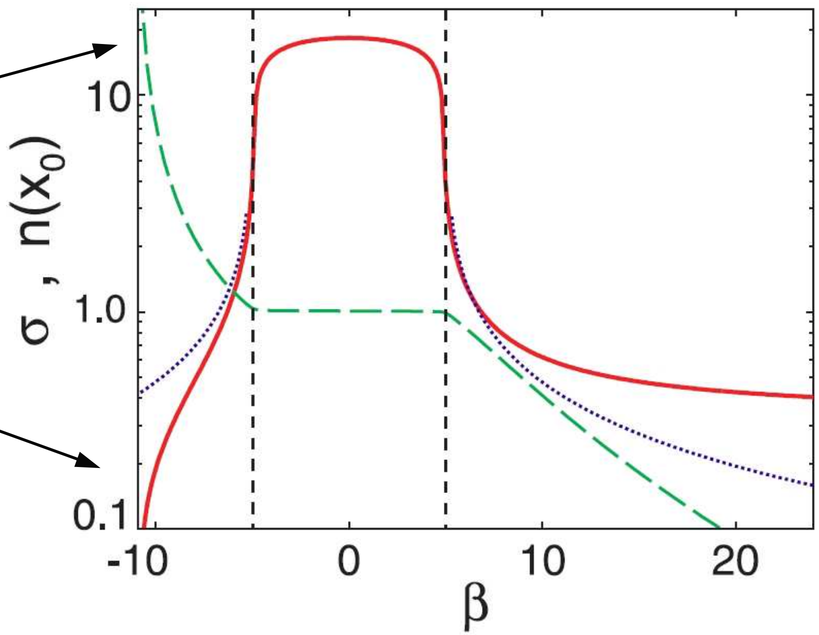
> Linearization accurate for small β
> Strong BEC deformation

2D numerical results

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

density diverges

width shrinks to zero



____ Localization length

.... Weak coupling

_ _ _ BEC density at impurity

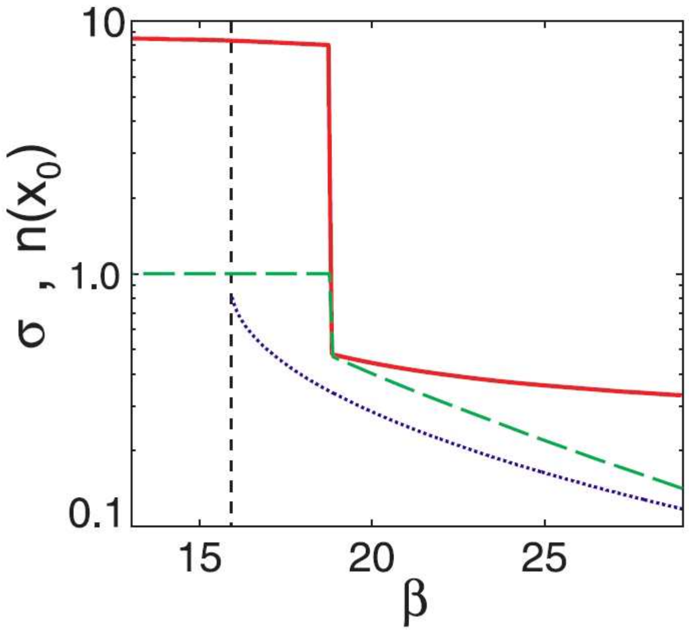
> Linearization accurate for small β

> Correct threshold for critical β

> Critical attractive coupling

3D numerical results

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



____ Localization length

.... Weak coupling

_ _ _ BEC density at impurity

> Linearization fails completely

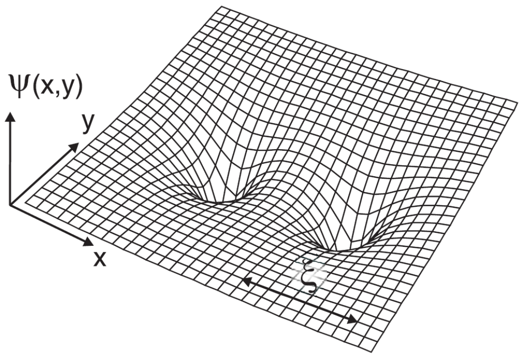
> Sharp jump to localized state

> No ground state for attractive impurities

BEC induced interactions

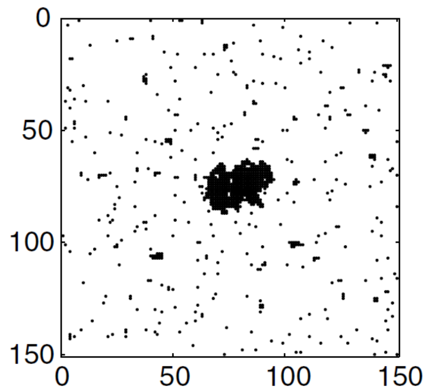
- Interaction caused by BEC deformation

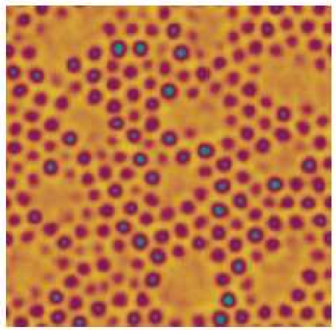
$$F[\chi] = \frac{\alpha}{2}\int \mathrm{d}\mathbf{r}|\nabla\chi|^2 - \underbrace{\beta^2\gamma^D\int \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'|\chi(\mathbf{r})|^2 G(\mathbf{r}-\mathbf{r}')|\chi(\mathbf{r}')|^2}_{\text{interaction energy}}$$

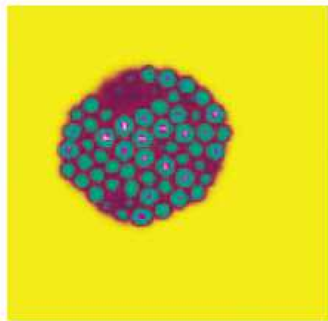


Short range repulsion
+ Induced attraction

Cluster formation



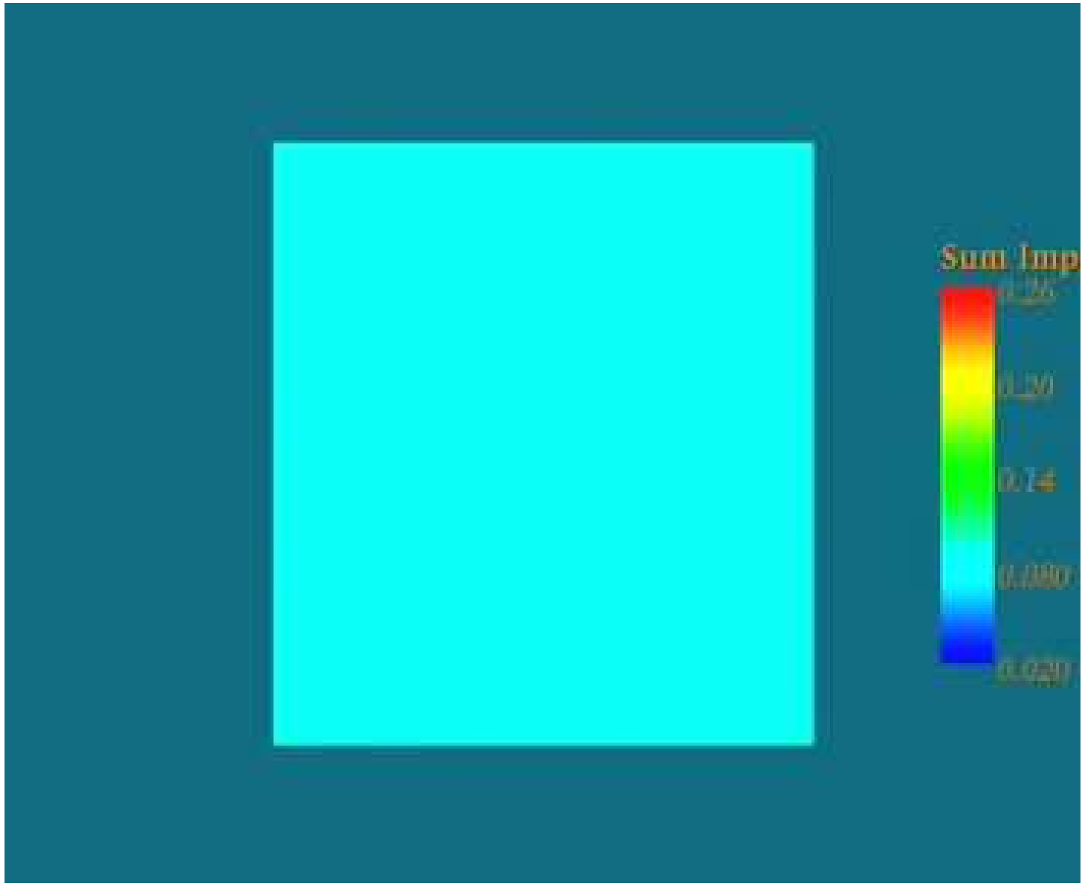




A. Klein, MB, S. R. Clark and D. Jaksch, New J. Phys. **9**, 411 (2007)
MB, A. Klein, S. R. Clark and D. Jaksch, New J. Phys. **10**, 033015 (2008)
D.C. Roberts and S. Rica, Phys. Rev. Lett. **102**, 025301 (2009)

BEC induced interactions

- Dynamics of impurtiy cluster

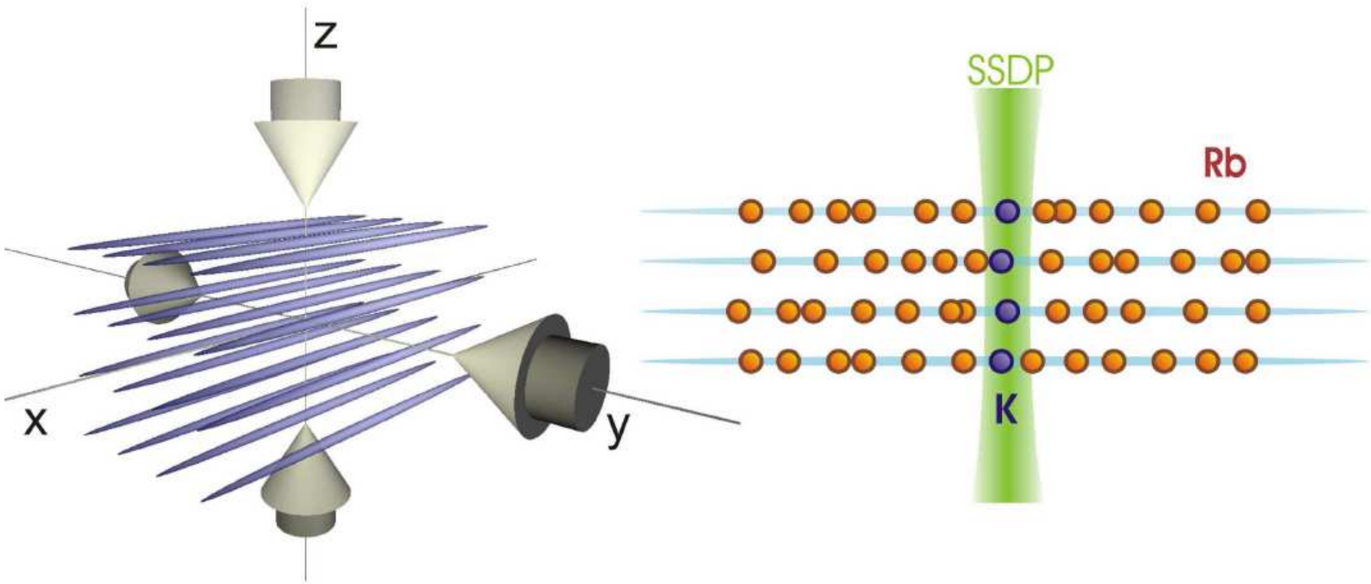


Cheerios effect

D.C. Roberts and S. Rica, Phys. Rev. A **80**, 013609 (2009)

Dynamic Impurities

Experiment by Inguscio Group

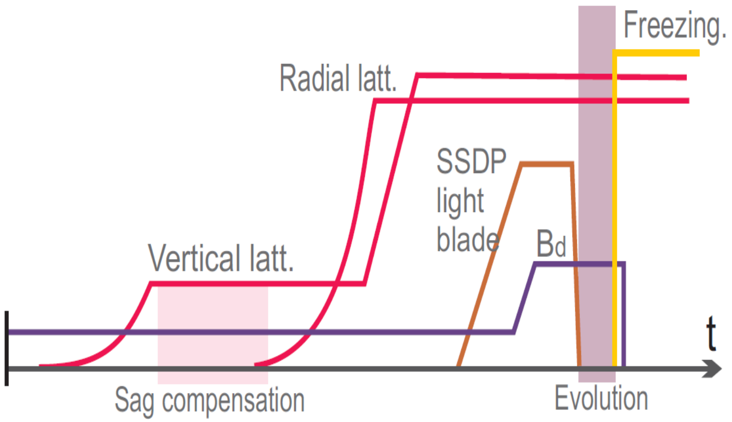


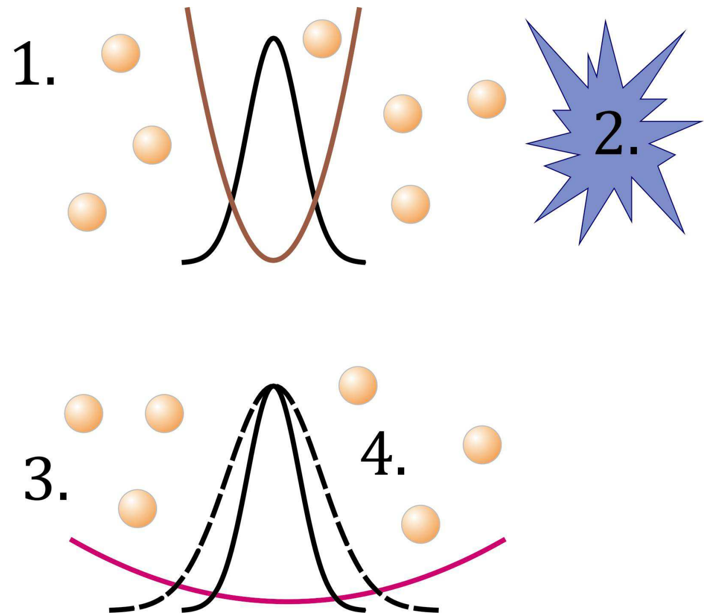
- Bose gas in one-dimensional tubes
- Impurity in a tight dipole potential
- Tune interactions between Bose gas and impurity

Inguscio Group, Phys. Rev. A **85**, 023623 (2012)

Experimental procedure

- Sequence of trapping potentials and interactions

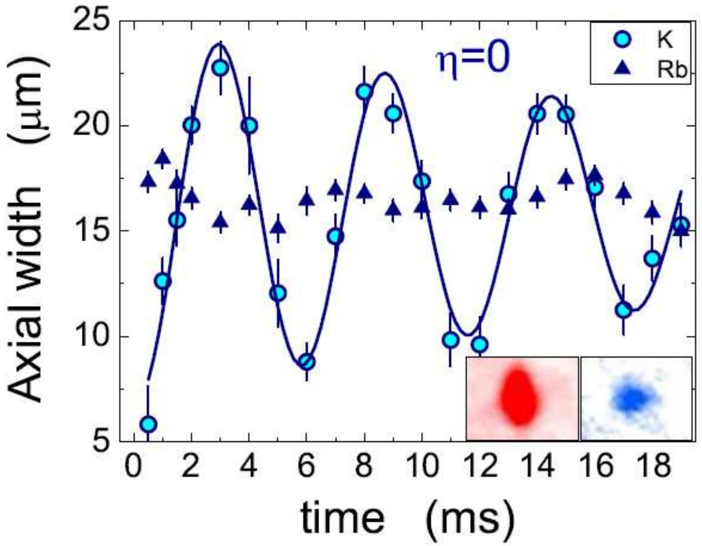


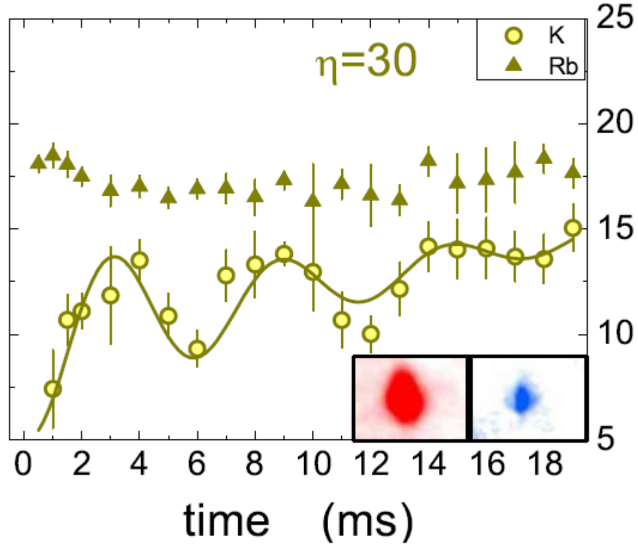


1. Impurity is tightly trapped
2. Impurity-Bose gas interactions are switched on
3. Tight impurity trap switched off at time t = 0
4. Breathing oscillations in shallow potential t > 0

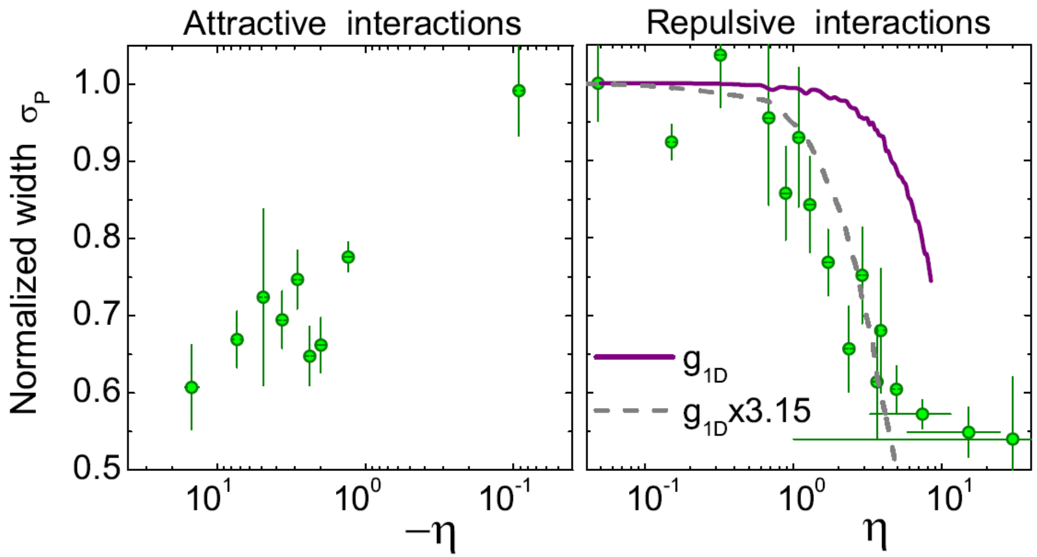
Experimental observations

- Properties of breathing oscillations



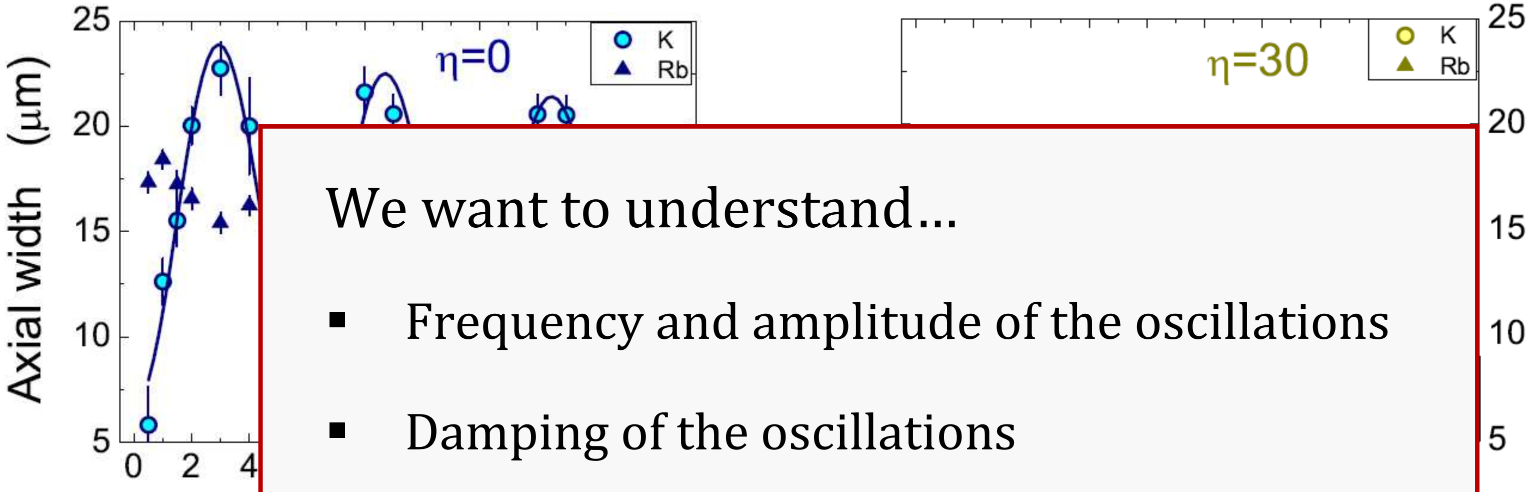


Amplitude depends on interaction η



Experimental observations

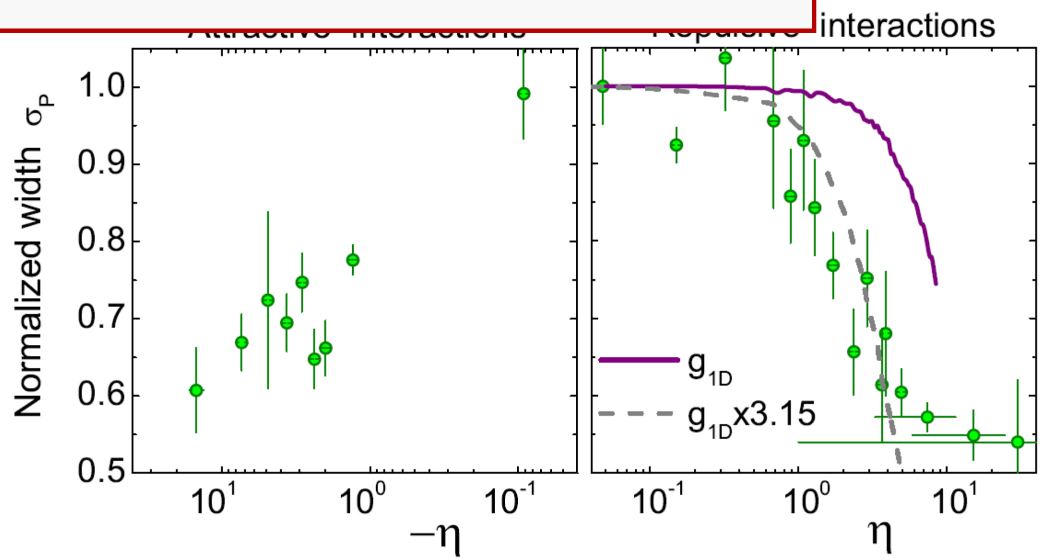
- Properties of breathing oscillations



We want to understand…

- Frequency and amplitude of the oscillations
- Damping of the oscillations
- Supression of amplitude by interactions

Amplitude depends on interaction η



Coupled GPS equations

- Model for experiment at zero temperature

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

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

Switch Ω_a from large to small at time t=0

- 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

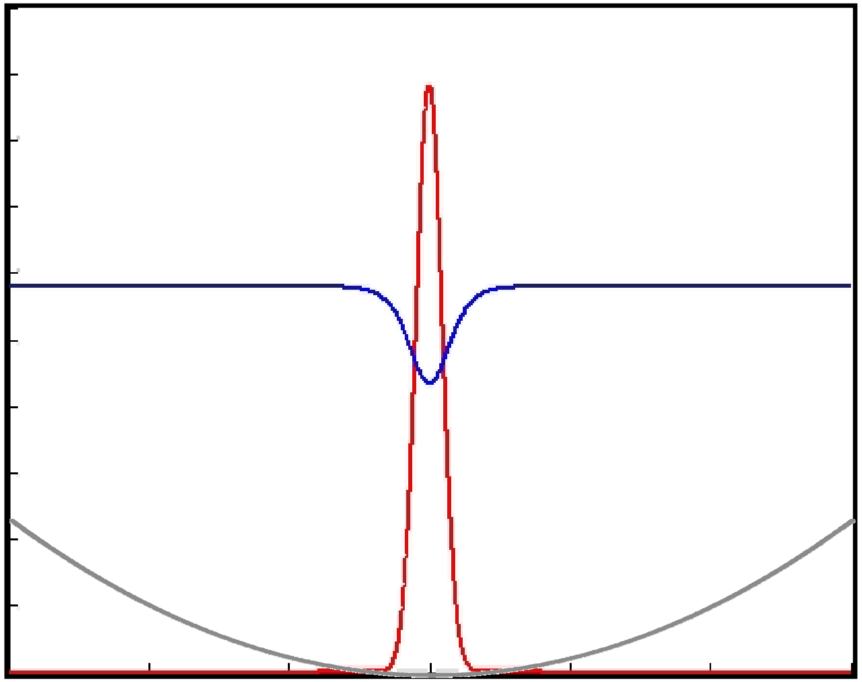
W. Bao and D. Jaksch, SIAM J. Numer. Anal. **41**, 1406 (2003)

W. Bao and Q. Du, SIAM J. Sci. Comput. **25**, 1674 (2004)

T. H. Johnson, MB, Y. Cai, S. R. Clark, W. Bao and D. Jaksch, EPL **98,** 26001 (2012)

Damped oscillations

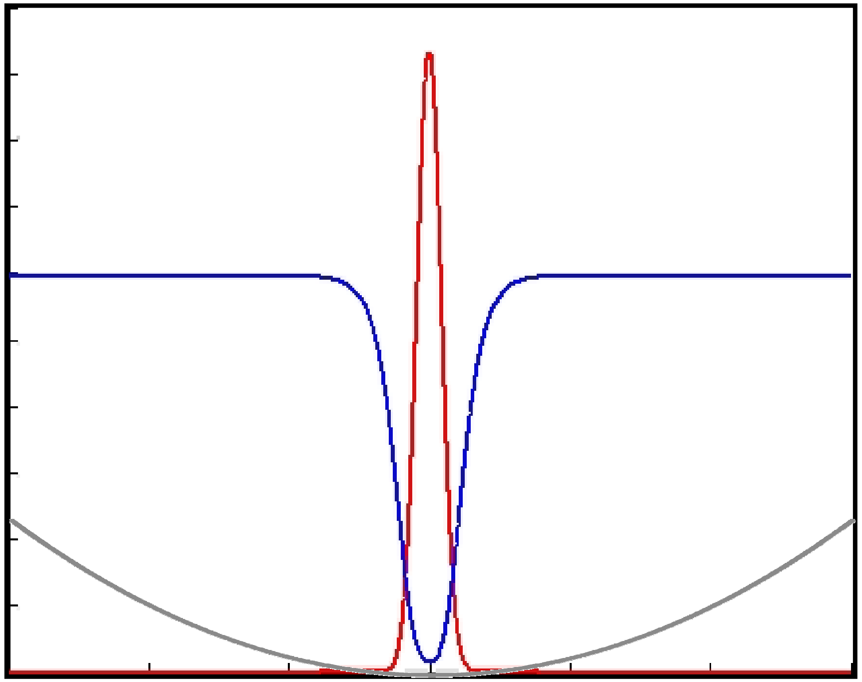
- Weak K-Rb interactions
- Excitation of the Bose gas => damped oscillations



- Impurity density
- Bose gas density

Dynamic self-trapping

- Strong K-Rb interactions
- Strong interactions => self-trapping => small amplitudes



- Impurity density
- Bose gas density

attractive impurites
=> density bulge

Oscillations in the TF-regime

- Coupled GPS equations

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

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

- Thomas-Fermi approximation for Bose gas (no damping)
- Self-focusing non-linear Schrödinger equation

$$i\hbar\frac{\partial\chi}{\partial t} = \left(-\frac{\hbar^2\nabla^2}{2m_a} + \eta g n_0 - \eta^2 g|\chi|^2 + \frac{m_a}{2}\Omega_a^2 r^2\right)\chi$$

- Inhomogeneity => linear term η
- Self-trapping => quadratic term η^2

Oscillations in the TF-regime

- Coupled GPS equations

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

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

- Thomas-Fermi approximation for Bose gas (no damping)
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$$i\hbar\frac{\partial\chi}{\partial t} = \left(-\frac{\hbar^2\nabla^2}{2m_a} + \eta g n_0 - \eta^2 g|\chi|^2 + \frac{m_a}{2}\Omega_a^2 r^2\right)\chi$$

- Inhomogeneity => linear term η
- Self-trapping => quadratic term η²

Evolution of impurity width

- Gaussian ansatz for impurity wave function

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

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

$$m_a\ddot{\sigma} = -\frac{\partial V(\sigma)}{\partial\sigma} \qquad \gamma = -m_a\dot{\sigma}/2\hbar\sigma$$

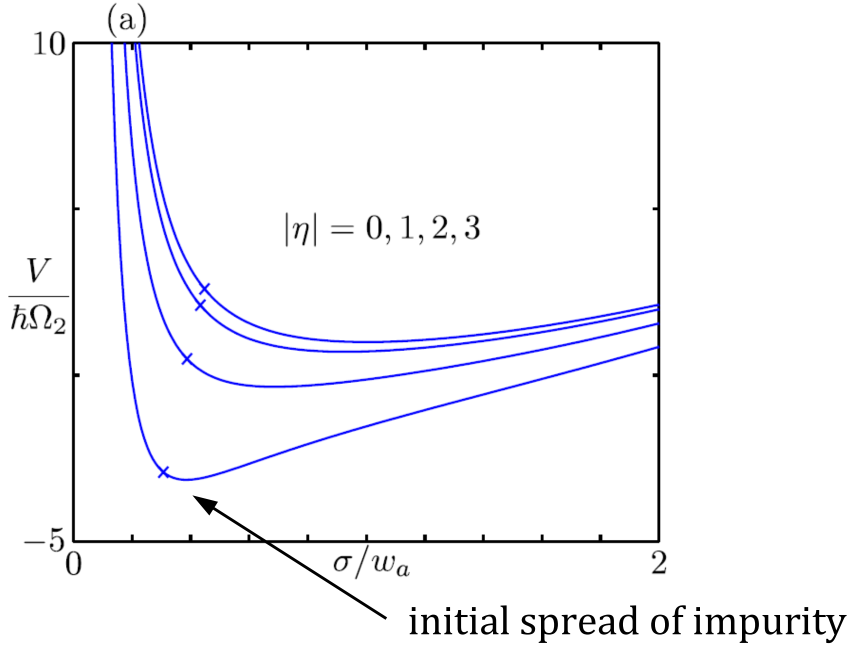
(1) $$V_0(\sigma) = \frac{\hbar^2}{2m_a\sigma^2} + \frac{m_a}{2}\Omega_a^2\sigma^2$$ "free" oscillation of Gaussian

(2) $$V_{\mathrm{st}}(\sigma) = -\frac{\eta^2 g}{d(2\pi)^{d/2}\sigma^d}$$ self-trapping potential ~ η^2

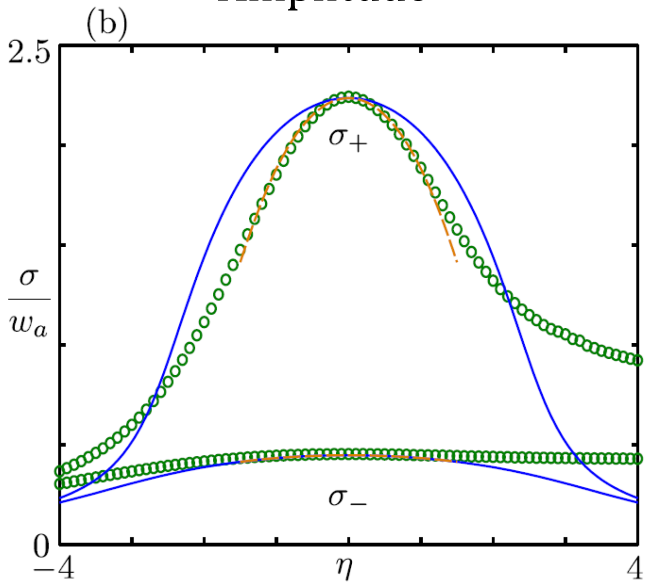
(3) $$V_{\mathrm{inh}}(\sigma) = \eta\mu_b\left[\frac{2}{d}\tilde{\Gamma}\left(\frac{d}{2},\frac{R^2}{\sigma^2}\right) - \frac{\sigma^2}{R^2}\tilde{\Gamma}\left(1+\frac{d}{2},\frac{R^2}{\sigma^2}\right)\right]$$ inhomogeneous background ~ η

Homogeneous Bose gas

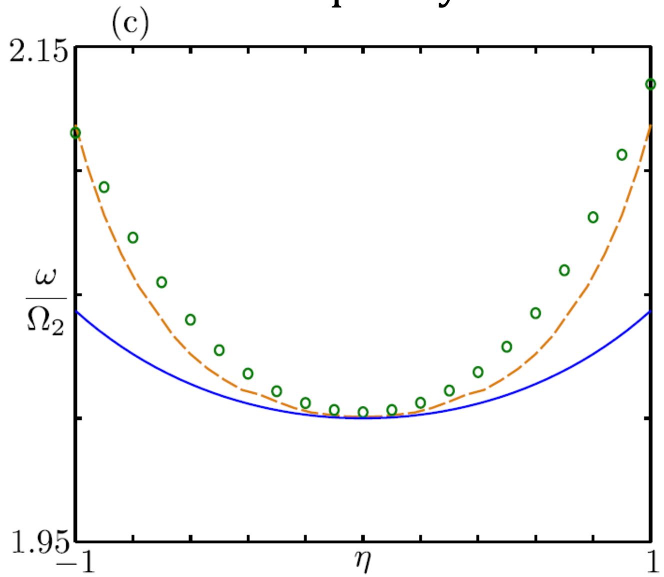
Potential



Amplitude



Frequency

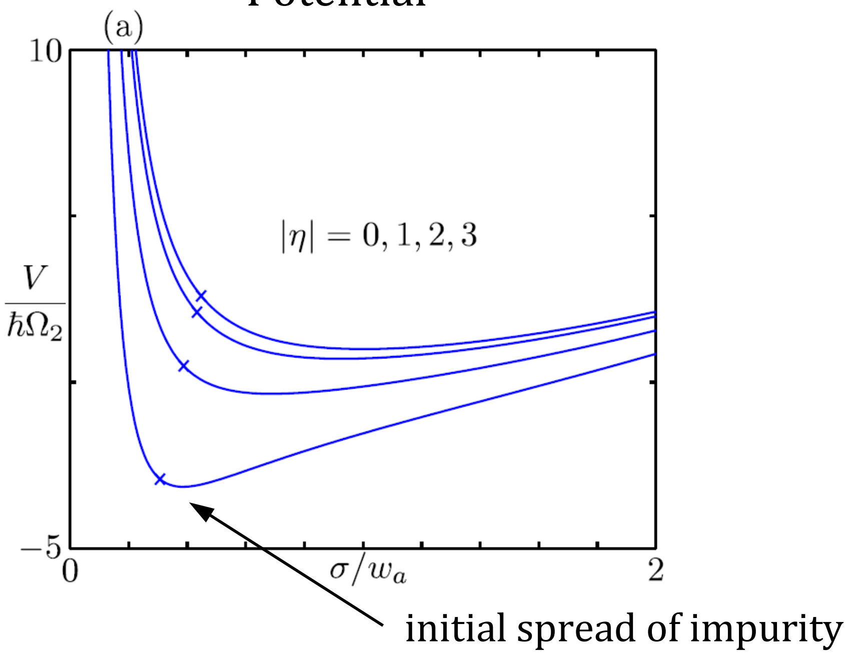


Strong interaction η results in

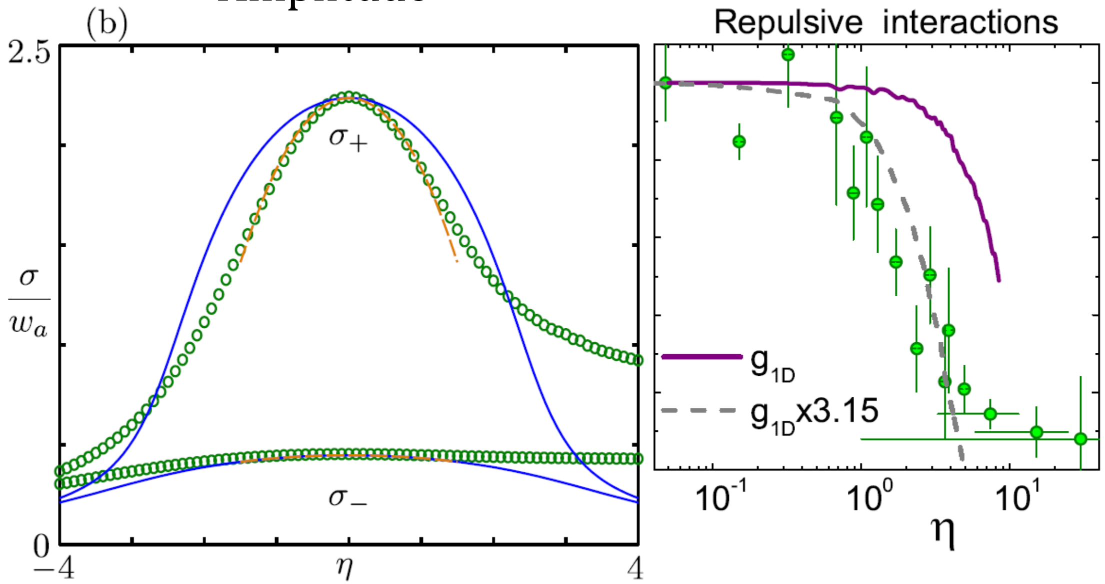
- deeper effective potenial V(σ)
- significantly smaller ampliutes
- higher oscillation frequency

Homogeneous Bose gas

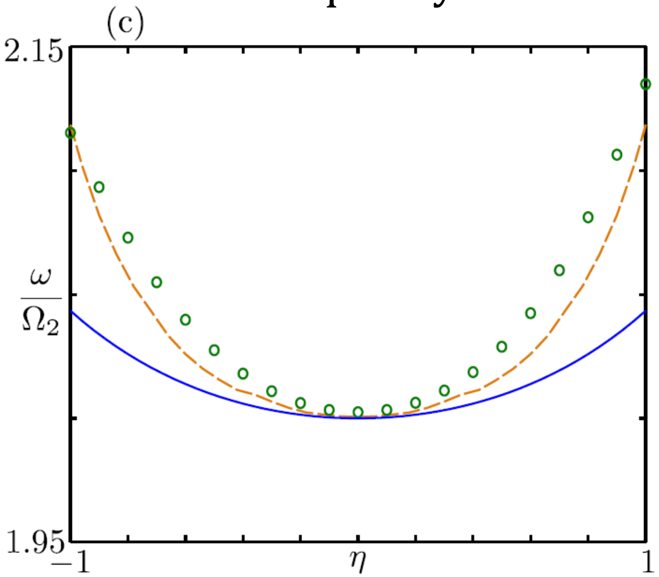
Potential



Amplitude



Frequency



Strong interaction η results in

- deeper effective potenial V(σ)
- significantly smaller ampliutes
- higher oscillation frequency

Damping by phonons

- Include Bogoliubov-phonons of the Bose gas

$$\hat{H}_b = E_0 + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \hat{b}^\dagger_{\mathbf{q}} \hat{b}_{\mathbf{q}}$$

- Impurity acts as classical driving force

$$\hat{H}_{ab} = \eta g n_0 + \eta g \sum_{\mathbf{q}\neq 0} (\hat{b}^\dagger_{\mathbf{q}} + \hat{b}_{\mathbf{q}})\, f_{\mathbf{q}}$$

$$f_{\mathbf{q}} = \sqrt{\frac{n_0 \epsilon_{\mathbf{q}}}{\mathcal{V}\hbar\omega_{\mathbf{q}}}} \int \mathrm{d}\mathbf{r} |\chi(\mathbf{r})|^2 \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}$$

Valid for sufficiently weak interactions η

- Coherent-state ansatz for ground state and evolution

$$|\Psi\rangle = |\sigma, \gamma\rangle \otimes |\{\alpha_{\mathbf{q}}\}\rangle$$

$$|\{\alpha_{\mathbf{q}}\}\rangle = \bigotimes_{\mathbf{q}} \mathrm{e}^{-|\alpha_{\mathbf{q}}|^2/2} \mathrm{e}^{\alpha_{\mathbf{q}} \hat{b}^\dagger_{\mathbf{q}}} |0\rangle$$

coherent states of phonon modes

$$L = \langle\Psi|\big(\mathrm{i}\hbar\partial_t - \hat{H}\big)|\Psi\rangle$$

$$S = \int \mathrm{d}t\, L$$

Energy loss of impurities

- Energy loss of impurity with linear phonon spectrum

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

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

- Non-Markovian effects decaying on time scale σ/c
- Strong damping if impurity is highly localized

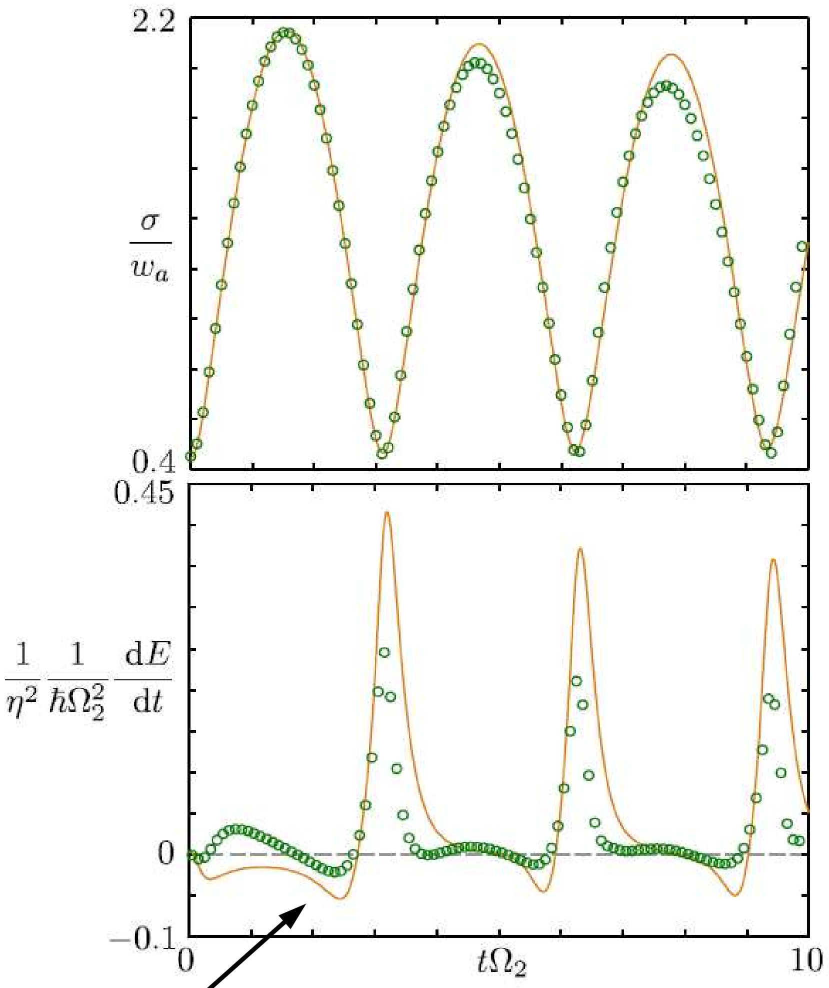
$$\frac{\mathrm{d}E}{\mathrm{d}t} \sim \eta^2 \cdot \frac{gn_0}{\hbar} \cdot \frac{g}{\xi} \cdot \left(\frac{\xi}{\ell}\right)^2$$

healing length

size of impurity

Energy loss of impurities

- Solve equation for σ(t) including loss



Impurity absorbs energy from Bose gas

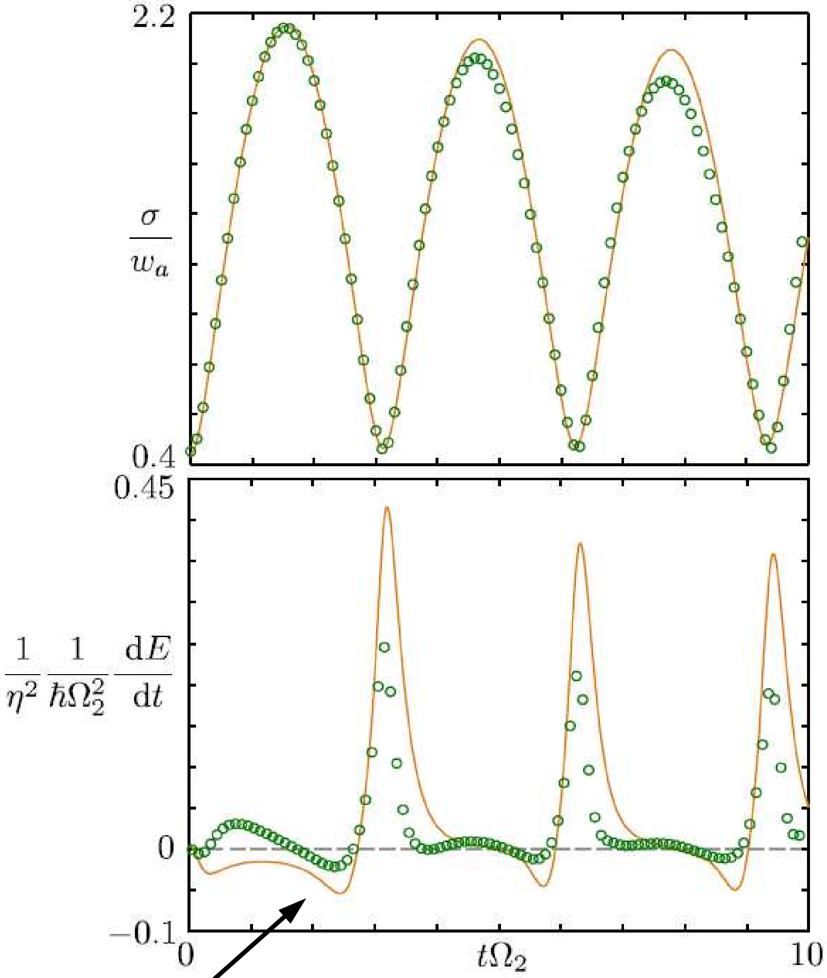
- Analytic results
- Numerical solution of coupled GPS equation

Very different from "standard" damping

- Non-Markovian
- Partly reversable exchange of energy

Energy loss of impurities

- Solve equation for σ(t) including loss



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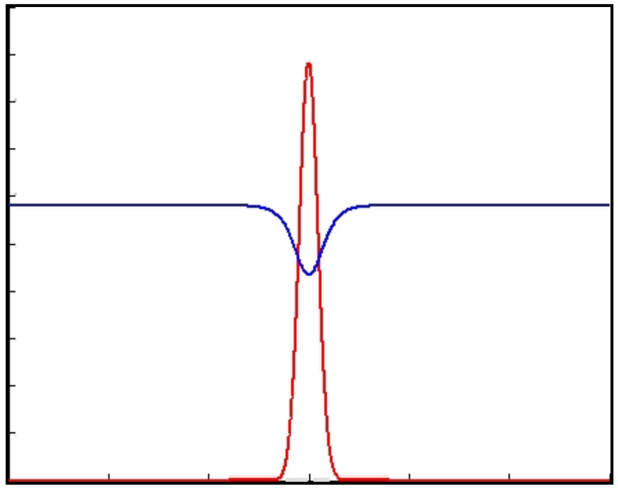

Energy loss of impurities

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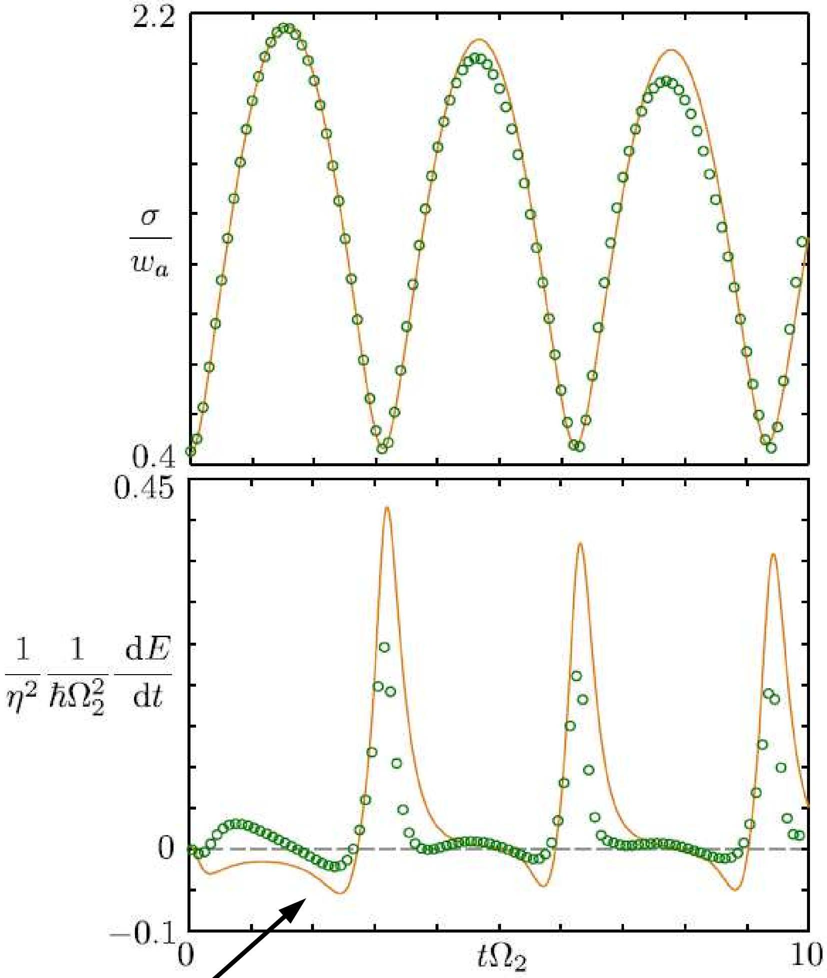

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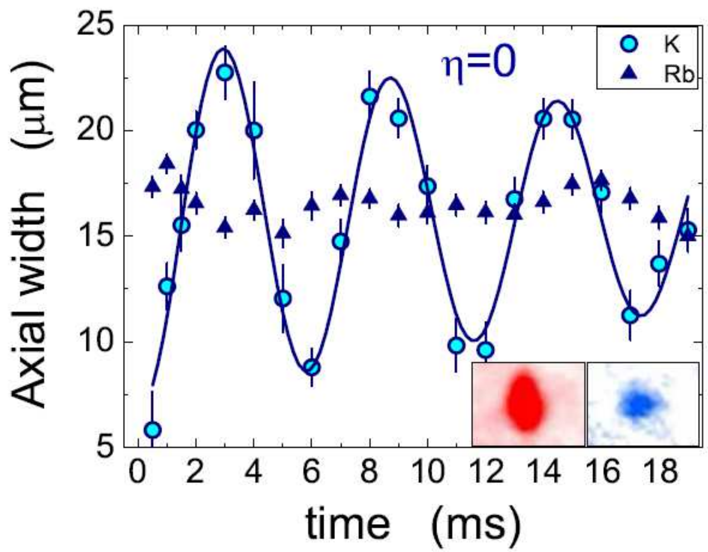
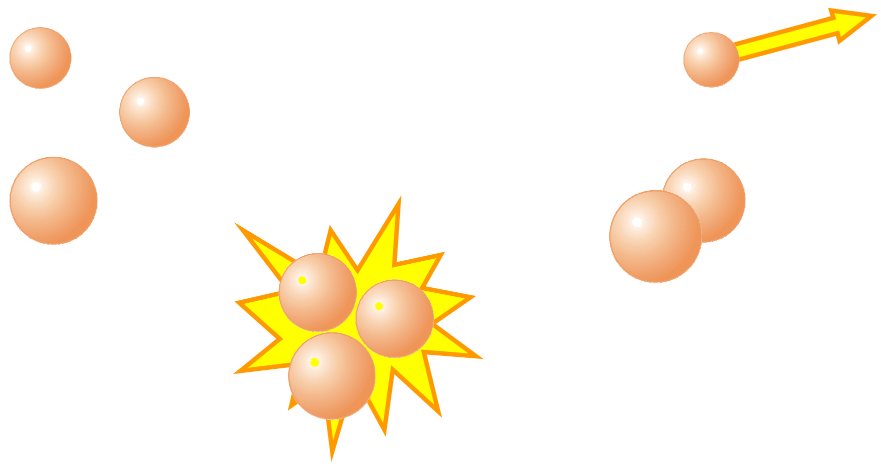


Three-body recombination

Three-body recombination

- Realistic BEC suffers from three-body recombination



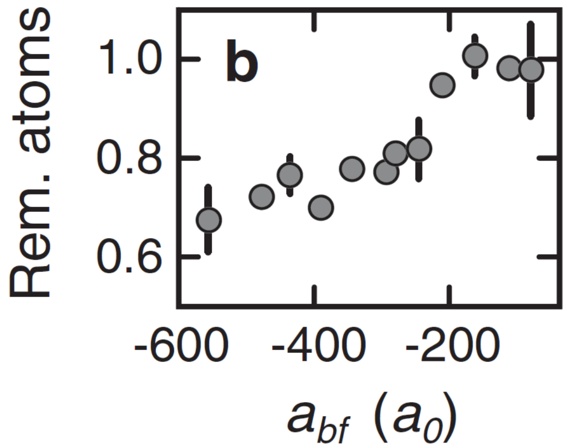
$$\frac{\mathrm{d}N}{\mathrm{d}t} = -K_3 \int \mathrm{d}\mathbf{r}\, n^3(\mathbf{r}, t)$$

$$-\,\mathrm{i}\hbar\frac{K_3}{2}|\psi|^4\psi$$

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)

Widera Group, Phys. Rev. Lett. **109**, 235301 (2012)

Three-body recombination

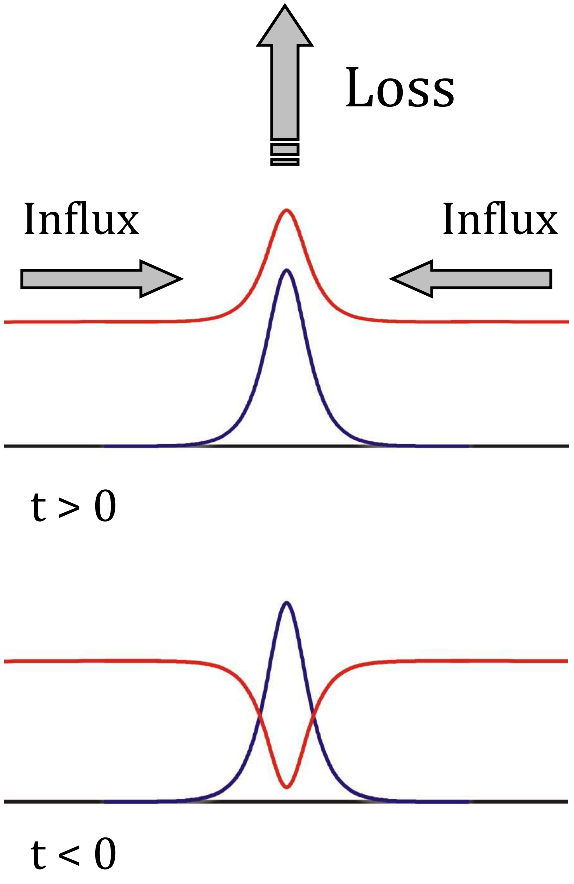
- Solve time-dependent system by using TSSP method

$$
\begin{aligned}
i\hbar\partial_t\psi &= -\frac{\hbar^2}{2m_b}\nabla^2\psi + \kappa|\chi|^2\psi + g|\psi|^2\psi - i\hbar\frac{K_3}{2}|\psi|^4\psi \\
i\hbar\partial_t\chi &= -\frac{\hbar^2}{2m_a}\nabla^2\chi + \kappa|\psi|^2\chi
\end{aligned}
$$

- Find non-equilibrium steady-state for attractive interactions κ < 0

- Compare loss depending on interaction κ with experimental results

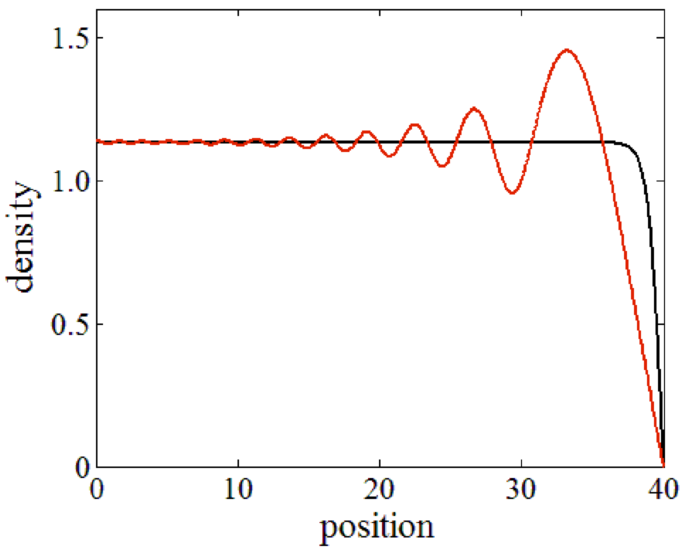
W. Bao and D. Jaksch, SIAM J. Numer. Anal. **41**, 1406 (2003)

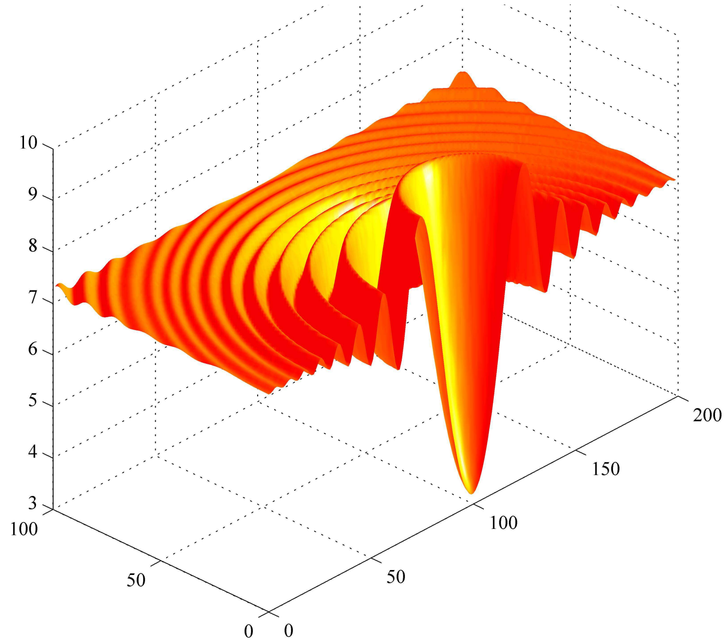


Three-body recombination

- 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 $K_3 > 0$

Main insights

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.

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Variational ansatz yields conceptual understanding of exact numerical results.

Impurities are the new vortices!

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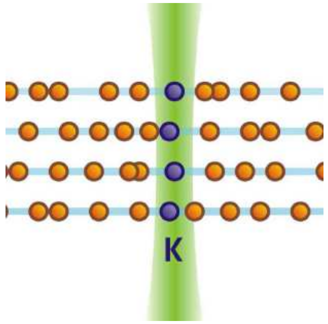

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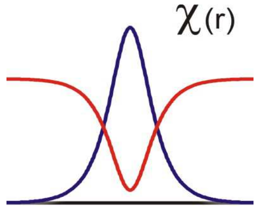

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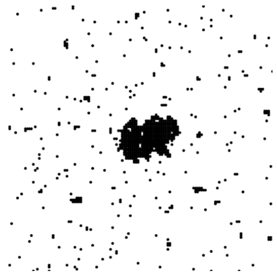

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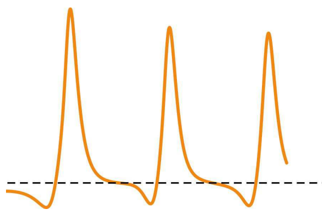

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Classical Theory of Boson Wave Fields

E. P. Gross

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

$$i\hbar\dot{\Phi}(\mathbf{q}, t) = -\frac{\hbar^2}{2m}\nabla^2\Phi + \Phi\int U(|\mathbf{q}-\mathbf{x}|)\psi^+(\mathbf{x}, t)\psi(\mathbf{x}, t)\, d^3x,$$

$$i\hbar\dot{\psi} = -\frac{\hbar^2}{2M}\nabla^2\psi + \psi\int V(\mathbf{x}-y)\psi^+(\mathbf{y})\psi(\mathbf{y})\, d^3y \qquad (53)$$

$$+\psi\int V(\mathbf{x}-\mathbf{q})\Phi^*(\mathbf{q}, t)\Phi(\mathbf{q}, t)\, d^3q$$

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