Analytical and Numerical Study of Localized Impurity in Bose-Einstein Condensate

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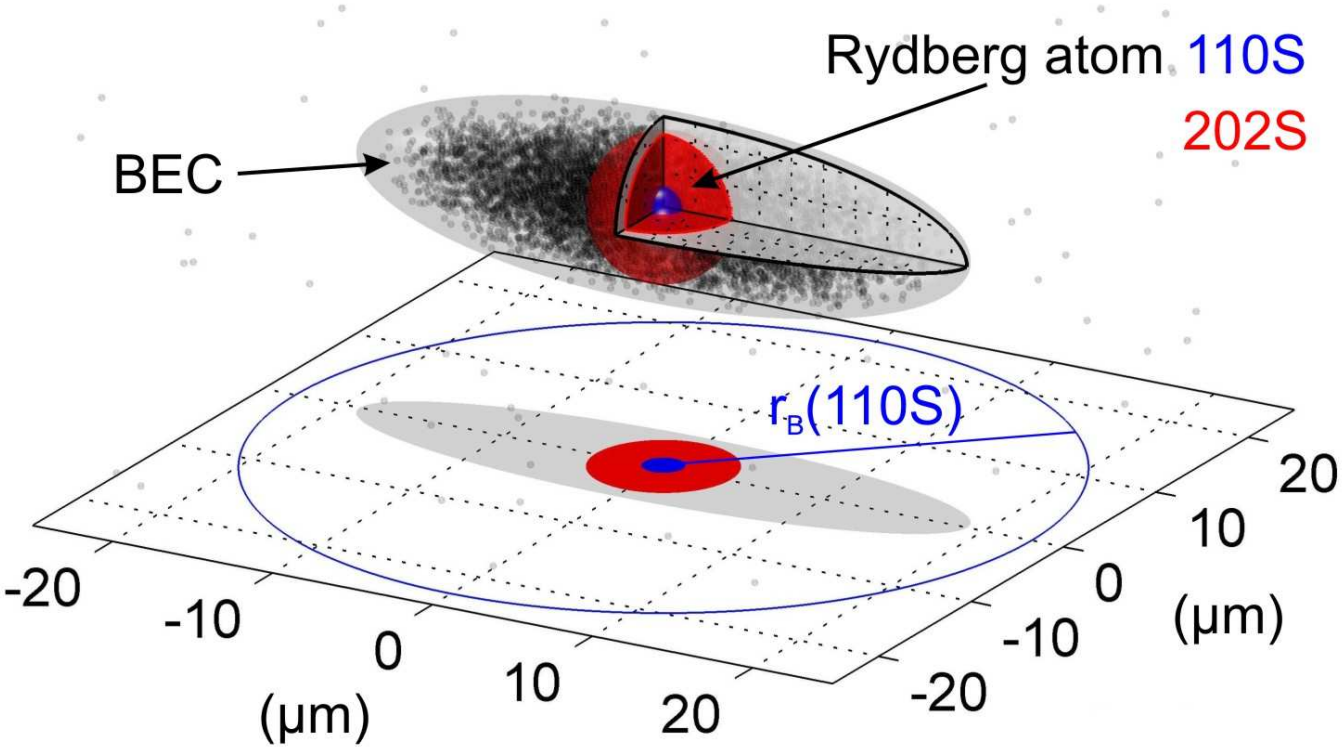
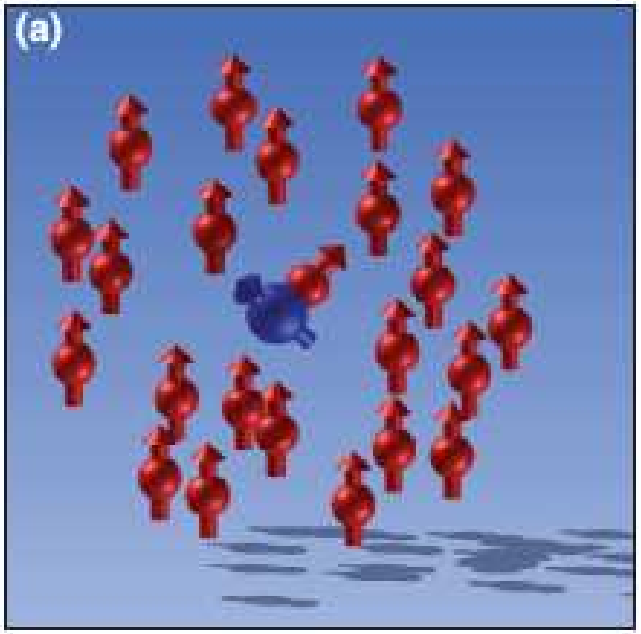
New year seminar, 2015

- First Experiment: Coupling a single-electron/Rydberg atom to a Bose-Einstein condensate,



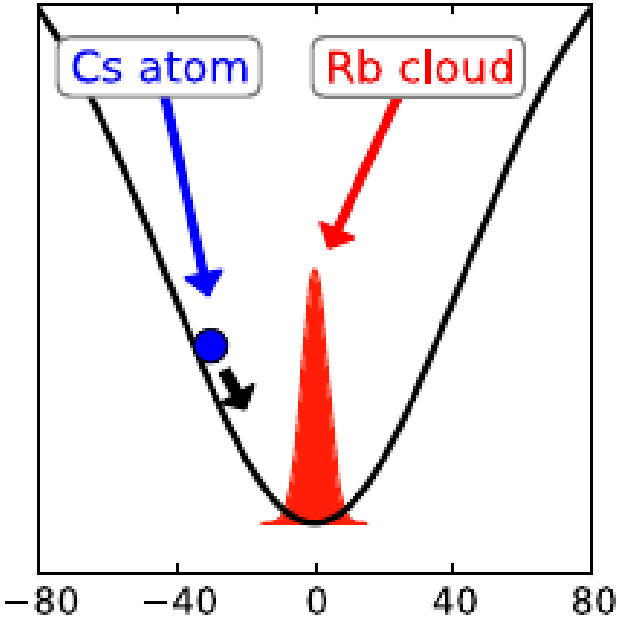
J.B. Balewski, et al., Nature **502**, 664 (2013).

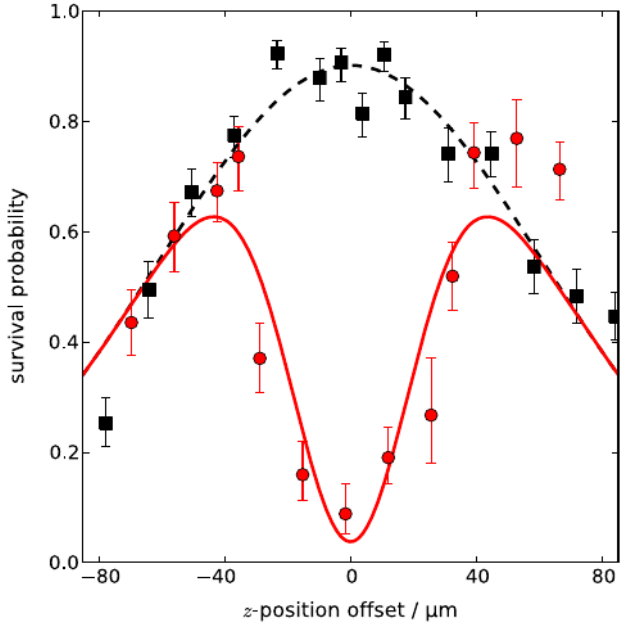
- Second Experiment: Coupling a single-ion (Ytterbium-Yb^+) to a Bose-Einstein condensate,



L. Ratschbacher, et al., Phys. Rev. Lett. **110**, 160402 (2013).

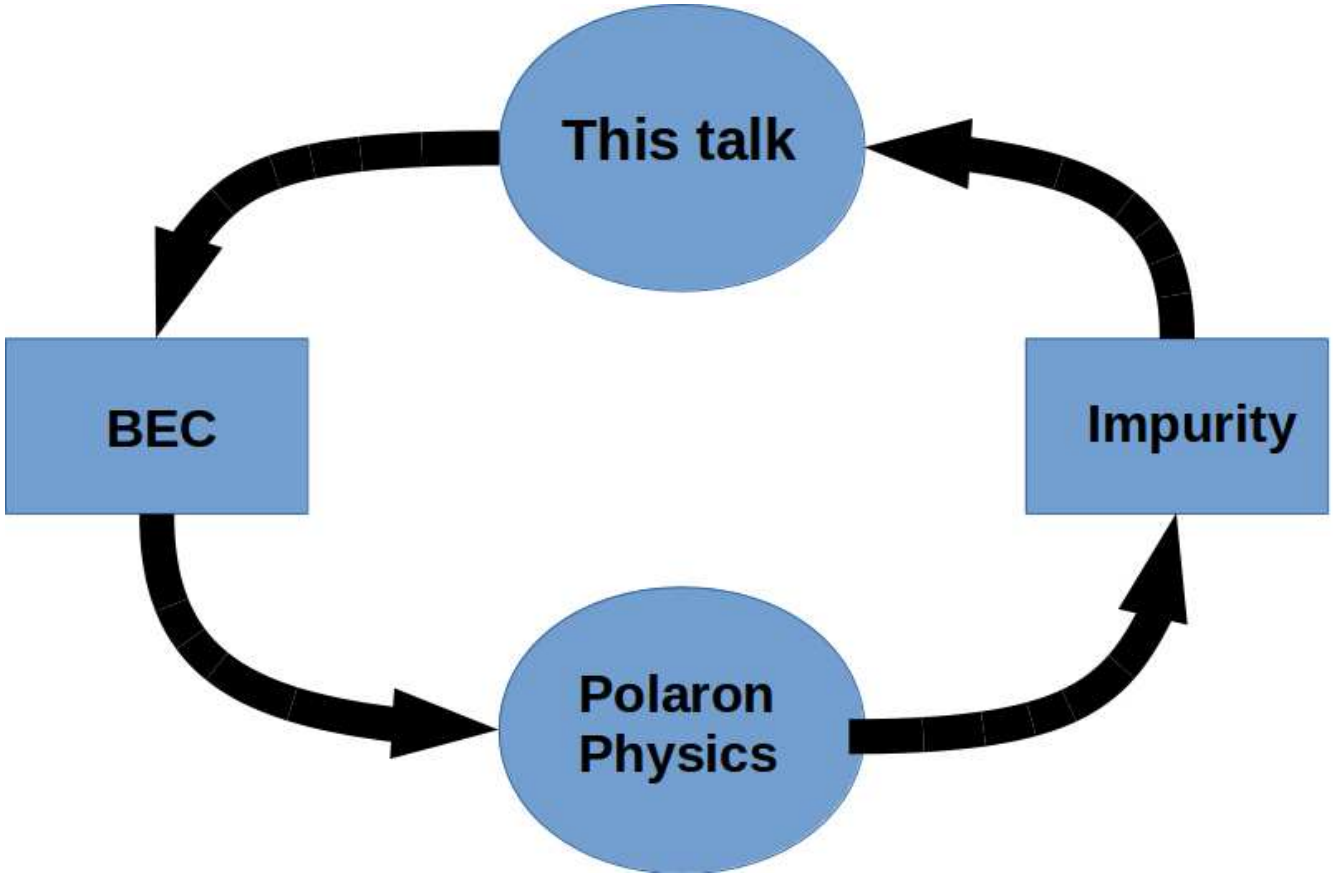
- Third experiment: Coupling a single-Cs atom to a Bose-Einstein condensate,





N. Spethmann, et al., Phys. Rev. Lett. **109**, 235301 (2012).

- This talk-outlook



3D Lagrangian

$$\mathcal{L}_{3D} = \frac{i\hbar}{2}\left(\psi^{\star}(\mathbf{r},t)\frac{\partial\psi(\mathbf{r},t)}{\partial t} - \psi(\mathbf{r},t)\frac{\partial\psi^{\star}(\mathbf{r},t)}{\partial t}\right) + \frac{\hbar^2}{2m_{\mathrm{B}}}\psi^{\star}(\mathbf{r},t)\triangle\psi(\mathbf{r},t) - V(\mathbf{r})\psi^{\star}(\mathbf{r},t)\psi(\mathbf{r},t) - \frac{G_{\mathrm{B}}^{3\mathrm{D}}}{2}\|\psi(\mathbf{r},t)\|^4 - G_{\mathrm{IB}}^{3\mathrm{D}}\|\psi_{\mathrm{I}}(\mathbf{r},t)\|^2\|\psi(\mathbf{r},t)\|^2$$

- $G_{\mathrm{B}}^{3\mathrm{D}} = \frac{N4\pi\hbar^2 a_{\mathrm{B}}}{m_{\mathrm{B}}}$
- $G_{\mathrm{IB}}^{3\mathrm{D}} = \frac{2\pi\hbar^2 a_{\mathrm{IB}}}{m_{\mathrm{IB}}}$ and $m_{\mathrm{IB}} = \frac{m_{\mathrm{I}}m_{\mathrm{B}}}{m_{\mathrm{I}}+m_{\mathrm{B}}}$

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Derivation of Lagrangian from 3D to 1D

- $\omega_z \ll \omega_r$ and $V(\mathbf{r}) = \frac{m_B \omega_z^2 z^2}{2} + \frac{m_B \omega_r^2 \left(x^2+y^2\right)}{2}$
- $\psi(\mathbf{r}, t) = \psi(z, t)\phi(r_\perp, t)$

Wave-functions

$$\phi(r_\perp, t) = \frac{e^{-\frac{x^2+y^2}{2l_r^2}}}{\sqrt{\pi} l_r} e^{-i\omega_r t}$$

$$\phi_l(r_\perp, t) = \frac{e^{-\frac{x^2+y^2}{2l_{rl}^2}}}{\sqrt{\pi} l_{rl}} e^{-i\omega_{rl} t}$$

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1D Lagrangian

$$\mathcal{L}_{1D} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathcal{L}_{3D} dxdy.$$

$$\begin{aligned}\mathcal{L}_{1D} =& \frac{i\hbar}{2}\left(\psi^{\star}(z,t)\frac{\partial\psi(z,t)}{\partial t} - \psi(z,t)\frac{\partial\psi^{\star}(z,t)}{\partial t}\right)\\ &+ \frac{\hbar^2}{2m_{\mathrm{B}}}\psi^{\star}(z,t)\frac{\partial^2\psi(z,t)}{\partial z^2} - V(z)\psi^{\star}(z,t)\psi(z,t)\\ &- \frac{G_{\mathrm{B}}}{2}\parallel\psi(z,t)\parallel^4 - G_{\mathrm{IB}}\parallel\psi_{\mathrm{I}}(z,t)\parallel^2\parallel\psi(z,t)\parallel^2\end{aligned}$$

- $G_{\mathrm{B}} = 2N_{\mathrm{B}}a_{\mathrm{B}}\hbar\omega_{\mathrm{r}}$
- $G_{\mathrm{IB}} = \frac{2\hbar^2 a_{\mathrm{IB}}}{m_{\mathrm{IB}}\left(l_{\mathrm{r}}^2+l_{\mathrm{rI}}^2\right)}$, how we can increase or decrease G_{IB} (next slide)

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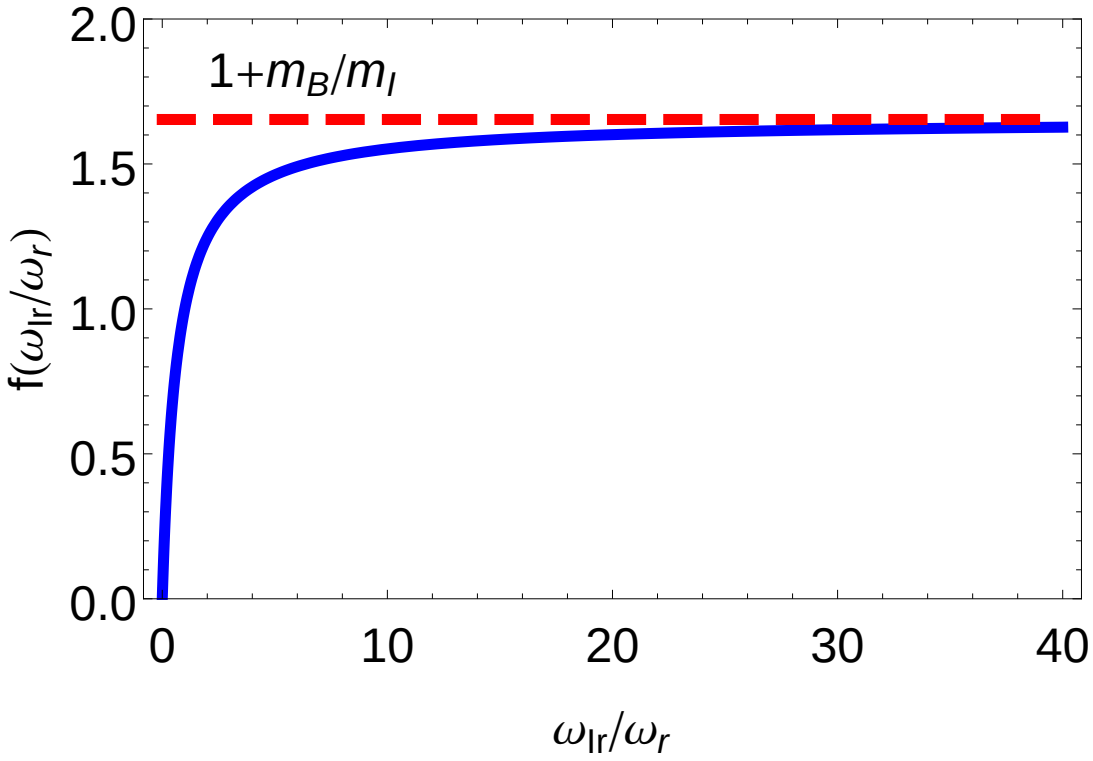
Derivation of Lagrangian from 3D to 1D

- $G_{\mathrm{IB}} = 2a_{\mathrm{IB}}\hbar\omega_{\mathrm{r}} f\left(\omega_{\mathrm{Ir}}/\omega_{\mathrm{r}}\right)$
- Geometric function $f\left(\omega_{\mathrm{Ir}}/\omega_{\mathrm{r}}\right) = \frac{1+\frac{m_{\mathrm{B}}}{m_{\mathrm{I}}}}{1+\frac{m_{\mathrm{B}}\omega_{\mathrm{r}}}{m_{\mathrm{I}}\omega_{\mathrm{Ir}}}}$



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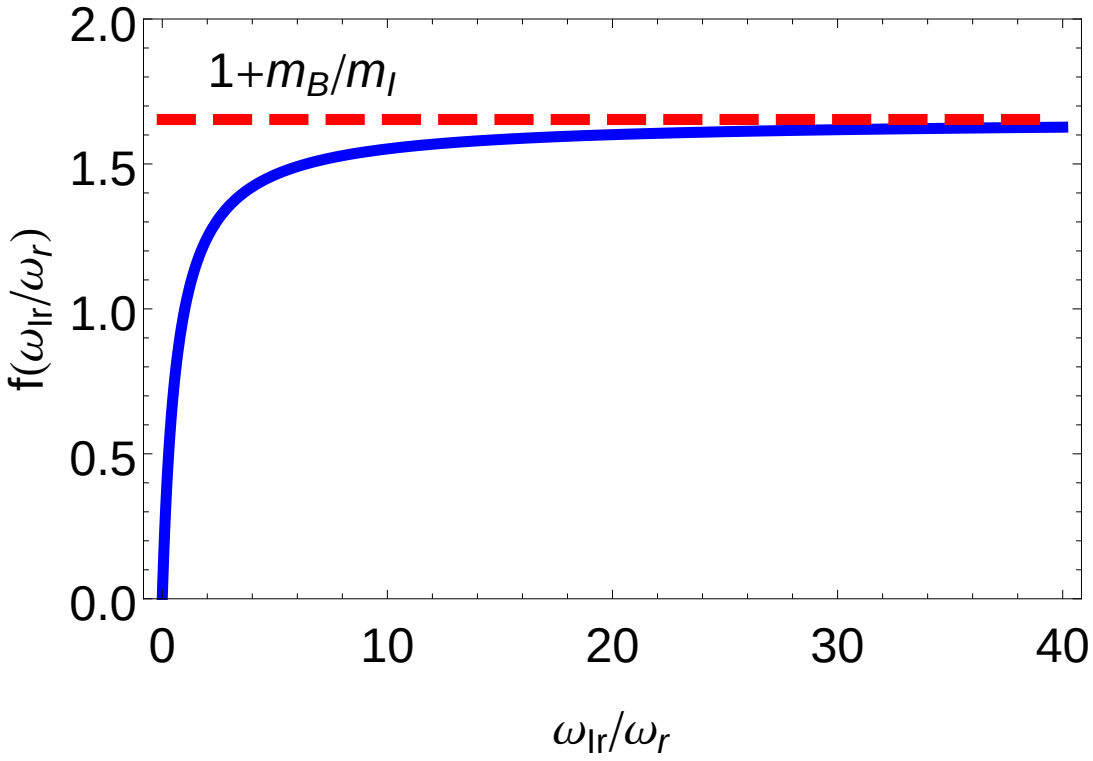

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Euler-Lagrangian equation

$$\frac{\delta \mathcal{A}\left[\psi^{\star}, \psi\right]}{\delta \psi^{\star}(z, t)} = \frac{\partial \mathcal{L}_{1D}}{\partial \psi^{\star}(z, t)} - \frac{\partial}{\partial z} \frac{\partial \mathcal{L}_{1D}}{\partial \frac{\partial \psi^{\star}(z,t)}{\partial z}} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}_{1D}}{\partial \frac{\partial \psi^{\star}(z,t)}{\partial t}} = 0$$

1D Gross-Pitaevskii equation (1DGPE)

$$i\hbar \frac{\partial}{\partial t} \psi(z, t) =$$
$$\left\{ -\frac{\hbar^2}{2m_B} \frac{\partial^2}{\partial z^2} + \frac{m_{\mathrm{B}} \omega_z^2 z^2}{2} + G_{\mathrm{IB}} \parallel \psi_{\mathrm{I}}(z, t) \parallel^2 + G_{\mathrm{B}} |\psi(z, t)|^2 \right\} \psi(z, t)$$

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1D Dimensionless Gross-Pitaevskii equation

$$i\frac{\partial}{\partial\tau}\tilde{\psi}\left(\tilde{z}\right) = \left\{-\frac{1}{2}\frac{\partial^2}{\partial\tilde{z}^2} + \frac{\tilde{z}^2}{2} + \tilde{G}_{\mathrm{IB}}|\tilde{\psi}_{\mathrm{I}}\left(\tilde{z}\right)|^2 + \tilde{G}_{\mathrm{B}}|\tilde{\psi}\left(\tilde{z}\right)|^2\right\}\tilde{\psi}\left(\tilde{z}\right)$$

Dimensionless parameters

- $\tau = \omega_z t$, $\tilde{z} = z/l_z$ and $\tilde{\psi} = \psi/\sqrt{l_z}$
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- where $l_z = \sqrt{\hbar/m_{\mathrm{B}}\omega_z}$ is the oscillator length
- From here on, we will drop the tildes for simplicity.

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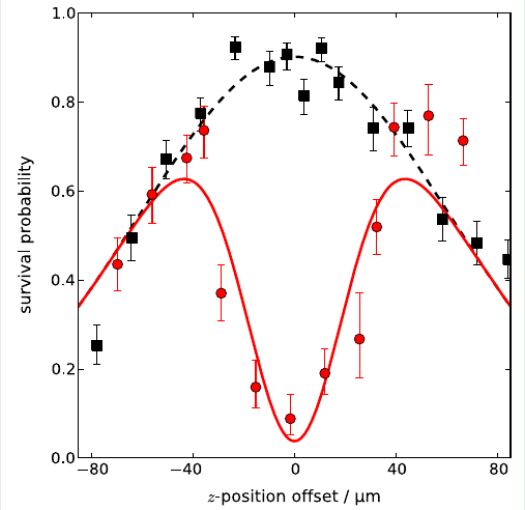
Impurity wave function in experimental realization



N. Spethmann, et al., Phys. Rev. Lett. **109**, 235301 (2012).

Impurity wave function in dimensionless form

$$\psi_I(z) = \frac{1}{\sqrt{\sqrt{\pi}\alpha}} e^{-\frac{z^2}{2\alpha^2}}$$

Here $\alpha = l_{zI}/l_z$

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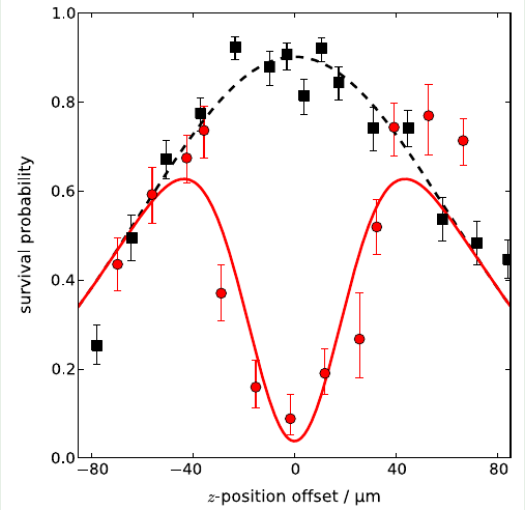

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Thomas-Fermi variational ansatz

- $\psi(z) = \sqrt{\frac{\mu}{G_B}\left(1 - \frac{z^2}{2\mu} - \frac{Ge^{-\frac{z^2}{\alpha^2}}}{\mu\sqrt{\pi}\alpha}\right)\Theta\left(1 - \frac{z^2}{2\mu} - \frac{Ge^{-\frac{z^2}{\alpha^2}}}{\mu\sqrt{\pi}\alpha}\right)}$
- Here μ and G are variational parameters

Extremizing energy with respect to μ and G yields:

- $\left.\begin{array}{l}\mu = \frac{1}{2}\left(\frac{3}{2}\right)^{2/3}(G_B + G)^{2/3} \\ G = G_{IB}\end{array}\right\} \Longrightarrow$ Thomas-Fermi solution

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Numerical Method

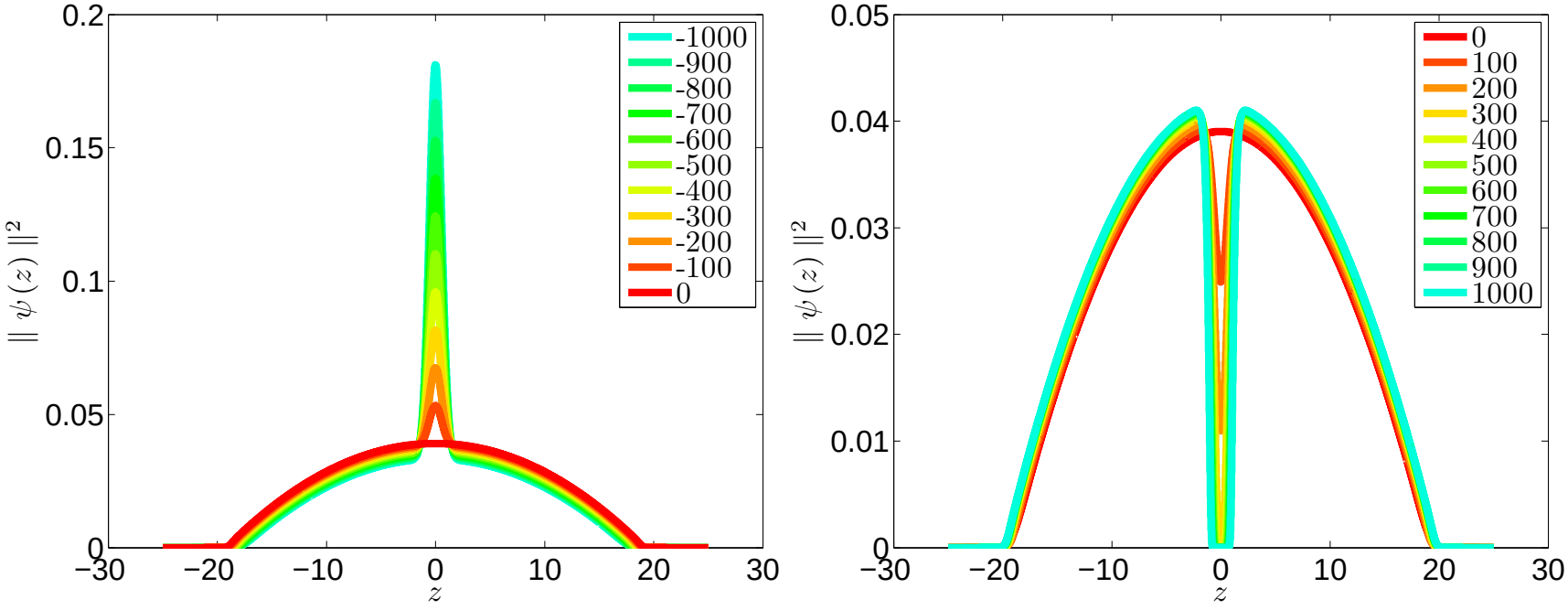
- Our numerical calculation based on the split operator method
- $H = T + V$, here $T = K.E$ and $V = P.E + I.E$
- $\psi(z, \tau + \Delta\tau) = e^{-\frac{T\Delta\tau}{2}} e^{-V\Delta\tau} e^{-\frac{T\Delta\tau}{2}} \psi(z, \tau) + \mathcal{O}\left(\Delta\tau^3\right)$
- $\psi(z, \tau) = e^{-\tau H} \psi(z, 0) = \sum_j e^{-\tau E_j} c_j \phi_j$

J. Javanainen, et al., J. Phys. A: Math. Gen. **39**, L179 (2006).
R. Barnett, et al., New Journal of Physics **12**, 043004 (2010).
D. Vudragovic, et al., Comput. Phys. Commun. **183**, 2021 (2012).

Imaginary time evolution

Movie

Density profile of BEC



Here we plotted numerically the density profile of the system for different values of the G_{IB}.

Impurity height/depth (IHD)

- $$\mathrm{IHD} = \begin{cases} |\Psi(0)|^2_{G_{\mathrm{IB}}} - |\Psi(0)|^2_{G_{\mathrm{IB}}=0} & G_{\mathrm{IB}} \leq 0 \\ \mathrm{Max}\left(|\Psi(z)|^2_{G_{\mathrm{IB}}}\right) - |\Psi(0)|^2_{G_{\mathrm{IB}}} & G_{\mathrm{IB}} > 0 \end{cases}$$

Impurity full width half maximum width (IW) defined as

- $$|\Psi(\mathrm{IW})|^2_{G_{\mathrm{IB}}} = \begin{cases} \left(|\Psi(0)|^2_{G_{\mathrm{IB}}} + |\Psi(0)|^2_{G_{\mathrm{IB}}=0}\right)/2 & G_{\mathrm{IB}} \leq 0 \\ \left(\mathrm{Max}\left(|\Psi(z)|^2_{G_{\mathrm{IB}}}\right) + |\Psi(0)|^2_{G_{\mathrm{IB}}}\right)/2 & G_{\mathrm{IB}} > 0 \end{cases}$$

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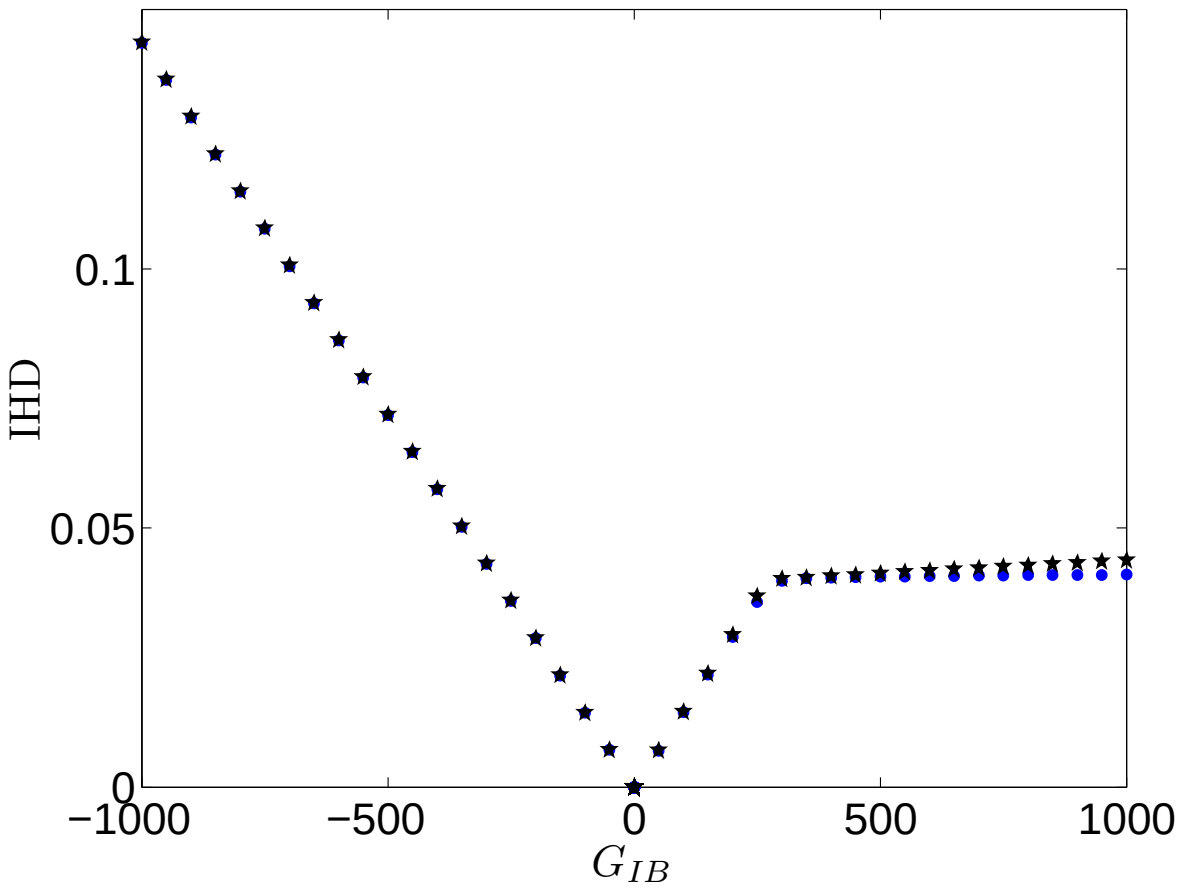
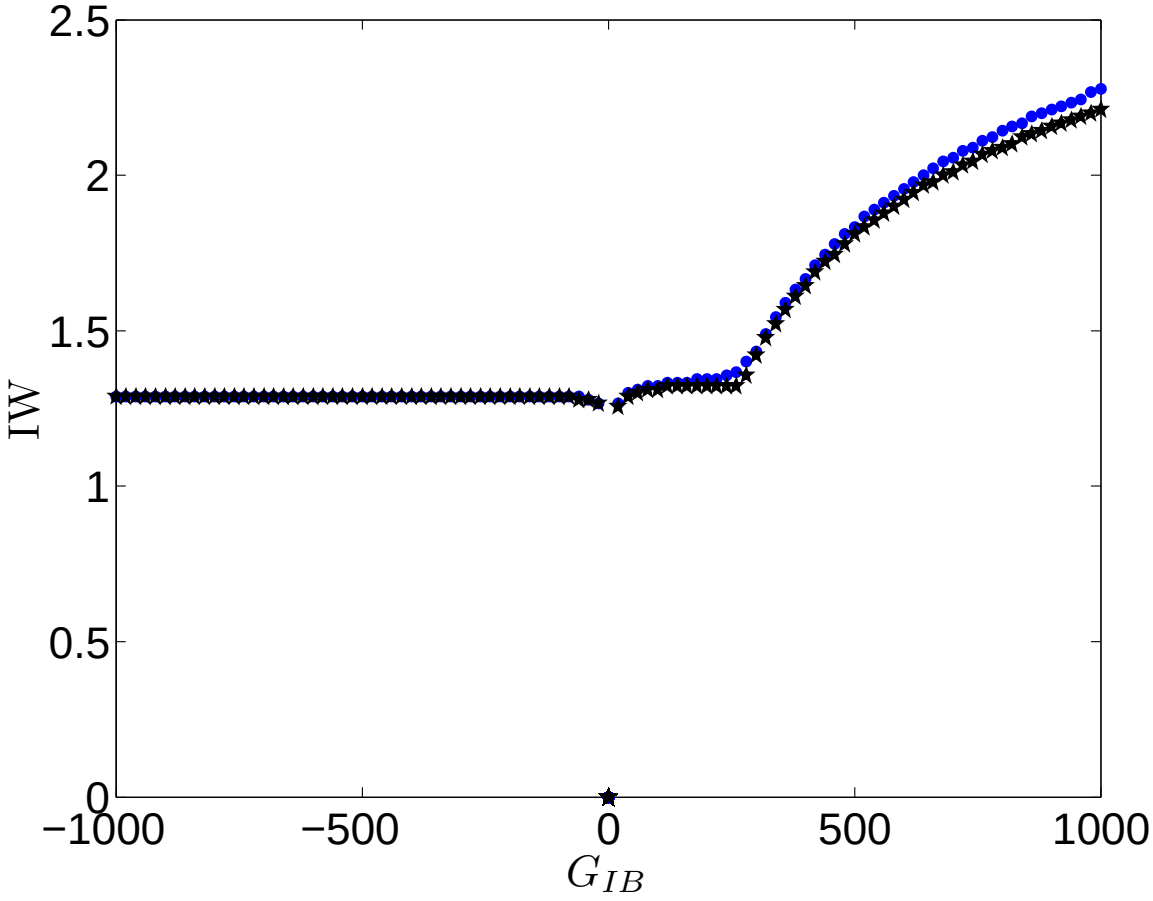


Height/depth of impurity bump/dip versus impurity-BEC coupling constant G_{IB} for the BEC coupling constant $G_{\mathrm{B}} = 4718.15$.

Impurity full width half maximum width (IW)



Width of impurity bump/dip versus impurity-BEC coupling constant G_{IB} for the BEC coupling constant $G_{\mathrm{B}} = 4718.15$.

Critical impurity-BEC coupling constant

For a specific value of G_{IB} when no more ^{87}Rb atoms left at the center of the trap, the Impurity dip reaches its maximum value, we called this value critical impurity-BEC coupling constant G_{IBc}.

$$G_{\mathrm{IBc}} = \sqrt{\pi}\alpha/2\,(3/2)^{2/3}\,(G_{\mathrm{B}} + G_{\mathrm{IBc}})^{2/3}$$

$$G_{\mathrm{IBc}} \overset{\text{Variational}}{=} 275 \overset{\text{Numerical}}{\simeq} 286$$

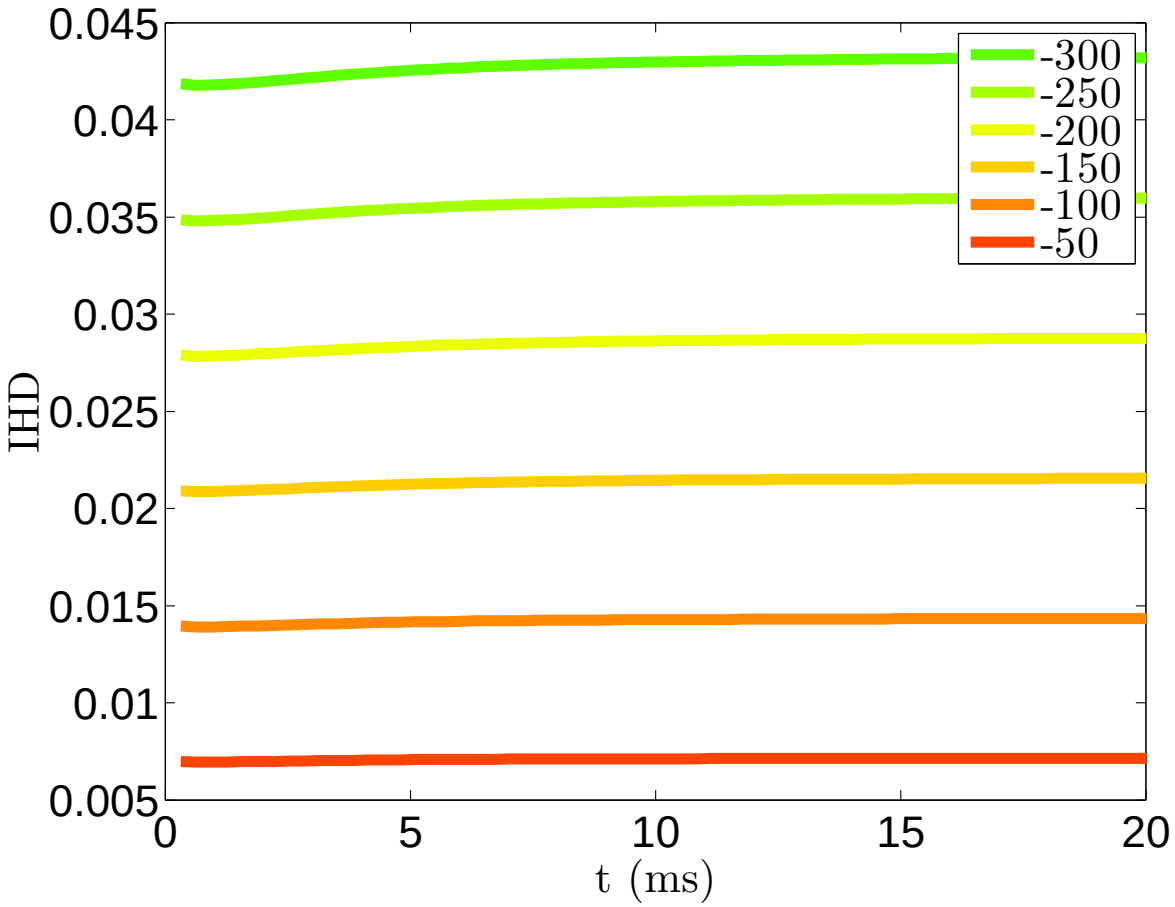
$$\mathrm{IHD_c} = G_{\mathrm{IBc}}/\sqrt{\pi}\alpha G_{\mathrm{B}} \overset{\text{Variational}}{=} 0.0401 \overset{\text{Numerical}}{\simeq} 0.0393$$

$$\mathrm{IW_c} \overset{\text{Variational}}{=} 1.3444 \overset{\text{Numerical}}{\simeq} 1.400$$

Real time evolution

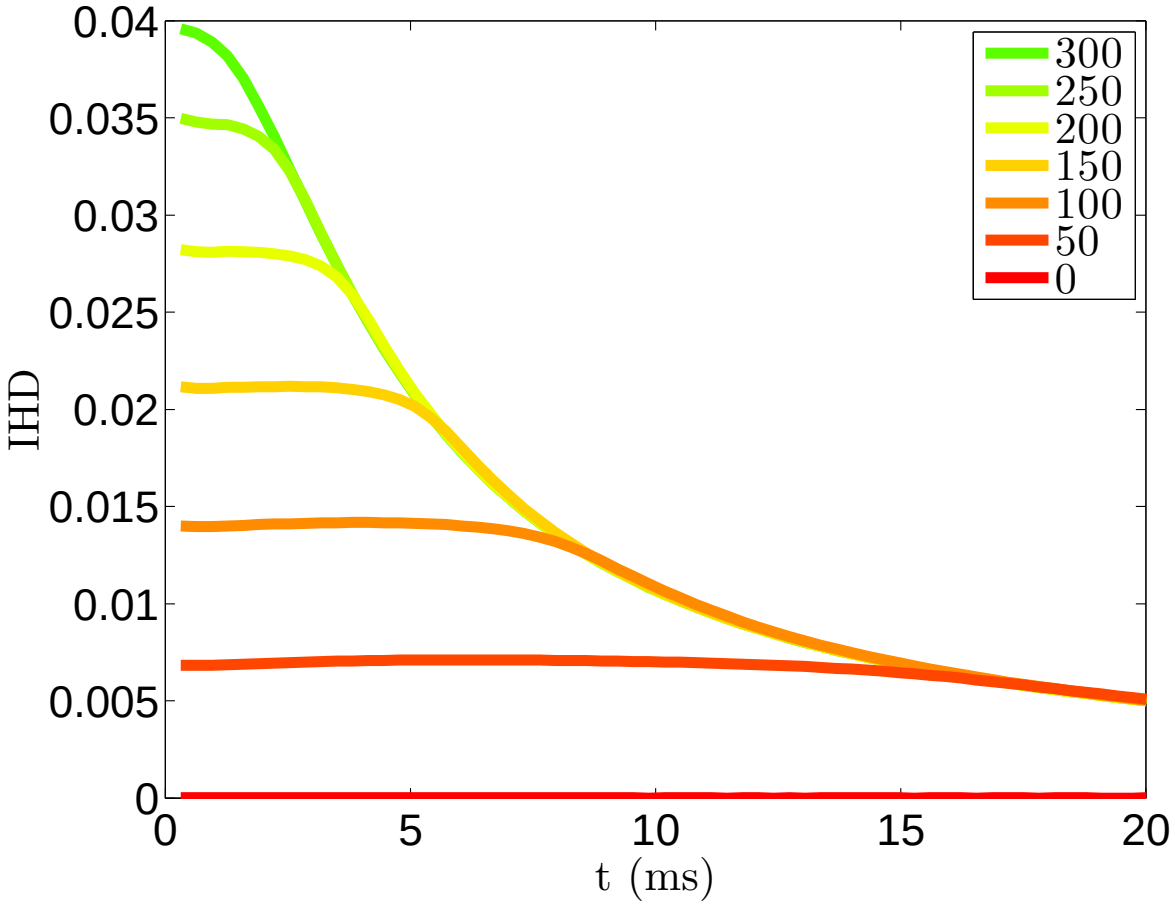
Movie

Impurity height/depth (IHD)



We plotted the IHD vs time for different values of impurity-BEC coupling constant G_{IB}.

Impurity height/depth (IHD)



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We will work out more realistic models by exploring in more detail the properties of a 2D and 3D system.

Study the Impurity and vortex interaction

Emergence of Phonons by moving Impurity

Move vortex with using Impurity

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Impurity and the three-body recombination

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Bloch Group, Phys. Rev. Lett. **102**, 030408 (2009).
Widera Group, Phys. Rev. Lett. **109**, 235301 (2012).

Impurity and far field vortex-vortex interaction

R. Navarro, et al., Phys. Rev. Lett. **110**, 225301 (2013).

Solve two coupled GPEs for 100 ^{137}Cs atoms as an Impurity and 10^6 ^{87}Rb atoms as a BEC

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Solve two coupled GPEs for 100 ^{137}Cs atoms as an Impurity and 10^6 ^{87}Rb atoms as a BEC

Impurity and the three-body recombination

$$i\hbar\frac{\partial}{\partial t}\psi(z,t) = \left\{-\frac{\hbar^2}{2m_B}\frac{\partial^2}{\partial z^2} + \frac{m_B\omega_z^2 z^2}{2}\right.$$
$$\left. + G_{IB} \parallel \psi_I(z,t) \parallel^2 + G_B|\psi(z,t)|^2 - i\hbar\frac{K_3}{2}|\psi(z,t)|^4\right\}\psi(z,t)$$

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Impurity and far field vortex-vortex interaction

R. Navarro, et al., Phys. Rev. Lett. **110**, 225301 (2013).

Solve two coupled GPEs for 100 ^{137}Cs atoms as an Impurity and 10^6 ^{87}Rb atoms as a BEC

Thanks