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

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Motivation

Motivated by the recent experimental work of Refs. [1,2], we investigate a localized ^{133}Cs impurity in the center of a trapped ^{87}Rb Bose-Einstein condensate. Within a zero-temperature Gross-Pitaevskii mean-field description we provide a one-dimensional physically intuitive model, which we solve by both a time-independent variational approach and numerical calculations. With this we predict at first equilibrium results for the emerging condensate wave function which reveals an impurity-induced dip or bump in case of a repulsive or an attractive Rb-Cs interaction strength. Afterwards, we show that the impurity-induced dip or bump in the condensate wave function remains even present during a time-of-flight (TOF) expansion after having switched off the harmonic confinement. All these results are useful for extracting the Rb-Cs interaction strength from experimental TOF expansion data.

Impurity in one-dimensional BEC

- Lagrangian density for three-dimensional case

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

- Here $\psi_\mathrm{I}(\mathbf{r},t)$ represents the impurity and $\psi(\mathbf{r},t)$ describes the BEC wave-function. We set $\omega_\mathrm{z} \ll \omega_\mathrm{r}$ for quasi one-dimensional setting, so the one-dimensional Lagrangian is defined via $\mathcal{L}_{1D} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathcal{L}_{3D}dxdy$
- We decompose the wave-function as $\psi(\mathbf{r},t) = \psi(z,t)\phi(r_\perp,t)$ with $r_\perp = (x,\ y)$
- We define $\phi(r_\perp,t) = e^{-\frac{x^2}{2l_\mathrm{r}^2}-\frac{y^2}{2l_\mathrm{r}^2}-i\omega_\mathrm{r}t}/\sqrt{\pi}l_\mathrm{r}$, and $\phi_\mathrm{I}(r_\perp,t) = e^{-\frac{x^2}{2l_\mathrm{Ir}^2}-\frac{y^2}{2l_\mathrm{Ir}^2}-i\omega_\mathrm{Ir}t}/\sqrt{\pi}l_\mathrm{Ir}$ here $l_\mathrm{r} = \sqrt{\frac{\hbar}{m_\mathrm{B}\omega_\mathrm{r}}}$ and $l_\mathrm{Ir} = \sqrt{\frac{\hbar}{m_\mathrm{I}\omega_\mathrm{Ir}}}$ so

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

  - ⁕ ^{87}Rb coupling constant $G_\mathrm{B} = 2N_\mathrm{B}a_\mathrm{B}\hbar\omega_\mathrm{r}$, here $N_\mathrm{B} = 20\times10^4$ and s-wave scattering length is $a_\mathrm{B} = 87\ a_0$.
  - ⁕ Effective ^{87}Rb and ^{133}Cs coupling constant $G_\mathrm{IB} = 2a_\mathrm{IB}\hbar\omega_\mathrm{r}f(\omega_\mathrm{r}/\omega_\mathrm{Ir})$, here s-wave scattering length for impurity-BEC coupling $a_\mathrm{IB} = 650\ a_0$ and geometric function $f(\omega_\mathrm{r}/\omega_\mathrm{Ir}) = \frac{1+m_\mathrm{B}/m_\mathrm{I}}{1+(m_\mathrm{B}/m_\mathrm{I})(\omega_\mathrm{r}/\omega_\mathrm{Ir})}$

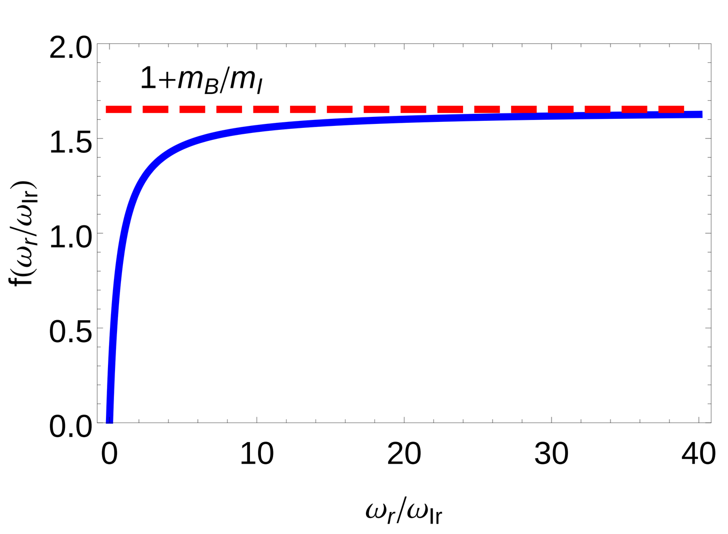

Fig. 1: Geometric function $f(\omega_\mathrm{r}/\omega_\mathrm{Ir})$ reaches its maximum value at $1+m_\mathrm{B}/m_\mathrm{I}$ for the frequency ratio $\omega_\mathrm{r}/\omega_\mathrm{Ir} \geq 20$. In calculations we are using $\omega_\mathrm{r}/\omega_\mathrm{Ir} = 1$, from where the geometric function becomes equal to one.

- For one-dimensional dimensionless GPE, we have with $\tau = \omega_z t$, $\tilde{z} = z/l_z$, $l_z = \sqrt{\hbar/m_\mathrm{B}\omega_z}$, and $\tilde{\psi} = \psi/\sqrt{l_z}$

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

- Resulting dimensionless interaction strengths $\tilde{G}_\mathrm{B} = 2N_\mathrm{B}\omega_\mathrm{r}a_\mathrm{B}/\omega_z l_z$ and $\tilde{G}_\mathrm{IB} = 2a_\mathrm{IB}\omega_\mathrm{r}f(\omega_\mathrm{r}/\omega_\mathrm{Ir})/\omega_z l_z$
- Resulting dimensionless experimental parameters in 1D model
  - ⁕ ^{87}Rb and ^{133}Cs longitudinal trap frequencies are $\omega_z = \omega_{\mathrm{I}z} = 2\pi\times0.050$ kHz and radial trap frequencies are $\omega_r = \omega_{\mathrm{I}r} = 2\pi\times0.179$ kHz
  - ⁕ BEC dimensionless coupling constant is $\tilde{G}_\mathrm{B} = 4718.15$
  - ⁕ Impurity-BEC dimensionless coupling constant is $\tilde{G}_\mathrm{IB} = 0.16$ and the value of $\alpha = l_{\mathrm{I}z}/l_z = 0.808$
- From now on, we will drop the tildes for simplicity.

Variational approach

- Here we use the variational ansatz

$$\psi(z) = \sqrt{\frac{\mu}{G_\mathrm{B}}\left(1-\frac{z^2}{2\mu}-\frac{Ge^{-\frac{z^2}{\alpha^2}}}{\mu\sqrt{\pi}\alpha}\right)}\,\Theta\left(1-\frac{z^2}{2\mu}-\frac{Ge^{-\frac{z^2}{\alpha^2}}}{\mu\sqrt{\pi}\alpha}\right)$$

- Extremizing energy with respect to μ and G yields:

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

- Impurity height/depth (IHD) and full width half maximum width (IW) defined as

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

Numerical density profiles

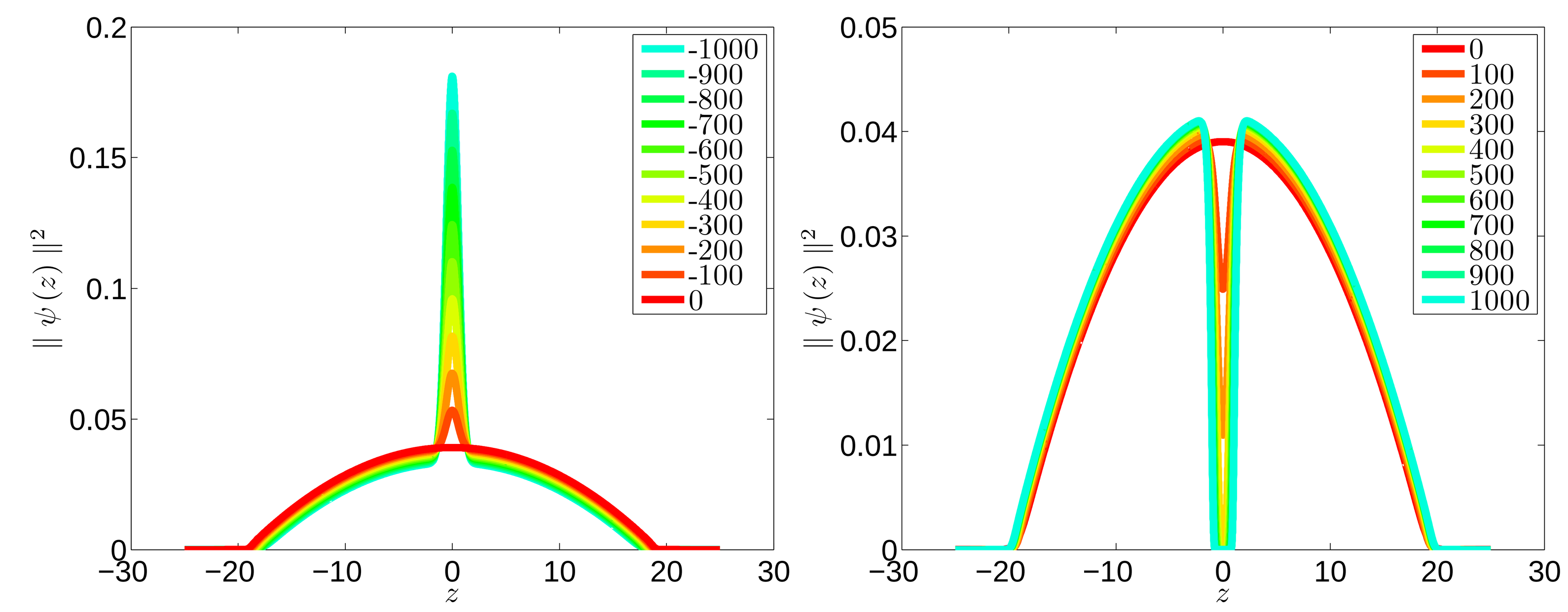

Fig. 2: Density profile of the system for different values of G_IB as mentioned in the figures, for the BEC coupling constant $G_\mathrm{B} = 4718.15$.

Impurity height/depth and width of impurity bump/dip

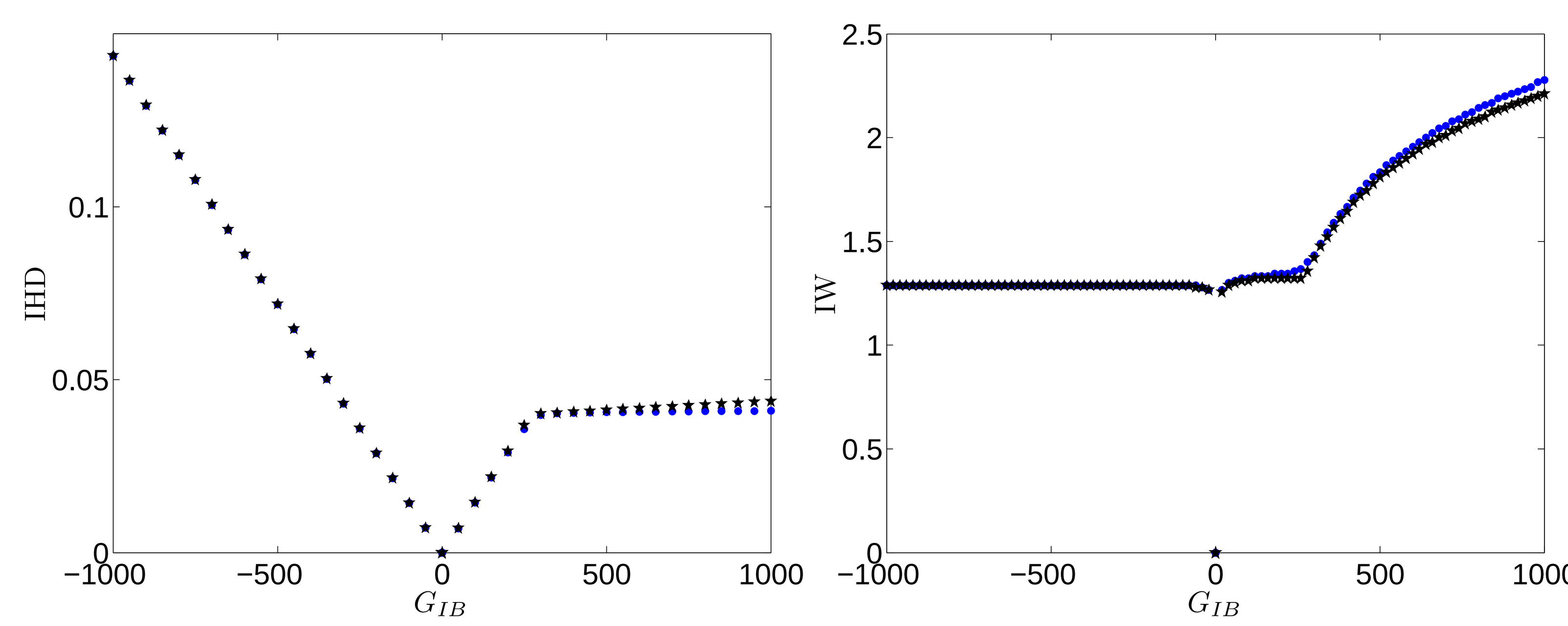

Fig. 3: (a) Height/depth and (b) width of impurity bump/dip versus impurity-BEC coupling constant G_IB for the BEC coupling constant $G_\mathrm{B} = 4718.15$ calculated from variationally (black stars) and numerically (blue circles) by solving GPE.

- Critical values:

$$\left\{\begin{array}{l}G_\mathrm{IBc} = \sqrt{\pi}\alpha/2\,(3/2)^{2/3}(G_\mathrm{B}+G_\mathrm{IBc})^{2/3}\Longrightarrow G_\mathrm{IBc} = 275\\ \mathrm{IHD_c} = G_\mathrm{IBc}/\sqrt{\pi}\alpha G_\mathrm{B} \overset{\text{Variational}}{=} 0.0401 \overset{\text{Numerical}}{\backsimeq} 0.0384\\ \mathrm{IW_c} \overset{\text{Variational}}{=} 1.3444 \overset{\text{Numerical}}{\backsimeq} 1.3889\end{array}\right.$$

Time of flight (TOF)

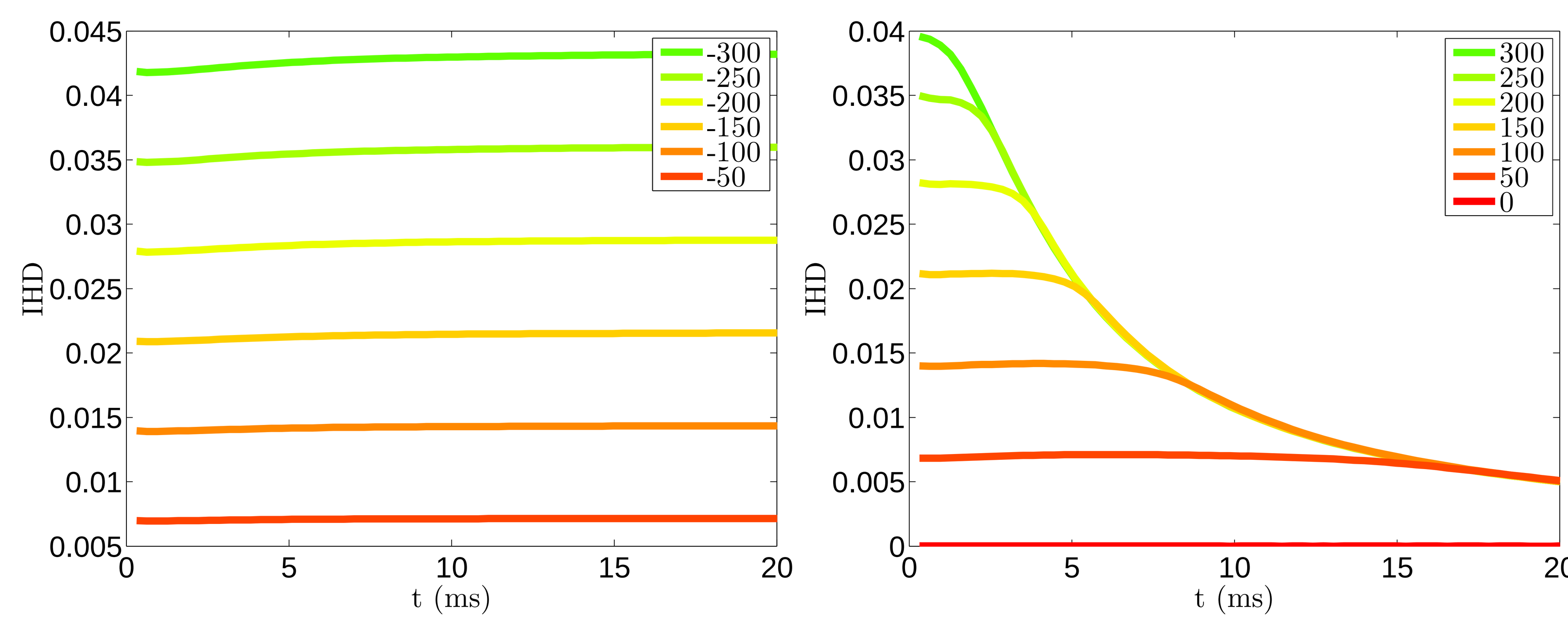

Fig. 4: IHD versus time during time-of-flight expansion for the BEC coupling constant $G_\mathrm{B} = 4718.15$.

- In free expansion for the negative values of G_IB IHD stays constant.
- And for positive G_IB it starts decreasing.

Acknowledgment

We would like to acknowledge Ednilson Santos and Artur Widera for their insightful comments. This work was supported in part by the German-Brazilian DAAD program under the project name: "Dynamics of Bose-Einstein Condensates Induced by Modulation of System Parameters".

DAAD Deutscher Akademischer Austausch Dienst German Academic Exchange Service

References

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