

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

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**Abstract** – We study the interaction-induced localization —the so-called self-trapping— of a neutral impurity atom immersed in a homogeneous Bose-Einstein condensate (BEC). Based on a Hartree description of the BEC we show that —unlike repulsive impurities— attractive impurities have a singular ground state in 3d and shrink to a point-like state in 2d as the coupling approaches a critical value  $\beta^*$ . Moreover, we find that the density of the BEC increases markedly in the vicinity of attractive impurities in 1d and 2d, which strongly enhances inelastic collisions between atoms in the BEC. These collisions result in a loss of BEC atoms and possibly of the localized impurity itself.

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Impurities immersed in liquid helium have proven to be a valuable tool for probing the structure and dynamics of a Bose-condensed fluid [1]. An example is the use of impurities for the direct visualization of quantized vortices in superfluid  $^4\text{He}$  [2]. Recently, the experimental realization of impurities in a BEC [3,4] and the possibility to produce quantum degenerate atomic mixtures [5,6] have generated renewed interest in the physics of impurities. In particular, it was pointed out that single atoms can get trapped in the localized distortion of the BEC that is induced by the impurity-BEC interaction [7–11]. More precisely, the impurity becomes self-trapped if its interaction with the BEC is sufficiently strong to compensate for the high kinetic energy of a localized state, an effect akin to the self-trapping of impurities in liquid helium [1].

However, there are two fundamental differences between liquid helium and a BEC. First, for typical experimental parameters the healing length of a BEC is three orders of magnitude larger than for liquid helium [12], and thus the so-called “bubble” model [13] cannot be applied. A second important difference is that the impurity-BEC interactions are tunable by an external magnetic field in the vicinity of Feshbach resonances [14,15]. In view of recent experimental progress [16] it thus seems possible to

investigate the self-trapping problem in the same physical system over a wide range of interaction strengths —for both attractive and repulsive impurities.

In the present paper we study the self-trapping properties of impurities for strong attractive and repulsive impurity-BEC coupling within the framework of a Hartree description of the BEC. This necessitates the use of an essentially non-perturbative approach, which is in contrast to previous analytical studies [7–9] where the effect of the impurities on the BEC was treated as a small perturbation. We first consider the effect of a highly localized  $\delta$ -impurity on the BEC in one dimension. This approach indicates that the density of the BEC is substantially increased in the vicinity of an attractive impurity, which enhances inelastic collisions and may result in the loss of the impurity atom. In addition, we bring forward a scaling argument to show that attractive impurity-BEC interactions can lead to a point-like ground state of the impurity in 2d and 3d. Specifically, the ground state is singular for arbitrarily small attractive coupling in 3d, which seemingly contradicts the known perturbative results. Finally, in order to extend our analytical findings we present numerical results stemming from the exact solutions for the ground state of the system, where unlike in previous numerical studies [10,11] neither the impurity nor the BEC are subject to an external trapping potential.

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Our analysis of the self-trapping problem is based on the model suggested by Gross [1,17] describing the impurity wave function  $\chi(\mathbf{x}, t)$  interacting with the condensate wave function  $\psi(\mathbf{x}, t)$  in the Hartree approximation. The model is given by the coupled equations

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m_b}\nabla^2\psi + \kappa|\chi|^2\psi + g|\psi|^2\psi, \quad (1)$$

$$i\hbar\partial_t\chi = -\frac{\hbar^2}{2m_a}\nabla^2\chi + \kappa|\psi|^2\chi, \quad (2)$$

where the impurity-BEC interaction and the repulsive interaction among the BEC atoms have been approximated by the contact potentials  $\kappa\delta(\mathbf{x} - \mathbf{x}')$  and  $g\delta(\mathbf{x} - \mathbf{x}')$ , respectively. Here,  $m_a$  is the mass of the impurity,  $m_b$  is the mass of a boson in the BEC and the coupling constants  $\kappa$  and  $g > 0$  depend on the respective  $s$ -wave scattering lengths [18,19]. The functions  $\psi(\mathbf{x}, t)$  and  $\chi(\mathbf{x}, t)$  are normalized as

$$\int d\mathbf{x}|\psi(\mathbf{x})|^2 = N \quad \text{and} \quad \int d\mathbf{x}|\chi(\mathbf{x})|^2 = 1, \quad (3)$$

where  $N$  is number of atoms in the BEC. We tacitly assume that the properties of the BEC, *e.g.* the density far away from the impurity, are fixed. The interaction strength  $\kappa$ , on the other hand, is considered to be an adjustable parameter, since it may be easily changed in experiments.

As a starting point we briefly review and systematically extend the perturbative results on the self-trapping problem [7–9] based on a variational approach. This method, however, yields results that are of second order in  $\kappa$ , and hence is not adequate to capture the differences between attractive and repulsive impurities. In the main part of the paper, we present our non-perturbative and numerical results in order to reveal these fundamental differences. Finally, we conclude with a discussion of the physical implications of our findings.

**Perturbative results.** – To start we reformulate eqs. (1) and (2) in terms of dimensionless quantities for a homogeneous BEC with density  $n_0$ . The two relevant length scales in the model are the healing length  $\xi = \hbar/\sqrt{gn_0m_b}$  and the average separation of the condensate atoms  $s = n_0^{-1/d}$ , where  $d$  is the dimension of the system. Introducing the dimensionless quantities  $\tilde{\mathbf{x}} = \mathbf{x}/\xi$ ,  $\tilde{\psi} = \psi s^{d/2}$  and  $\tilde{\chi} = \chi \xi^{d/2}$  one obtains the time-independent equations

$$\tilde{\psi} = -\frac{1}{2}\nabla^2\tilde{\psi} + \beta\gamma^d|\tilde{\chi}|^2\tilde{\psi} + |\tilde{\psi}|^2\tilde{\psi}, \quad (4)$$

$$\varepsilon\tilde{\chi} = -\frac{\alpha}{2}\nabla^2\tilde{\chi} + \beta|\tilde{\psi}|^2\tilde{\chi}. \quad (5)$$

Here,  $\alpha = m_b/m_a$  is the mass ratio,  $\beta = \kappa/g$  is the relative coupling strength,  $\gamma = s/\xi$  and  $\varepsilon$  is the energy of the impurity. The energy of the condensate  $E_{\text{bec}}$ , the interaction energy  $E_{\text{int}}$  and the kinetic energy of the impurity

$E_{\text{kin}}$  are given by

$$E_{\text{bec}} = \gamma^{-d} \int d\mathbf{x} \left( \frac{1}{2}|\nabla\psi|^2 - |\psi|^2 + \frac{1}{2}|\psi|^4 \right), \quad (6)$$

$$E_{\text{int}} = \beta \int d\mathbf{x} |\chi|^2 |\psi|^2, \quad (7)$$

$$E_{\text{kin}} = \frac{\alpha}{2} \int d\mathbf{x} |\nabla\chi|^2, \quad (8)$$

where all energies are measured in units of  $gn_0$  and we dropped the tilde for notational convenience, as in the remainder of the paper. Equations (4) and (5) have a trivial solution with  $|\psi|^2 = 1$  and  $\varepsilon = \beta$ , which corresponds to a delocalized impurity.

*Thomas-Fermi approximation.* If the density of the BEC changes smoothly we can apply the Thomas-Fermi approximation, *i.e.* neglect the term  $\nabla^2\psi$  in eq. (4). In this regime we immediately find that  $|\psi(\mathbf{x})|^2 = 1 - \beta\gamma^d|\chi(\mathbf{x})|^2$ , and thus  $\chi(\mathbf{x})$  obeys the self-focusing non-linear Schrödinger equation

$$\varepsilon'\chi = -\frac{1}{2}\nabla^2\chi - \zeta|\chi|^2\chi, \quad (9)$$

with the self-trapping parameter  $\zeta = \beta^2\gamma^d/\alpha$  and  $\varepsilon' = (\varepsilon - \beta)/\alpha$ . In one dimension eq. (9) admits the exact solution [7,20]  $\chi_\lambda(x) = (2\lambda)^{-1/2}\text{sech}(x/\lambda)$ , with the localization length  $\lambda = 2/\zeta$  and the energy  $\varepsilon' = -\zeta^2/8$ . In addition, numerical solutions of eq. (9) show that the wave function of the form  $\chi_\lambda(\mathbf{x}) = N_\lambda\text{sech}(|\mathbf{x}|/\lambda)$ , with  $N_\lambda$  the normalization constant, is also an accurate approximation to the exact solution in two and three dimensions [20,21]. However, these solutions can self-focus and become singular in finite time [20].

A comparison of the individual terms in  $E_{\text{bec}} + E_{\text{int}}$  shows that the Thomas-Fermi approximation is valid for  $\zeta \ll 1$ , which is a rather stringent condition on the system parameters. However, the merit of eq. (9) lies in the fact that it yields an almost exact wave function for weakly localized impurities with  $\ell_{\text{loc}} \gg 1$ , where  $\ell_{\text{loc}}$  is the localization length of the impurity. In addition, we see from the solution of eq. (9) that self-trapping occurs for arbitrarily small coupling in 1d for both types of impurities.

*Weak-coupling approximation.* An alternative approach is to linearize the equation for  $\psi(\mathbf{x})$  by considering small deformations  $\delta\psi(\mathbf{x}) = \psi(\mathbf{x}) - 1$  of the condensate [7–9]. This corresponds to a consistent expansion of eqs. (4) and (5) in  $\beta$ , which results in the linear equations

$$\left(-\frac{1}{2}\nabla^2 + 2\right)\delta\psi = -\beta\gamma^d|\chi|^2, \quad (10)$$

$$\left(-\frac{\alpha}{2}\nabla^2 + 2\beta\delta\psi\right)\chi = (\varepsilon - \beta)\chi, \quad (11)$$

where we assumed that  $\delta\psi$  is real for simplicity. It can be seen from eq. (10) that the linearization of eq. (4) is valid in the regime  $|\beta|\gamma^d/\ell_{\text{loc}}^d \ll 1$ . The solution of eq. (10) is given in terms of the Green's function  $G(\mathbf{x})$  satisfying the

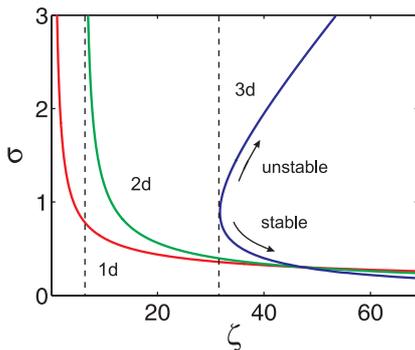


Fig. 1: The localization length  $\sigma$  (solid lines) as a function of the self-trapping parameter  $\zeta$  obtained by using a Gaussian variational wave function. Self-trapping occurs for arbitrarily small  $\zeta$  in 1d, for  $\zeta > 2\pi$  in 2d and for  $\zeta \gtrsim 31.7$  in 3d (vertical dashed lines). From the two self-trapping solutions for a given  $\zeta$  in 3d, only the more localized state is stable.

Helmholtz equation. One finds by inserting the solution of eq. (10) into eq. (11) that  $\chi$  obeys the non-local non-linear Schrödinger equation

$$\left( -\frac{1}{2}\nabla^2 - 2\zeta \int d\mathbf{x}' G(\mathbf{x} - \mathbf{x}') |\chi(\mathbf{x}')|^2 \right) \chi = \varepsilon' \chi. \quad (12)$$

Equation (12) minimizes the energy functional  $F[\chi] = E_{\text{kin}} + E_{\text{def}}$ , with

$$E_{\text{def}} = -\beta^2 \gamma^d \int d\mathbf{x} d\mathbf{x}' |\chi(\mathbf{x})|^2 G(\mathbf{x} - \mathbf{x}') |\chi(\mathbf{x}')|^2, \quad (13)$$

which has been discussed in the context of liquid helium by Lee and Gunn [7]. We see from eqs. (8) and (13) that the self-trapping parameter  $\zeta$  is proportional to  $E_{\text{def}}/E_{\text{kin}}$ , *i.e.* the ratio between the potential energy gained by deforming the BEC and the kinetic energy of the impurity.

In order to estimate the critical parameters for which self-trapping occurs we insert the harmonic-oscillator ground state

$$\chi_\sigma(\mathbf{x}) = (\pi\sigma^2)^{-d/4} \prod_{j=1}^d \exp(-x_j^2/2\sigma^2), \quad (14)$$

with  $\sigma$  the harmonic-oscillator length, as a variational wave function into the functional  $F[\chi]$ . The resulting energy  $f(\sigma)$  is given by

$$f(\sigma) = \frac{\alpha d}{4\sigma^2} - \beta^2 \gamma^d h(\sigma), \quad (15)$$

with the functions

$$h_{1d}(\sigma) = \frac{1}{2} \exp(2\sigma^2) \text{erfc}(\sqrt{2}\sigma), \quad (16)$$

$$h_{2d}(\sigma) = -\frac{1}{2\pi} \exp(2\sigma^2) \text{Ei}(-2\sigma^2), \quad (17)$$

$$h_{3d}(\sigma) = \frac{1}{\pi} \left[ \frac{1}{\sqrt{2\pi}\sigma} - \exp(2\sigma^2) \text{erfc}(\sqrt{2}\sigma) \right], \quad (18)$$

where  $\text{erfc}(x)$  is the complementary error function and  $\text{Ei}(x)$  the exponential integral. The impurity localizes if  $f(\sigma)$  has a minimum for a finite value of  $\sigma$ , which depends only on the self-trapping parameter  $\zeta$ .

The explicit expression for  $f(\sigma)$ , which appears to be a novel result, allows us to determine the self-trapping threshold, *i.e.* the critical coupling strength above which self-trapping occurs, and the size of the self-trapped state even for highly localized self-trapping solutions as long as  $|\beta|\gamma^d/\sigma^d \ll 1$ . Figure 1 shows the localization length  $\sigma$  as a function of the self-trapping parameter  $\zeta$  in 1d, 2d and 3d. Specifically, in 1d we find by asymptotically expanding  $f(\sigma)$  in the limit  $\sigma \gg 1$  that there exists a self-trapping solution for arbitrarily small  $\zeta$  with  $\sigma = \sqrt{2\pi}/\zeta$ . The same expansion yields a critical value  $\zeta_{\text{crit}} = 2\pi$  above which self-trapping occurs in 2d. In the 3d case, numerical minimization of  $f(\sigma)$  shows that the critical value is  $\zeta_{\text{crit}} \simeq 31.7$ , where the corresponding state is highly localized with  $\sigma \simeq 0.87$ . Interestingly, there exist two self-trapping solutions for a given  $\zeta$  in 3d, however only the more localized state is stable.

**Beyond perturbation theory.** – We now consider the self-trapping problem in the regime of strong impurity-BEC interactions, *i.e.* the case of a localized self-trapping state accompanied by a possibly strong deformation of the BEC. We first illustrate the effect of higher-order terms in  $\beta$  for a 1d system and subsequently discuss 2d and 3d systems based on a scaling argument.

*The  $\delta$ -approximation in 1d.* In order to find approximate solutions of eqs. (4) and (5) we assume that the impurity is highly localized due to the strong impurity-BEC interaction. More precisely, we consider the regime where the effect of the impurity on the BEC is essentially the same as for a  $\delta$ -impurity with  $|\chi(x)|^2 = \delta(x)$ . This approximation is valid provided that  $\ell_{\text{loc}} \ll 1$ , *i.e.* the localization length is much smaller than the healing length of the BEC, which is achieved for sufficiently large  $|\beta|$ . Our approach focuses only on the deformation of the BEC caused by the impurity. Nevertheless, the  $\delta$ -approximation allows us to illustrate the differences between attractive and repulsive impurities, which are also present in higher dimensions.

We first calculate the condensate wave function  $\psi(x)$  in the presence of a  $\delta$ -impurity at position  $x_0$ , which is determined by the equation

$$\left[ -\frac{1}{2}\partial_{xx} - 1 + |\psi(x)|^2 + \beta\gamma\delta(x-x_0) \right] \psi(x) = 0, \quad (19)$$

with the boundary conditions  $\psi(x) = 1$  and  $\partial_x \psi(x) = 0$  in the limit  $x \rightarrow \pm\infty$ . Using the known solutions of eq. (19) for  $\beta = 0$  and taking  $x_0 = 0$  for simplicity we obtain  $\psi(x) = \coth(|x| + c)$  and  $\psi(x) = \tanh(|x| + c)$  for attractive and repulsive impurities, respectively, with  $c$  a constant. Given that the derivative of  $\psi(x)$  has a discontinuity at  $x_0$  it

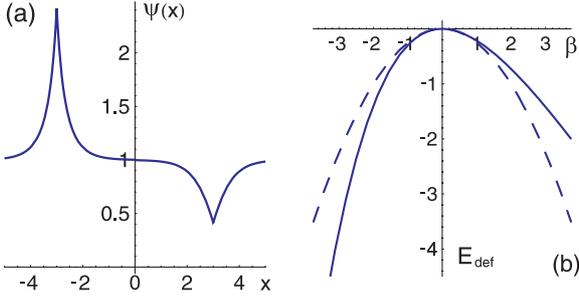


Fig. 2: (a) Deformation of the BEC for an attractive (left) and repulsive (right)  $\delta$ -impurity with the same interaction strength  $\gamma|\beta|=1$ . (b) Deformation energy  $E_{\text{def}}$  for a  $\delta$ -impurity as a function of the interaction strength  $\beta$  (solid line) compared to the weak-coupling approximation (dashed line) for  $\gamma=0.5$ . Attractive (repulsive) impurities have lower (higher) energy than predicted by the weak-coupling approximation.

follows that in both cases  $1 - [\psi(x_0)]^2 = \beta\gamma\psi(x_0)$  and thus

$$\psi(x_0) = -\frac{\beta\gamma}{2} + \sqrt{1 + \left(\frac{\beta\gamma}{2}\right)^2}, \quad (20)$$

which fixes the constant  $c$ . We note that  $\psi(x_0) \in (0, 1]$  for  $\beta \geq 0$  and  $\psi(x_0) \in (1, \infty)$  for  $\beta < 0$ . Thus, the density of the condensate  $n(x_0) \equiv [\psi(x_0)]^2$  at the position of the impurity  $x_0$  is not bounded for attractive interactions. The enhanced deformation of the BEC due to an attractive  $\delta$ -impurity is already visible for a moderate interaction strength as illustrated in fig. 2(a).

The solution of eq. (19) allows us to determine the deformation energy  $E_{\text{def}}$  to all orders of  $\beta$ . Using eqs. (6) and (7) we find that for both types of impurities

$$E_{\text{def}} = \frac{4}{3}\gamma^{-1} \left\{ 1 - \left[ 1 + \left(\frac{\beta\gamma}{2}\right)^2 \right]^{3/2} + \left(\frac{\beta\gamma}{2}\right)^3 \right\}. \quad (21)$$

We note that the non-perturbative result for  $E_{\text{def}}$  is consistent with the weak-coupling approximation since in the limit  $\sigma \rightarrow 0$  we find from eq. (16) that  $\beta^2\gamma h_{1d}(\sigma) \rightarrow \beta^2\gamma/2$ . Figure 2(b) shows the deformation energy  $E_{\text{def}}$  as a function of the interaction strength  $\beta$  in comparison with the weak-coupling result. It can be seen that attractive impurities have lower energy than predicted by the weak-coupling approximation, whereas repulsive impurities have higher energy.

**Impurity collapse.** The results in the previous section indicate that the ground state of the impurity and the BEC strongly depend on the sign of  $\beta$ . We now show that the sign of  $\beta$  has a crucial effect on the ground state in 2d and 3d by using a scaling argument based on a variational wave function for  $\psi(\mathbf{x})$  and  $\chi(\mathbf{x})$ .

Let us consider the total energy of the system  $E_{\text{tot}} = E_{\text{bec}} + E_{\text{int}} + E_{\text{kin}}$ , which is clearly bounded from below for  $\beta > 0$  but not necessarily for  $\beta < 0$ . We now analyze the scaling of the individual terms in  $E_{\text{tot}}$  depending on the localization length of the impurity and the deformation of

the BEC. To this end we insert the Gaussian trial function  $\chi_\sigma(\mathbf{x})$  for the impurity and  $\psi_\sigma(\mathbf{x}) = 1 + \delta\psi_\sigma(\mathbf{x})$  for the condensate into  $E_{\text{tot}}$ , where

$$\delta\psi_\sigma(\mathbf{x}) = \frac{a}{\sigma^{\delta/2}} \prod_{j=1}^d \exp(-x_j^2/b\sigma^2), \quad (22)$$

with  $a$ ,  $b$  and  $\delta$  positive constants. In what follows we are particularly interested in the limit  $\sigma \rightarrow 0$  and only consider finite deformations of the BEC. Consequently, we add the constraint  $\delta \leq d$  to assure that  $\int d\mathbf{x} |\delta\psi(\mathbf{x})|^2 \sim \sigma^{d-\delta}$  is finite. We note that  $\chi_\sigma(\mathbf{x})$  and  $\psi_\sigma(\mathbf{x})$  have the correct asymptotic behavior required for them to be valid physical states of the system; however, they may not be a good approximation for the ground state. We obtain that the individual energy contributions scale as  $E_{\text{int}} \sim \sigma^{-\delta}$ ,  $E_{\text{kin}} \sim \sigma^{-2}$  and

$$E_{\text{bec}} \sim c_0\sigma^{d-\delta-2} + \sum_{j=1}^4 c_j \sigma^{d-j\delta/2}, \quad (23)$$

where the  $c_j > 0$  depend on the system parameters.

Comparing the terms above one finds that for a three-dimensional system  $E_{\text{tot}}$  is not bounded from below in the limit  $\sigma \rightarrow 0$  for a fixed  $\delta$ , *i.e.* the energy of the system becomes arbitrarily low if the impurity collapses to a point. Explicitly, in the 3d case we have  $E_{\text{bec}} \sim c_0\sigma^{1-\delta} + c_1\sigma^{3-\delta/2} + \dots + c_4\sigma^{3-2\delta}$  and hence a comparison of the exponents yields that  $|E_{\text{int}}| > E_{\text{kin}} + E_{\text{bec}}$  for  $2 < \delta < 3$  in the limit  $\sigma \rightarrow 0$ . Moreover, in the same limit  $\int d\mathbf{x} |\delta\psi_\sigma(\mathbf{x})|^2 \rightarrow 0$ , *i.e.* the deformation of the BEC is vanishingly small despite the collapse of the impurity. We note that the above argument holds for arbitrarily small  $\beta$ , and thus the weak-coupling approximation in 3d is valid for  $\beta > 0$  only since for  $\beta < 0$  there is always a state of lower energy with  $\sigma \rightarrow 0$ .

In the 2d case it is not possible to find a value for  $\delta$  such that the total energy  $E_{\text{tot}}$  is dominated by  $E_{\text{int}}$  in the limit  $\sigma \rightarrow 0$ . Nevertheless, for  $\delta=2$  we obtain  $E_{\text{int}} \sim E_{\text{kin}} \sim E_{\text{bec}} \sim \sigma^{-2}$ , which implies that the collapse of the impurity depends on the particular system parameters, *e.g.* the coupling strength  $\beta$ . In contrast to the 3d case this collapse is accompanied by a sizeable deformation of the BEC since  $\int d\mathbf{x} |\delta\psi_\sigma(\mathbf{x})|^2$  is finite in the limit  $\sigma \rightarrow 0$  for  $\delta=2$ . Finally, for a one-dimensional system similar considerations lead to result that  $|E_{\text{int}}| < E_{\text{kin}} + E_{\text{bec}}$  in the limit  $\sigma \rightarrow 0$  for any valid  $\delta$ , and hence our variational approach does not predict a collapse of the impurity.

**Numerical results.** – We have determined the ground state of the impurity and the BEC numerically by using the normalized gradient flow method [22,23] in order to extend the analytical results. To make eqs. (4) and (5) amenable to computational modelling we assumed that both the impurity and the condensate were enclosed in a sphere of zero potential with infinitely high potential walls at its radius  $R$ . The system parameters for the numerical calculations were set to  $\alpha = 1.0$  and  $\gamma = 0.5$ , whereas  $\beta$  was varied over a large range.

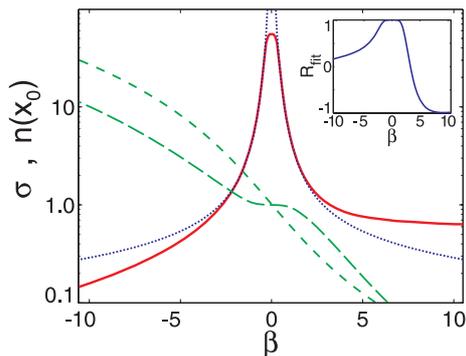


Fig. 3: The localization length  $\sigma$  (solid line) and the density of the condensate  $n(x_0)$  (long-dashed line) at the impurity position  $x_0$  as a function of the interaction strength  $\beta$  in 1d. The weak-coupling approximation (dotted line) accurately reproduces  $\sigma$  in the regime  $|\beta|\gamma/\sigma \ll 1$ . The localization length saturates to a finite value  $\sigma \sim 60$  as  $\beta \rightarrow 0$  because of the finite system size. The deformation of the BEC is qualitatively described by the  $\delta$ -approximation (short-dashed line). The inset shows the smooth transition from a sech-type ( $R_{\text{fit}}=1$ ) to a Gaussian ( $R_{\text{fit}}=-1$ ) self-trapping state for repulsive impurities.

A quantitative measure for the localization length  $l_{\text{loc}}$  was found by fitting the functions  $\chi_\sigma(\mathbf{x})$  and  $\chi_\lambda(\mathbf{x})$  to the exact impurity wave function yielding the values  $\sigma$  and  $\lambda$ . In addition, we compared the corresponding fitting errors  $S_\sigma$  and  $S_\lambda$  and evaluated the quantity  $R_{\text{fit}} = (S_\sigma - S_\lambda) / (S_\sigma + S_\lambda)$ . Accordingly,  $R_{\text{fit}} = -1$  indicates that the self-trapped state is accurately described by a Gaussian  $\chi_\sigma(\mathbf{x})$ , whereas for  $R_{\text{fit}} = 1$  the impurity is rather in a sech-type state  $\chi_\lambda(\mathbf{x})$ . One would expect that  $R_{\text{fit}} \approx -1$  for a highly localized impurity with  $l_{\text{loc}} \ll 1$  since the impurity sees only the harmonic part of the effective potential  $|\psi(\mathbf{x})|^2$ . On the other hand,  $R_{\text{fit}} \approx -1$  for a weakly localized impurity with  $l_{\text{loc}} \gg 1$  according to the Thomas-Fermi approximation.

As can be seen in fig. 3, in the 1d case there is no self-trapping threshold in agreement with the weak-coupling result, which accurately reproduces the localization length  $\sigma$  in the regime  $|\beta|\gamma/\sigma \ll 1$ . However, we see that for large  $|\beta|$  attractive impurities are more localized than the repulsive ones. Moreover, repulsive impurities undergo a smooth transition from a sech-type to a Gaussian self-trapping state for increasing  $\beta$  as indicated by  $R_{\text{fit}}$ . The deformation of the condensate  $n(x_0)$  at the position of the impurity  $x_0$  is qualitatively described by the  $\delta$ -approximation with a strong increase in the density of the BEC for attractive impurities.

In two dimensions, the impurity localizes for  $|\beta| > \beta_{\text{crit}}$ , where  $\beta_{\text{crit}}$  is correctly predicted by the weak-coupling result, as shown in fig. 4. This is not accidental since the localization length  $\sigma$  diverges close to  $\beta_{\text{crit}}$  in 2d, as can be seen in fig. 1, and thus the criterion  $|\beta|\gamma^2/\sigma^2 \ll 1$  for the validity of the linearization of eqs. (4) and (5) is always met near  $\beta_{\text{crit}}$ . In contrast, for large  $|\beta|$  the localization length  $\sigma$  strongly deviates from the weak-coupling result.

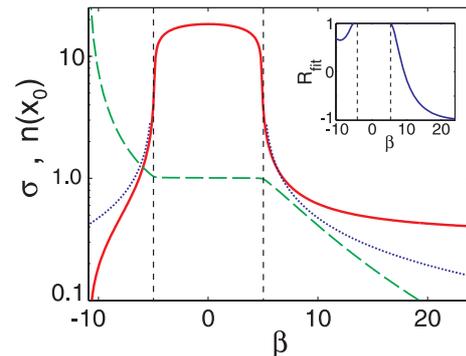


Fig. 4: The localization length  $\sigma$  (solid line) and the density of the condensate  $n(x_0)$  (dashed line) at the impurity position  $x_0$  as a function of the interaction strength  $\beta$  in 2d. The weak-coupling approximation (dotted lines) accurately predicts the self-trapping threshold at  $\beta_{\text{crit}} = \sqrt{8\pi}$  (vertical dashed lines). The localization length saturates to a finite value  $\sigma \sim 20$  for  $|\beta| < \beta_{\text{crit}}$  because of the finite system size. Attractive impurities shrink to a point-like state and the density of the BEC  $n(x_0)$  diverges as  $\beta$  approaches a critical value  $\beta^* \sim -10$  in agreement with our scaling argument. The behavior of  $R_{\text{fit}}$  (inset) is similar to the 1d case.

In particular, attractive impurities shrink to a point-like state and the density of the condensate  $n(x_0)$  diverges as  $\beta$  approaches a critical value  $\beta^*$ , which is in agreement with the scaling argument in the previous section. The behavior of  $R_{\text{fit}}$  is similar to the 1d case.

For a 3d system we are able to obtain numerical results for  $\beta > 0$  only, which in view of our scaling argument was to be expected. The localization length  $\sigma$  and the density of the condensate  $n(x_0)$  for repulsive impurities are shown in fig. 5. We see that the weak-coupling approximation underestimates the exact value  $\beta_{\text{crit}}$  since in 3d we have that  $\sigma \sim 1$  even close to  $\beta_{\text{crit}}$  and thus  $\beta\gamma^3/\sigma^3$  is not necessarily small. As shown in the inset of fig. 5 the transition from a sech-type to a Gaussian self-trapping state is slower than in 1d and 2d.

**Discussion and conclusion.** – In our analytical and numerical investigation of the self-trapping problem we have shown, in particular, that an attractive impurity-BEC interaction leads to a strong deformation of the BEC in 1d and 2d and to a singular ground state of the impurity in 2d and 3d. However, both the high density of the BEC and the point-like state of the impurity entail additional physical effects, which were initially small and not taken into account in our model.

The high density of the BEC near the impurity enhances inelastic collisions that lead to two- and three-body losses of the condensate atoms [24]. Specifically, the inelastic collisions might cause the loss of the impurity atom itself. However, provided that the impurity is not affected by inelastic collisions one can account for the loss of the condensate atoms by adding damping terms of the form  $-i\Gamma_2|\psi(\mathbf{x})|^2\psi(\mathbf{x})$  and  $-i\Gamma_3|\psi(\mathbf{x})|^4\psi(\mathbf{x})$  to eq. (1), where the positive constants  $\Gamma_2$  and  $\Gamma_3$  are two- and

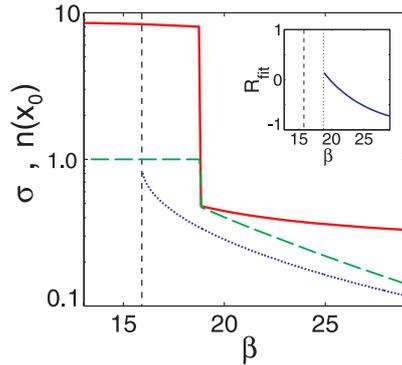


Fig. 5: The localization length  $\sigma$  (solid line) and the density of the condensate  $n(x_0)$  (dashed line) at the impurity position  $x_0$  as a function of the interaction strength  $\beta$  in 3d. There is no well-defined ground state for  $\beta < 0$  in 3d in agreement with our scaling argument. The weak-coupling approximation (dotted line) predicts a self-trapping threshold at  $\beta_{\text{crit}} \simeq 15.9$  (vertical dashed line), which is lower than the numerical result  $\beta_{\text{crit}} \simeq 18.8$ . The localization length saturates to a finite value  $\sigma \sim 10$  for  $\beta < \beta_{\text{crit}}$  because of the finite system size. The convergence of the impurity wave function to a Gaussian self-trapping state is slower than in 1d and 2d as indicated by  $R_{\text{fit}}$  (inset).

three-body loss rates, respectively. We note that these additional terms would require the simulation of the full dynamics of the system [25] and may have a non-trivial effect on the self-trapping process.

Moreover, the contact potential approximation is valid as long as the various length scales of the system, *e.g.* the localization length  $\ell_{\text{loc}}$ , are large compared to the characteristic range of the exact interaction potential [18]. Thus the interaction between the condensate atoms and the impurity is no longer correctly described by the contact potential  $\kappa\delta(\mathbf{x}-\mathbf{x}')$  in the limit  $\ell_{\text{loc}} \rightarrow 0$  where the influence of higher partial waves becomes important. The resulting repulsion would of course lead to a finite width of the impurity wave function. We note that with the above proviso our results are also valid for ionic impurities with positive charge [26,27] in the regime where the ion-boson scattering is dominated by the *s*-wave contribution [28,29].

Finally, we conclude with the remark that our model is also applicable if the BEC is confined to a harmonic trap [10] provided that the harmonic-oscillator length of the potential is much larger than the localization length  $\ell_{\text{loc}}$  of the impurity and the healing length  $\xi$  of the BEC.

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