Strong-Coupling Polarons in Dilute Gas Bose-Einstein Condensates

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A neutral impurity atom immersed in a dilute Bose-Einstein condensate (BEC) can have a bound ground state in which the impurity is self-localized. In this polaronlike state, the impurity distorts the density of the surrounding BEC, thereby creating the self-trapping potential minimum. We describe the self-localization in a strong-coupling approach.

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Experimentalists are pursuing the localization and transportation of individual atoms in dilute gas Bose-Einstein condensates (BECs) [1,2]. Their motives are manifold: the transportation of particles into and out of a localized state would realize a quantum-dot-like single particle device. The rate at which the localized state receives or emits particles could determine the local density of states like a scanning tunneling microscope (STM). The motion of a localized atom could test superfluid dynamics [3], and its acceleration the Unruh effect [4]. Light resonant with multiple localized particles could itself exhibit localization [5]. The spins of localized particles could make up a quantum register of movable qubits. However, the challenge of localizing a neutral atom by means of a steep external potential is daunting [2]. In this Letter, we propose an alternative strategy: an impurity self-localizes within a region smaller than the BEC-healing length when the magnitude of the impurity-boson scattering length is increased above a critical value. Similar to the electron self-localization in a polar crystal (forming a so called strong-coupling large polaron), the BEC impurity localizes because the interaction energy gain (stemming from the local distortion of the boson field) outweighs the kinetic energy cost. Observing this phenomenon in cold atoms may require a Feshbach resonance (to alter the impurity-boson interaction) and impurity creation (either by a Raman process or by trapping a different atom species), but these techniques have been demonstrated [6]. This experiment would create a novel class of self-localized particles: polarons with mass comparable to or possibly larger than that of the boson particles.

In the context of condensed ^{4}He fluids, Miller *et al.* [7] remarked on impurity self-localization and mentioned the polaron connection. They advocated a perturbation treatment (weak-coupling theory) by demonstrating the similarity of the perturbed wave function with the variational one proposed by Feynman and Cohen to include "backflow" [8]. The weak-coupling description predicts that phonon-drag increases the impurity mass from m_I to $m_I^* = m_I/[1-\alpha]$, where α is a dimensionless coupling constant. Its value depends on the BEC density ρ_B, the impurity-boson interaction potential V_q, the boson mass m_B, and the excitation energy E_q^B of the boson modes of momentum q:

$$\alpha = \frac{4}{3}\left(\frac{m_B}{m_I}\right)\frac{\rho_B}{(2\pi)^3}\int d^3q \frac{|V_q(\hbar^2q^2/2m_B)|^2}{E_q^B[E_q^B + \hbar^2q^2/2m_I]^3}. \quad (1)$$

For a dilute BEC and an impurity-boson contact interaction of scattering length a_{IB}, $V_q \to \lambda_{IB} = 2\pi\hbar^2(1/m_B + 1/m_I)a_{IB}$ and $E_q^B \to \hbar c_B q\sqrt{1+(\xi q)^2}$. Here, ξ is the BEC-healing length which depends on the boson-boson scattering length a_{BB}, $\xi = 1/\sqrt{16\pi\rho_B a_{BB}}$, and c_B denotes the BEC velocity of sound, $c_B = \hbar/(2m_B\xi)$, so that

$$\alpha = \frac{8}{3\sqrt{\pi}}\sqrt{\frac{\rho_B a_{IB}^4}{a_{BB}}}\left(1+\frac{m_B}{m_I}\right)^2\left(\frac{m_B}{m_I}\right)F\left(\frac{m_B}{m_I}\right), \quad (2)$$

where $F(y) = \int_0^\infty x^5/[\sqrt{1+x^2}(x\sqrt{1+x^2}+yx^2)^3]$. As in polaron physics, the effective mass divergence at $\alpha = 1$ indicates self-localization, even though the weak-coupling description breaks down when $\alpha \sim 1$ [9].

We describe the self-localized impurity in a strong-coupling treatment—similar to the Landau-Pekar description of polarons [10]—using a product wave function for the ground state:

$$\Psi_{1,N}(\mathbf{r},\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N) \simeq \chi(\mathbf{r})\psi(\mathbf{x}_1)\psi(\mathbf{x}_2)\ldots\psi(\mathbf{x}_N), \quad (3)$$

where $\chi(\mathbf{r})$ represents the impurity wave function and ψ denotes the single particle state occupied by the N indistinguishable bosons of position $\mathbf{x}_j$. We substitute Eq. (3) into the Hamiltonian eigenvalue equation and multiply in one instance by $\psi^*(\mathbf{x}_1)\psi^*(\mathbf{x}_2)\ldots\psi^*(\mathbf{x}_N)$, and in another instance by $\chi^*(\mathbf{r})\psi^*(\mathbf{x}_2)\ldots\psi^*(\mathbf{x}_N)$. Integrating the first equation over $\mathbf{x}_1\mathbf{x}_2\ldots\mathbf{x}_N$, the second over $\mathbf{r}\ \mathbf{x}_2\ldots\mathbf{x}_N$, and choosing the ground state wave function to be real valued (e.g., $|\chi|^2 = \chi^2$) we obtain [11]

$$E_I\chi(\mathbf{r}) = -\frac{\hbar^2\nabla_{\mathbf{r}}^2}{2m_I}\chi(\mathbf{r}) + \lambda_{IB}\varphi^2(\mathbf{r})\chi(\mathbf{r}) \quad (4a)$$

$$\mu_B\varphi(\mathbf{x}) = -\frac{\hbar^2\nabla_{\mathbf{x}}^2}{2m_B}\varphi(\mathbf{x}) + \lambda_{BB}\varphi^3(\mathbf{x}) + \lambda_{IB}\chi^2(\mathbf{x})\varphi(\mathbf{x}), \quad (4b)$$

where $\lambda_{BB} = [4\pi\hbar^2/m_B]a_{BB}$ and φ is the condensate field, $\varphi = \sqrt{N}\psi$. If $E_{1,N}$ and $E_{0,N}$ are the ground state energies of N bosons in the presence of one or zero impurity atoms, respectively, the BEC chemical potential is $\mu_B = E_{1,N} - E_{1,N-1}$, and the impurity energy is $E_I = E_{1,N} - E_{0,N}$.

Since the BEC experiences the density of only a single impurity, its field may be altered only slightly for sufficiently weak boson-impurity coupling, $\varphi(\mathbf{r}) = \sqrt{\rho_B^0} + \delta\varphi(\mathbf{r})$. Using $\mu_B \approx \lambda_{BB}\rho_B^0$, the corresponding linearization of Eqs. (4) gives

$$E_b\chi(\mathbf{r}) = -\frac{\hbar^2}{2m_I}\nabla_{\mathbf{r}}^2\chi(\mathbf{r}) + 2\lambda_{IB}\sqrt{\rho_B^0}\delta\varphi(\mathbf{r})\chi(\mathbf{r}) \tag{5a}$$

$$[\nabla_{\mathbf{x}}^2 - \xi^{-2}]\delta\varphi(\mathbf{x}) = \frac{2m_B\lambda_{IB}\sqrt{\rho_B^0}}{\hbar^2}\chi^2(\mathbf{x}), \tag{5b}$$

where $E_b = E_I - \lambda_{IB}\rho_B^0$ is the binding energy.

As a modified Helmoltz equation, we solve Eq. (5b) in terms of the Green function $G_\xi(\mathbf{r}) = (4\pi)^{-1}e^{-|\mathbf{r}|/\xi}/|\mathbf{r}|$,

$$\delta\varphi(\mathbf{x}) = -\frac{1}{2\sqrt{\rho_B^0}}\frac{\lambda_{IB}}{\lambda_{BB}\xi^2}\int d\mathbf{r}G_\xi(\mathbf{x}-\mathbf{r})\chi^2(\mathbf{r}). \tag{6}$$

The excess number of BEC atoms in the impurity region is then $\int d\mathbf{r}2\sqrt{\rho_B^0}\delta\varphi(\mathbf{r}) = -(\lambda_{IB}/\lambda_{BB})$, in agreement with [12] where this number, induced by a general potential, was determined from thermodynamic arguments. The substitution of (6) into (5a) results in the wave equation of a particle that self-interacts through an attractive Yukawa (or screened Coulomb) potential. Exploiting the Coulomb analogy, we introduce an effective charge Q, where $Q^2 = [\lambda_{I,B}\rho_B^0]a_{I,B} \times 2(1 + m_B/m_I)$,

$$E_b\chi(\mathbf{r}) = -\frac{\hbar^2}{2m_I}\nabla_{\mathbf{r}}^2\chi(\mathbf{r}) - \left[\int d\mathbf{x}\frac{Q^2}{|\mathbf{r}-\mathbf{x}|}e^{-|\mathbf{r}-\mathbf{x}|/\xi}\chi^2(\mathbf{x})\right]\chi(\mathbf{r}). \tag{7}$$

Incidentally, $V_{\rm med}(\mathbf{r}) = -Q^2e^{-|\mathbf{r}|/\xi}/|\mathbf{r}|$ is also the BEC-mediated interaction experienced by distinguishable particles immersed in a BEC, as calculated from perturbation theory [13,14]. The Coulomb analogy also suggests natural units E_0, the effective Rydberg energy, and R_0, an effective Bohr radius, $Q^2/R_0 = \hbar^2/m_IR_0^2 = 2E_0$,

$$E_0 = [\lambda_{IB}\rho_B^0][a_{IB}^3\rho_B^0] \times 4\pi\left(\frac{m_B}{m_I}\right)^2\left(1+\frac{m_I}{m_B}\right)^3$$
$$R_0 = \frac{1}{4\pi a_{IB}^2\rho_B^0} \times \frac{m_Im_B}{(m_B+m_I)^2}, \tag{8}$$

which set the relevant energy (E_0), time ($\hbar/E_0$), and length (R_0) scales. Note that $[4\pi a_{IB}^2\rho_B^0]^{-1}$ is the mean free path of an impurity moving among hard-sphere scatterers distributed at the BEC density.

The polaron corresponds to solutions of (7) with negative eigenvalue E_b. We break translational symmetry by hand and solve (7) iteratively for an s-wave impurity wave function centered on the origin. At each iteration step, we solve the eigenvalue problem for an impurity particle experiencing an effective potential $u(r) = [\int d\mathbf{x}\frac{-Q^2}{|\mathbf{r}-\mathbf{x}|}e^{-|\mathbf{r}-\mathbf{x}|/\xi}\chi^2(\mathbf{x})]$, in which we substitute the impurity density $\chi^2(\mathbf{x})$ obtained from the previous iteration. By using the spherical symmetry of the wave function and defining $\beta = \xi/R_0$, in natural units (8) $u(r)$ reads

$$u(r) = \frac{-8\pi\beta}{r}\left[e^{-r/\beta}\int_0^r dr'\sinh\left(\frac{r'}{\beta}\right)r'\chi^2(r') + \sinh\left(\frac{r}{\beta}\right)\int_r^\infty dr'e^{-r'/\beta}r'\chi^2(r')\right], \tag{9}$$

where β represents the only density/interaction dependence that remains, thereby becoming the relevant dimensionless coupling constant,

$$\beta = \frac{\xi}{R_0} = \sqrt{\pi}\sqrt{\frac{a_{IB}^4}{a_{BB}}\rho_B^0}\left(1+\frac{m_B}{m_I}\right)\left(1+\frac{m_I}{m_B}\right). \tag{10}$$

Another candidate is the effective fine-structure coupling constant, $Q^2/[\hbar c_B]$, which turns out simply proportional, $Q^2/[\hbar c_B] = 2(m_B/m_I)\beta$. In Fig. 1 we show the iteratively obtained $\chi(r)$ functions, whereas the inset shows the corresponding binding energies (in units of E_0), for several β values. Thus, this strong-coupling description predicts that the impurity self-localizes if $\beta > 4.7$. The deeply bound variational wave function ($\beta > 20$) with width $\sigma = 3\sqrt{\pi/2}$, shown by the bold line of Fig. 1, is remarkably similar to the iterative function [15].

When $\beta \geq 20$, the impurity state converges to that of a particle bound by a pure Coulomb-self-interaction with energy $E_b = -0.316E_0$ and extent $\sqrt{\langle r^2\rangle} = 4.64R_0$.

To understand the interesting "transition" regime, $4.7 < \beta \leq 20$, which exhibits an intricate interaction depen-

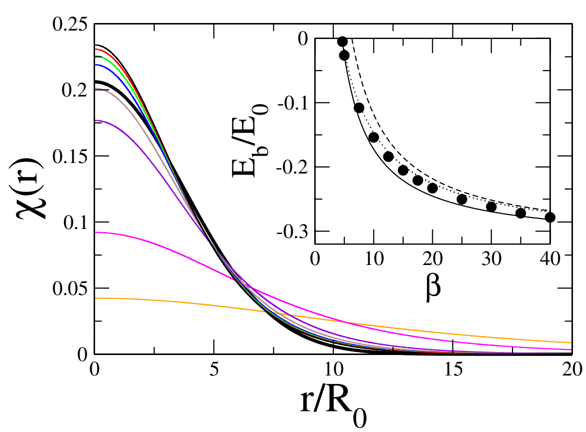

FIG. 1 (color online). Radial wave function obtained through the iterative procedure for $\xi/R_0 = 4.7, 5, 10, 20, 30, 40$ (from bottom to top). In bold black line, the initial Gaussian guess. In the inset, the energy of the ground wave function vs ξ (dots). In dotted line, the variational result obtained numerically. The expansion for large ξ/R_0 is in dashed line, and the best fit $E_b/E_0 \simeq -1/\pi + 3R_0/2\xi$ in solid line.

dence, we approximate the impurity wave function variationally. The effective impurity Eq. (7) is equivalent to minimizing the functional $E_V = T + V/2$ [16], where T denotes the kinetic energy $T = -(\hbar^2/2m_I) \times \int d\mathbf{r}\chi(\mathbf{r})\nabla^2\chi(\mathbf{r})$ and V the self-interaction energy $V = \int d\mathbf{r}\chi^2(\mathbf{r})u(\mathbf{r})$, with respect to variations of the real-valued normalized wave function, $\chi(\mathbf{r})$. Choosing a Gaussian trial wave function, $\chi(\mathbf{r}) = \exp(-|\mathbf{r}|^2/2\sigma^2)/(\pi\sigma^2)^{3/4}$, the functional, written in natural units, becomes

$$E_V = \frac{3}{2\sigma^2} - \sqrt{\frac{2}{\pi}}\frac{f(\sigma/\beta)}{\sigma}, \quad (11)$$

where $f(a) = \int drre^{-ra}e^{-r^2/2}$. Numerical minimization of (11) with respect to σ gives a binding energy that agrees well with the iterative solution of (7), shown in dotted line in the inset of Fig. 1. The dashed line plots the energy obtained by expanding (11) for large β, $E_b/E_0 \simeq -1/\pi + 2/\beta$, showing reasonable agreement with the iterative solution but slightly overestimating the minimal β value for self-localization. A fit that gives better agreement over the whole β range is $E_b/E_0 \simeq -1/\pi + 1.5/\beta$ (solid line in inset of Fig. 1). With $E_0 = [\lambda_{BB}\rho_B^0]2(m_B/m_I)\beta^2$, E_b also equals

$$E_b \approx [\lambda_{BB}\rho_B^0]2(m_B/m_I)\left[\frac{3}{2}\beta - \frac{\beta^2}{\pi}\right], \quad (12)$$

reminiscent of the strong-coupling energy of traditional polarons, proportional to the square of the coupling constant [9].

In Fig. 2 we compare the corresponding minimal $\sqrt{\rho_B^0 a_{IB}^4/a_{BB}}$ value for localization as a function of (m_B/m_I) predicted by the weak ($\alpha > 1$) [7] and strong ($\beta > 4.7$) coupling descriptions. Although neither treatment should be quantitatively correct, they give comparable results for $1 < (m_B/m_I) < 10$.

In an inhomogeneous BEC confined by a trapping potential $V_B(\mathbf{r})$, the impurity-free density $\rho_B^0(\mathbf{r})$ varies spatially. Assuming that $\rho_B^0(\mathbf{r})$ varies slowly on the scale of R_0 ($R_0|\nabla\rho_B^0|/\rho_B^0 \ll 1$), we describe the self-localized impurities (which appear pointlike to the BEC) as immersed in a locally homogeneous superfluid. If the impurities localize on a time scale shorter than the time for the impurity to move appreciable ($E_0/\hbar \gg \omega_{\text{trap}}$), or for the impurities to attract each other (which depends on the average impurity density), we can describe the subsequent impurity dynamics as that of classical point particles subject to an effective potential. This potential energy $V_I^{\text{eff}}(\mathbf{r})$ is the sum of the external impurity potential $V_I^{\text{ext}}(\mathbf{r})$, the mean-field energy $\lambda_{IB}\rho_B^0(\mathbf{r})$, and the local binding energy $E_b[\rho_B^0(\mathbf{r})]$ of Eq. (12). Computing $\rho_B^0(\mathbf{r})$ in the Thomas-Fermi approximation, we find

$$V_I^{\text{eff}}(\mathbf{r}) = V_I^{\text{ext}}(\mathbf{r}) + \mu_B[1 - V_B(\mathbf{r})/\mu_B] \times \left\{\frac{\lambda_{IB}}{\lambda_{BB}} + 2\frac{m_B}{m_I}\left(\frac{-\beta^2(\mathbf{r})}{\pi} + \frac{3\beta(\mathbf{r})}{2}\right)\right\}, \quad (13)$$

where

$$\beta(\mathbf{r}) = \sqrt{\pi}\left(1 + \frac{m_B}{m_I}\right)\left(1 + \frac{m_I}{m_B}\right) \times \sqrt{\frac{a_{IB}^4}{a_{BB}}\rho_B^0(\mathbf{r} = 0)}\sqrt{1 - \frac{V_B(\mathbf{r})}{\mu_B}}. \quad (14)$$

Even when $V_I^{\text{ext}} = 0$ and the impurity-BEC interaction is repulsive $\lambda_{IB} > 0$—so that the boson mean-field [the first term in the {} bracket of Eq. (13)] would expel the impurity from the trap center—the binding energy [the other terms in the {} bracket of Eq. (13)] can give an overall potential that attracts the impurities to the trap middle. This behavior is illustrated in Fig. 3 for typical experimental parameters for ^{6}Li impurities in a ^{87}Rb BEC ($m_B/m_I = 14.5$). Even if in the true ground state the impurity would hover at the

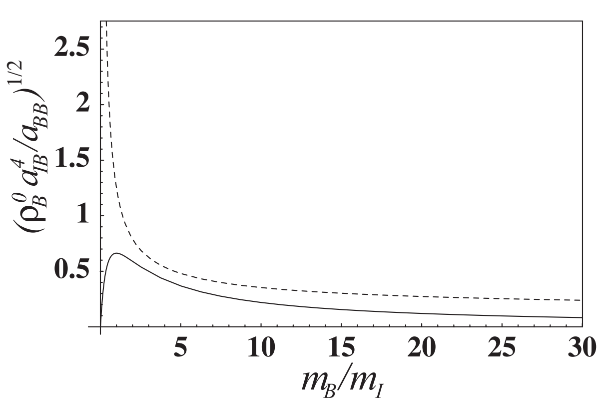

FIG. 2. Minimal $\sqrt{\rho_B^0 a_{IB}^4/a_{BB}}$ value for localization of the impurity as a function of the mass ratio m_B/m_I obtained from weak coupling ($\alpha > 1$) [7] and strong coupling [Eq. (7) and $\beta > 4.7$] descriptions, dashed and solid line, respectively.

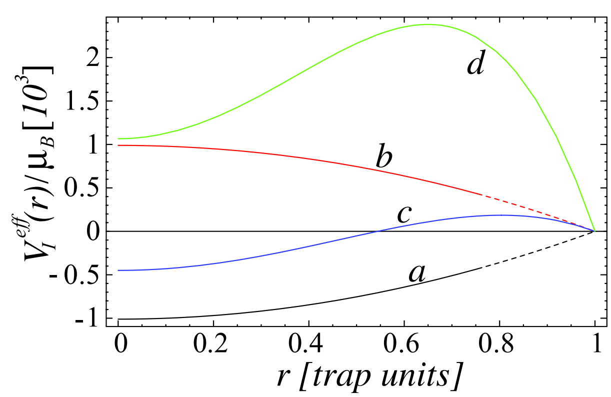

FIG. 3 (color online). Effective potential of the impurity as a function of distance to the trap center for (a) attractive and (b) repulsive boson-impurity interaction, using $\rho_B^0(0)|a_{IB}^3| = 10^{-3}$, $|a_{IB}|/a_{BB} = 10^3$, and $m_I = m_B$. (c), (d) have $a_{IB} > 0$, but the former has $\rho_B^0(0)|a_{IB}^3| = 0.05$ and $m_I = m_B$, while in the latter $\rho_B^0(0)|a_{IB}^3| = 10^{-3}$ and $m_B = 14.5m_I$ (^{6}Li impurities in a ^{87}Rb BEC). The dashed lines show the values at which the localization condition, $\beta > 4.7$, is not fulfilled.

edge of the BEC, the self-localization can form a metastable state with long tunneling times. In any case, $V_I^{\rm ext}$ can keep the impurities within the BEC, and $\lambda_{BI} > 0$ impurities tend to gather in the trap center.

A question remains regarding the accuracy of the product state (3) when $m_B/m_I \sim 1$, although $|E_b| \gg \mu_B$ implies a separation of time scales that justifies the lack of impurity-BEC correlations. For $|E_b| \lesssim \mu_B$, a more sophisticated description could be useful: we expect the above results to serve as a benchmark for future calculations.

When is the linearization of φ justified? With $\chi(\mathbf{r}) = e^{-r^2/2\sigma^2}/(\pi\sigma^2)^{3/4}$, the ratio of the peak-value of the impurity-induced fluctuation, $\delta\varphi(\mathbf{r}=0)$, to its spatial average, $\sqrt{\rho_B^0}$, equals $\delta\varphi(\mathbf{r}=0)/\sqrt{\rho_B^0} = -(1/\sqrt{\pi}) \times (1 + m_B/m_I)(a_{IB}/\sigma)f(\sigma/[\sqrt{2}\xi])$. Assuming a deeply bound polaron, $f(\sigma/[\sqrt{2}\xi]) \approx 1$ and $\sigma \approx 3\sqrt{\pi/2}R_0$, the condition $|\delta\varphi(\mathbf{r}=0)/\sqrt{\rho_B^0}| < 1/10$ takes the form

$$|\rho_B^0 a_{IB}^3| < \frac{m_I^2 m_B}{(m_B + m_I)^3}\frac{1}{1.89}\frac{1}{10}. \tag{15}$$

A large increase in a_{IB} above the critical value for self-localization could collapse the system when the linearization condition $\delta\rho_B/\rho_B^0$ is violated, as found in [11]. We speculate that in this regime $\lambda_{IB} > 0$ impurities could "phase separate," creating a hole in the BEC density.

In addition, the self-localization condition, $\beta > 4.7$, gives a lower bound to $|\rho_B^0 a_{IB}^3|$ and

$$\frac{m_I^2 m_B}{(m_B + m_I)^3}\frac{1}{18.9} > |\rho_B^0 a_{IB}^3| > 7.0\left(\frac{a_{BB}}{a_{IB}}\right)\frac{m_I^2 m_B^2}{(m_B + m_I)^4}, \tag{16}$$

defines the regime in which the linearization assumption holds and the strong-coupling description predicts self-localization. Furthermore, the (a_{IB}/a_{BB}) ratio is subject to conditions stemming from the validity of the contact description of the impurity-boson interactions, $|\rho_B^0 a_{IB}^3| \ll 1$, and from the outermost inequalities of (16), giving, respectively,

$$\left|\frac{a_{IB}}{a_{BB}}\right| \gg \frac{7.0 m_I^2 m_B^2}{(m_B + m_I)^4}, \quad \text{and} \quad \left|\frac{a_{IB}}{a_{BB}}\right| > \frac{132 m_B}{(m_B + m_I)}. \tag{17}$$

These conditions may require a Feshbach resonance, but this can be achieved with existing technology.

Time of flight measurements or diffraction of light resonant with impurities can detect polaron formation. In the former case, the tightly bound impurity wave function can expand faster and further than if the impurity were not self-bound [17]. In the latter case, the opening angle θ of the cone in which light of momentum k is scattered coherently, $2\sin(\theta/2) \sim 1/[k\sqrt{\langle r^2\rangle}]$, for $k \sim R_0^{-1}$ widens abruptly when the impurity self-localizes. Another detection/control scheme could use excited bound states of the impurity. Such states would entail exciting new applications like the creation of artificial atoms. Thus, their properties and conditions for existence deserve further investigation.

In summary, we have pointed out that a neutral impurity atom immersed in a homogeneous (or large) BEC can self-localize in a region smaller than the BEC-healing length. In a strong-coupling description with BEC linearization, the localizing BEC distortion gives rise to an attractive self-interaction with a spatial dependence identical to the BEC-mediated impurity-impurity interaction. Roughly, binding occurs when the range of the self-interaction range exceeds the extent of the bound impurity—more precisely, when $\beta > 4.7$, a condition that can be fulfilled experimentally. Using a variational Gaussian impurity wave function, we construct an analytical approximation to the binding energy from which we obtained the effective potential energy experienced by self-localized impurities in a trapped BEC.

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