Small polarons in dilute gas Bose-Einstein condensates

F. M. Cucchietti and E. Timmermans

T-4, Theory Division, Los Alamos National Laboratory, Los Alamos, NM 87545
(Dated: June 11, 2018)

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 small polaron-like 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.

PACS numbers: 03.75.Hh, 67.40.Yv

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 small 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 He-fluids, Miller et al. [6] 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 wavefunction with the variational one proposed by Feynman and Cohen to include ‘backflow’ [3]. The weak-coupling description predicts that phonon-drag increases the impurity mass from $m_I$ to $m_I^f = m_I/(1 - \alpha)$, where $\alpha$ is a dimensionless coupling constant. Its value depends on the BEC density $\rho_B$, 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 $q$:

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

For a dilute BEC and an impurity-boson contact interaction of scattering length $a_{IB}, V_q \rightarrow \lambda_{IB} = 2\pi h^2 (1/m_B + 1/m_I) a_{IB}$ and $E_q^B \rightarrow \hbar c_B q^3 / (1 + (\xi q)^2)$. Here, $\xi$ is the BEC-healing length which depends on the boson-boson scattering length $a_{BB}, \xi = 1/\sqrt{16\pi c_B \rho_B a_{BB}}$, and $c_B$ denotes the BEC velocity of sound, $c_B = \hbar/(2m_B \xi)$, so that

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

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

We describe the self-localized impurity in a strong-coupling treatment—similar to the Landau-Peierls description of small polarons [10]—using a product wavefunction:

$$
\Psi_{1,N}(r, x_1, x_2, ..., x_N) \sim \chi(r) \psi(x_1) \psi(x_2) ... \psi(x_N), \tag{3}
$$

where $\chi(r)$ represents the impurity wavefunction and $\psi$ denotes the single particle state occupied by the $N$ indistinguishable bosons of position $x_j$. We substitute Eq. (3) into the Hamiltonian eigenvalue equation and multiply first by $\psi^*(x_1) \psi^*(x_2) ... \psi^*(x_N)$, then by $\chi^*(r) \psi^*(x_2) ... \psi^*(x_N)$. Integrating the first equation over $x_1 x_2 ... x_N$, the second over $r$, choosing the ground state wavefunction to be real valued (e.g. $|\chi|^2 = \chi^2$) we obtain

$$
E_I \chi(r) = -\frac{h^2 \nabla \chi^2}{2m_I} \chi(r) + \lambda_{IB} \varphi^2(r) \chi(r), \tag{4a}
$$

$$
\mu_B \psi(x) = -\frac{h^2 \nabla \psi \psi(x) + \lambda_{BB} \varphi^3(x) + \lambda_{IB} \chi^2(x) \varphi(x)}, \tag{4b}
$$
where $\lambda_{BB} = \frac{4\pi \hbar^2}{m_B} a_{BB}$ and $\varphi$ 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, the BEC chemical potential is $\mu_B = E_{1,N} - E_{0,N}$, 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, $\varphi(r) = \sqrt{\rho_B^0} + \delta \varphi(r)$. Using $\mu_B \approx \lambda_{BB}^0$, the corresponding linearization of Eqs. 4 gives

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

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

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

As a modified Helmholtz equation, we solve Eq. 5b in terms of the Green function $G_\xi(r) = (4\pi)^{-1} e^{-r/\xi}/r$, where this number, induced by a general potential, was determined from thermodynamic arguments. The substitution of $\delta \varphi$ into $E_b \chi$ 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 $Q^2 = [\lambda_{IB} \lambda_{BB}^0] a_{IB} \times [1 + m_B/m_I]$,

$$E_b \chi(r) = -\frac{\hbar^2}{2m_I} \nabla^2_r \chi(r) \tag{6}$$

$$- \int dx Q^2 \frac{e^{-r/\xi}}{|x|} \chi^2(x) \chi(r).$$

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

$$E_0 = \left[ \lambda_{IB} \lambda_{BB}^0 \right] a_{IB}^3 \times 4\pi \left( \frac{m_B}{m_I} \right)^2 \left( 1 + \frac{m_I}{m_B} \right)^3$$

$$R_0 = \frac{1}{4\pi a^2_{BB} \lambda_{BB}^0} \times \frac{m_I m_B}{(m_B + m_I)^2},$$

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

The small polaron then corresponds to solutions of 4 with negative eigenvalue $E_b$. We break translational symmetry by hand and solve 4 iteratively for an s-wave impurity wavefunction centered on the origin. At each iteration step, we solve the eigenvalue problem for an impurity particle experiencing an effective potential $u(r) = \int dx \frac{\phi(x)}{r} e^{-r/\xi} \chi^2(x)$, in which we substitute the impurity density $\chi^2(x)$ obtained from the previous iteration. Spherical symmetry $u(r)$ to a one-dimensional integral. Working in natural units 5 and defining $\beta = \xi/R_0$, $u(r)$ reads

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

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

$$\beta = \frac{\xi}{R_0} = \sqrt{\pi} \frac{a_{IB}^3 m_B}{a_{BB} \rho_B^0} \left( 1 + \frac{m_I}{m_B} \right) \left( 1 + \frac{m_I}{m_B} \right). \tag{10}$$

Another candidate, $Q^2/[\hbar c_B^2] = 2(m_B/m_I)^3$. 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 $\beta$-values. Thus, this strong-coupling description predicts 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.

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 $\sqrt{\tau^2} = 4.64R_0$.

To understand the interesting ‘transition’ regime, $4.7 < \beta \leq 20$, which exhibits an intricate interaction dependence, we approximate the impurity wavefunction variationally. The effective impurity equation 4 is equivalent to minimizing the functional $E_V = T + V/2$ 14, where $T$ denotes the kinetic energy $T = -\frac{\hbar^2}{2m_I} \int d\chi(r) \nabla^2 \chi(r)$ and $V$ the self-interaction energy $V = \int d\chi^2(r) u(r)$, with respect to variations of the real-valued normalized wavefunction, $\chi(r)$. Choosing a Gaussian trial wavefunction, $\chi(r) = \exp (-|r|^2/2\sigma^2)/\left(\pi\sigma^2\right)^{3/4}$, the functional, written in natural units, becomes

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

where $f(a) = \int dr \, r e^{-r^2} e^{-r^2/2}$. Numerical minimization of 11, with respect to $\sigma$ gives a binding energy that agrees well with the iterative solution of 4, shown in dotted line in the inset of Fig. 1. The dashed line
mating the minimal that gives better agreement over the whole \( \beta \) plots the energy obtained by expanding (11) for large \( \beta > 4.7 \) and \( \beta > 4.7 \) 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 \( V_B(r) \), the impurity-free density \( \rho^0_B(r) \) varies spatially. Assuming that \( \rho^0_B(r) \) varies slowly on the scale of \( R_0 \) (\( R_0 | \nabla \rho^0_B(r)/\rho^0_B(r) | < 1 \)), we describe the self-localized impurities (which appear point-like 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 (\( E_0/\hbar >> \omega_{trap} \)), 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 \( V_{eff}(r) \) is the sum of the external impurity potential \( V_{ext}(r) \), the mean-field energy \( \lambda IB \rho^0_B(r) \), and the local binding energy \( E_b[\rho^0_B(r)] \) of Eq. (12). Computing \( \rho^0_B(r) \) in the Thomas-Fermi approximation, we find

\[
V_{eff}(r) = V_{ext}(r) + \mu_B \left( 1 - \frac{V_B(r)}{\mu_B} \right) \times \left\{ \frac{\lambda IB}{\lambda BB} + \frac{2 m_B}{m_I} \left( \frac{-\beta^2(r)}{\pi} + \frac{3 \beta(r)}{2} \right) \right\}, \tag{13}
\]

where

\[
\beta(r) = \sqrt{\pi} \left( 1 + \frac{m_B}{m_I} \right) \left( 1 + \frac{m_I}{m_B} \right) \sqrt{\frac{\alpha^2_{IB} \rho^0_B(r=0)}{\alpha^2_{BB} \rho^0_B(r)} \times \frac{1 - V_B(r)}{\mu_B}}. \tag{14}
\]

Even when \( V_{ext} = 0 \) and the impurity-BEC interaction is repulsive \( \lambda IB > 0 \) – so that the boson mean-field (the first

\[
E_b \approx [\lambda BB \rho^0_B]^2 (m_B/m_I) \left[ \frac{3}{2} - \frac{\beta^2}{\pi} \right], \tag{12}
\]

reminiscent of the strong coupling energy of traditional polarons, proportional to the square of the coupling constant \(|\alpha|\). In Fig. 2 we compare the corresponding minimal \( \sqrt{\rho^0_B a^2_{IB}/a_{BB}} \)-value for localization as a function of \( (m_B/m_I) \) predicted by the weak (\( \alpha > 1 \)) \( r \) and strong (\( \beta > 4.7 \)) coupling descriptions.

FIG. 1: Radial wavefunction 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 wavefunction vs \( \xi \) (dots). In dotted line, the variational result obtained numerically. The expansion for large \( \xi/R_0 \) is in dashed line, and the best fit \( E_b/E_0 \approx -1/\pi + 3R_0/2\xi \) in solid line.

FIG. 2: Minimal \( \sqrt{\rho^0_B a^2_{IB}/a_{BB}} \)-value for localization of the impurity as a function of the mass ratio \( m_B/m_I \) obtained from weak coupling (\( \alpha > 1 \)) \( r \) and strong coupling (Eq. (14) and \( \beta > 4.7 \)) descriptions, dashed and solid line respectively.

plots the energy obtained by expanding \( r \) for large \( \beta \), \( E_b/E_0 \approx -1/\pi + 2/\beta \), showing reasonable agreement with the iterative solution but slightly overestimating the minimal \( \beta \)-value for self-localization. A fit that gives better agreement over the whole \( \beta \)-range is \( E_b/E_0 \approx -1/\pi + 1.5/\beta \) (solid line in inset of Fig. 1). With \( E_0 = [\lambda BB \rho^0_B]^2 (m_B/m_I) \beta^2 \), \( E_b \) also equals

\[
E_b \approx [\lambda BB \rho^0_B]^2 (m_B/m_I) \left[ \frac{3}{2} - \frac{\beta^2}{\pi} \right], \tag{12}
\]

FIG. 3: Effective potential of the impurity as a function of distance to the trap center for (a) attractive and (b) repulsive boson-impurity interaction, using \( \rho^0_B(0) |a^2_{IB}| = 10^{-3} \), \( |a_{IB}|/a_{BB} = 10^3 \) and \( m_B = m_I = \mu_B \). (c) and (d) have \( a_{IB} > 0 \), but the former has \( \rho^0_B(0) |a^2_{IB}| = 0.05 \) and \( m_B = m_I \), while in the latter \( \rho^0_B(0) |a^2_{IB}| = 10^{-3} \) and \( m_B = 14.5 m_I \) (Li impurities in a \( ^{87}\text{Rb} \) BEC). The dashed lines show the values at which the localization condition, \( \beta > 4.7 \), is not fulfilled.
term in the {\-bracket} would expell the impurity from the trap center – the binding energy (the other terms in the {\-bracket}) 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 Li impurities in a \(R\) BEC (\(m_B/m_I = 14.5\)). Even if in the true ground state the impurity would hover at the edge of the BEC, the self-localization can form a metastable state with long tunneling times. In any case, \(V_T^{xt}\) can keep the impurities within the BEC, and \(\lambda_B > 0\) impurities tend to gather in the trap center.

A question remains regarding the accuracy of the product state \(\lambda\) when \(m_B/m_I \sim 1\), although \(|E_\beta| \gg \mu_B\) implies a separation of time scales that justifies the lack of impurity-BEC correlations. For \(|E_\beta| \lesssim \mu_B\), 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 \(\varphi\) justified? With \(\chi(r) = e^{-r^2/2\sigma^2}/(\pi \sigma^2)^{3/4}\), the ratio of the peak-value of the impurity-induced fluctuation, \(\delta \varphi(r = 0)\), to its spatial average, \(\sqrt{\rho_B}\), equals \(\delta \varphi(r = 0)/\sqrt{\rho_B} = -\l(1/(\sqrt{\pi})\r(1 + m_B/m_I)\l(\varphi(\sigma)/\sigma\r)\r.\) Assuming a deeply bound polaron, \(f(\sigma/\sqrt{2}K) \approx 1\) and \(\sigma \approx 3\sqrt{\pi}/2\kappa_0\), the condition \(|\delta \varphi(r = 0)/\sqrt{\rho_B}| < 1/10\) takes the form

\[
|\rho_B^{1/2}a_B^3| < \frac{m_B^2 m_B}{(m_B + m_I)^3} \frac{1}{1.89} \times 10. (15)
\]

A large increase in \(a_B\) 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 \(\lambda_B > 0\) 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 \(|\rho_B^{1/2}a_B^3|\) and

\[
|a_B| > \frac{7.0 m_B^2}{(m_B + m_I)^3}, \quad \frac{a_B}{a_{BB}} > \frac{132 m_B}{(m_B + m_I)}. (16)
\]

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 small 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 \(\theta\) of the cone in which light of momentum \(k\) is scattered coherently, \(2\sin(\theta/2) \sim 1/(k\sqrt{r^2})\), for \(k \sim R_0^{-1}\) widens abruptly when the impurity self-localizes.

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 wavefunction, 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.

\[\text{References}\]

[1] R. B. Diener, Biao Wu, M. G. Raizen, and Qian Niu, Phys. Rev. Lett. 89, 070401 (2002).
[2] C. A. Sackett and B. Deissler, J. Opt. B: Quantum Semiclass. Opt. 6 15 (2004).
[3] G. E. Astrakharchik and L. P. Pitaevskii, Phys. Rev. A 70, 013608 (2004).
[4] Unruh, W.G., Phys. Rev. D 14, 870 (1976).
[5] D. S. Wiersma, M. P. van Albada, B. A. van Tiggelen, and A. Lagendijk, Phys. Rev. Lett. 74, 4193 (1995).
[6] Chikkatur AP, et al., Phys. Rev. Lett., 85, 483 (2000); Hadzibabic Z. et al., Phys. Rev. Lett., 88, 160401 (2002).
[7] A. Miller, D. Pines and P. Nozieres, Phys. Rev., 127, 1452 (1962).
[8] R. P. Feynman, M. Cohen, Phys. Rev., 102, 1189 (1956).
[9] Chapter 6 in G. D. Mahan, 'Many-Particle Physics', Plenum Press, New York and London, 2nd edition (1990).
[10] Landau L. D., Pekar S. I., Zh Eksp. Teor. Fiz. 16 (1946).
[11] We became aware of work by R.M. Kalas and D. Blume, cond-mat/0512031 solving Eqs. 3 with a BEC-trapping potential to characterize \(|a_{BB}| < 0\) impurities trapped by their interactions with the BEC. They also observed self-localization (as a sudden decrease of the impurity extent below \(\xi\) at high \(|a_{BB}|\)-values and collapse at higher \(|a_{BB}|\)-values.
[12] L. Viverit, C. J. Pethick, and H. Smith, Phys. Rev. A, 61, 053605 (2000).
[13] M. J. Bijlsma, B. A. Heringa, and H. T. C. Stoof, Phys. Rev. A., 61, 053601 (2000).
[14] As opposed to the energy, \((T + V)\), the factor \(1/2\) prevents double counting when varying with respect to \(\chi(r)\).
[15] P. Massignan, C. J. Pethick, and H. Smith, Phys. Rev. A. 71, 023606 (2005).
[16] The success of the Gaussian wavefunction is paralleled in the description of traditional small polarons, see 3.
[17] Malcom Boshier, private communication.