Self-localized impurities embedded in a one-dimensional Bose-Einstein condensate and their quantum fluctuations

Krzysztof Sacha[1,2] and Eddy Timmermans[1]
[1]*T-4, Theory Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków, Poland*
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We consider the self-localization of neutral impurity atoms in a Bose-Einstein condensate in a one-dimensional model. Within the strong coupling approach, we show that the self-localized state exhibits parametric soliton behavior. The corresponding stationary states are analogous to the solitons of nonlinear optics and to the solitonic solutions of the Schrödinger-Newton equation (which appears in models that consider the connection between quantum mechanics and gravitation). In addition, we present a Bogoliubov-de Gennes formalism to describe the quantum fluctuations around the product state of the strong coupling description. Our fluctuation calculations yield the excitation spectrum and reveal considerable corrections to the strong coupling description. The knowledge of the spectrum allows a spectroscopic detection of the impurity self-localization phenomenon.

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I. INTRODUCTION

Recent work pointed out that neutral impurity atoms immersed in a dilute gas Bose-Einstein condensate (BEC) can spontaneously self-localize [1,2]. Repeated measurements of the impurity position would observe this particle's wave function to have a finite extent, even if its average position cannot be predicted *a priori* (at least if the BEC were homogeneous in the absence of the impurity). In three dimensions (3D), the BEC-impurity physics is akin to that of an electron moving in a polar crystal (a polaron) [3]. In 3D, the self-localization of a neutral atom BEC impurity occurs when the magnitude of the impurity-boson scattering length exceeds a minimal value (regardless of the sign of that interaction). The self-localized BEC impurity state resembles that of a small polaron. Traditional (i.e., electronic) small polarons have been successfully described in the strong coupling limit by the Landau-Pekar treatment [4] which assumes a wave function that is the product of a single electron wave function and a bosonic phonon state. The self-localized BEC impurity has been described similarly [1,2] by the product of a single-particle impurity wave function and a BEC state. Linearizing the BEC response to the impurity density then gives an effective impurity equation of a single particle experiencing an attractive Yukawa self-interaction potential [1]. While the ensuing analysis is elegant, the validity of the starting point (i.e., the product state) is much more questionable than in the description of traditional polarons. In the latter case, the large mass difference of crystal ions and electrons implies a clear separation of time scales which justifies the product state — one can always think of the slow (boson) field adjusting itself to the time-averaged field of the fast (electron) particle. In the cold atom BEC impurity, the boson and impurity atoms tend to have similar masses and the time scales do not separate. Hence, we can expect the deviations from the product state, the fluctuations that describe the entanglement of the impurity and boson degrees of freedom, to become much more significant.

In this paper, we describe the one-dimensional analogue of the BEC impurity, realizable in quasi-one-dimensional BEC's. For this system and for a specific choice of the parameters, we find an exact solution to the strong coupling equations and we solve for the quantum fluctuations as a function of the impurity-boson mass ratios. The explicit solution to the strong-coupling equations are parametric solitons, which establishes that the one-dimensional (1D) analogues of self-localized BEC impurities are optical solitons. Specifically, the impurity soliton solutions resemble the solitons that appear when a quadratic nonlinearity is responsible for second-harmonic generation [5,6]. The Schrödinger-Newton equation that models the gravitational interaction, while preventing the quantum-mechanical spreading of the center-of-mass position of macroscopic objects [7–9], as well as the mean-field equations of coupled atomic-molecular BEC's [10,11] possess similar parametric soliton solutions. The connection with these very different fields of physics further extends the scope of the BEC-impurity physics.

The experimental realization of the BEC-impurity systems requires the creation of distinguishable atoms in BECs. This feat has been realized by converting a fraction of the BEC atoms with a two-photon Raman transition to a different spin state in order to observe the superfluid suppression of slow impurity scattering by the BEC [12], or by trapping distinct species of atoms [13,14] or isotopes [15]. In this paper, we describe a BEC trapped in a 1D box. Our predictions apply to atomic traps with strong confinement in the two transverse directions (quasi-1D). A 1D box potential was recently achieved experimentally [16], but our calculations should also describe the physics of quasi-1D BEC's with trapping potentials that vary slowly in the longitudinal direction.

The paper is organized as follows: In Sec. II, we introduce the model and work within the product state description. Section III presents a formalism that goes beyond the product state ansatz by means of a Bogoliubov description of the quantum fluctuations. In Sec. IV, we discuss our numerical results, and we conclude in Sec. V.

II. STRONG COUPLING APPROACH

We consider M impurity bosonic atoms immersed in a homogeneous BEC in a 1D model. The Hamiltonian of the system reads

$$\hat{H} = \int dx \left\{ \hat{\varphi}^{\dagger}(x) \left[-\frac{\hbar^2 \partial_x^2}{2m_B} + \frac{\lambda_{BB}}{2} \hat{\varphi}^{\dagger}(x)\hat{\varphi}(x) - \mu_B \right] \hat{\varphi}(x) + \hat{\psi}^{\dagger}(x) \times \left[-\frac{\hbar^2 \partial_x^2}{2m_I} - E_I \right] \hat{\psi}(x) \quad + \lambda_{IB}\hat{\varphi}^{\dagger}(x)\hat{\varphi}(x)\hat{\psi}^{\dagger}(x)\hat{\psi}(x), \right. \quad (1)$$

where $\hat{\varphi}(x)$ and $\hat{\psi}(x)$ stand for the condensate boson and impurity atom field operators, respectively; m_B and m_I are the boson and impurity masses, while μ_B and E_I represent the chemical potentials of the BEC and impurity systems. We assume contact boson-boson and impurity-boson interactions characterized by λ_{BB} and λ_{IB}, respectively. We neglect the mutual interactions of impurity atoms in the assumption that their number and local density remains sufficiently small.

In the strong coupling treatment [1,4], we describe the system in terms of a product state,

$$\Psi = \eta(y_1) \cdots \eta(y_M)\zeta(x_1) \cdots \zeta(x_N), \quad (2)$$

where $\eta(x)$ is the wave function occupied by the M impurity atoms and $\zeta(x)$ is the single particle state occupied by the N bosons. The expectation value of the Hamiltonian (1) for the product state (2) gives an energy that reaches its minimal value when the following equations are satisfied:

$$\left[-\frac{\hbar^2 \partial_x^2}{2m_B} + \lambda_{BB}\varphi^2(x) + \lambda_{IB}\psi_0^2(x) \right] \varphi(x) = \mu_B \varphi(x),$$

$$\left[-\frac{\hbar^2 \partial_x^2}{2m_I} + \lambda_{IB}\varphi^2(x) \right] \psi_0(x) = E_I \psi_0(x), \quad (3)$$

where

$$\varphi(x) = \sqrt{N}\zeta(x),$$

$$\psi_0(x) = \sqrt{M}\,\eta(x), \quad (4)$$

and we have assumed that both $\varphi(x)$ and $\psi_0(x)$ are real valued — an assumption that is permitted since we wish to describe a ground state. We also assume that M, the number of impurity atoms is small, so that we may expect only a slight modification of the boson wave function $\varphi(x)$ with respect to the homogeneous BEC solution $\sqrt{\rho}$, where ρ is the BEC density. Therefore, we substitute

$$\varphi(x) = \sqrt{\rho} + \phi_0(x), \quad (5)$$

into Eq. (3) and keep linear terms in $\phi_0(x)$ only,

$$\left[-\frac{\hbar^2 \partial_x^2}{2m_B} + 2\lambda_{BB}\rho \right] \phi_0(x) + \lambda_{IB}\sqrt{\rho}\psi_0^2(x) = 0, \quad (6)$$

$$\left[-\frac{\hbar^2 \partial_x^2}{2m_I} + 2\lambda_{IB}\sqrt{\rho}\phi_0(x) \right] \psi_0(x) = \tilde{E}_I \psi_0(x), \quad (7)$$

where $\mu_B \approx \lambda_{BB}\rho$ and $\tilde{E}_I = E_I - \lambda_{IB}\rho$ [1]. This approximation is valid provided,

$$\frac{\phi_0(x)}{\sqrt{\rho}} \ll 1. \quad (8)$$

Then, Eq. (6) can be solved in terms of the Green function of the 1D Helmholtz equation,

$$\phi_0(x) = -\frac{m_B \lambda_{IB}\sqrt{\rho}}{\hbar^2 \chi} \int dy\, \psi_0^2(y) e^{-\chi|x-y|}, \quad (9)$$

where

$$\chi = \frac{2\sqrt{m_B \lambda_{BB}\rho}}{\hbar}, \quad (10)$$

represents the BEC-coherence length. The substitution of Eq. (9) into Eq. (7) gives an equation that describes impurity atoms self-interacting through an attractive exponential potential. Note the difference with the three-dimensional situation in which the self-interaction takes place through a Yukawa (screened Coulomb) potential [1].

Equations similar to Eqs. (6) and (7) occur in nonlinear optics [5,6], in mean-field descriptions of coupled atomic-molecular BEC's [10,11] and in the Schrödinger-Newton model [8]. These equations are known to possess parametric soliton solutions. In the present case, an analytical solution exists for a particular value of the condensate density. For

$$\rho = \frac{M^2 m_I^2 \lambda_{IB}^4}{36\hbar^2 m_B \lambda_{BB}^3}, \quad (11)$$

the Eqs. (6) and (7) transform into

$$\left[-\frac{\partial_x^2}{2} + \frac{M}{3} \right] \phi_0(x) + \left(\frac{M}{6} \right)^{1/4} \sqrt{\frac{m_B}{m_I}}\, \mathrm{sgn}(\lambda_{IB}) \psi_0^2(x) = 0,$$

$$\left[-\frac{\partial_x^2}{2} + 2\left(\frac{M}{6} \right)^{1/4} \sqrt{\frac{m_I}{m_B}}\, \mathrm{sgn}(\lambda_{IB}) \phi_0(x) \right] \psi_0(x) = E\psi_0(x). \quad (12)$$

These coupled equations possess a solitonic solution,

$$E = -\frac{M}{3},$$

$$\phi_0(x) = -\,\mathrm{sgn}(\lambda_{IB}) \sqrt{\frac{3M^{3/2} m_B}{8\sqrt{6} m_I}} \cosh^{-2}\left(\sqrt{\frac{M}{6}} x \right),$$

$$\psi_0(x) = \sqrt{\frac{3M^{3/2}}{4\sqrt{6}}} \cosh^{-2}\left(\sqrt{\frac{M}{6}} x \right). \quad (13)$$

In Eqs. (12) and (13), we have scaled energy and length by E_0 and x_0 where

$$E_0 = \frac{\lambda_{IB}^2}{\hbar}\sqrt{\frac{m_B\rho}{\lambda_{BB}}},$$

$$x_0 = \left(\frac{\hbar^6\lambda_{BB}}{m_I^2 m_B \rho \lambda_{IB}^4}\right)^{1/4}. \tag{14}$$

The soliton (13) describes a bound state of the impurity-BEC system with an impurity extent of the order $\sqrt{6/M}$, which is precisely the BEC-healing length since

$$\frac{\xi}{x_0} = \frac{\hbar}{x_0\sqrt{m_B\lambda_{BB}\rho}} = \sqrt{\frac{6}{M}}. \tag{15}$$

The self-localization takes place for either sign of the impurity-BEC interaction ($\lambda_{IB}>0$ and $\lambda_{IB}<0$). In addition to and caused by the impurity localization, the condensate is deformed. The BEC exhibits a dip in the density if the impurity and BEC-particles mutually repel ($\lambda_{IB}>0$), and exhibits a hump if the they attract ($\lambda_{IB}<0$).

We have shown there exists a class of analytical solutions for a particular choice of parameters of the 1D BEC-impurity system. In general, one can solve the coupled equations numerically. Using the Gaussian ansatz for $\psi_0(x)$, one can also show that there is impurity self-localization in the 1D model even as $\lambda_{IB}\to 0$ [17]. This is markedly different from the 3D situation for which the impurity-BEC interaction must be sufficiently strong before self-localization sets in [1].

III. QUANTUM FLUCTUATIONS

Hamiltonian (1) describes a small number of bosonic impurity particles immersed in a BEC in a 1D-model with interparticle interactions of the contact type. Assuming that the presence of the impurity atoms does not significantly perturb the condensate, we may decompose the bosonic field operator into

$$\hat{\varphi}(x) \approx \sqrt{\rho} + \hat{\phi}(x), \tag{16}$$

where $\sqrt{\rho}$ denotes the stationary mean-field solution for a condensate wave function in the absence of impurities, and $\hat{\phi}(x)$ describes the small perturbations of the condensate caused by the impurity (or impurities). We substitute Eq. (16) into the Hamiltonian (1) and keep terms that are quadratic in the $\hat{\phi}$ operator only. Next, we replace the condensate boson-boson interaction term in the Hamiltonian by

$$\frac{\lambda_{BB}}{2}\rho(\hat{\phi}\hat{\phi} + 4\hat{\phi}^\dagger\hat{\phi} + \hat{\phi}^\dagger\hat{\phi}^\dagger) \approx 3\lambda_{BB}\rho\hat{\phi}^\dagger\hat{\phi}. \tag{17}$$

This approximation implies that we neglect the depletion of the BEC induced by the interactions between condensate particles. The BEC depletion that we compute is then caused entirely by the interactions with the impurities. We expect that this approximation will not greatly affect the impurity physics. It does, however, modify the description of long-wavelength BEC excitations. In the absence of impurities, approximation (17) corresponds to the Hartree-Fock approximation. This approach predicts a gap in the BEC-excitation spectrum, contrary to the Goldstone (or Hugenholtz-Pines) theorem, and different from the Bogoliubov spectrum [18]. The final effective Hamiltonian in the units (14) reads

$$\hat{H}_{\text{eff}} = \int dx\left\{\hat{\phi}^\dagger(x)\left[-\frac{m_I\partial_x^2}{2m_B} + \alpha\right]\hat{\phi}(x) + \hat{\psi}^\dagger(x)\left[-\frac{\partial_x^2}{2} - E\right]\hat{\psi}(x) + \gamma\left[\hat{\phi}^\dagger(x) + \hat{\phi}(x)\right]\hat{\psi}^\dagger(x)\hat{\psi}(x)\right\}, \tag{18}$$

where

$$\alpha = \frac{2\hbar}{\lambda_{IB}^2}\sqrt{\frac{\lambda_{BB}^3\rho}{m_B}},$$

$$\gamma = \text{sgn}(\lambda_{IB})\left(\frac{\hbar^2\lambda_{BB}^3 m_{\text{I}}^2\rho}{\lambda_{IB}^4 m_B^3}\right)^{1/8}. \tag{19}$$

We treat the resulting Hamiltonian (18) with a Bogoliubov approximation [18]: First, we solve the mean-field equations, then we construct the quantum fluctuations around the mean-field solutions. To this end, we expand the field operators as

$$\hat{\phi}(x) \approx \phi_0(x) + \delta\hat{\phi}(x),$$

$$\hat{\psi}(x) \approx \psi_0(x) + \delta\hat{\psi}(x). \tag{20}$$

In zeroth order in the $\delta\hat{\phi}$ and $\delta\hat{\psi}$ operators, one obtains the mean-field equations,

$$\left[-\frac{m_{\text{I}}\partial_x^2}{2m_B} + \alpha\right]\phi_0(x) + \gamma|\psi_0(x)|^2 = 0,$$

$$\left[-\frac{\partial_x^2}{2} + \gamma\{\phi_0(x) + \phi_0^*(x)\}\right]\psi_0(x) = E\psi_0(x), \tag{21}$$

identical to Eqs. (6) and (7), written in the units of Eq. (14).

While the mean-field description of coupled atomic-molecular BECs gives solitonic solutions that are identical to Eq. (13) [10,11], the Hamiltonian of the atomic-molecular BECs is different from Eq. (18). The coupled atomic-molecular BEC Hamiltonian contains terms that convert molecules into atoms and vice versa, rather than the interaction term $\gamma[\hat{\phi}^\dagger(x)+\hat{\phi}(x)]\hat{\psi}^\dagger(x)\hat{\psi}(x)$. The latter term can be found in models where bosonic particles $\hat{\psi}$ feel a long-range force caused by the exchange of a mesonlike particle $\hat{\phi}$ [11].

Given that $\psi_0(x)$ and $\phi_0(x)$ satisfy the mean-field equations (21), the first-order terms in the $\delta\hat{\phi}$ and $\delta\hat{\psi}$ operators cancel. The second-order term gives an effective Hamiltonian that takes the form

$$\hat{H}_{\mathrm{eff}} \approx \frac{1}{2}\int dx(\delta\hat{\phi}^{\dagger},-\delta\hat{\phi},\delta\hat{\psi}^{\dagger},-\delta\hat{\psi})\mathcal{L}\begin{pmatrix}\delta\hat{\phi}\\ \delta\hat{\phi}^{\dagger}\\ \delta\hat{\psi}\\ \delta\hat{\psi}^{\dagger}\end{pmatrix}, \quad (22)$$

where

$$\mathcal{L}=\begin{pmatrix} h_{\phi} & 0 & \gamma\psi_0^*(x) & \gamma\psi_0(x)\\ 0 & -h_{\phi} & -\gamma\psi_0^*(x) & -\gamma\psi_0(x)\\ \gamma\psi_0(x) & \gamma\psi_0(x) & h_{\psi} & 0\\ -\gamma\psi_0^*(x) & -\gamma\psi_0^*(x) & 0 & -h_{\psi}\end{pmatrix}, \quad (23)$$

and

$$h_{\phi}=-\frac{m_1\partial_x^2}{2m_B}+\alpha$$

$$h_{\psi}=-\frac{\partial_x^2}{2}+\gamma\{\phi_0(x)+\phi_0^*(x)\}-E. \quad (24)$$

The problem of diagonalizing Hamiltonian (22) reduces to the problem of diagonalizing the non-Hermitian operator $\mathcal{L}$ (i.e., to solving equations of the Bogoliubov-de Gennes type). The $\mathcal{L}$–operator possesses two symmetries (similar to the symmetries of the original Bogoliubov-de Gennes equations [19]),

$$u_1\mathcal{L}u_1=-\mathcal{L}^*,$$

$$u_3\mathcal{L}u_3=\mathcal{L}^{\dagger}, \quad (25)$$

where

$$u_1=\begin{pmatrix}\sigma_1 & 0\\ 0 & \sigma_1\end{pmatrix},\quad u_3=\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix}, \quad (26)$$

and

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad (27)$$

are the first and third Pauli matrices, respectively.

Suppose that all eigenvalues of the $\mathcal{L}$–operator are real. Symmetries (25) imply that if

$$|\Psi_k^R\rangle=\begin{pmatrix}|u_k^{\phi}\rangle\\ |v_k^{\phi}\rangle\\ |u_k^{\psi}\rangle\\ |v_k^{\psi}\rangle\end{pmatrix}, \quad (28)$$

is a right eigenvector of the $\mathcal{L}$-operator with eigenvalue ε_k, then $|\Psi_k^{\mathrm{L}}\rangle=u_3|\Psi_k^R\rangle$ is a left eigenvector of the same eigenvalue ε_k, and $u_1|\Psi_k^{R*}\rangle$ is a right eigenvector with eigenvalue $-\varepsilon_k$. Except for the eigenstates corresponding to zero eigenvalue, the eigenstates of the $\mathcal{L}$–operator can be divided into two families "+" and "–",

$$\langle\Psi_k^R|u_3|\Psi_{k'}^R\rangle=\pm\delta_{k,k'}. \quad (29)$$

We apply the Bogoliubov transformation,

$$\begin{pmatrix}\delta\hat{\phi}(x)\\ \delta\hat{\phi}^{\dagger}(x)\\ \delta\hat{\psi}(x)\\ \delta\hat{\psi}^{\dagger}(x)\end{pmatrix}=\sum_{k\in\text{“+”}}[\hat{b}_k\Psi_k^{\mathrm{R}}(x)+\hat{b}_k^{\dagger}u_1\Psi_k^{\mathrm{R}*}(x)], \quad (30)$$

with quasi-particle operators that can be written as

$$\hat{b}_k^{\dagger}=-\langle v_k^{\phi*}|\hat{\phi}\rangle+\langle u_k^{\phi*}|\hat{\phi}^{\dagger}\rangle-\langle v_k^{\psi*}|\hat{\psi}\rangle+\langle u_k^{\psi*}|\hat{\psi}^{\dagger}\rangle,$$

$$\hat{b}_k=\langle u_k^{\phi}|\hat{\phi}\rangle-\langle v_k^{\phi}|\hat{\phi}^{\dagger}\rangle+\langle u_k^{\psi}|\hat{\psi}\rangle-\langle v_k^{\psi}|\hat{\psi}^{\dagger}\rangle, \quad (31)$$

and that fulfill the bosonic commutation relation $[\hat{b}_k,\hat{b}_{k'}^{\dagger}]=\delta_{k,k'}$. This transformation gives an effective Hamiltonian that is diagonal

$$\hat{H}_{\mathrm{eff}}\approx\sum_{k\in\text{“+”}}\varepsilon_k\hat{b}_k^{\dagger}\hat{b}_k. \quad (32)$$

To obtain the energy eigenvalues and eigenstates of effective Hamiltonian (22), one has to solve mean-field equations (21), then diagonalize operator (23). For a specific value of the average BEC-density, given by Eq. (11), we obtain solitonic solution (13) of the mean-field equations. In that case, the eigenstates of the $\mathcal{L}$–operator corresponding to the zero eigenvalue take on the form

$$\begin{pmatrix}0\\ 0\\ \cosh^{-2}\left(\sqrt{\frac{M}{6}}x\right)\\ -\cosh^{-2}\left(\sqrt{\frac{M}{6}}x\right)\end{pmatrix},\quad \begin{pmatrix}-\sqrt{\frac{m_B}{2m_I}}\\ -\sqrt{\frac{m_B}{2m_I}}\\ \mathrm{sgn}(\lambda_{IB})\\ \mathrm{sgn}(\lambda_{IB})\end{pmatrix}\partial_x\cosh^{-2}\left(\sqrt{\frac{M}{6}}x\right), \quad (33)$$

where the first eigenvector corresponds to the breaking of the U(1) symmetry in the BEC-Bogoliubov theory [19], while the second eigenvector corresponds to the breaking of the translational symmetry, indicating that the translation of the soliton costs no energy. There is another zero-momentum eigenstate which has a nonzero eigenvalue. This eigenvalue and its eigenvector take on simple analytical forms:

$$\varepsilon = \frac{Mm_I}{3m_B}, \quad \Psi^R(x) = \begin{pmatrix} \mathrm{sgn}(\lambda_{IB}) \\ 0 \\ \frac{3}{2}\sqrt{\frac{m_B}{2m_I}}\cosh^{-2}\left(\sqrt{\frac{M}{6}}x\right) \\ -\frac{3}{2}\sqrt{\frac{m_B}{2m_I}}\cosh^{-2}\left(\sqrt{\frac{M}{6}}x\right) \end{pmatrix} \frac{1}{\sqrt{L}}, \tag{34}$$

where L is the size of the 1D box. Other eigenstates can be found numerically. In the next section, we present numerical results for realistic parameter values.

IV. NUMERICAL RESULTS

We consider eight impurity ^{85}Rb atoms, i.e., $M=8$, immersed in a BEC of ^{23}Na atoms in an elongated trap that is a box in the axial direction, while in the transverse directions there is a harmonic trap of frequency $\omega_\perp$. The transverse $\omega_\perp$-confinement is so strong that only the ground states of the transverse degrees of freedom are relevant. In this quasi-1D regime, the system is effectively 1D and confined by a 1D-box potential. The coupling constants of Hamiltonian (1) read

$$\lambda_{IB} = 2\pi\hbar^2 a_{IB}\left(\frac{1}{m_I}+\frac{1}{m_B}\right)\frac{1}{\pi(\sigma_B^2+\sigma_I^2)} = 2\,\hbar\,\omega_\perp a_{IB},$$

$$\lambda_{BB} = \frac{4\pi\hbar^2 a_{BB}}{m_B}\frac{1}{2\pi\sigma_B^2} = 2\,\hbar\,\omega_\perp a_{BB}, \tag{35}$$

where the s-wave scattering lengths $a_{BB}=3.4$ nm and $a_{IB}=16.7$ nm [20]. The $\sigma_B=\sqrt{\hbar/m_B\omega_\perp}$ and $\sigma_I=\sqrt{\hbar/m_I\omega_\perp}$ lengths represent the ground state extents of a single BEC-boson particle and of a single impurity atom confined by the two-dimensional harmonic trap in the transverse direction with frequency $\omega_\perp$. We take the transverse trapping frequency to be equal to $\omega_\perp = 2\pi\times 500$ Hz. Assuming that the size of the box in the longitudinal direction is equal to 100 μm (in units (14), this length corresponds to a box size $L\approx 80$), we confine 11,000 atoms in the BEC. These parameters correspond to the specific value of the condensate density (11) and are well within the experimental range [16].

Figure 1 shows the excitation spectra that were calculated numerically with periodic boundary conditions. Note that the dispersion shows two branches. Each excitation of the lower branch delocalizes an impurity atom, except for the very lowest level, which corresponds to an excitation that leaves the impurity atom localized, as shown in Fig. 2. The upper branch corresponds to particlelike BEC excitations, in which the impurity remains localized, as shown in Fig. 3. The highest curves of Fig. 3 show the mode of Eq. (34). In Fig. 1, we have also plotted the BEC spectrum calculated within the Hartree-Fock approximation [18],

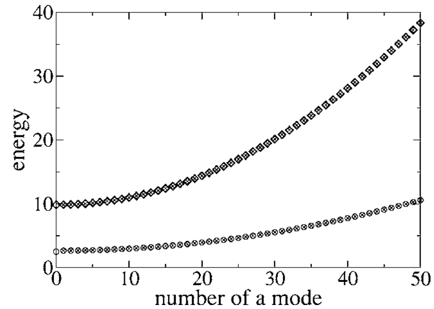

FIG. 1. Excitation spectrum of the quasi-1D ^{23}Na BEC with eight ^{85}Rb atom impurities, in the energy units of Eq. (14). The upper branch corresponds to BEC-particlelike excitations, while the impurities remain localized. This branch coincides with the Hartree-Fock spectrum of the BEC without the impurity atoms (diamonds) given by Eq. (36). The lower branch corresponds to excitations that delocalize the impurity atoms (except for the lowest-energy level, as can be seen in Fig. 2). Circles denote even solutions and crosses show solutions of odd symmetry.

$$\varepsilon_n^{\mathrm{HF}} = \frac{m_I}{m_B}\left[\frac{2\pi^2}{L^2}n^2 + \frac{M}{3}\right], \tag{36}$$

where $n=0,1,\ldots$ Actually, to obtain Eq. (36), we have used Hamiltonian (18) in which we neglected terms involving the $\hat{\psi}(x)$ operator. The Hartree-Fock spectrum (36) provides the relevant comparison for the model since the terms neglected in Eq. (17) correspond to the Hartree-Fock description of the single BEC. Figure 1 shows that the upper energy branch is nearly identical to the Hartree-Fock BEC spectrum in the absence of impurities. The lower energy branch describes

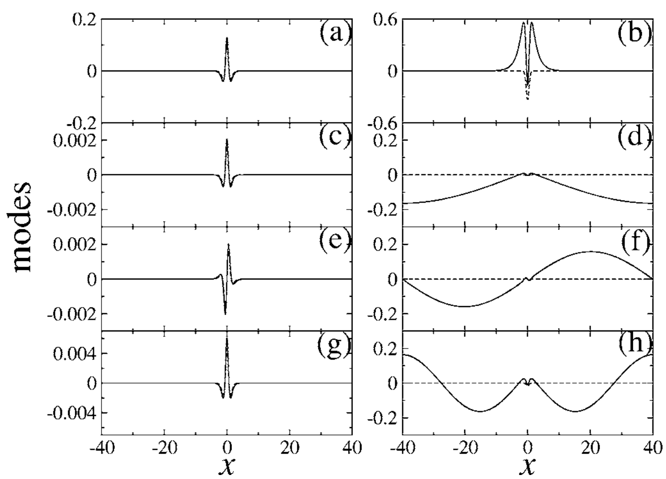

FIG. 2. The eigenstates of the $\mathcal{L}$-operator, Eq. (23), corresponding to the lower-energy branch of the Hamiltonian (32), see Fig. 1. Left column is related to condensate modes, i.e., u_k^ϕ (solid lines) and v_k^ϕ (dashed lines — hardly visible behind the solid lines), while the right column is related to impurities modes, i.e., u_k^ψ (solid lines) and v_k^ψ (dashed lines). There are four lowest-energy eigenstates presented in the figure, i.e., (a)-(b) is the lowest one, (c)-(d), (e)-(f), and (g)-(h) are shown in order of increasing energy. The states describe the excitation of eight self-localized ^{85}Rb atoms embedded in a quasi-1D ^{23}Na BEC.

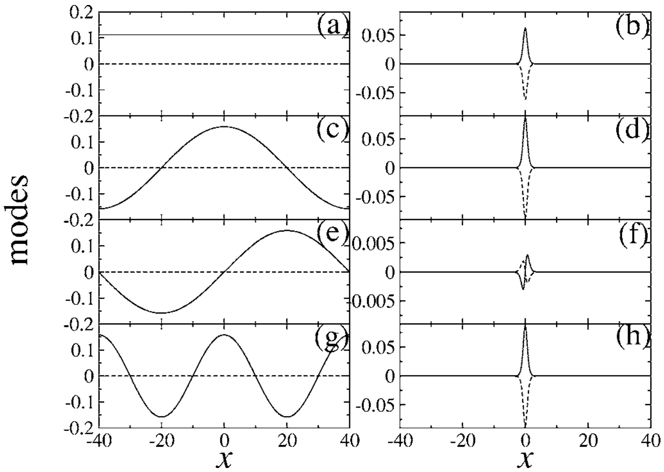

FIG. 3. The same as in Fig. 2 but for the upper energy branch of the Hamiltonian (32), see Fig. 1. The modes shown in panels (a)-(b) correspond to the solution given by Eq. (34).

impurity excitations with negligible excitation of the BEC, see Fig. 2). We interpret the energy gap in the lower-energy branch (as the wave number tends to zero) as the minimal energy needed to break the self-localization bond of the many-body BEC-impurity system. This gap is then a characteristic feature of impurity self-localization. Its detection by means of Bragg spectroscopy [21], for instance, can serve as a smoking-gun signal for the observation of BEC-impurity self-localization.

The ground state of the system is the Bogoliubov vacuum state $|0\rangle$, i.e., the state annihilated by all $\hat{b}_k$ operators in Eq. (31). We can estimate the quantum fluctuation corrections to the product state by calculating the density of the impurity atoms:

$$\langle 0|\hat{\psi}^{\dagger}(x)\hat{\psi}(x)|0\rangle = \psi_0^2(x) + \langle 0|\delta\hat{\psi}^{\dagger}(x)\delta\hat{\psi}(x)|0\rangle = \psi_0^2(x) + \sum_{k\in\text{“+”}} [v_k^{\psi}(x)]^2. \quad (37)$$

In Fig. 4, we plot $\psi_0^2(x)$ and $\Sigma_k[v_k^{\psi}(x)]^2$. The quantum fluctuation contribution to the impurity density is

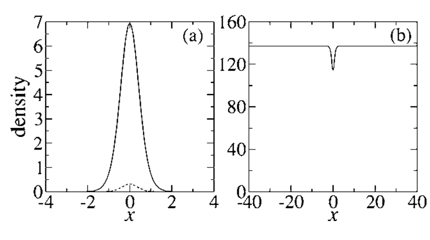

FIG. 4. Panel (a): solid line denotes the density of the impurity atoms, $\psi_0^2(x)$, calculated within the product state ansatz, dashed line is the correction to this density, i.e. $\langle 0|\delta\hat{\psi}^{\dagger}(x)\delta\hat{\psi}(x)|0\rangle = \Sigma_k[v_k^{\psi}(x)]^2$, obtained within the formalism that goes beyond the product state approximation. Panel (b): BEC density given by Eq. (39). The results are related to eight ^{85}Rb atoms immersed in a BEC of ^{23}Na atoms. The length is given in the units of Eq. (14).

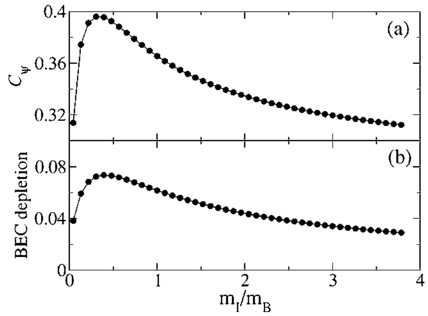

FIG. 5. Integral (38) [panel (a)] and condensate depletion [panel (b)] as a function of the impurity mass m_I. Note that the maximal values of the C_ψ and condensate depletion correspond to $m_I/m_B \approx 0.5$.

$$C_\psi = \int dx \sum_{k\in\text{“+”}} [v_k^{\psi}(x)]^2 = 0.31, \quad (38)$$

as compared to the value of 8 for the integral of $\psi_0^2(x)$, which shows that the fluctuation corrections to the product state are not insignificant. In the case of a single impurity, i.e., $M=1$, keeping the other parameters fixed, $C_\psi=0.30$ and the fluctuation corrections turn out to be more dramatic. The condensate density (see Fig. 4) reads:

$$\langle 0|\hat{\varphi}^{\dagger}(x)\hat{\varphi}(x)|0\rangle = \left[\sqrt{x_0\rho} + \phi_0(x)\right]^2 + \langle 0|\delta\hat{\phi}^{\dagger}(x)\delta\hat{\phi}(x)|0\rangle \approx x_0\rho + 2\sqrt{x_0\rho}\,\phi_0(x), \quad (39)$$

where we have introduced approximations due to the facts that $\phi_0(x)/\sqrt{x_0\rho} \leqslant 0.083$ [that also justify the linearization (5) or (16)] and $\langle 0|\delta\hat{\phi}^{\dagger}(0)\delta\hat{\phi}(0)|0\rangle/\phi_0^2(0) \approx 0.03$.

Decreasing the mass of the impurity atom, while keeping all other parameters fixed, integral (38) and the BEC depletion increase and reach their maximal values for $m_I/m_B \approx 0.5$, see Fig. 5. This shows that when the impurity mass is half that of the BEC-bosons, the product state approximation needs the largest corrections. Qualitatively, this behavior agrees with the time scale separation argument, which predicts that the large and small mass ratio regimes are well described by a product state [4].

V. CONCLUSIONS

We have considered the self-localization of neutral bosonic impurity atoms embedded in a dilute gas Bose-Einstein condensate in a 1D model. We have analyzed the system within a Bogoliubov formalism that describes the quantum fluctuations around the strong coupling product state approximation previously made in the cold-atom literature [1,2]. Our description gives an excitation spectrum that consists of two branches. The lower-energy branch corresponds to excitations that delocalize the impurity atoms (with the exception of the lowest-energy excitation). The higher-energy branch corresponds to BEC-particlelike excitations (and coincides, in our approximation, with the Hartree-Fock spectrum of the BEC in the absence of the impurity atoms), while the impurities remain self-localized.

The energy gap in the lower-energy branch (i.e., the branch that corresponds to the excitation of impurity atoms with negligible excitation of the BEC) suggests a spectroscopic means (Bragg spectroscopy [21]) for detecting BEC-impurity self-localization.

The parameters of our calculation are well within the experimental range. An extension of this approach to the three-dimensional BEC-impurity system appears straightforward. One can extend the formalism to account for the presence of a larger number of impurity atoms by including a nonlinear term in Hamiltonian (1) to account for interactions among the impurity atoms. Also, the depletion of the BEC caused by the interactions among condensate particles (neglected in the present calculations) can be included.

Furthermore, our calculations reveal the close analogy of 1D BEC-impurity self-localization with parametric solitons known in nonlinear optics [5,6], in the Schrödinger-Newton model [7–9], and in the coupled atomic-molecular BEC system [10,11]. The problem of impurity atoms immersed in an atomic BEC offers intriguing opportunities for experimentally realizing the phenomena predicted in these fields.

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