Self-localized state and solitons in a Bose-Einstein-condensate–impurity mixture at finite temperature

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(Received 1 April 2014; published 29 July 2014)

We study the properties of a Bose-Einstein-condensate (BEC)–impurity mixture at finite temperature employing the time-dependent Hartree-Fock Bogoliubov (TDHFB) theory which is a set of coupled nonlinear equations of motion for the condensate and its normal and anomalous fluctuations on the one hand and for impurity on the other. The numerical solutions of these equations in the static quasi-one-dimensional regime show that the thermal cloud and the anomalous density are deformed as happens to the condensate and the impurity becomes less localized at nonzero temperatures. Effects of the BEC fluctuations on the self-trapping state are studied in homogeneous weakly interacting BEC-impurity at low temperature. The self-trapping threshold is also determined in such a system. The formation of solitons in the BEC-impurity mixture at finite temperature is investigated.

DOI: 10.1103/PhysRevA.90.013628 PACS number(s): 67.85.Hj, 05.30.Jp, 67.85.Bc

I. INTRODUCTION

During recent years, a revived interest in Bose-Einstein-condensate (BEC)–impurity mixtures has been stimulated by the experimental works of the authors of Refs. [1–4]. In particular, it has been proven that single atoms can get trapped in the localized distortion of the BEC that is induced by the impurity-BEC interaction [5–7]. Recently, Catani *et al.* [8] created a harmonically trapped impurity suspended in a separately trapped Bose gas and they studied the dynamics of such a system following a sudden lowering of the trap frequency of the impurity. Very recently, an important experimental study of the quantum dynamics of a deterministically created spin-impurity atom propagated in a one-dimensional (1D) lattice system has been realized in Ref. [9].

Theoretically, the self-trapping impurities in BEC with strong attractive and repulsive coupling have been studied in homogeneous and harmonically trapped condensate [10,11]. The quasiparticle excitation spectrum and quantum fluctuations around the product state that describes the entanglement of the impurity and boson degrees of freedom have been calculated in a homogeneous case [12]. In such a system, the formation of a parametric soliton behavior has also been predicted [10]. Moreover, it has been shown that the self-localized BEC-impurity state resembles that of a small polaron which has been described successfully in the strong coupling limit using both the Landau-Pekar treatment [13] and the Fröhlich-Bogoliubov Hamiltonian within the Feynman path integral [14,15]. Then, this study was generalized to two polaron flavors and multi-impurity polarons in a dilute BEC by Tempere *et al.* [14] and Blinova *et al.* [16]. Furthermore, the dynamics and the breathing oscillations of a trapped impurity as well as the impurity transport through a strongly interacting bosonic quantum gas are investigated in Refs. [17,18]. Additionally, the properties of the impurity-BEC in a double-well potential are discussed in Ref. [19].

Although these theories give good results at zero temperature, they completely ignore the behavior of the BEC-impurity at finite temeprature. The effects of the temperature are so important, in particular on the fluctuations, on the expansion of the condensate, and on the thermodynamics of the system. Certainly, the dynamics of the BEC-impurity at nonzero temperatures is a challenging problem as for example the Bogoliubov approximation becomes invalid, at least at large times, and large thermal phase fluctuations have to be taken into account even at low temperatures where density fluctuations are small. It is therefore instructive to derive a self-consistent approach to describe the static and the dynamic behavior of BEC-impurity mixtures at finite temperature especially because all experiments actually take place at nonzero temperatures.

Our approach is based on the time-dependent Balian-Vénéroni (BV) variational principle [20]. This variational principle requires first the choice of a trial density operator. In our case, we consider a Gaussian time-dependent density operator. This ansatz belongs to the class of the generalized coherent states. The BV variational principle is based on the minimization of an action which involves two variational objects: one is related to the observables of interest and the other is akin to a density matrix [21]. This leads to a set of coupled time-dependent mean-field equations for the condensate, the noncondensate, the anomalous average, and the impurity. This approach is called time-dependent Hartree-Fock-Bogoliubov (TDHFB).

The original numerical implementation of this theory [22] successfully addressed the issue of the condensate and the thermal cloud formation at finite temperature. Likewise, the TDHFB equations have been used to study the properties of the so-called anomalous density in three- and two-dimensional homogeneous and trapped Bose gases [23,24]. The results of this analysis present an overall good agreement with recent experimental and theoretical works and highly coincide with the Monte Carlo simulation. The TDHFB theory yields also remarkable agreement with various experiments, e.g., hydrodynamic collective modes and vortex nucleation at finite temperature [25].

The rest of this paper is organized as follows. In Sec. II, we review the main steps used to derive the TDHFB equations from the BV variational principle. In Sec. III, the TDHFB

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equations are applied to a trapped BEC-impurity system to derive a set of coupled equations governing the dynamics of the condensate, the noncondensate, the anomalous average, and the impurity. We then restrict ourselves to solve these equations numerically in a static quasi-1D case and we therefore look at how much the impurity enhances the condensate fluctuations and how much it may be localized. In Sec. IV, we discuss the effects of the condensate fluctuations on the self-trapping impurity using the linearized TDHFB equations in a homogeneous quasi-1D case. Formulas of some thermodynamic quantities of such a system are also given. Section V is devoted to studying the behavior and the formation of solitons in BEC-impurity mixtures in quasi-1D geometry. In this section we analyze numerically the different scenarios that emerge in our model, as well as the temperature effects on the depth and on the creation of solitons. Finally we present our conclusions in Sec. VI.

II. TDHFB EQUATIONS

The Gaussian density operator $\mathcal{D}(t)$ is completely characterized by the partition function $\mathcal{Z}(t) = \mathrm{Tr}\,\mathcal{D}(t)$, the one boson field expectation value $\langle\hat\psi\rangle(\mathbf{r},t) = \mathrm{Tr}\,\hat\psi(\mathbf{r})\,\mathcal{D}(t)/\mathcal{Z}(t)$, and the single-particle density matrix is defined as

$$\rho_j(\mathbf{r},\mathbf{r}',t) = \begin{pmatrix} \langle\hat{\bar\psi}^+\hat{\bar\psi}\rangle & -\langle\hat{\bar\psi}\hat{\bar\psi}\rangle \\ \langle\hat{\bar\psi}^+\hat{\bar\psi}^+\rangle & -\langle\hat{\bar\psi}\hat{\bar\psi}^+\rangle \end{pmatrix}_j (\mathbf{r},\mathbf{r}',t), \tag{1}$$

where j refers to the BEC atoms as B and to the impurity neutral atoms as I.

In the preceding definitions, $\hat\psi_j$ and $\hat\psi_j^+$ are the boson destruction and creation field operators (in the Schrödinger representation), respectively, satisfying the usual canonical commutation rule $[\hat\psi_j(\mathbf{r}),\hat\psi_j^+(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}')$, and $\hat{\bar\psi}_j(\mathbf{r}) = \hat\psi_j(\mathbf{r}) - \Phi_j(\mathbf{r})$ is the noncondensed part of the field operator with $\Phi_j = \langle\hat\psi_j(\mathbf{r})\rangle$.

Upon introducing these variational parameters into the BV principle, one obtains dynamical equations for the expectation values of the one- and two-boson field operators [21–23]:

$$i\hbar\frac{d\Phi_j}{dt} = \frac{d\mathcal{E}}{d\Phi_j}, \tag{2}$$

$$i\hbar\frac{d\rho_j}{dt} = \left[\rho_j, \frac{d\mathcal{E}}{d\rho_j^+}\right]. \tag{3}$$

One of the most noticeable properties of these equations is the unitary evolution of the one-body density matrix ρ_j, which means that the eigenvalues of ρ_j are conserved. This immediately leads to the expression

$$\rho_j(\rho_j+1) = (I_j - 1)/4, \tag{4}$$

where I known as the Heisenberg invariant. Therefore, Eq. (4) involves the conservation of the von Neumann entropy $S = \mathrm{Tr}\,\mathcal{D}\ln\mathcal{D}$. Indeed, parameter (4) is related to the degree of mixing (see Appendix A of Ref. [26]). For pure state and at zero temperature, $I = 1$.

Among the advantages of the TDHFB equations is that they should yield the general time, space, and temperature dependence of the various densities. Furthermore, they satisfy the energy and number conserving laws. Interestingly, our TDHFB equations can be extended to provide self-consistent equations of motion for the triplet correlation function by using the post-Gaussian ansatz.

III. APPLICATION TO THE BEC-IMPURITY SYSTEM

We consider N_I impurity atoms of mass m_I in an external trap $V_I(\mathbf{r})$ and identical bosons of mass m_B trapped by an external potential $V_B(\mathbf{r})$. The impurity-boson interaction and boson-boson interactions have been approximated by the contact potentials $g_B\delta(\mathbf{r}-\mathbf{r}')$ and $g_{IB}\delta(\mathbf{r}-\mathbf{r}')$, respectively. We neglect the mutual interactions of impurity atoms under the assumption that their number and local density remains sufficiently small [10,11]. The many-body Hamiltonian for the combined system which describes bosons, impurity, and impurity-boson gas coupling is given by

$$\begin{aligned}\hat H &= \hat H_B + \hat H_I + \hat H_{IB}\\ &= \int d\mathbf{r}\hat\psi_B^+(\mathbf{r})\left[-\frac{\hbar^2}{2m_B}\Delta + V_B(\mathbf{r}) + \frac{g_B}{2}\hat\psi_B^+(\mathbf{r})\hat\psi_B(\mathbf{r})\right]\hat\psi_B(\mathbf{r})\\ &\quad + \int d\mathbf{r}\hat\psi_I^+(\mathbf{r})\left[-\frac{\hbar^2}{2m_I}\Delta + V_I(\mathbf{r})\right]\hat\psi_I(\mathbf{r})\\ &\quad + g_{IB}\int d\mathbf{r}\hat\psi_I^+(\mathbf{r})\hat\psi_I(\mathbf{r})\hat\psi_B^+(\mathbf{r})\hat\psi_B(\mathbf{r}),\end{aligned} \tag{5}$$

where $\hat\psi_B(\mathbf{r})$ and $\hat\psi_I(\mathbf{r})$ are the boson and impurity field operators.

The total energy $\mathcal{E} = \mathcal{E}_B + \mathcal{E}_I + \mathcal{E}_{IB} = \langle\hat H\rangle$ can be easily computed yielding the following:

$$\begin{aligned}\mathcal{E}_B &= \int d\mathbf{r}\left(-\frac{\hbar^2}{2m_B}\Delta + V_B\right)(|\Phi_B|^2 + \tilde n)\\ &\quad + \frac{g_B}{2}\int d\mathbf{r}\big(|\Phi_B|^4 + 4\tilde n|\Phi_B|^2\\ &\quad + 2\tilde n^2 + |\tilde m|^2 + \tilde m^*\Phi_B^2 + \tilde m\Phi_B^{*2}\big),\end{aligned} \tag{6a}$$

$$\mathcal{E}_I = \int d\mathbf{r}\left[\left(-\frac{\hbar^2}{2m_I}\Delta + V_I\right)(|\Phi_I|^2 + \tilde n_I)\right], \tag{6b}$$

$$\mathcal{E}_{IB} = g_{IB}\int d\mathbf{r}(|\Phi_I|^2 + \tilde n_I)(|\Phi_B|^2 + \tilde n), \tag{6c}$$

where Φ_B and Φ_I stand for the condensate and the impurity wave functions, respectively. The noncondensed density $\tilde n$ and the anomalous density $\tilde m$ are identified, respectively, with $\langle\hat{\bar\psi}_B^+\hat{\bar\psi}_B\rangle$ and $\langle\hat{\bar\psi}_B\hat{\bar\psi}_B\rangle$ and $\tilde n_I = \langle\hat{\bar\psi}_I^+\hat{\bar\psi}_I\rangle$ is the impurity fluctuation.

Expressions (6) for the energy allow us to write down Eqs. (2) and (3) more explicitly as

$$\begin{aligned}i\hbar\dot\Phi_B &= \bigg(-\frac{\hbar^2}{2m_B}\Delta + V_B + g_B(|\Phi_B|^2 + 2\tilde n)\\ &\quad + g_{IB}(|\Phi_I|^2 + \tilde n_I)\bigg)\Phi_B + g_B\tilde m\Phi_B^*,\end{aligned} \tag{7a}$$

$$i\hbar\dot\Phi_I = \left(-\frac{\hbar^2}{2m_I}\Delta + V_I + g_{IB}(|\Phi_B|^2 + \tilde n)\right)\Phi_I, \tag{7b}$$

$$i\hbar\dot{\tilde n} = g_B\big(\tilde m^*\Phi_B^2 - \tilde m\Phi_B^{*2}\big), \tag{7c}$$

$$i\hbar\dot{\tilde{n}}_I = 0, \tag{7d}$$

$$i\hbar\dot{\tilde{m}} = g_B(2\tilde{n}+1)\Phi_B^2 + 4\left(-\frac{\hbar^2}{2m_B}\Delta + V_B + 2g_B n + \frac{g_B}{4}(2\tilde{n}+1) + g_{IB}(|\Phi_I|^2+\tilde{n}_I)\right)\tilde{m}, \tag{7e}$$

where $n = |\Phi_B|^2 + \tilde{n}$ is the total density in the BEC. Putting $g_{IB} = 0$ (i.e., neglecting the mean-field interaction energy between bosons and impurity components) one recovers the usual TDHFB equations [22–25] describing a degenerate Bose gas at finite temperature and the Schrödinger equations describing a noninteracting impurity system. In the case when $\tilde{n} = \tilde{m} = 0$, Eqs. (7) becomes similar to those derived in Ref. [27] for Bose-Fermi mixtures with fermions playing the role of the impurity.

Interestingly, we see from Eq. (7d) that the noncondensed density of the impurity is constant while the anomalous density which describes correlations between pairs does not exist in such a system. Indeed, the absence of the anomalous density in the impurity is due to the neglect of the interaction between impurity atoms. One should mention also at this level that Eq. (7e), which describes the behavior of the anomalous density-impurity, has no analog in the literature.

A useful link between the noncondensed and the anomalous densities of BEC can be given via Eq. (4):

$$I_B = (2\tilde{n}+1)^2 - 4|\tilde{m}|^2. \tag{8}$$

Equation (8) clearly shows that $\tilde{m}$ is larger than $\tilde{n}$ at low temperature, so the omission of the anomalous density in this situation is principally an unjustified approximation and wrong from the mathematical point of view.

Notice that for a thermal distribution, $I_k = \coth^2(\varepsilon_k/T)$, where ε_k is the excitation energy of the system. The expression of I allows us to calculate in a very useful way the dissipated heat for the d-dimensional BEC-impurity mixture as $Q = (1/n)\int E_k I_k d^dk/(2\pi)^d$ with $E_k = \hbar^2k^2/2m$ [24]. It is necessary to stress also that our formalism provides an interesting formula for the superfluid fraction $n_s = 1 - 2Q/dT$ [24], which reflects the importance of the parameter I.

Equations (7) in principle cannot be used as they stand since they do not guarantee to give the best excitation frequencies. Indeed it is well know [23,28,29] that the inclusion of the anomalous average leads to a theory with a (unphysical) gap in the excitation spectrum. The standard treatment in calculations for trapped gases has been to neglect $\tilde{m}$ in the above equations, which restores the symmetry and hence leads to a gapless theory. This is often reminiscent of the Popov approximation. In addition, one finds that the anomalous average is divergent if one uses a contact interaction. To go beyond Popov, one has to renormalize the anomalous average to circumvent this ultraviolet divergence. Following the method described in Ref. [28], we get from Eq. (7a):

$$g_B|\Phi_B|^2\Phi_B + g_B\tilde{m}\Phi_B^* = g_B\left(1+\tilde{m}/\Phi_B^2\right)|\Phi_B|^2\Phi_B = U|\Phi_B|^2\Phi_B. \tag{9}$$

This is similar to the so-called $G2$ approximation based on the T-matrix calculation [28].

At very low temperature where $\tilde{m}/\Phi_B^2 \ll 1$, the new coupling constant U reduces immediately to g_B. Inserting U in Eqs. (7a) and (7b) and using $2\tilde{n}+1 \approx 2\tilde{m}$ [25], this approximation is valid at very low temperature where $\tilde{m} \geqslant \tilde{n}$ as we have mentioned above. After some algebra we obtain

$$i\hbar\dot{\Phi}_B = \left\{-\frac{\hbar^2}{2m_B}\Delta + V_B + g_B[\beta|\Phi_B|^2 + 2\tilde{n} + \gamma(|\Phi_I|^2+\tilde{n}_I)]\right\}\Phi_B, \tag{10a}$$

$$i\hbar\dot{\tilde{m}} = \left\{-\frac{\hbar^2}{2m_B}\Delta + V_B + g_B[2G\tilde{m} + 2n + \gamma(|\Phi_I|^2+\tilde{n}_I)]\right\}\tilde{m}, \tag{10b}$$

where $\beta = U/g_B$, $G = \beta/4(\beta-1)$, and $\gamma = g_{IB}/g_B$.

Let us now reveal the significance of parameter β. First of all, β accounts for finite-temperature effects (dissipation); it scales with temperature T according to the formula (8). Futhermore, for $\beta = 1$, i.e., $\tilde{m}/\Phi_B^2 = 0$, Eq. (10a) reduces to the well-known HFB-Popov equation, which is safe from all ultraviolet and infrared divergences and thus provides a gapless spectrum. For $0 < \beta < 1$, G is negative, while for $\beta > 1$, G is positive. At this level, we note that for large values of β, one gets a BEC with strong interactions and high correlations. So, in order to guarantee the diluteness of the system, β should vary as $\beta = 1 \pm \epsilon$ with ϵ being a small value.

In what follows we consider a single impurity $N_I = 1$, which means that there is no impurity fluctuation ($\tilde{n}_I = 0$), immersed in elongated (along the x direction) BEC and confined in a highly anisotropic trap (such that the longitudinal and transverse trapping frequencies are $\omega_{Bx}/\omega_{B\perp} \ll 1$). In such a case, the system can be considered as quasi-1D and, hence, the coupling constants of the Hamiltonian (5) effectively take their 1D form, namely, $g_B = 2\hbar\omega_{B\perp}a_B$ and $g_{IB} = 2\hbar\omega_{B\perp}a_{IB}$, where a_B and a_{IB} are the scattering lengths describing the low-energy boson-boson and impurity-boson scattering processes.

The time-independent TDHFB equations can be easily obtained within the transformations: $\Phi_B(x,t) = \Phi_B(x)\exp(-i\mu_B t/\hbar)$, $\tilde{m}(x,t) = \tilde{m}(x)\exp(-i\mu_{\tilde{m}} t/\hbar)$, and $\Phi_I(x,t) = \Phi_I(x)\exp(-i\mu_I t/\hbar)$, where μ_B, $\mu_{\tilde{m}}$, and μ_I are, respectively, the chemical potential of the condensate and of the anomalous density and of the impurity. Strictly speaking $\mu_{\tilde{m}}$ is also associated with the thermal cloud density since $\tilde{n}$ and $\tilde{m}$ are related to each other by Eq. (8). Then the static TDHFB equations read

$$\mu_B\Phi_B = \left[-\frac{\hbar^2}{2m_B}\Delta + \frac{1}{2}m_B\omega_{Bx}^2x^2 + g_B(\beta|\Phi_B|^2 + 2\tilde{n} + \gamma|\Phi_I|^2)\right]\Phi_B, \tag{11a}$$

$$\mu_{\tilde{m}}\tilde{m} = \left[-\frac{\hbar^2}{2m_B}\Delta + \frac{1}{2}m_B\omega_{Bx}^2x^2 + g_B(2G\tilde{m} + 2n + \gamma|\Phi_I|^2)\right]\tilde{m}, \tag{11b}$$

$$\bar{\mu}_I \Phi_I = \left[-\frac{\hbar^2}{2m_I}\Delta + \frac{1}{2} m_I \omega_{Ix}^2 x^2 + g_B(\gamma|\Phi_B|^2 + \gamma\tilde{n}) \right] \Phi_I. \tag{11c}$$

To gain insight into the behavior of the thermal cloud and the anomalous densities in the BEC-impurity system at finite temperature, we solve numerically Eqs. (11) using the finite-differences method. In the numerical investigation, we use $a_0 = \sqrt{\hbar/m_B\omega_{Bx}}$ and $\hbar\omega_{Bx}$ as the length (the ground state extent of a single BEC-boson particle) and the energy units, respectively, and we end up with $\alpha = m_B/m_I$ being the ratio mass and $\Omega = \omega_{Bx}/\omega_{Ix}$. The parameters are set to $N_I = 1$ of ^{85}Rb impurity atom, $N = 10^5$ of ^{23}Na bosonic atoms, $a_B = 3.4$ nm, $a_{IB} = 16.7$ nm, the transverse trapping frequency is $\omega_{B\perp} = 2\pi \times 500$ Hz [10], the longitudinal trapping frequency is $\omega_{Bx} = 2\pi \times 5$ Hz, $\gamma = 4.91$, and $\Omega = 0.2$.

Our numerical simulations show that for repulsive interactions, the condensate is distorted by the impurity and forms a dip near the center of the trap. The impurity is focused inside the condensate forming a self-localized state as is illustrated in the left panel of Fig. 1 which is in good agreement with existing theoretical results. One can see also from Fig. 1 (right panel) that the density of the condensate and of the impurity is lowered for $\beta = 1.1$. In addition, the thermal cloud is deformed away from the impurity, as happens to the condensate cloud. The density of the impurity reduces and becomes less localized when the temperature grows as shown in the same figure. Indeed, this decay arises from the fact that at nonzero temperatures the condensate coexists with both a noncondensed cloud and an anomalous density composed of thermally excited quasiparticles. Therefore, interactions between condensed and noncondensed atoms on the one hand and interactions of the impurity with atoms of the surrounding condensate on the other hand lead to dissipation, so that the impurity loses energy and delocalizes.

A qualitative difference can be observed between anomalous density with impurity and anomalous density without impurity. Figure 2, shows that the dip in the neighborhood of the center of the trap, which arises from the interactions between atoms of the condensate and those of the thermal cloud [23], becomes deeper in the presence of the impurity. This clearly confirms that the anomalous density is also distorted in an analogous manner with the condensate.

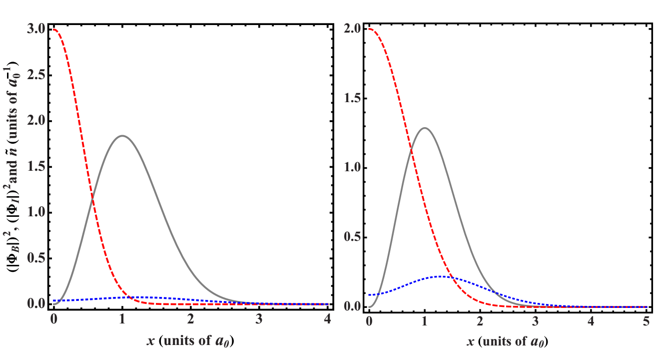

FIG. 1. (Color online) Condensed (gray lines), noncondensed (red-dashed lines), and impurity (blue-dotted lines) densities as functions of the radial distance for $\beta = 0$ (left panel) and for $\beta = 1.1$ (right panel) for the above parameters.

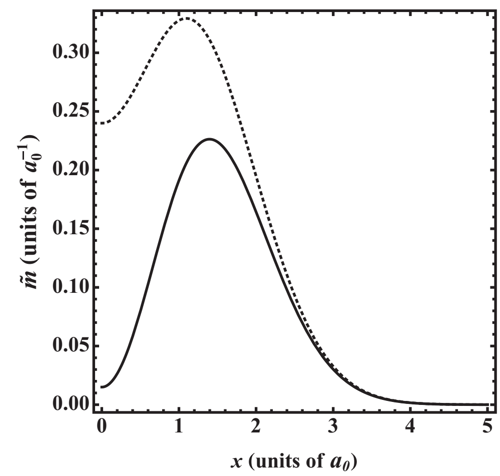

FIG. 2. Anomalous density as a function of the radial distance for $\beta = 1.1$ with the same parameters as in Fig. 1. Solid lines: in the presence of the impurity. Dotted lines: without impurity.

IV. EFFECTS OF BEC FLUCTUATIONS ON THE SELF-TRAPPING IMPURITY

In order to study effects of BEC fluctuations on the self-trapping problem of weakly BEC-impurity interactions in the homogeneous case ($V_B = V_I = 0$), it is convenient to linearize Eqs. (11a) and (11b) by considering the small deformations [14] $\delta\Phi_B = \Phi_B - 1$ and $\delta\tilde{m} = \tilde{m} - 1$ of the condensate and of the anomalous density, respectively. Assume that $\delta\Phi_B$ and $\delta\tilde{m}$ are real for simplicity. The linear equations take the following forms:

$$\left(-\frac{1}{2}\Delta + A\right)\delta\Phi_B = -C|\Phi_I|^2, \tag{12a}$$

$$\left(-\frac{1}{2}\Delta + B\right)\delta\tilde{m} = -C|\Phi_I|^2, \tag{12b}$$

$$\left[-\frac{1}{2}\Delta + \frac{\gamma}{\alpha}(2\delta\Phi_B + \delta\tilde{m})\right]\Phi_I = \bar{\varepsilon}\Phi_I, \tag{12c}$$

where $A = 2 + 2(\beta - 2) + \bar{\mu}_B$, $B = 2 + 4G + \bar{\mu}_{\tilde{m}}$, $C = \gamma/\xi n$, $\xi = \hbar/\sqrt{m_B n g_B}$ is the healing length, $\bar{\varepsilon} = (\bar{\mu}_I - 3\gamma/2)/\alpha$, $\bar{\mu}_B = \mu_B/ng_B$, $\bar{\mu}_{\tilde{m}} = \mu_{\tilde{m}}/ng_B$, and $\bar{\mu}_I = \mu_I/ng_B$.

Equation (12c) constitutes a natural extention of that used in the literature [11,14] since it contains the condensate and its fluctuation. The solution of this equation allows us to study not only the self-localizing problem at finite temperature but also enables us to see how the condensate fluctuation enhances the thermodynamics of the impurity such as the chemical potential and the compressibility.

It can be seen from Eqs. (12a) and (12b) that the linearization of Eqs. (11) is valid in the regime $C \ll 1$. The solution of Eqs. (12a) and (12b) is given in terms of the Green's function $G(x)$. Inserting this solution into Eq. (12c) with the assumption that $\delta\tilde{m}/\delta\Phi_B \ll 1$ at low temperature, one finds that Φ_I obeys the nonlocal nonlinear Schrödinger equation

$$\left[-\frac{1}{2}\Delta - 2\zeta \int dz' G(z,z')|\Phi_I(z')|^2\right]\Phi_I = \bar{\varepsilon}\Phi_I, \quad (13)$$

where $\zeta = \gamma C/\alpha$ is the self-trapping parameter.

Multiplying Eq. (13) by $\Phi_I^*(z)$, integrating over z, and making use of the normalization condition, we obtain

$$\begin{aligned}\bar{\varepsilon} &= \bar{\varepsilon}_{\mathrm{kin}} + \bar{\varepsilon}_{\mathrm{def}} \\ &= -\frac{1}{2}\int dz \Phi_I^*(z)\Delta\Phi_I(z) \\ &\quad - \zeta \int dz \int dz' |\Phi_I(z)|^2 G(z,z')|\Phi_I(z')|^2, \quad (14)\end{aligned}$$

where $\bar{\varepsilon}_{\mathrm{def}}$ is the energy gained by deforming the BEC.

To estimate the critical parameters for which self-trapping occurs, we insert the normalized Gaussian wave function $\Phi_I(z) = (1/\sqrt{\pi q^2})^{1/4}\exp(-z/2q)^2$. A straightforward calculation yields

$$\bar{\varepsilon} = \frac{1}{4q^2} - \zeta f(q), \quad (15)$$

where $f(q) = (1/2)\exp(-2q^2)\mathrm{erfc}(\sqrt{2}q)$ with $\mathrm{erfc}(x)$ being the complementary error function. Equation (15) provides a useful expression for the impurity chemical potential

$$\bar{\mu}_I = \frac{\alpha}{4q^2} + \gamma\left[\frac{3}{2} - Cf(q)\right]. \quad (16)$$

It is clearly seen from Eq. (16) that, for $q > 1$, $\bar{\mu}_I$ is linearly increasing with γ. Importantly, Eq. (16) shows that the variational impurity chemical potential differs by a factor of $3/2$ compared to the ordinary zero temperature case, i.e., without fluctuations. We then infer that the presence of thermal fluctuations of the condensate leads to corrections of the chemical potential of the impurity.

The above chemical potential implies the following expression for the impurity compressibility $\kappa_I^{-1} = n^2\partial\bar{\mu}_I/\partial n$:

$$\kappa_I^{-1} = \frac{1}{2}\frac{\gamma^2}{\xi}f(q). \quad (17)$$

The compressibility (17) remains finite and increases with γ.

If $q \gg 1$, we can Taylor-expand f as $f \approx 1/2 - \sqrt{2/\pi}q$. In this limit, the impurity energy $\bar{\varepsilon} = 1/(4q^2) + \zeta q/\sqrt{2\pi} - \zeta/2$ attains a minimum at $q = 0.85\,\zeta^{-1/3}$. Therefore, the self-trapping occurs for small ζ in quasi-1D BEC-impurity, which is in agreement with the theoretical results of Ref. [11]. We conclude that the condensate fluctuations do not have considerable effects on the occurrence of the self-tapping at low temperature. It is worth noting that our model is also applicable in harmonically trapped BEC.

V. SOLITONS IN THE BEC-IMPURITY SYSTEM

Our aim in this section is in a sense twofold. On the one hand, we aim to study the formation of matter-wave solitons in BEC-impurity mixtures at finite temperature in an experimentally relevant and realizable setting. On the other hand, we are aiming to see what are the effects of the temperature or the dissipation on the generation of solitons.

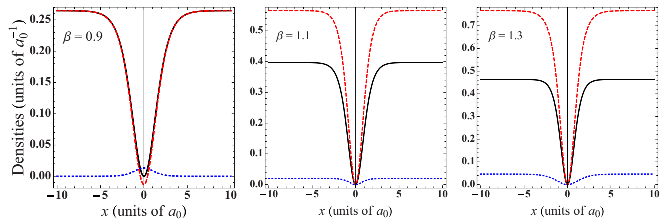

FIG. 3. (Color online) Density profiles for solitons in the BEC-impurity mixture with the same parameters as in Fig. 1. Solid lines: ordinary soliton. Red-dashed lines: impurity soliton. Blue-dotted lines: anomalous soliton.

What is advantageous in our model (11) is that the anomalous density is treated dynamically on the same footing as the condensate, which leads us to predict a new kind of soliton, namely, an anomalous soliton. This soliton occurs generically in the thermal equilibrium state of a weakly interacting Bose gas irrespective of the presence or not of the impurity. At this point, one should mention that the previous analysis of parameter β highlights the emergence of, at least, two different cases for BEC with repulsive interactions($g_B > 0$): bright anomalous soliton for $0 < \beta < 1$ and dark anomalous soliton for $\beta > 1$.

To investigate in more detail the formation of solitons in a weakly repulsive BEC-impurity under the presence of thermal fluctuations, we consider a quasi-1D (elongated along the x direction) geometry which is the most favorable for the appearance of solitons. Again, we solve numerically Eqs. (11), employing appropriate boundary conditions with the same experimental values corresponding to Fig. 1.

Figure 3 depicts clearly the formation of dark solitons in the condensed and the impurity components and a bright soliton in the anomalous density for $\beta = 0.9$. The situation is inverted for $\beta = 1.1$ where a spontaneous dark anomalous soliton is generated, without any external forcing or perturbations, which is in good accordance with our previous analysis. This soliton becoming widespread and deep as temperature rises unlike to the condensed (ordinary) and impurity solitons where they become narrower and deeper at higher temperatures because they lose energy due to the dissipation. A similar behavior has been predicted in Ref. [30] for thermal solitons in a quasi-1D Bose gas. Also, a careful observation of the same figure shows that the impurity soliton is deeper than the condensed one and the depth of these three solitons increases with increasing temperature. Another important remark is that the impurity soliton is localized inside the ordinary one especially for values of $\beta > 1$ and both solitons are localized in the core of the anomalous soliton. Consequently, the width of the anomalous soliton is larger than that of the ordinary soliton whatever the range of the temperature. This is in fact natural since the anomalous soliton is related to the thermal cloud and this latter surrounds the condensate as it was shown in earlier BEC experiments.

It is understood also that for the BEC-impurity with attractive interactions ($g_B < 0$), bright anomalous solitons can be produced at higher temperature (for $\beta > 1$).

We turn now to analyze the dynamics of the anomalous solitons. Usually, solitons can be moved by shaking slightly the

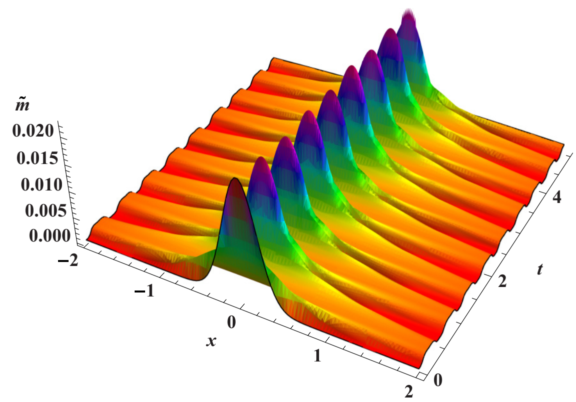

FIG. 4. (Color online) Evolution of the anomalous soliton for $\beta = 0.9$ with the same parameters as in Fig. 3. Here we measure time in units of ω_{Bx}^{-1}, the position in units of a_0, and the density of a_0^{-1}.

trapping potential. In such a situation, the anomalous soliton obeys the time-dependent TDHFB equations. For $\beta = 0.9$, we observe from Fig. 4 that a bright anomalous soliton propagates with almost constant amplitude reflecting the robustness and the stability of this soliton during its evolution. This behavior persists also for dark anomalous solitons.

An interesting question that begs to be asked is what kind of solitons will exist in the BEC-impurity mixture with attractive boson-boson interactions and repulsive boson-impurity interactions or inversely? For example, for Bose-Fermi gas mixtures, it has been shown that bright solitons are produced as a result of a competition between two interparticle interactions: boson-boson repulsion versus boson-fermion attraction [27]. The response to this question and others related to the formation and the behavior of soliton molecules in BEC-impurity systems will be given elsewhere.

VI. CONCLUSION

In this paper we have derived from the time-dependent BV variational principle a set of coupled equations for the BEC-impurity mixture. These equations govern in a self-consistent way the dynamics of the condensate, the thermal cloud, the anomalous average, and the impurity. The numerical simulations of the TDHFB equations in the harmonically trapped quasi-1D model showed that the thermal cloud and the anomalous density are distorted by the impurity as happens with the condensate. Additionally, the impurity is reduced and becomes less localized with increasing temperature.

Furthermore, we have investigated effects of BEC fluctuations on the self-trapping impurity in homogeneous weak interaction regimes at low temperature. We have found that these fluctuations may enhance the chemical potential and the compressibility of the impurity, while they do not affect the occurrence of the self-trapping state. We have shown that the self-trapping takes place for small values of ζ in agreement with the case of zero temperature.

Moreover, we have studied the formation of matter-wave solitons in repulsively quasi-1D BEC-impurity mixtures in the presence of thermal effects. Our formalism reveals the formation of stable solitons. Depending of parameter β, the system contains much more than the standard picture. A dark soliton is created in condensed and impurity parts of the system, whereas a bright soliton is formed in the anomalous density. A dark anomalous soliton is willingly generated at higher temperatures without the need of any external perturbations or squeezing of the geometry. This anomalous soliton is shown to be stable and robust during its time evolution. Our formalism allows us to explain the temperature dependence of the appearance of deep solitons in the BEC-impurity.

An important step for future theoretical studies in the finite-temperature regime is to fully include the interaction part of the impurity atoms in the total Hamiltonian of the system [31]. This permits us to study in a self-consistent way, within the TDHFB formalism, fluctuations of the impurity and their effects on the formation of solitons and vortices in such a system.

ACKNOWLEDGMENTS

We gratefully acknowledge Tomi Johnson for discussion and comments on this paper. This work was supported by the Algerian government under Research Grant No. CNEPRU-D00720130045.

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