Bosonic impurity in a one-dimensional quantum droplet in the Bose–Bose mixture

F Kh Abdullaev¹,² and R M Galimzyanov¹,³

¹ Physical-Technical Institute of the Academy of Sciences, Chingiz Aitmatov Street 2-b, 100084, Tashkent-84, Uzbekistan
² Physics Department, National University of Uzbekistan, University Street 4, 100174, Tashkent-174, Uzbekistan
E-mail: ravil_galimzyanov@yahoo.com

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Abstract
We study an impurity immersed in the mixture of Bose ultracold gases in the regime where a quantum droplet (QD) exists. The quasi-one-dimensional geometry is considered. We find an effective attractive potential, which acts by the QD onto the impurity. The bound states of the impurity in this potential are investigated. These impurity-bound states can provide potential probes for the presence of quantum fluctuation effects on the droplet properties. In the case of strong impurity–Bose–Einstein condensate coupling we study the properties of the nonlinear local modes on the impurity induced by the quantum fluctuations.

Keywords: quasi-one-dimensional BEC, quantum droplet, impurity, quantum fluctuations, bound states, effective potential

1. Introduction

A lot of attention has recently been devoted to the investigation of self-supported quantum droplets (QDs) in ultracold quantum gases [1–6]. They represent new states of quantum liquids, and in the distinction from droplets in the liquid helium, can exist at densities that are lower by a few orders. The possibility of tuning parameters of Bose–Einstein condensate (BEC) in the wide region opens up new possibilities for studying the QDs.

The existence of these droplets in BEC with attractive two-body interaction is connected with the stabilizing role being played by quantum fluctuations [7]. The contribution to the ground energy from quantum fluctuations was first calculated by Lee–Huang–Yang (LHY) [8] and has the repulsive character in 3D. In quasi-1- or 2D systems it can be either attractive or repulsive, depending on the density [9]. Theoretical investigation of the dynamics of droplets in a quasi-1D setup is carried out in [10–12]. Balance between the residual mean field attractive nonlinearity, produced by interaction of a attractive inter-species and repulsive intra-species, and repulsive LHY term, leads to the existence of QDs. At the present time they are theoretically predicted for Bose–Bose (BB) mixtures [7], dipolar condensates [13], Bose–Fermi (BF) mixtures [14], and spin–orbit coupled BEC [15,16]. The QDs have recently been observed in BB mixtures [5], dipolar condensates [2,3], and probably in BF mixtures [17]. QDs formed by atoms of different atomic species have been reported in [18]. Dynamics of the Faraday waves under action of the quantum fluctuations are investigated in recent work [11].

It should be noted that QDs in ultracold gases resemble ones in liquid helium. Interaction of an impurity with the droplet in liquid helium leads to rich phenomena as creation clusters with confinement of single molecules inside or on the surface of free droplets and so on [19].

Using this analogy we can expect that an impurity immersed into the QD may have new interesting properties like the generation of quantum polarons (see e.g. [20–25]). Such an investigation has recently been performed in the case of the fermionic impurity embedded into the dipolar condensate [26]. It is shown that this type of impurity provides a unique probe for analysis of the properties of the QD.
In the present work we will study another system, namely a neutral Bose-impurity, immersed in a quasi-1D Bose–Bose mixture. We study self-localization of the impurity and find the bound state energies in the effective potential induced by a QD. We will also investigate the case of strong coupling of an impurity with BEC when the localized state of the impurity is accompanied by strong deformation of the BEC [28, 29]. Note that in these works the problem has been investigated without taking into account quantum fluctuations.

The structure of the work is as follows: in section 2 we give basic equations describing BB mixture and an impurity immersed there. In section 3 we find effective potentials and calculate energy levels of bound states of an impurity at different values of the system parameters. In section 4 the case of strong coupling of the δ-impurity with BEC is investigated. We find nonlinear localized modes on the impurity and compare analytical predictions with results of numerical simulations of the full GP equation.

2. Model

The analysis is based on the model describing the interaction of an impurity with the BEC. The system of equations for wave functions of the one-component condensate and an impurity has been previously introduced in [27, 28].

This system can be generalized for a two-component case, where components correspond to different isotopes or hyperfine states. Dynamics of an impurity immersed in the mixture of two Bose gases taking into account quantum fluctuations in the LHY form [9] is described by the coupled system of equations for wave functions of the BB mixture Ψ1, Ψ2 and the impurity Φ

\[ i\hbar \Psi_{1,1} + \frac{\hbar^2}{2m_1} \Psi_{1,xx} - (g_{11} |\Psi_1|^2 + g_{12} |\Psi_2|^2) \Psi_1 + \frac{\sqrt{mg_{11}}}{\pi \hbar} (g_{11} |\Psi_1|^2 + g_{22} |\Psi_2|^2)^{1/2} |\Psi_1 - g_{IB1} |\Phi|^2 \Psi_1 = 0, \]  

(1)

\[ i\hbar \Psi_{2,2} + \frac{\hbar^2}{2m_2} \Psi_{2,xx} - (g_{22} |\Psi_2|^2 + g_{21} |\Psi_1|^2) \Psi_2 + \frac{\sqrt{mg_{22}}}{\pi \hbar} (g_{11} |\Psi_1|^2 + g_{22} |\Psi_2|^2)^{1/2} |\Psi_2 - g_{IB2} |\Phi|^2 \Psi_2 = 0, \]  

(2)

\[ i\hbar \Phi_{1} + \frac{\hbar^2}{2m_I} \Phi_{xx} - (g_{IB1} |\Psi_1|^2 + g_{IB2} |\Psi_2|^2) \Phi = 0, \]  

(3)

where a subscript notation, ‘y’, is used for the partial derivative with respect to a generic variable y, g_{ij} = 2\hbar\omega_{ij}a_{ij}, with \omega_{ij} being the transverse frequency of the trap (BECs and impurities are supposed to have the same transverse frequency) a_{ij} is the intra- and inter-species atomic scattering lengths, and g_{IB1,2} is the impurity-Boson scattering lengths. The scattering lengths can be tuned by using the Feshbach resonance technique [30]. Hereafter we assume g_{11} = g_{22} = g, m_1 = m_2 = m_I = m and g = |g_{12}| + δg, g_{IB1} = g_{IB2} = g_{IB}.

Then we can suppose \psi_1 = \psi_2 = \psi so the system of equations takes the form

\[ i\hbar \Psi_1 + \frac{\hbar^2}{2m} \Psi_{xx} - g \delta |\Psi|^2 \Psi - g_{IB} |\Phi|^2 \Psi + g_{QF} |\Psi|^2 \Psi = 0, \]  

(4)

\[ i\hbar \Phi_1 + \frac{\hbar^2}{2m_I} \Phi_{xx} - 2g_{IB} |\Psi|^2 \Phi = 0, \]  

(5)

where \( g_{QF} = \sqrt{2mg_{IB}^3}/(\pi \hbar) \). Note that in the case of one dimension, quantum fluctuations lead to the effective attraction effect. Then, for existence of the QD in this limit, we should choose the small residual two-body repulsion, i.e. \( \delta g > 0 \).

Defining characteristic units of length \( x_0, \) time \( t_0, \) wave function \( \Psi_0 \) and energy \( E_0 \) (see e.g. [10])

\[ x_0 = \sqrt{\frac{\hbar^2 \delta g_{IB}^{1/2}}{2mg_{IB}^{3/2}, \ t_0 = \sqrt{\frac{\hbar^2 \delta g_{IB}^{3/2}}{2mg_{IB}^3}, \ E_0 = \frac{2mg_{IB}^{3}}{\pi^2 \hbar^2 \delta g_{IB}}}, \]  

(6)

where \( \delta g_{IB} \) is a fixed value of the detuning of inter- and intra-species scattering lengths, and rescaling \( x' = x/x_0, t' = t/t_0, \psi' = \psi/\psi_0, \) we get the following dimensionless system of equations (the primes are omitted)

\[ i\psi_1 + \frac{1}{2} \psi_{xx} - |\psi|^2 \psi + |\psi| \psi + f_1 |\phi|^2 \psi = 0, \]  

(7)

\[ i\phi + \frac{1}{2} \phi_{xx} + f_1 |\psi|^2 \phi = 0, \]  

(8)

where \( \gamma = \frac{\delta g}{\delta g_{IB}}, f_1 = -N_{IB}g_{IB}/(N_0 \delta g_{IB}), f_2 = -2g_{IB}/\delta g_{IB}. \)

Let us consider the case when \( f_1 = f_2 = 0 \) corresponds to an uncoupled system. The exact solution for the droplet (\( \gamma = 1 \)) has the form

\[ \psi(x) = \frac{3\mu}{1 + \sqrt{1 - 9\mu/2 \cosh(\sqrt{2\mu} x)}. \]  

(9)

The number of atoms in this wavepacket

\[ N = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 4 \left[ \ln \left( \sqrt{9\mu/2 + 1} - 1 \right) \right] = \frac{9\mu}{2}. \]  

(10)

For small \( N \ll 1 \) the droplet profile is well described by the Gaussian function, and for \( N \gg 1 \) the profile turns into the flat top one, extending with increasing \( N. \) When \( N \ll 1, \) chemical potential \( \mu \approx 0.382N^{2/3} \) and \( \mu \approx 2/9 \) for \( N \gg 1 \) [10].

3. Effective potential and energy levels for an impurity trapped by the QD

Now we consider the case when the back action of the impurity on the BEC can be neglected (i.e. \( f_1 = 0 \)). From equation (8) we can see that the impurity is in the effective potential induced by a QD

\[ V_{eff}(x) = -f_2 |\psi(x)|^2 = -f_2 \frac{9\mu^2}{(1 + \sqrt{1 - 9\mu/2 \cosh^2(\sqrt{2\mu} x)})^2}. \]  

(11)

There are two limits
**3.1. Effective potential and energy levels when \( \gamma = 0 \) (i.e. \( \delta g = 0 \))**

In this important case the residual mean field term vanishes, i.e. the inter- and intra-species interactions balance each other. The leading effect in the formation of the droplet is given by the LHY term, and the effects of quantum fluctuations dominate. The exact solution for a QD has the form \[ \psi(x) = \frac{3\tilde{\mu} e^{i\tilde{\mu}x}}{2 \cosh^2 \left( \sqrt{\frac{\tilde{\mu}}{2}}x \right)}, \]

where the chemical potential \( \tilde{\mu} \) may take values \( 0 < \tilde{\mu} < \infty \).

Interaction between the QD (12) and an impurity is determined by an effective potential \[ V_{\text{0,eff}}(x) = -f_2 \frac{9\tilde{\mu}^2}{4 \cosh^4 \left( \sqrt{\frac{\tilde{\mu}}{2}}x \right)}. \]

The energy level for this potential is difficult to find analytically; therefore we will use an approximation of it by a potential of the solvable form.

It turns out that the function \( y(z) = 1/\cosh^4(x) \) is well approximated by the expression \( a/\cosh^2(bx) \) with fitting parameters \( a \) and \( b \). Then effective potential \( V_{\text{0,eff}}(x) \) can be well approximated by the new one

\[ V_{\text{0,eff}}(x) \approx V_{\text{0,app}}(x) = -a f_2 \frac{9\tilde{\mu}^2}{4 \cosh^2 \left( \sqrt{\frac{\tilde{\mu}}{2}}(bx) \right)}. \]

Effective potential \( V_{\text{0,eff}}(x) \) and its approximated variant \( V_{\text{0,app}}(x) \) are shown in figure 1. Here the dotted line is for the exact effective potential \( V_{\text{0,eff}} \) equation (13) and the solid line is for its fitted variant. We can see that the curves are in good agreement with each other.

Introducing new parameter

\[ \lambda = \frac{1}{2} + \sqrt{\frac{1}{4} + f_2^2 \frac{9\tilde{\mu}a}{b^2}}, \]

approximating potential \( V_{\text{0,app}}(x) \) can be transformed to the modified Pöschl–Teller potential \[ V_{\text{0,Poschl–Teller}} = -\frac{1}{2} \left( \sqrt{\frac{\tilde{\mu}}{2}b} \right)^2 \lambda (\lambda - 1), \]

Everywhere fitting parameters are: \( a = 1.022 \) and \( b = 1.523 \).

All this makes it possible to get approximated analytical expressions for \( n \) levels in the potential \( V_{\text{0,eff}} \) equation (13),

\[ E_n = -\frac{1}{2} b^2 \left( \sqrt{\frac{\tilde{\mu}}{2}b} \right)^2 (\lambda - n)^2, \]

where \( n < \lambda - 1 \) [34].

The distance between energy levels can be found from equation (16) as

\[ \Delta E_n = E_n - E_{n-1} = b^2 \frac{\tilde{\mu}}{2} \left( \lambda - n - \frac{1}{2} \right), \quad n < \lambda - 1. \]

We can conclude that properties of the bound states are strongly defined by quantum fluctuation effects, so measuring the energy spectrum we can probe the quantum fluctuations in BEC.

**3.2. Effective potential and energy levels when \( \gamma \neq 0 \) (i.e. \( \delta g \neq 0 \), \( f_1 = 0 \) and \( f_2 = 10 \))**

Let us consider the case when \( \delta g \neq 0 \). Here it is difficult to find an analytical expression for all energy levels, so we will perform numerical simulations. In our calculations all physical values are dimensionless ones in correspondence with equation (6). In figure 2 the forms of the effective potential induced by the QD consisting of \( N \) atoms are shown (\( N \) is directly determined by the parameter \( \mu \)). We can see that the closer \( \mu \) to the threshold value \( \mu = 2/9 \) the closer the form of the droplet effective potential to a wide rectangular well. Figure 3 depicts energy levels of the impurity depending on different values of the chemical potential \( \mu \). The first four eigenfunctions are shown in figure 4 for the case \( \mu = 0.222 \) (dimensionless number of atoms, \( N = 4.2 \)). The eigenfunctions are not normalized and have the same amplitude.

Now we turn to the case when the number of atoms \( N \) in the system is large. The dependence of \( N \) on the value of chemical potential \( \mu \) is determined by equation (10). At large number of atoms \( \mu \rightarrow 2/9 \) and may be expressed in terms of \( N \) as in reference [10]

\[ \mu \approx \frac{2}{9} \left[ 1 - \exp(-2 - \frac{3}{2}N) \right]. \]
As shown in work [12], the stationary QD solution equation (9) may be presented as the sum of two kink solutions

\[ \psi(x) = \sqrt{\frac{\mu}{2}} \left[ \tanh \left( \frac{\mu}{2} (x + x_0(\mu)) \right) + \tanh \left( \frac{\mu}{2} (-x + x_0(\mu)) \right) \right] e^{int}, \]

where

\[ x_0(\mu) = \frac{1}{\sqrt{2\mu}} \arctanh \left( \sqrt{\frac{\mu}{2}} \right). \]

Effective potential induced by the QD is determined by equation (11), \( V_{eff}(x) = -f_2 |\psi(x)|^2. \) When the number of atoms is large and \( N \gg 1 \) with \( \mu \to 2/9 \), the form of the potential \( V_{eff}(x) \) turns into a rectangular well potential with the fixed depth \( V_0 = -f_2 2\mu \) and the width \( 2x_0 = 2.25N + 3 \). We should be reminded that \( N \) and \( x_0 \) are dimensionless values in accordance with equation (6).

Figures 2, 3, 4.

Figure 2. Forms of the droplet effective potential equation (11) at different chemical potentials \( \mu \). Dotted line is for \( \mu = 0.08 \), dashed dotted line is for \( \mu = 0.2 \), dashed line is for \( \mu = 0.222 \), and solid line is for \( \mu = 0.222222 \). Everywhere \( f_2 = 10 \).

Figure 3. The impurity energy levels at different \( \mu \). Asterisks are for ground states, filled circles are for the second energy levels, circles with crosses are for the third energy levels and crosses are for the fourth energy levels. Everywhere \( f_2 = 10 \).

Figure 4. Stationary wave packets of the impurity for \( \mu = 0.222 \) corresponding to \( N = 4.2 \). The line with asterisks is for the ground state wave packet, the line with filled circles is for a wave packet of the second energy level, the line with circles containing crosses inside is for the wave packet of the third energy level and the line with crosses is for the wave packet of the fourth energy level. The wave packets are of the same amplitude and they are not normalized.

Transitions between first nearest deep energy levels in the potential are determined as

\[ \Delta E_n = E_n - E_{n-1} = f_2 \frac{\pi}{8x_0} (2n + 1), \]

where \( n \) is the level number.

The level spectrum may be measured by periodical variation in time of the scattering length \( a_{1n} = a_0 + a_1 \sin(\omega t) \) with the frequency \( \omega = \Delta E/h \), which induces resonant transitions between levels [26, 27, 38] with \( \Delta E \approx (50 \div 100) \text{Hz} \) (see below). Also for measurements of the impurity spectrum, the radio-spectroscopy method [39] can be used.

Let us estimate the parameters for the experiment. We can consider binary \(^{85}\text{Rb} \) atoms BEC in the cigar type quasi-1D trap with the transverse oscillator length \( l_\perp \approx 0.6 \mu \text{m} \). The atomic scattering lengths can be chosen as \( a_{11} = a_{22} = 2000 \mu \text{m}, a_{12} \approx -(0.95 \div 0.99) a_{11} \), that corresponds to \( f_2 = 20 \div 100 \). In this case the characteristic scale of the length is \( l_0 \sim (1 \div 0.4) \mu \text{m} \), the time scale is \( t_0 \sim (0.8 \div 0.2) \mu \text{s} \) and the atom’s number is \( N_0 \approx 40 \sim 450 [12] \). The energy scale \( E_0 = \hbar/t_0 \) is of the order \((50 \div 100) \text{Hz} \) for the above data.

4. Strong coupling of an impurity with BEC

Next we consider the effect of strong coupling on the BEC deformation by an impurity. In the mean field approximation for one-component BEC, self-trapping properties of impurities for strong attractive and repulsive cases have been investigated in [29]. We can approximate the impurity action by considering it as

\[ \phi(x)^2 = \phi_0(x), \]

i.e. as the \( \phi \)-impurity. This approximation is valid when the localization scale \( l \ll l_0 \), where \( l_0 \) is the healing length. The \( \phi \)-impurity is placed at the point \( x = 0 \). So the BEC wave function is described by a
stationary GP equation, which follows from equation (7) (note that \( \Psi(x,t) = \psi(x) \exp(\mu t) \))

\[
-\mu \psi + \frac{1}{2} \psi_{xx} - |\psi|^2 \psi + |\psi| \psi - \Delta(x) \psi = 0,
\]

where \( A \) is the strength of the \( \delta \)-potential. We look for a solution in the form

\[
\psi(x) = \psi_0(x + x_0), \quad x < 0,
\]

\[
\psi(x) = \psi_0(x - x_0), \quad x > 0,
\]

where \( \psi_0(x) \) is a stationary solution of equation (7)

\[
\psi_0(x) = \frac{3\mu}{1 + \sqrt{1 - 9\mu/2} \cosh(\sqrt{2\mu}x)}.
\]

for some given value of the chemical potential \( \mu \).

Integrating equation (20) once around the point \( x = 0 \) we obtain

\[
\psi_1(0) - \psi_1(-0) = -2A \psi_0(x_0). \tag{22}
\]

Substituting solution (21) into equation (22), we come to an equation for the parameter \( x_0 \)

\[
\frac{\sqrt{2\mu} \sqrt{1 - 9\mu/2} \sinh(\sqrt{2\mu} x_0)}{1 + \sqrt{1 - 9\mu/2} \cosh(\sqrt{2\mu} x_0)} = A. \tag{23}
\]

This equation has an exact solution for a localized mode with respect to \( x_0 \)

\[
x_0 = \sqrt{2/\mu} \arctanh \left( \frac{1 + \sqrt{1 + \frac{4\mu}{9\mu - 2\mu}}}{A(1 - \sqrt{1 - 9\mu/2})} \right).
\tag{24}
\]

From equation (23) follows the inequality

\[ |A| < \sqrt{2\mu} \]

which determines an existence domain of stationary solutions of equation (20).

The number of atoms in the nonlinear localized mode is determined as

\[
N_c = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 2\sqrt{2\mu} \times \left[ 2 \sqrt{\frac{2}{9\mu}} \left( \arctanh \left( \sqrt{\frac{a}{a + b}} \right) + \arctanh \left( \sqrt{\frac{a}{a + b}} \tanh(x_0') \right) \right) - \left( 1 + \frac{b \sinh(x_0') \cosh(x_0')}{a + b \cosh^2(x_0')} \right) \right]. \tag{25}
\]

where

\[ a = 1 - \sqrt{1 - 9\mu/2}, \quad b = 2\sqrt{1 - 9\mu/2}, \quad x_0' = \sqrt{\mu/2} x_0. \]

The dependence \( N_c \) versus \( \mu \) is depicted in (figure 5) for two values of the strength, \( A = +0.15 \) (dotted line) and \( A = -0.15 \). According to the Vakhitov–Kolokolov (VK) criterion [35], a positive slope of the curve \( N_c(\mu) \) corresponds to the stability of the stationary solution \( \psi(x) \). We can see that the slope is positive over the entire range of values of the parameter \( \mu \) for both cases. Thus it should follow that both our solutions must be stable. Further we will demonstrate that the problem of stability is more complicated.

In (figure 6) stationary solutions of the governing equation (20) are shown: (a) a single-peaked solution for the attractive impurity, \( A = -0.15 \) and (b) a double-peaked solution for the repulsive impurity, \( A = +0.15 \). In both cases the chemical potential \( \mu = 0.15 \). The region of parameters exists (e.g. \( A < 0, A^2/2 < \mu < 2/9 \)), where the solution is stable. Single-peaked solutions are localized on an impurity corresponding to the attractive \( \delta \)-potential. Such a solution with \( A = -0.15 \) \( (\mu = 0.15) \) is depicted in figure 7(a). It remains stable in the entire time-interval of the numerical simulations.

Double-peaked solutions are localized on an impurity corresponding to the repulsive \( \delta \)-potential. The numerical simulations show that the stability of these solutions, as was mentioned above, is complicated. For instance, as shown in figure 7(c), the solution for positive \( A = +0.15 \) is stable at the value of the chemical potential \( \mu = 0.21 \).
Figure 7. Stationary solutions of equation (20). Evolution of stationary solutions: (a) stable solution for the attractive $\delta$-potential with $A = -0.15$ and $\mu = 0.15$; (b) unstable solution for the repulsive delta-potential with $A = 0.15$ and $\mu = 0.15$; (c) stable solution for the same repulsive delta-potential with $A = 0.15$ but another $\mu = 0.21$.

The Vakhitov–Kolokolov slope criterion gives the necessary stability condition for the localized solution. However, this condition is insufficient for the case when the solution is centered at the potential maximum. The wavepacket can drift away from its initial location and the drift instability will develop [36]. We have performed numerical simulation for the case when $A = +0.15, \mu = 0.15$ and observed the drift instability of the solution for a repulsive impurity (see figure 7(b)). Detailed analysis of this instability requires separate investigation of the spectral condition [37] for equation (20).

5. Conclusion

In conclusion, we have studied properties of a neutral bosonic impurity immersed into a quantum droplet (QD). We have found an effective potential acting on the impurity from the side of the QD. We have calculated energy levels for bound states of the impurity in this potential for cases of dominating quantum fluctuations, as well as effects of the mixed mean field and quantum fluctuations. In the case of strong coupling of the impurity with BEC we have shown the existence of the nonlinear local mode of the impurity produced by the balanced mean field nonlinearities and quantum fluctuations. We have found the strength threshold of the impurity for the existence of nonlinear localized modes in BEC. In our numerical simulations we have demonstrated the appearance of drift instability of the solution for the repulsive impurity.

In future, it will be interesting to study the bound states of an impurity immersed in a 3D droplet as well as interaction of an impurity with quantum 2D vortices. The problem of stability and the existence of nonlinear localized modes of 2D and 3D systems also requires consideration.

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ORCID iDs

R M Galimzyanov © https://orcid.org/0000-0003-3235-9889

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