Localization of a dipolar Bose–Einstein condensate in a bichromatic optical lattice

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Received 17 June 2010, in final form 29 July 2010
Published 4 October 2010
Online at stacks.iop.org/JPhysB/43/205305

Abstract

By numerical simulation and variational analysis of the Gross–Pitaevskii equation we study the localization, with an exponential tail, of a dipolar Bose–Einstein condensate (DBEC) of $^{52}\text{Cr}$ atoms in a three-dimensional bichromatic optical lattice (OL) generated by two monochromatic OLs of incommensurate wavelengths along three orthogonal directions. For a fixed dipole–dipole interaction, a localized state of a small number of atoms ($\sim 1000$) could be obtained when the short-range interaction is not too attractive or not too repulsive. A phase diagram showing the region of stability of a DBEC with a short-range interaction and dipole–dipole interaction is given.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The localization of a non-interacting wave form in a disordered potential, predicted by Anderson [1], has been the topic of vigorous research in different areas. Localization has been observed experimentally in diverse contexts [2] including Bose–Einstein condensates (BEC) [3, 4]. Billy et al [3] demonstrated the localization of a cigar-shaped interacting $^{87}\text{Rb}$ BEC released into a one-dimensional (1D) waveguide with controlled disorder created by a laser speckle. Roati et al [4] observed the localization of a non-interacting $^{39}\text{K}$ BEC in a bichromatic quasi-periodic optical-lattice (OL) potential created by superposing of two standing-wave polarized laser beams of incommensurate wavelengths. The non-interacting BEC was created [4] by tuning the atomic scattering length $a$ to zero near a Feshbach resonance [5]. The disorder in a quasi-periodic OL potential is deterministic, in contrast to the complete disorder in an optical speckle potential. Localization in such a quasi-periodic potential is a special case of Anderson localization in a fully disordered potential and is well described by the Aubry–André model [6]. Such a localization is often termed Aubry–André localization. However, these two mechanisms of localization are distinct. While the Anderson localization of wavefunctions with exponential tails is a pure quantum effect, the Aubry–André localization may occur in a classical phase space [7]. The localization of a BEC in a disordered potential has been the subject matter of various theoretical [8–12] and experimental [2–4] studies.

In the presence of strong disorder one has strong Anderson localization [3, 4], where the localized state could be quite similar to a localized state of the Gaussian shape in an infinite potential or a potential of very high barriers. Then the quantum state cannot escape the strong barriers of the disordered potential. However, the more interesting case of localization is in the presence of a weak disorder when the system is localized due to the quasi-periodic (disordered) nature of the potential [3, 4] and not due to the strength of the lattice. Localization takes place due to cancellation of waves coming after multiple scattering from many barriers of the random potential. When this happens, the localized state acquires a pronounced exponential tail.

The usual dilute BEC with negligible dipole moment interacting via short-range interaction is described by the mean-field Gross–Pitaevskii (GP) equation. More recently, it has been possible [13] to obtain a BEC of $^{52}\text{Cr}$ atoms with large dipole moment leading to a long-range dipole–dipole (dipolar) interaction superposed on the usual short-range interaction, which can be varied using a Feshbach resonance [5]. This allows us to study the dipolar BEC.
The cigar- and pancake-shaped localized DBEC are obtained by considering bichromatic OL potentials of different strengths along the orthogonal directions. A localized DBEC, without short-range interaction, can be achieved in a bichromatic OL trap for a small number of atoms by tuning [13] the atomic scattering length to zero near a Feshbach resonance [5]. For a cigar-shaped DBEC, without short-range interaction, as the number of atoms increases it becomes highly attractive and suffers from collapse instability. In the presence of a repulsive short-range interaction, the effect of the attractive dipolar interaction in the cigar shape can be compensated leading to a localized DBEC for a small number of atoms; delocalization may take place due to excess of repulsion for a large number of atoms. For a pancake-shaped DBEC, the dipolar interaction is repulsive and a localized DBEC is obtained for a small number of atoms. For a large number of atoms excess of repulsion should lead to delocalization. From a variational analysis of the localization of a DBEC, a phase diagram illustrating its stability for different short-range interactions, number of atoms and the geometry of the bichromatic OL is given. To obtain localization, the short-range interaction should be small. As in 1D [9, 10, 28], a large repulsive short-range interaction destroys the localization and the localized state escapes to infinity in all cases. A large attractive short-range interaction leads to collapse instability and destroys the localization.

In section 2 we present a brief account of the modified GP equation with the bichromatic OL potential in the presence of a dipolar interaction together with a Gaussian variational analysis. In section 3 we present numerical and variational studies of the localization of a dipolar interaction in the presence and absence of a short-range interaction. In section 4 we present a brief summary of the present investigation.

2. Analytical formulation

We study the localization of the DBEC of \( N \) atoms, each of mass \( m \), using the following mean-field GP equation with the bichromatic OL potential \( V(\mathbf{r}) \) [13]:

\[
\frac{m}{\hbar^2} \mu \phi(\mathbf{r}) = \left[ -\frac{1}{2} \nabla^2 + V(\mathbf{r}) + 4\pi a N|\phi(\mathbf{r})|^2 + \int U_{dd}(\mathbf{r} - \mathbf{r}') |\phi(\mathbf{r}')|^2 d\mathbf{r}' \right] \phi(\mathbf{r}),
\]

with

\[
U_{dd}(\mathbf{r}) = 3Na_{dd}(1 - 3 \cos^2 \theta)/r^3
\]

and

\[
V(\mathbf{r}) = \sum_{l=1}^{2} A_l \left[ v_\rho \sin^2(k_l x) + \sin^2(k_l y) \right] + v_z \sin^2(k_l z)
\]

where \( \phi(\mathbf{r}) \) is the DBEC wavefunction of the normalization \( \int |\phi(\mathbf{r})|^2 d^3\mathbf{r} = 1 \), \( \mu \) is the chemical potential, \( a \) is the atomic scattering length, \( \theta \) is the angle between \( \mathbf{r} \) and the direction of polarization, here taken along the \( z \) axis, \( A_l = k_l^2 s_l/2, \lambda_l \) are the wavelengths, \( k_l = 2\pi/\lambda_l \) are the wave numbers and \( s_l \) are...
the strengths of the OL potentials. The parameters \( v_r \) and \( v_z \) control the relative strengths of the OLs in different directions and can be varied to achieve the pancake- \((v_z > 1, v_r = 1)\) and cigar-shaped \((v_r > 1, v_z = 1)\) DBEC. The constant \( a_{dd} = \mu_0 \bar{μ}^2 m/(12\pi \hbar^2) \) in the dipolar interaction \( U_{dd} \) is a length characterizing the strength of the dipolar interaction and its experimental value for \( ^{35} \text{Cr} \) atoms is \( 15 \bar{a}_0 \) [13], with \( \bar{a}_0 \) being the Bohr radius, \( \bar{μ} \) the (magnetic) dipole moment of a single atom and \( \mu_0 \) the permeability of free space.

The GP equation (1) can be solved variationally by minimizing the energy functional [13]

\[
\frac{m}{\hbar^2} E[\phi] = \int \left[ \frac{1}{2} |\nabla \phi|^2 + V(\rho) \phi^2 + 2\pi a N \phi^4 \right] + \frac{\phi^2}{2} \int U_{dd}(\rho - r')|\phi(r')|^2 \, dr',
\]

(4)

with the following Gaussian ansatz for \( \phi(\rho) \) [29]:

\[
\phi(\rho) = \left( \frac{\pi^{-3/2}}{w_\rho^2 w_z^2} \right)^{1/2} \exp \left( -\frac{\rho^2}{2w_\rho^2} - \frac{z^2}{2w_z^2} \right),
\]

(5)

where \( w_\rho \) is the width in the radial direction \( \rho \) and \( w_z \) is the width in the axial direction \( z \). We have assumed circular symmetry in the \( x\text{-}y \) plane. Equations (4) and (5) lead to [29]

\[
\frac{m}{\hbar^2} E = \frac{1}{4} \left[ \frac{2}{w_\rho^2} + \frac{1}{w_z^2} \right] + \frac{N}{\sqrt{2\pi}} \frac{1}{w_\rho w_z} [a - a_{dd} \phi(\kappa)]
\]

\[
+ \frac{1}{2} \sum_{l=1}^{2} A_l [2v_\rho + v_z - 2v_\rho E_{\rho,l} - v_z E_{z,l}],
\]

(6)

\[
f(\kappa) = \frac{1 + 2\kappa^2}{1 - \kappa^2} - \frac{3\kappa^2 \text{atanh} \sqrt{1 - \kappa^2}}{(1 - \kappa^2)^{1/2}}, \quad \kappa \equiv \frac{w_\rho}{w_z},
\]

(7)

To compare the numerical results with variational analysis, we only consider localized states mostly occupying a single site of the bichromatic OL. Throughout this study the strength parameters of the two components of the bichromatic OL are taken as \( s_1 = s_2 = 4 \) and the corresponding wavelengths are taken as \( \lambda_1 = 5 \mu m, \lambda_2 = 0.862\lambda_1 \). The relative strengths of the radial and axial bichromatic OLs are varied by adjusting the parameters \( v_\rho \) and \( v_z \) in equation (3). To demonstrate that with these sets of parameters we are in the limit of localization with an exponential tail in a weak potential, we solve the 1D linear Schrödinger equation in dimensionless variables [31]

\[
-\frac{1}{2} \phi''(x) + \sum_{l=1}^{2} \frac{2\pi^2 s_l}{\lambda_l^2} \sin^2 \left( \frac{2\pi}{\lambda_l} x \right) \phi(x) = E \phi(x), \quad (13)
\]

with the above sets of parameters, where the prime denotes the \( x \)-derivative and \( E \) denotes the energy. In the limit of zero nonlinearity \( (a = 0) \) and zero dipolar interaction \( (a_{dd} = 0) \), (1) decouples into three equations like (13). In Figures 1(a) and (b) we plot the density \( \phi^2(x) \) of (13) versus \( x \) in linear and log scales together with its Gaussian variational counterpart \( \phi_\text{var}(x) = \exp(-x^2/w^2)/(\sqrt{\pi}w^2) \), with \( w = 0.4865 \) being the variational width, and the exponential fit \( \phi_\text{ex}(x) = \exp(-\text{abs}(x)/I_{\text{loc}})/(0.4865\pi^{1/2}) \), with \( I_{\text{loc}} = 0.75 \) being the localization length [3], providing a measure of the exponential tail. For a strong localization with a strong bichromatic potential \( I_{\text{loc}} \to 0 \) and the localized state has a

3. Numerical study

We perform a full 3D numerical simulation in Cartesian \( x, y, z \) variables using the imaginary- and real-time propagations with the Crank–Nicolson discretization [30] employing small space (~0.025) and time (~0.0001) steps necessary for obtaining converged results. For this purpose we use the FORTRAN programs provided in [31] after transforming (1) into a time-dependent form by replacing \( m\mu/h^2 \) by \( i\partial/\partial t \), where \( t \) is the time. The dipolar interaction term is evaluated by the usual fast Fourier transformation technique [14]. The imaginary- and real-time propagations lead essentially to the same localized states. This not only ensures the correctness of the calculational scheme, but also guarantees that the localized states are stationary and not a result of dynamical self-trapping [32]. (The imaginary-time propagation can only find the stationary localized states and cannot obtain the dynamical self-trapped states.) The stability of the localized state was tested by the real-time propagation allowing small perturbations of potential or interaction parameters. (In the absence of the dipolar interaction, the localized states have been demonstrated explicitly to be stable in one [10] and two [12] dimensions.) The accuracy of the numerical simulation was tested by varying the size of space and time steps and the total number of space and time steps.

To demonstrate that with these sets of parameters we are in the limit of localization with an exponential tail in a weak potential, we solve the 1D linear Schrödinger equation in dimensionless variables [31]

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\frac{1}{2} \phi''(x) + \sum_{l=1}^{2} \frac{2\pi^2 s_l}{\lambda_l^2} \sin^2 \left( \frac{2\pi}{\lambda_l} x \right) \phi(x) = E \phi(x), \quad (13)
\]

with the above sets of parameters, where the prime denotes the \( x \)-derivative and \( E \) denotes the energy. In the limit of zero nonlinearity \( (a = 0) \) and zero dipolar interaction \( (a_{dd} = 0) \), (1) decouples into three equations like (13). In Figures 1(a) and (b) we plot the density \( \phi^2(x) \) of (13) versus \( x \) in linear and log scales together with its Gaussian variational counterpart \( \phi_\text{var}(x) = \exp(-x^2/w^2)/(\sqrt{\pi}w^2) \), with \( w = 0.4865 \) being the variational width, and the exponential fit \( \phi_\text{ex}(x) = \exp(-\text{abs}(x)/I_{\text{loc}})/(0.4865\pi^{1/2}) \), with \( I_{\text{loc}} = 0.75 \) being the localization length [3], providing a measure of the exponential tail. For a strong localization with a strong bichromatic potential \( I_{\text{loc}} \to 0 \) and the localized state has a
pure Gaussian tail. However, when $l_{\text{loc}} > x_{\text{rms}}$ with $x_{\text{rms}}$ being the root mean square size, the exponential tail is pronounced and the limit of localization in a weak quasi-periodic potential is attained [3, 4]. In the present example, $x_{\text{rms}} = 0.53$ and $l_{\text{loc}} = 0.75$, and hence we are in the limit of localization in a weak potential. This is clear from figure 1(b), where the central part of the localized state is fitted to the variational Gaussian solution, whereas the large-$x$ parts are fitted to an exponential function with a large localization length over about nine orders of magnitude. In figure 1(b), one can identify several minor peaks in successive wells of the bichromatic OL potential. The state of figure 1 is localized by the weak bichromatic lattice and if we substantially reduce the strength of the potential, no localized state will emerge. In the experiments of [3, 4] and in some other studies on localization [9] in a weak potential, localized states with a pronounced undulating tail over many wells of the localization potential were considered. However, a weak limit of localization with an exponential tail can also be achieved in the absence of a pronounced undulating tail, as we have shown here. In this paper we consider localization in the presence of a pronounced Gaussian peak and a weak undulating tail as can be seen from figure 1(b). The existence of a pronounced Gaussian peak will be turned to good advantage in predicting accurate analytical variational results for the localized state and for an analytical understanding of the localization. We also consider the localization in the presence of a short-range interaction and dipolar interaction. The inclusion of a repulsive short-range interaction will in general destroy localization by increasing the localization length and thus creating a more pronounced exponential tail [9]. The inclusion of the dipolar interaction will have an effect on localization, which we study here, and such inclusion should not destroy the exponential tail of localization as illustrated in figure 1(b).

A variational analysis is useful for a qualitative understanding of the problem and we present the same before considering a numerical solution of (1). In figure 2 we plot the variational widths $w_\rho$ and $w_z$ for a DBEC of 170 $^{52}$Cr atoms in the cigar and pancake shapes. This figure shows the evolution of the widths from the pancake to cigar shapes while the radial width $w_\rho$ reduces and the axial width $w_z$ increases as expected. For $a = 0$, the axial width $w_z$ does not increase with the increase of $v_x$, as in the cigar shape the dipolar interaction becomes attractive and does not permit the increase of $w_z$.

Next we study, using (6), the set of values of the parameters for which the energy can have a minimum and allows a stable localized DBEC. The region of stability for the dipole strengths $a_{dd} = 0$ and $15a_0$ is shown in figure 3 for (a) 170 and (b) 500 $^{52}$Cr atoms as a phase plot of $a/\alpha_0$ versus the relative strengths of the bichromatic OL $v_\rho$ and $v_z$ in the radial and axial directions. The stability of a DBEC in a harmonic trap has also been studied [14]. For a fixed $a_{dd}$ and $N$ the stability region lies between the two corresponding lines in figure 3. Above the upper line the system becomes too repulsive (positive $Na/\alpha_0$) to be confined by the weak bichromatic OL. Below the lower line the system becomes too attractive (negative $Na/\alpha_0$) and suffers from collapse instability. The localization of a BEC (without dipolar interaction) is controlled by the nonlinearity $4\pi aN$ alone of (1) and the effect of the dipolar interaction on the stability of the DBEC is clearly exhibited in figure 3. In these figures we also plot numerical results for collapse instability with negative (attractive) scattering length (the lower limit of the stability in this figure), which agree well with the variational
Figure 3. Stability region in the $a/a_0$ versus $\nu_\rho$ and $\nu_z$ (relative strengths of the bichromatic OL in the radial and axial directions) phase plots for (a) 170 and (b) 500 atoms for $a_{dd} = 15a_0$ ($^{52}$Cr atoms) and $a_{dd} = 0$ variational—var (lines), numerical—num (points). Localization is possible between the upper and lower lines of the same data set.

Figure 4. Numerical (num) and variational (var) energies $E$ versus relative strengths of the bichromatic OLs $\nu_\rho$ and $\nu_z$ for (a) 170 and (b) 500 $^{52}$Cr atoms.

results. Starting from a stable localized state, the stability lines (points) are obtained by slowly changing the scattering length $a$ at a fixed trap symmetry (by fixing the parameters $\nu_\rho$ and $\nu_z$) until no localized state is obtained (by numerical or variational means). On the pancake side the dipolar interaction is repulsive and the localization is destroyed for a smaller value of the repulsive scattering length compared to the case where the dipolar interaction is absent, as can be seen in figure 3. The opposite happens on the cigar side where the dipolar interaction is attractive. On the cigar side the dipolar interaction is attractive and the localization is destroyed for a larger value of the repulsive scattering length compared to the case where the dipolar interaction is absent, as can be seen in figure 3(b) for 500 atoms. This effect is smaller in figure 3(a) for 170 atoms.

From (7) we find that $f(\kappa)$ is positive for the cigar shape leading to an attractive contribution to energy (6), whereas it is negative in the pancake shape leading to a repulsive term in energy. For $N = 170$ there is a symmetric state with $w_z = w_\rho$ and $f(\kappa) = 0$ near $\nu_\rho = 1, \nu_z \approx 1.3$ where the dipolar interaction does not contribute and where the DBEC is most stable at the maxima as shown in figure 3(b). At this point the DBEC acts like a ‘normal BEC’ and the $Na/a_0$ value at the maximum is independent of $N$. In the pancake shape, the localization of the DBEC can be easily destroyed due to a large repulsive dipolar interaction in the weak bichromatic OL. In the cigar shape, the large attractive dipolar interaction may lead to the collapse of the localized DBEC more easily than in the absence of the dipolar interaction. These aspects are clearly illustrated in figure 3(b). For $N = 500$ the interactions are stronger than for $N = 170$ and the domain of the allowed localization in terms of the number of atoms has reduced.

In figures 4(a) and (b) we compare the numerical and variational energies of the $^{52}$Cr DBEC of 170 atoms with $a = 0$ and $20a_0$ and of 500 atoms with $a = 0$ and $10a_0$, respectively. A smaller value of $a$ is required for the stability of 500 atoms (see figure 3(b)). The agreement between variational and numerical results is good in general except for $\nu_z \to 100, \nu_\rho = 1$. In this limit the localized DBEC occupies two sites of the bichromatic OL and does not have a Gaussian shape. This justifies a small disagreement between the numerical and variational results in this limit. The variational result for $a = 10a_0$ in figure 4(b) only exists up to $\nu_z \approx 35$ (see figure 3(b)).

Next we study how the DBEC solely under the effect of the dipolar interaction ($a = 0$) changes its shape as we move from the cigar- to pancake-shaped configuration. In
The effect of the dipolar interaction is small in the symmetric case with \(v_z = v_\rho = 1\) and \(N = 500\) atoms. Nevertheless, due to the complicated dipolar interaction, the density \(\phi^2(x, 0, z)\) does not have a pure circular shape in this case (not explicitly shown). This density distribution will be circular for a BEC without dipolar interaction. (A nearly circular shape for this density is obtained for a DBEC with \(v_\rho = 1\) and \(v_z = 1.6\).) The numerical and variational energies for this state are 6.97 and 7.06, respectively.

We next consider the localization for \(v_z = 10\), \(v_\rho = 1\) and \(a = 0\). In this pancake shape, the dipolar interaction is repulsive and for 500 \(^{52}\text{Cr}\) atoms a localized DBEC is obtained. In figures 6(a) and (b) we show the numerical and variational 2D contour plots of the density \(\phi^2(x, y, 0)\) in the \(z = 0\) plane, respectively, for this DBEC. The numerical and variational 2D contour plots for the density \(\phi^2(x, y, 0)\) in the \(z = 0\) plane for the same DBEC is shown in figures 6(c) and (d), respectively. In this case, the dipolar interaction is repulsive in nature and hence the size of the DBEC is larger than the Gaussian variational shape (see figure 5 where the opposite happens for a DBEC with an attractive dipolar interaction.). The numerical and variational energies for this state are 14.16 and 14.26, respectively. The change from a cigar shape to a pancake shape of the localized DBEC as we move from \(v_\rho = 10\) and \(v_z = 1\) to \(v_\rho = 1\) and \(v_z = 10\) is obvious from the density distribution in figures 5(a) and 6(a). Although the variational and numerical energies (studied in figures 5 and 6) are quite close to each other, the numerically obtained matter density should have some peculiarities not obtainable from the variational calculation due to the anisotropic dipolar interaction. (The variational calculation is based on an axially symmetric Gaussian distribution.)
4. Summary and conclusion

We investigated the localization of a $^{52}$Cr DBEC in a weak bichromatic OL trap in the presence and absence of a short-range interaction using the numerical and variational solutions of the 3D GP equation (1). Of the two solutions, the numerical solution is the most precise and should be used in the case of disagreement with the variational solution. Although the density of the central part of the localized states has a near-Gaussian distribution, the density distribution also has a long exponential tail [3, 4]. The Gaussian distribution near the center permits a variational analysis of localization, which is used for an analytical understanding of the problem. A DBEC of a small number of atoms with a weak short-range interaction could be localized by a relatively weak bichromatic OL trap. From the variational solution we obtain a phase diagram (figure 3(b)) illustrating the effect of the dipolar interaction on the localization as a function of the strengths of the traps $\nu_r$ and $\nu_z$ in the axial and radial directions, respectively. We find that for $^{52}$Cr atoms, the dipolar interaction has a moderate effect on localization. (A larger effect will certainly appear for dipolar molecules where the dipole moment could be larger by an order of magnitude compared to the dipole moment of $^{52}$Cr atoms.) The numerical and variational energies of the DBEC, as well as the corresponding densities, are in reasonable agreement with each other. In the absence of a short-range interaction, the localized DBEC can accommodate the largest number of $^{52}$Cr atoms ($\sim$1000) in the spherical configuration and this number reduces for both cigar and pancake shapes due to the attractive and repulsive dipolar interaction, respectively. The attractive dipolar interaction leads to collapse and the repulsive dipolar interaction leads to leakage to infinity. We hope that this study will motivate experiments on the localization of a $^{52}$Cr DBEC in a bichromatic OL trap. The estimate of the number of localized $^{52}$Cr atoms, their radial and axial sizes and shapes, etc as predicted in the present study can be verified in the experiment.

Acknowledgments

FAPESP and CNPq (Brazil) and DST (India) provided partial support.

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