Partial delocalization of two-component condensates in optical lattices

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Abstract

We study management of localized modes in two-component (spinor) Bose–Einstein condensates embedded in optical lattices by means of changing interspecies interactions. By numerical integration of the coupled Gross–Pitaevskii equations, we find three different regimes of the delocalizing transition: (i) the partial delocalization when the chemical potential of one of the components collapses with a gap edge and the respective component transforms into a Bloch state, while the other component remains localized; (ii) the partial delocalization as a consequence of instability of one of the components; and (iii) the situation where a vector soliton reaches the limits of the existence domain. It is shown that there exists a critical value for the interspecies scattering length, below which solutions can be manipulated and above which one of the components is irreversibly destroyed.

1. Introduction

Management of matter waves in optical lattices (OLs) can be implemented in different ways, including variation of parameters of the periodic potential in time or change of the nonlinearity with the help of the Feshbach resonance. In particular, by changing the amplitude of the lattice one can achieve the delocalizing transition, which consists of transformation of an initially localized mode, also referred to as a gap soliton, into a spreading out atomic wave packet. Such a transition was predicted for two- and three-dimensional single-component Bose–Einstein condensates (BECs)\textsuperscript{[1, 2]} and can be achieved by adiabatically decreasing the amplitude of the periodic potential below some value, with subsequent restoration of the initial lattice profile. If the amplitude of the lattice reaches some critical value, the initially localized wave packet cannot be recovered at the end of the experiment and one observes a spreading out condensate. In a recent paper [3], it has been shown that the delocalizing transition can be observed also in one-dimensional (1D) systems, with the help of interplay between the linear and nonlinear lattices. This suggestion was based on the fact that the transition occurs in a system where small amplitude gap solitons cannot exist [2], i.e. where a minimal atomic number is necessary for the creation of a localized mode. From the physical point of view, the transition is related to modulational stability of the Bloch states bordering either the semi-infinite gap in the spectrum of Bogoliubov’s phonons or in a gap induced by the periodic potential [3].

The described results naturally raise questions about the existence of other 1D systems allowing for delocalizing transition and about other physical mechanisms resulting in delocalizing transition. A simple positive answer to the first of these questions readily follows from the fact that the quintic nonlinear Schrödinger equation with a periodic potential requires a critical number of particles for the creation of a gap soliton [4] and thus represents a system which can undergo the 1D delocalizing transition. The answer to the second question is also positive, and moreover, it offers a system allowing for a new type of delocalizing transition. To explain this, we recall that new factors affecting the existence of gap solitons appear when one considers multicomponent systems in periodic potentials, and, in particular, binary mixtures or spinor condensates loaded in OLs: a necessary condition for the existence of the modes is that the chemical potentials of both components must belong to the respective phonon gaps [5]. This condition may be violated being subjected to change of the system parameters, thus leading to destruction of two-component gap solitons. Generally speaking, in such a situation one does not necessarily expect...
complete delocalization of the condensate, because one of the chemical potentials may still belong to a gap, while the other one reaches the gap edge. Instead, in this situation, one may observe a partial delocalizing transition, where one of the components spreads out, while the other one stays localized. Detailed description of this phenomenon constitutes one of the main goals of the present paper.

Practical relevance of the formulated problem is justified by the fact that binary mixtures are experimentally available in laboratories (see, e.g., [6–10], for the rubidium spinor condensate). Theory of coherent structures emergent in spinor condensates embedded in OLs has also received a considerable deal of attention [5, 11, 12]. Moreover, being interested in the interplay between the induced periodicity and the varying nonlinearity, we mention that systems subjected to such conditions were addressed in [12–14], the latter dealing with the tight-binding approximation of the problem.

Before going into details, we briefly discuss other aspects of the formulated problem. First, transformation between two different states of a condensate represents not only fundamental but also practical interest, as it allows for selective and thus controllable separation of the initially localized components of mixtures of BECs. Its mathematical relevance is determined by the fact that the transition allows for experimental study of the limits of the existence of localized states.

Second, on the basis of preceding studies, the most direct approach to obtain the delocalizing transition would be the change of the parameters of the OL. However (this was checked by our extensive numerical simulations), the response of a binary mixture to such a change is very similar to that displayed by one-component BECs, and does not lead to the delocalizing transition. In particular, decreasing (increasing) of the potential results in expansion (narrowing) of vector gap solitons (cf [1, 2]). Essentially new phenomena can be found when management is performed by means of changing the interspecies interactions (for one-component BECs, the delocalizing transition induced by nonlinear management was suggested in [3]).

Third, it was also verified numerically that the delocalizing transition reveals qualitatively the same behaviour for binary mixtures of two different species of atoms and for spinor condensates. Therefore, in the present work we concentrate on the more simple dynamics of a spinor condensate induced by the change of the interspecies interaction.

Finally, since the adiabatic change of the parameters in practice represents a particular type of management of mixtures of BECs, it is particularly relevant to mention that, in [12], it was shown that interplay between the OL potential and the scattering length can assist building two-component gap solitons.

The paper is organized as follows. In section 2, we introduce the model and explain how the solutions are constructed and how its behaviour is studied. Section 3 is devoted to the case where all nonlinear coefficients are repulsive, the delocalization being achieved when the chemical potential of one of the components collapses with a gap edge. In section 4, nonlinear coefficients have different signs and delocalization is observed when gap solitons reach the limits of the existence domain or when dynamical instabilities are developed. Section 5 summarizes our results.

2. The model and numerical method

A diluted two-component mixture of spinor BECs in the mean-field approximation is described by the coupled Gross–Pitaevskii (GP) equations (see, e.g., [5, 6, 8, 15] and references therein), \( j = 1, 2 \)

\[
\begin{align*}
\hbar \frac{\partial \psi_j}{\partial t} &= -\frac{\hbar^2}{2m} \Delta \psi_j + U(x) \psi_j \\
+ \frac{4\pi \hbar^2}{m} &\left( a_{jj} |\psi_j|^2 + a_{i,j} |\psi_i|^2 |\psi_j|^2 \right) \psi_j,
\end{align*}
\]

(1)

where \( U(x) = U(x + d) \) is the external potential, which in our case is periodic along the x-direction with the lattice constant \( d \) and \( a_{ij} = a_{ji} \) are the s-wave scattering lengths of the binary interactions. Such condensates are available experimentally. Namely, mixtures of the hyperfine states \( |F = 2, m_F = 1 \rangle \) and \( |F = 2, m_F = 2 \rangle \) [6], \( |F = 1, m_F = -1 \rangle \) and \( |F = 2, m_F = 1 \rangle \) [7, 8], |F = 2, m_F = 2 \rangle |F = 1, m_F = 1 \rangle [9] and \( |F = 1, m_F = 0 \rangle \) and \( |F = 1, m_F = \pm 1 \rangle \) [10] of \(^{87}\text{Rb}\) atoms have already been reported.

Equation (1) takes into account that the two components of the mixture are different hyperfine states of the same atoms, therefore, the masses of both components are identical, i.e. \( m_1 = m_2 = m \). In this context, it is worth mentioning that our analysis has a general character and can be applied to any binary mixture of BECs, either of spinors (as done in the present paper) or of atoms of different species. In the latter case, however, distinct atomic masses \( m_1 \neq m_2 \) result in nonidentical band-gap structures of the associated linear problems, which requires technical adjustments of the numerical approaches developed below.

We assume that the lattice is produced by two counter-propagating monochromatic laser beams, resulting in a cos-like shape of the periodic potential \( U(x) \). Then, in the quasi-one-dimensional case, equation (1) can be rewritten in the dimensionless variables \( (j = 1, 2) \)

\[
\begin{align*}
\bar{\partial} \bar{\psi}_j \bar{\partial} \tau &= -\bar{\partial}^2 \bar{\psi}_j - V \cos(2\chi) \bar{\psi}_j \\
+ \left( \chi |\bar{\psi}_j|^2 + \chi |\bar{\psi}_{3-j}|^2 \right) \bar{\psi}_j.
\end{align*}
\]

(2)

Now the distance and the time are measured in the units of \( d/\pi \) and \( E_R/\hbar \), respectively, \( E_R = \hbar^2 \pi^2 / (2md^2) \) being the recoil energy, and \( V \) is the amplitude of the OL in units of the recoil energy. The link between the dimensionless order parameter \( \bar{\Psi}_j \) and the macroscopic wavefunction \( \psi_j \), as well as the explicit expressions (differing by a factor of 2) for the coefficients \( \chi_j \) and \( \chi \) through the scattering lengths \( a_{ij} \) can be found in [5]. Here, we only mention that the effective number of particles of the component \( j \) is calculated as \( N_j = \int |\bar{\Psi}_j|^2 d\bar{x} \) and is related to the real number of atoms, \( N_j \), by the simple formula \( N_j = gN_J \), where \( g \approx 10^{-3} \times 10^{-4} \) in the real experimental situation (see e.g. [6]).

Since we are interested in a situation where \( \chi = \chi(\bar{t}) \) is adiabatically changing in time, stationary localized solutions
of equation (2) play a prominent role. We thus make an ansatz
\[ \Psi_j(x, t) = \Psi_j(x) \exp(-i\mu_j t), \]
where \( \mu_j \) is the chemical potential of the jth component, in equation (2). Dropping the tildes over the dimensionless variables (the only ones used below) we obtain (\( j = 1, 2 \))
\[ \mu_j \Psi_j = -\frac{d^2 \Psi_j}{dx^2} - V \cos(2x) \Psi_j + (\chi_j |\Psi_j|^2 + \chi |\Psi_{3-j}|^2) \Psi_j. \] (3)
A diversity of localized modes supported by equation (3) and possessing a given symmetry were described in [5]. Here, we focus only on the particular case of fundamental symmetric modes (designated in [5] as OS–OS modes). Moreover, to simplify the construction of the initial states (we do this by the shooting method), as well as for their systematic exploration, we restrict the consideration to the case where
\[ (\chi_0 - \chi_1)(\chi_0 - \chi_3) > 0, \] (4)
\( \chi_0 \) defined as \( \chi_0 = \chi(t = 0) \). In this case, the simplest initial profile of a localized mode is characterized by equal chemical potentials \( \mu_1 = \mu_2 = \mu_0 \). Then \( \Psi_j = \alpha_j \Phi \), where \( \alpha_j = \sqrt{|\chi_0^2 - \chi_1 \chi_3|/|\chi_0 - \chi_{3-j}|} \) and the real function \( \Phi \) solves the equation
\[ \mu \Phi = -\Phi_{xx} - V \cos(2x) \Phi + \sigma \Phi^3, \] (5)
\( \sigma = \text{sgn}(\chi_0 - \chi_1 \chi_3)(\chi_0 - \chi_{3-j}) \) (we observe that due to the constrain of equation (4), it does not depend on \( j \)). A relation among the numbers of particles is given by
\[ \int |\Phi|^2 \, dx = N = \alpha_1^2 N_1 = \alpha_2^2 N_2. \] (6)
For each of the components, the OL results in a band spectrum, and the chemical potentials \( \mu_{1,2} \) must belong to the respective gaps. We further restrict our analysis to \( \mu_0 \) belonging either to the semi-infinite or to the first lowest gap. To be specific, we will also fix \( V = 1 \), which does not affect qualitatively the phenomenon.

As we investigate the behaviour of localized modes subjected to the adiabatic variation of \( \chi \), we first employ the Newton–Raphson (NR) method for constructing the branches of solutions, which ‘depart’ from the given \( \Psi_j \) and are constrained to fixed values of \( N_{1,2} \). When the strength of the interspecies interactions is changed, the chemical potentials of both components are changed as well, i.e. \( \mu_1 = \mu_2(\chi) \), provided that \( \mu_1(\chi_0) = \mu_2(\chi_0) = \mu_0 \), and can be computed using the formula (\( j = 1, 2 \))
\[ \mu_j = \frac{1}{N_j} \int_{-\infty}^{\infty} \left( \frac{d \Psi_j}{dx} \right)^2 - V \cos(2x) |\Psi_j|^2 + \chi_j |\Psi_j|^4 + \chi |\Psi_{3-j}|^4 |\Psi_j|^2 \right) \, dx. \] (7)
This formula can also be used to calculate ‘instant’ chemical potentials in the temporal adiabatic dynamics, when \( \chi = \chi(t) \), which is studied using the procedure as follows.

For a given \( \chi_0 \), we start with the solutions \( \Psi_j = \alpha_j^{-1} \Phi \) obtained from equation (5). For the sake of definiteness, the variation of the interspecies interaction is chosen as
\[ \chi(t) = (\chi_0 - \chi_m) \cos^2 \left( \frac{\pi t}{T} \right) + \chi_m, \] (8)
with \( \chi_m = \chi(T/2) \) and \( T \) being the total time of simulations. In other words, we first increase the nonlinearity until the maximal value \( \chi_m \) and then decrease it until the initial value \( \chi_0 \). Behaviour of this system is investigated by the direct integration of equation (2), with adiabatic variation of \( \chi(t) \), according to equation (8).

For management to be possible, the initial solutions must be experimentally feasible. Therefore, we test the dynamical stability of the initial \( \Psi_{1,2} \), by perturbing it with some addenda (in the presented results it is given by 0.05 \( \cos(0.5(x + \phi_j)) \)) \( \Psi_j \), where \( \phi_1 = 0.0 \) and \( \phi_2 = 0.3 \) and numerically integrating equation (2), with constant \( \chi = \chi_0 \).

3. Repulsive two-body interactions
First, we consider a binary mixture with all repulsive interactions. To be specific we choose \( \chi_1 = 1.0, \chi_2 = 0.5 \) and \( \chi_0 = 2.0 \), which corresponds to \( \alpha_1 \approx 1.53, \alpha_2 \approx 1.87 \) and \( \sigma = 1 \). We start with the existence of the stationary fundamental vector soliton for different \( \chi \), using the NR method, as explained above. From equation (6) it readily follows that, at \( \chi = \chi_0 \), we have \( N_2/N_1 = 0.66(6) \). The chemical potentials \( \mu_{1,2}(\chi) \) are depicted in figure 1 (the left top panel), where one can observe two important features.

First, even infinitesimal change of \( \chi = \chi_0 + \delta \chi \) results in increase of the chemical potentials and their splitting: \( \mu_j = \mu_0 + \delta \mu_j \), with \( \delta \mu_{1,2} > 0 \) and \( \delta \mu_1 \neq \delta \mu_2 \). Second, the chemical potential of the second component monotonously grows with \( \chi \) approaching the top of the first energy gap. The latter suggests that, at some \( \chi = \chi_{0a} \) between points B and C.
Dynamics of the densities of the first component in (b) and (d) and of the second component in (c) and (e) are presented.

Figure 2. (a) The number of particles of the first component along the first energy gap ($\mu \in [0.471; 1.467]$), with $\Psi_1 = 0$. The horizontal thin line represents $N_j \approx 1.95$ (i.e. the number of particles of the first component in the mixture analysed in figure 1). (b) The solid line represents the profile of $\Psi_1$ from figure 1C. The dashed line is obtained as a solution of equation (3), with $\Psi_1 = 0$ and $N_j = 1.95$ (the lines are indistinguishable on the figure scale). (c) The solid line corresponds to $\Psi_2$ taken at the point C of figure 1, compared with the Bloch wave (the dashed line) calculated at the lower edge of the second band ($\mu = 1.467$) and having an amplitude matching the solution $\Psi_2$.

(see the left top panel of figure 1), $\mu_2$ collapses with the gap edge. For $\chi > \chi_{cr}$, the vector soliton with given numbers of particles in each component does not exist, so according to the arguments exposed above, $\chi_{cr}$ must determine the critical value above which the delocalizing transition occurs. Moreover, one can predict that this is a partial delocalization because the chemical potential of the first component still belongs to the gap and thus the respective component persists.

Although we use a rather large spatial domain of calculation, $x \in [-48\pi; 48\pi]$, the provided analysis of the stationary solutions is not yet conclusive about the existence of the modes, because of boundaries possibly affecting the expanding second component. Indeed, from the profiles of $\Psi_j$ shown in figure 1, one observes tendency of the second component to the Bloch state of the upper band edge as $\chi$ exceeds $\chi_{cr}$. To check numerically whether the delocalization is authentic, i.e. that the second component does not represent, say, a small amplitude gap soliton, affected by the boundaries, we recall that $|\Psi_2|^2$ becomes small enough when $\chi$ tends to $\chi_{cr}$. Hence, the first component approximately solves equation (3) with $\Psi_2 = 0$. That is why, in figure 2, we constructed the lowest branch of the localized modes of the first component in the absence of the second component. For a given number of particles $N_1$, we found the chemical potential $\mu_1^*$ and constructed the one-component localized mode.

In figure 1 (left top panel), one can see that, indeed, $\mu_1 \rightarrow \mu_1^*$ (see the dashed line) in the domain where $\mu_2$ collapses with the second band. Direct comparison of the explicit shapes of the localized modes in the single-component BEC and the first component in the binary mixture is shown in figure 2(b), illustrating that the distribution of the first component is transformed into the one-component localized mode. At the same point, the second component becomes an extended Bloch state, as shown in figure 2(c).

Finally, we turn to the dynamical experiment. The results are shown in figure 3. Scanning values of $\chi_m$ between those corresponding to points B and C in figure 1, one observes complete restoring of the vector soliton if $\chi$ does not reach its critical value, which is found to be $\chi_{cr} \approx 2.6$, while the partial delocalization of the binary mode is observed when $\chi_m > \chi_{cr}$ (as predicted by the stationary analysis).

Additionally, we explored the case with all attractive interactions ($\chi \cdot x_j < 0$). Symmetric solutions are now located in the semi-infinite gap and, as $\chi$ adiabatically increased, the chemical potentials of both components grow, approaching the gap edge. However, we did not observe the delocalizing transition for negative values of $\chi$. It occurred only for $\chi > 0$, i.e. when $x_j \cdot \chi$ becomes negative. Therefore, next we focus on this case.

4. Cases $x_j \cdot \chi < 0$

Now we consider a binary mixture when intra- and interspecies interactions have different signs. To be specific, we investigate the case where $\chi_1 = -1.0$, $\chi_2 = -0.5$ and $\chi \geq 0$. In

Figure 3. In (a), time dependence of the intraspecies interaction is shown. Solid and dashes lines correspond to $\chi_m = 2.5$ and $\chi_m = 3$. Dynamics of the densities of the first component in (b) and (d) and of the second component in (c) and (e) are presented. $\chi_m = 2.5$ for [(b), (c)], and $\chi_m = 3.0$ for [(d), (e)]. Here, $\mu_0 = 1.3$ and $\chi_0 = 2.0$.
adiabatically increase the critical value of the interspecies interaction must coincide

\( \chi \), \ex \) are presented.

\( \alpha \) maximum strength for the repulsive interspecies interaction, splitting of the chemical potentials \( \alpha \) approaches the energy band edge, while the other component remains subjected to a sufficiently large change of the interspecies interaction. When all nonlinear interactions are repulsive, one of the components can be delocalized if subjected to a sufficiently large change of the interspecies scattering length, as its chemical potential collapses with the energy band edge, while the other component remains

with the bifurcation point \( \chi_{\text{ex}} \), where \( \mu_{1,2} \) belong to the gap but where \( \partial \mu_{1,2}/\partial \chi \approx \infty \). For the numbers of atoms as in figure 4, it was numerically found that \( \chi_{\text{ex}} \approx 0.0975 \). Passing to the dynamics, we integrated the GP equation (2). For different values of \( \chi_{\text{ex}} \) below the bifurcation point, \( \chi_{\text{ex}} < \chi_{\text{ex}} \), we found that the vector soliton can be restored to its initial shape, as shown in figures 5(b) and (c). However, if \( \chi \) overcomes the critical value \( \chi_{\text{ex}} \) (see figures 5(d) and (e)), one component (here \( \Psi_1 \)) breaks into two repelling wave packets moving outwards the centre, while the other component (here \( \Psi_2 \)) transforms into a stable single-component localized mode. The observed behaviour can also be interpreted as a kind of delocalizing transition. Its physical origin and, naturally, its manifestation are different from those reported in figure 4.

Additionally, instability of the vector soliton was observed for several values of \( \chi_{\text{ex}} < \chi_{\text{ex}} \). All such values are located in a region of the branch \( \mu_2(\chi) \) between its inflection point and \( \chi_{\text{ex}} \). We attribute this behaviour to the existence of domains of instability. From equation (8), we have that the velocity of \( \chi(t) \) at the point \( \chi_{\text{ex}} \) is zero (\( \dot{\chi} (\chi_{\text{ex}}) = 0 \)); therefore, a mode spends long enough time in the vicinity of \( \chi_{\text{ex}} \) for the instability to develop. This is what happens in figures 5(f) and (g), where one of the components of the vector soliton (here \( \Psi_1 \)) looses its stability, breaks from the second component and starts to move away from the centre, while the second component maintains its shape. In the case where \( \chi_{\text{ex}} > \chi_{\text{ex}} \), presented in figures 5(d) and (e), although we pass in the instability region, we do not observe instability. This can be explained by that fact that the time spent by the vector soliton in the instability region was not enough for instability to start developing.

5. Conclusions

We have studied the management of coupled gap solitons in a two-component spinor Bose–Einstein condensate embedded in an optical lattice, by means of the adiabatic variation of the interspecies interaction. When all nonlinear interactions are repulsive, one of the components can be delocalized if subjected to a sufficiently large change of the interspecies scattering length, as its chemical potential collapses with the energy band edge, while the other component remains

\begin{align*}
\text{Figure 4.} \quad &\text{The chemical potentials versus nonlinear coefficient } \chi \text{ (left top panel). The dotted line corresponds to the edge of the semi-infinite gap. In A, B and C, the profiles of stationary modes } \Psi_1 \text{ (solid lines) and } \Psi_2 \text{ (dashed lines) are shown. Here, } N_1 \approx 1.00 \text{ and } N_2 \approx 1.99. \text{ The initial chemical potential is } \mu_0 = -0.25. \text{ When } \chi \text{ approaches } \chi_{\text{ex}}, \text{ solutions B and C bifurcate.} \\
\end{align*}

\begin{align*}
\text{Figure 5.} \quad &\text{In (a), the time dependence of the interspecies interaction is shown. Solid, dash-dotted and dashed lines correspond to } \chi_{\text{ex}} = 0.02, \chi_{\text{ex}} = 0.08 \text{ and } \chi_{\text{ex}} = 0.15. \text{ Dynamics of the densities of the first component in (b), (d), (f) and of the second component in (c), (e), (g) are presented. } \chi_{\text{ex}} = 0.02 \text{ for [(b), (c)], } \chi_{\text{ex}} = 0.15 \text{ for [(d), (e)], and } \chi_{\text{ex}} = 0.08 \text{ for [(f), (g)]. Initial parameters are } \mu_0 = -0.25 \text{ and } \chi_0 = 0.0. \\
\end{align*}
localized. On the other hand, if the intra- and interspecies interactions have different signs, partial delocalization is achieved when solutions reach the limits of the existence domain. In this case, the manifestation of the phenomenon is different, as one of the components breaks in two gap solitons propagating outwards each other. Finally, we observed one more type of the delocalizing transition: the one caused by the instability of a vector soliton which develops more rapidly than the change of the scattering length occurs. In this case, one of the components splits out propagating in the form of a small amplitude gap soliton. In all the cases investigated the less populated component becomes delocalized while the more populated component maintains its shape.

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