Competition between attractive and repulsive interactions in two-component Bose-Einstein condensates trapped in an optical lattice

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We consider effects of inter-species attraction on two-component gap solitons (GSs) in the binary BEC with intra-species repulsion, trapped in the one-dimensional optical lattice (OL). Systematic simulations of the coupled Gross-Pitaevskii equations (GPEs) corroborate an assumption that, because the effective mass of GSs is negative, the inter-species attraction may split the two-component soliton. Two critical values, κ1 and κ2, of the OL strength (κ) are identified. Two-species GSs with fully overlapping wave functions are stable in strong lattices (κ > κ1). In an intermediate region, κ1 > κ > κ2, the soliton splits into a double-humped state with separated components. Finally, in weak lattices (κ < κ2), the splitting generates a pair of freely moving single-species GSs. We present and explain the dependence of κ1 and κ2 on the number of atoms (total norm), and on the relative strength of the competing inter-species attraction and intra-species repulsion. The splitting of asymmetric solitons, with unequal norms of the two species, is briefly considered too. It is found and explained that the splitting threshold grows with the increase of the asymmetry.

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I. INTRODUCTION AND THE MODEL

Self-supporting localized patterns in Bose-Einstein condensates (BECs), which are frequently called matter-wave solitons, have been the subject of many theoretical and experimental works. The solitons were first experimentally created in the condensate of 7Li atoms loaded in a strongly elongated (“cigar-shaped”) trap[1]. The use of the Feshbach-resonance (FR) technique[2] makes it possible to tune the scattering length of the inter-atomic collisions in the condensate to a small negative value, thus providing for the weak self-attractive nonlinearity, which is necessary for the creation of stable solitons. In another experiment, the solitons were observed in the 85Rb BEC remaining in the trap after the onset of collapse induced by the switch of the interaction between atoms from repulsive to attractive[3]. Potentially, the FR technique in combination with a quasi-one-dimensional optical lattice (OL, i.e., a spatially-periodic potential induced by a pair of counter-propagating laser beams) can be used to create solitons with a fully three-dimensional shape[4].

In most experiments, BEC is created in ultracold gases with repulsion between atoms. In this case, bright solitons were predicted as a result of the balance between the repulsive nonlinearity and negative effective mass of the matter waves, induced by the OL[5]. The corresponding gap solitons (GSs) emerge in finite bandgaps of the OL’s linear spectrum, where the negative effective mass is available. Theoretical models of matter-wave GSs were reviewed in Ref. [6], and their stability was analyzed in detail in Refs. [6, 7]. Additionally, in Ref. [8], the stability of the GS was also studied against quantum fluctuations, following the lines of the approach which was earlier developed for ordinary matter-wave solitons in Ref. [9]. Experimentally, GSs were created in the 87Rb condensate trapped in a cigar-shaped potential combined with an OL applied in the axial direction[10], with ≈ 250 atoms in the established soliton. An essential ingredient of the experiment was the acceleration of the condensate, with the aim to push the atomic waves into the spectral region featuring the negative effective mass. Another approach to the creation of the GS was proposed in Ref. [11]: one may add a strong parabolic trap to the OL potential, confining the entire condensate to a small spatial region, and then gradually relax the extra trap, which may allow the atomic cloud to remain in a relatively compact GS state. Besides that, one may expect that a chain of GSs may develop from the modulational instability of nonlinear quasi-periodic Bloch waves trapped in the OL[12].

Binary mixtures of BECs are also available as media in which various matter-wave patterns may be created. Most typically, the mixtures are formed by two different hyperfine states of the same atom, such as 87Rb[12] and 23Na[13]. Creation of a heteronuclear mixture of 41K and 87Rb was also reported[14]. As concerns the effective nonlinearity in the mixture, it is known that the sign and magnitude of the scattering lengths which characterize collisions between atoms belonging to different species may also be controlled by means of the FR technique[15].

In view of the latter possibility, it is reasonable to consider a binary BEC with the (natural) intra-species self-repulsion, while the inter-species interaction is switched to attraction. In recent theoretical works[16], it was proposed to use this setting to create symbiotic bright solitons: while self-repulsive species cannot support isolated solitons, the inter-species attraction may help to
create two-component solitons. Moreover, a similar perspective was discussed in the context of Bose-Fermi mixtures, where the interaction between bosons is repulsive, but the bosons and fermions attract each other [17]. Similarly, solitons in a binary degenerate Fermi gas, supported by the attraction between the fermion species, were predicted [18]. It was also proposed to use the attraction between fermions and bosons for making bosonic quantum dots that can trap fermion atoms (in particular, gap solitons in the BEC trapped in the OL may play the role of such dots) [19].

As mentioned above, a salient property of GSs is the negative effective mass, which should make their dynamical behavior drastically different from that of ordinary quasi-particles. In particular, both one- [21] and two-dimensional [22] GSs are expelled by the usual parabolic trapping potential, while being retained by the anti-trapping (inverted) potential. The negative effective mass may essentially affect the stability of two-component GSs. If the BEC species repel each other, the repulsive force, acting in combination with the negative effective mass, may actually keep the two components together. In Ref. [20], this possibility was verified, for two- and one-dimensional GSs of the binary BEC. It was demonstrated that, even with zero intra-species interaction, the repulsion between the components was sufficient to generate a family of symbiotic gap solitons. Adding nonzero intra-species repulsion expands the stability region of such GSs. Note that the symbiotic GSs found in Ref. [20] could be both of intragap and inter-gap types, i.e., with the chemical potentials of the two components belonging to the same or different finite bandgaps in the linear spectrum induced by the OL.

The objective of the present work is to consider effects of the attraction between BEC species on two-component GSs trapped in an OL, in the case when the intra-species interactions are repulsive. As mentioned above, the necessary signs and magnitudes of the respective nonlinear coefficients may be adjusted by means of the FR technique. Because of the negative sign of the effective GS mass, one may expect that the inter-species attraction destabilizes the two-component GSs, with a trend to split them into separate single-species solitons. This expectation is confirmed below, by means of systematic simulations of the coupled Gross-Pitaevskii equations (GPEs) for the macroscopic wave functions of the two components, \( \psi \) and \( \phi \).

In the normalized form (we set atomic mass, Planck’s constant, and the overall nonlinearity coefficient equal to 1, and the OL period equal to \( \pi \)), the coupled GPEs take the well-known form [23]:

\[
i\psi_t + (1/2)\psi_{xx} - \left[ (\cos \theta) |\psi|^2 + (\sin \theta) |\phi|^2 \right] \psi + \kappa \cos(2x)\psi = 0, \quad (1)
\]

\[
i\phi_t + (1/2)\phi_{xx} - \left[ (\cos \theta) |\phi|^2 + (\sin \theta) |\psi|^2 \right] \phi + \kappa \cos(2x)\phi = 0, \quad (2)
\]

where \( \kappa \) is the strength of the OL (actually measured in units of the corresponding recoil energy), and angle \( \theta \) is a parameter that determines the relative strength and sign of the inter- and intra-species interactions. The case of the intra-species repulsion and inter-species attraction, which we aim to consider in this work, corresponds to \( -\pi/2 < \theta < 0 \). If \( \psi \) and \( \phi \) represent two components of a spinor BEC (therefore, equal atomic masses are assumed in the two equations) with opposite \( z \)-components of the hyperfine spin, \( m_F = \pm 1 \), then \( \tan \theta = (a_0 + a_2) / (a_0 - a_2) \), with coefficients \( a_0 \) and \( a_2 \) accounting for the mean-field (spin-independent) and spin-exchange interactions between the atoms [24]. These coefficients may be, if necessary, controlled by means of the FR technique, as mentioned above.

Equations (1) and (2) conserve the corresponding Hamiltonian, and two norms (scaled numbers of atoms in the different species), \( N_{\psi,\phi} \equiv \int_{-\infty}^{\infty} \left| \psi(x) \right|^2 \, dx \). We will chiefly consider symmetric GS complexes, with \( N_{\psi} = N_{\phi} \equiv N \) (Section II); asymmetric states with unequal norms will also be considered, but briefly, in Section III.

II. RESULTS: SYMMETRIC GAP SOLITONS

Stationary soliton solutions to Eqs. (1) and (2) are looked for as

\[
\psi(x,t), \phi(x,t) = e^{-i\mu t} \Psi(x), e^{-i\nu t} \Phi(x), \quad (3)
\]

where \( \mu \) and \( \nu \) are chemical potentials of the two components. In this work, we focus on the two-component GSs of the most fundamental type, with both \( \mu \) and \( \nu \) falling in the first finite bandgap of the linear spectrum. The starting point is the symmetric soliton with identical components, \( \mu = \nu \) and \( \Psi(x) = \Phi(x) \), where the real wave function, \( \Psi(x) \), obeys the ordinary stationary equation for the single-component BEC,

\[
\mu \Psi + (1/2)\Psi'' - \sqrt{2} (\sin (\theta + \pi/4)) \Psi^3 + \kappa \cos(2x)\Psi = 0. \quad (4)
\]

This equation has GS solutions provided that \( \sin (\theta + \pi/4) > 0 \), which actually implies \( -\pi/4 < \theta < 0 \), since we are interested in \( \theta < 0 \) (the inter-species attraction), as said above. The remaining interval, \( -\pi/2 \leq \theta < -\pi/4 \), corresponds to the ordinary symbiotic solitons [10] trapped in the OL, with \( \mu \) falling in the semi-infinite gap.

Equation (4) can be solved by means of known numerical methods [2, 21] (the variational approximation [20], which was first used in the framework of the GPE in Ref. [23], becomes quite cumbersome if applied to GSs [27] therefore we do not resort to this method here). We tested the stability of symmetric solitons, generated by Eq. (4), against small random perturbations (which include a small initial separation between the components) by means of direct simulations of Eqs. (1) and (2). In
agreement with the expectation that the effective negative mass of the GS can make the two-component bound state unstable against the splitting under the action of the inter-species attraction, we have observed three different scenarios of the perturbation-induced dynamics, depending on the OL strength, \(\kappa\). As shown in Figs. 1a) and c), the bound state splits into two freely moving single-species solitons in the weak lattice, and remains stable in the strong OL. In the intermediate case, Fig. 1b), the bound states also splits, but the components cannot move freely; instead, they get pinned at a finite distance between them. As concerns the free motion of the single-component soliton, in Ref. [21] it was demonstrated that the GS moves without any tangible loss if its amplitude does not exceed a certain maximum value, above which the moving soliton is being braked by the underlying lattice.

A typical example of the stable symmetric soliton with separated centers of its two components is displayed in Fig. 2. In addition, the separation between centers of the two species in the stable solitons of this type, generated by the splitting of the unstable soliton with overlapping wave functions, \(\Psi = \Phi\), is shown in Fig. 3. According to Fig. 1, the separation is zero at \(\kappa > 0.46\), as the overlapping bound state is stable in that case, while at \(\kappa < 0.29\) the split components do not come to a halt (i.e., the separation is infinite).

As suggested by Fig. 3, two critical values, \(\kappa_1\) and \(\kappa_2\), of OL strength \(\kappa\) may be identified, for given \(\theta\) and norm \(N\): at \(\kappa < \kappa_1\), the original soliton, with \(\Psi(x) = \Phi(x)\), is unstable and splits, and at \(\kappa < \kappa_2\) (with \(\kappa_2 < \kappa_1\)) the splinters (single-component GSs) are not pinned by the lattice, but rather move freely. The dependence of both critical values on the norm of the initial overlapping bound state is shown in Fig. 4 (to interpret the results in physical terms, recall that \(\kappa\) shown in these plots is measured in units of the recoil energy). The decrease of \(\kappa_1\) and \(\kappa_2\) with increase of \(N\) is easy to understand, because the solitons with larger \(N\) are narrower, hence they are stronger pinned by the lattice [21].

In addition, Fig. 5 shows the dependence of \(\kappa_1\) and \(\kappa_2\)
FIG. 4: (Color online) Critical values of the lattice depth, $\kappa_1$ (solid line), below which the solitons with the overlapping wave functions, $\Psi = \Phi$, start to split, and $\kappa_2$ (dashed line), below which the single-component solitons generated by the splitting move freely, are shown as functions of norm $N$ of each component.

FIG. 5: (Color online) The critical lattice strengths, $\kappa_1$ (solid) and $\kappa_2$ (dashed), as functions of angle $\theta$, which determines the relative strength of the inter-species attraction and intra-species repulsion.

FIG. 6: (Color online) A stable unsplit soliton, with unequal norms in the two components: $N_\Psi = 1.5, N_\Phi = 1.6$, and $\theta = -0.3, \kappa = 1$.

FIG. 7: (Color online) Spontaneous splitting of an asymmetric soliton below the threshold, $\kappa_1$, for $N_\Psi = 1.5, N_\Phi = 1.6$, $\theta = -0.3$, and $\kappa = 0.5$ (in this case, $\kappa_1$ is slightly larger than 0.5, see Fig. 5). Total evolution time is $t = 1000$.

III. ASYMMETRIC GAP SOLITONS

We have also investigated the dynamics of asymmetric solitons, with different norms of the two components, $N_\Psi \neq N_\Phi$. An example of a stable soliton of that type, with coinciding centers of its components, is displayed in Fig. 6.

Similarly to the symmetric case, the asymmetric solitons become unstable against the splitting of the two components if the lattice strength falls below the threshold value, $\kappa_1$, see an example in Fig. 7. In the simulations, the splitting follows onset of oscillations of the solitons, with a significant amplitude.

Naturally, $\kappa_1$ depends on the asymmetry parameter, $(N_\Psi - N_\Phi) / (N_\Psi + N_\Phi)$, as shown in Fig. 8. The growth of the splitting threshold with the increase of the asymmetry can be readily explained. Indeed, as the norm of component $\Phi$ becomes smaller, its width increases. On the other hand, the effective pinning force (the amplitude of the effective Peierls-Nabarro potential [28]) acting on the soliton exponentially decays with the increase of the soliton’s width, hence a higher strength of the OL is required to prevent the splitting instability of the two-component asymmetric soliton.
We have considered effects of the attraction between two species in the binary BEC with intra-species repulsion, trapped in the OL (optical lattice), on the two-component GSs (gap solitons), supported by the balance between the repulsion and negative effective mass induced by the OL potential. Systematic simulations confirm the prediction suggested by the fact that the effective mass of the gap soliton is negative: if the OL is not strong enough, the inter-species attraction results in splitting of the two-component GS. We have identified two threshold values, $\kappa_1$ and $\kappa_2$, of the OL strength ($\kappa$), for the two-component GS with equal norms of its components. The unsplit solitons (with fully overlapping wave functions, $\Psi = \Phi$) are stable in strong lattices, with $\kappa > \kappa_1$; they split into a stationary symmetric state with separated components in interval $\kappa_1 > \kappa > \kappa_2$, and, in weak lattices, with $\kappa < \kappa_2$, the splitting generates a pair of freely traveling single-species GSs. The dependences of $\kappa_1$ and $\kappa_2$ on the norm of the original overlapping soliton, and on the relative strength of the inter-species attraction and intra-species repulsion ($\theta$) were found and explained. We have also considered, in a brief form, the dynamics of asymmetric solitons, with unequal norms of the two species. In particular, it was found (and explained) that the splitting threshold, $\kappa_1$, grows with the increase of the relative asymmetry.

The model introduced in this work calls for further analysis. In particular, it may be interesting to explore effects of intra-species attraction on symbiotic GSs supported by the inter-species repulsion (such as two-component GSs found in Ref. [20]), i.e., the case exactly opposite to that considered above. Another relevant generalization may be to study similar effects in two-dimensional GSs build of two species.

IV. CONCLUSIONS

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