Soliton molecules in dipolar Bose-Einstein condensates

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Dipolar interactions support the formation of intersite soliton molecules in a stack of quasi-one-dimensional (quasi-1D) traps. We show that the stability and properties of individual solitons and soliton molecules in such a geometry crucially depend on the interplay between contact and dipolar interactions. In particular, two different quasi-1D soliton regimes are possible: a one-dimensional (1D) soliton characterized by purely repulsive dipole-dipole interactions (DDI) and a three-dimensional (3D) soliton for which a sufficiently large dipole moment renders the DDI attractive. Furthermore, we find that in contrast to the dimers of polar molecules the soliton dimers exhibit a nontrivial behavior of the elementary excitations that stems from the competition between onsite and intersite DDI. Finally, we prove the existence of soliton trimers in a regime where molecular trimers do not occur. We demonstrate that the soliton molecules that we report are well feasible under realistic experimental conditions.

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I. INTRODUCTION

Recent developments in experiments on ultracold polar molecules [1–3], atoms with large magnetic dipole moment [4–7], and Rydberg atoms [8] open new promising perspectives in the rapidly progressing research on dipolar quantum gases. Interestingly, the presence of long-range and anisotropic dipole-dipole interactions essentially modifies the behavior of quantum gases leading to a wealth of new physics [9,10].

Dipolar effects are particularly relevant to what concerns the nonlinear properties of dipolar Bose-Einstein condensates (BECs). Crucially, whereas nondipolar BECs present a local Kerr-like type of nonlinearity, the nonlinearity in dipolar BECs exhibits a nonlocal character, similar to that in plasmas [11], photorefractive media [12,13], and nematic liquid crystals [14,15]. Interestingly, this nonlocality results in novel physical phenomena, including stabilization of two-dimensional solitons [16,17].

The long-range character of the DDI plays a substantial role in the physics of dipolar gases in optical lattices, even in the absence of intersite hopping. While a nondipolar gas in such a deep lattice may be considered as a system of mutually independent gases, nondipole intersite interactions in a dipolar gas couple the disjoint sites. In particular, in the physics of polar molecules this feature gives rise to a variety of unprecedented few-body bound states such as intersite dimers [18,19], trimers [20,21], and filaments [22,23].

The intersite interactions play also a key role in the behavior of a dipolar condensate in an optical lattice. Specifically, they have been found to fundamentally modify the BEC excitation spectrum [24,25] and to affect significantly the stability of the condensate [26,27]. Moreover, intersite interactions may lead to a correlated modulational instability, in which a locked density modulation pattern is shared among nonoverlapping sites, after a quench of a condensate into instability. Interestingly, such correlated modulational instability may result in the dynamical formation of soliton filaments and crystalline structures [28].

In this paper we analyze in detail the physics of dipolar bright solitons in a stack of quasi-1D condensates. We focus on the stability and properties of soliton dimers and trimers, which constitute the building blocks of the above-mentioned soliton filaments and crystals, respectively. These two- and three-soliton bound states are an example of the so-called soliton molecules. Recently, an optical equivalent of such objects has been realized experimentally in optical fibers [29,30] and a variety of theoretical proposals to create atomic soliton molecules have been presented [31–33]. Soliton dimers share some properties with molecular dimers. However, as we discuss in detail below, intrasoliton interactions (of course absent in the case of individual polar molecules) are decisive for their stability and elementary excitations. Moreover, whereas molecular trimers may be found (in the absence of any additional lattice [21]) only for a rather narrow window of the dipole moment orientations [20], soliton trimers may exist for the orientations for which trimers of individual polar molecules are precluded.

The paper is structured as follows. Section II introduces the general formalism. In Sec. III we compute the universal stability diagram for a single dipolar soliton in a quasi-1D trap and we show that such geometry supports two stable soliton regimes differing substantially in the character of the dipolar interactions. Section IV is devoted to the study of properties of the soliton dimers. We discuss the intersoliton binding potential and the nontrivial dependence of the dimer elementary excitations on the dipolar coupling. In Sec. V we analyze the trimer case, showing that soliton trimers may be found in a regime where molecular trimers would be unstable. We conclude in Sec. VI.

II. MODEL

In the following we consider a dipolar BEC loaded in a stack of $M$ parallel quasi-1D traps (tubes), formed by a two-dimensional optical lattice with sites located at $y_j = j \Delta$ (Fig. 1). The intertube potential barrier is considered...
obtain the energy of the system:

\[
E(l_x, l_y, l_z) = \frac{\hbar^2}{4m} \sum_{i=x,y,z} \frac{1}{l_i^4} + \frac{\omega_i^2}{4} \sum_{i=x,y} l_i^2 + \frac{N}{4\sqrt{2\pi^{3/2}l_x l_y l_z}} \left[ g + \frac{2}{3} g_d K \left( \frac{l_z}{l_x}, \frac{l_z}{l_y} \right) \right],
\]

with the function

\[
K(r_x, r_y) = \int_0^{2\pi} d\phi \int_0^1 du \frac{(1 - u^2)[2r_x^2 - (r_x^2 + 2r_y^2) \cos^2 \phi] - u^2}{(1 - u^2)[r_y^2 + (r_y^2 - r_x^2) \cos^2 \phi] + u^2}
\]

that in the cases of our interest may be evaluated analytically in terms of elliptic integrals \[34\]. A stable soliton solution corresponds to a minimum in the energy functional \( E(l_x, l_y, l_z) \) at finite nonzero values of the soliton widths. In Fig. 2 we present the universal stability diagram as a function of the dimensionless parameters \( g^* = g N/2\pi \hbar \omega, l_x^3 \) and \( g_d^* = g_d N/2\pi \hbar \omega, l_x^3 \).

Interestingly, we find two different soliton regimes, which differ remarkably in their properties and stability for growing \( g_d > 0 \). For sufficiently small \(|g^*| < |g_d^*|\), with \(|g_1^*| \approx 1\), a soliton may be considered as purely 1D, i.e., \( l_z = l_y = l_0 = \sqrt{\hbar/m \omega_z}\), whereas \( l_x \gg l_z \). For such soliton, the DDI remain repulsive for any \( g_d^* \). In consequence, the soliton width \( l_z \) increases monotonically for growing \( g_d^* \), until divergence at a critical value at which the soliton delocalizes. The condition for soliton stability against the expansion may be then found analytically from Eq. (3), \(|g^*|/g_d^* > 2/\pi\) (straight solid line in Fig. 1). In contrast, for \(|g^*| > |g_d^*|\) the atomic cloud cannot be considered any more as 1D, since \( l_z \) becomes comparable with the transverse widths and thus a stable soliton solution that occurs displays clearly a 3D character. In this regime, the DDI interaction changes its sign from repulsive to attractive at a finite \( g_d^* > 0 \) value, and hence for further growing \( g_d^* \), the soliton width decreases until the soliton becomes unstable against 3D collapse. Furthermore, we note that in the vicinity of \(|g_1^*|\) the stability diagram presents an interesting reentrant
character as a function of $g_d$, first expanding, then rebinding, and finally collapsing (Fig. 3). Interestingly, in contrast to the soliton-expansion transition, where the soliton width smoothly diverges, the rebinding transition is first-order-like, since the soliton abruptly rebinds at a finite width.

IV. SOLITON DIMERS

We assume in the following that a soliton in each tube is in the 1D regime discussed in Sec. III (this condition is self-consistently verified). At the end of this section we briefly comment on the case of solitons in the 3D regime. In the 1D regime, the wave functions factorize $\Psi_j(r) = \phi_j^{(x,y)}(x,y)\psi_j(z)$, with $\phi_j^{(x,y)}$ the ground-state wave function of the transverse harmonic oscillator in a site $j$. Employing the convolution theorem [35] and integrating Eq. (1) with respect to $x$ and $y$, we arrive at the dimensionally reduced system of equations:

$$i\hbar \partial_t \psi_j(z) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \frac{g N}{2\pi l_z^2} n_j(z) + \frac{g_d N}{3} \sum_{m=0}^{M-1} \int dk_z e^{ik_z \hat{n}_m(k_z)} F_{m-j}(k_z) \right] \psi_j(z),$$

with $\hat{n}_m(k_z)$ the Fourier transform of the axial wave-function density $n_m(z) = |\psi_m(z)|^2$ in a site $m$ and

$$F_j(k_z) = \int \frac{dk_x dk_y}{\pi} \left( \frac{3k_x^2}{k_x^2 + k_y^2 + k_z^2} - 1 \right) e^{-i(k_x^2 + k_y^2 - k_z^2)(z_j - z)}.$$

For stable individual solitons the intersite DDI may result for $g_d > 0$ in a binding of two solitons in different quasi-1D tubes into a soliton dimer (Fig. 4). Such dimer resembles recently reported dimers of individual polar molecules. However, as discussed below, in the physics of the soliton dimer the interplay between intrasoliton interactions and intersoliton interactions leads to nontrivial effects, which do not occur in the case of molecular dimers due to the absence of onsite DDI.

Two solitons localized in neighboring quasi-1D tubes ($j = 0, 1$) and with a relative displacement $z_r$ along the axis direction $z$ (Fig. 4) experience an interaction potential:

$$E_D(z_r) = \frac{g_d N}{3} \int dz n_1(z-z_r) \int dk_z e^{ik_z \hat{n}_1(k_z)} F_1(k_z).$$

We calculate $E_D(z_r)$ evolving Eq. (5) in imaginary time to obtain the ground state of the dimer $\psi_0^*(z)$ and then shifting the solitons to the distance $z_r$. Due to the anisotropy of the DDI the intersoliton potential is maximally attractive for $z_r = 0$, and becomes repulsive for large $z_r$ (Fig. 4). Naturally, the binding potential $E_D(z_r)$ calculated for actual soliton wave packets is considerably weaker than that expected for pointlike particles $E_D^0(z_r) = g_d N(z_r^2 - 2\Delta^2)/(\varepsilon_0^2 + \Delta^2)^{5/2}$. Nevertheless, we note that even for the case of the relatively small dipole moment of $^{52}\text{Cr}$, which we employed in our calculations for Fig. 4, the energy scale of the binding remains significant ($\sim 100$ Hz). Obviously, the binding would be stronger for condensates of atoms with larger dipole moment, such as dysprosium [6] and erbium [7], or in the case of polar molecules [1–3].

We now focus on the essential properties of the soliton dimer. First, following the imaginary time evolution of Eq. (5), for a given $\Delta/l_z$, we compute the width $l_z$ of the solitons forming the dimer, as a function of $g^*$ and $g_d^*$ [see Fig. 5 (top)]. Since we consider the 1D soliton regime, with an overall repulsive intrasoliton DDI, an increase of $g_d^*$ results in a broadening of the solitons, and eventually in the instability of the solitons against expansion. Note, however, that the attractive intersoliton interactions, while providing the binding mechanism itself, induce a trapping of each soliton by its neighbor, which contributes to stabilization of each soliton against expansion. This mechanism increases the stability threshold found in Sec. III for an individual soliton, as shown by the straight dashed line (at $|g^*|/g_d^* = 1.78$) in Fig. 2, obtained from a similar 3D variational calculation as that of the previous section.

FIG. 3. (Color online) Reentrant character of the soliton stability in a single quasi-1D trap in the vicinity of $g^*_c$. Here, $|g^*_c| = 0.95$.

FIG. 4. (Color online) Intersoliton binding potential for the case of the soliton dimer. The red dashed line represents the potential calculated within the pointlike approximation $E_D^0$. The blue solid line shows the actual potential computed numerically with Eq. (7). Here, we consider the case of a $^{52}\text{Cr}$ condensate ($\mu = 6 \mu_B$, with $\mu_B$ the Bohr magneton), $a_{sc} = -7.1 a_0$ (with $a_0$ the Bohr radius), $N = 100$, $\Delta = 6l_z = 512$ nm, and the lattice potential depth $s = 13.3 E_0$ (recoil energy). These parameters refer to $\omega_z = 26.7$ kHz and $(g^*, g_d^*) = (-0.88, 0.45)$. Inset: schematic depiction of the soliton dimer arrangement.
FIG. 5. (Color online) (Top) Width of the soliton dimer as a function of $g^*_d$ for $|g^*| = 0.6$ (blue dashed line) and $|g^*| = 0.8$ (green dot-dashed line), for the same parameters as in Fig. 4. The vertical dashed lines indicate the dimer expansion threshold. (Bottom) Frequency of the elementary excitations of the soliton dimer for the same parameters. Inset: scheme of the dimer elementary excitation mode.

The properties of the soliton dimer must be compared with those of intersite dimers formed by individual polar molecules. In the latter case, the localization of each molecular wave packet is solely due to the attractive intersite DDI, which induce a mutual trapping of both molecules. This means, in particular, that for $g^*_d = 0$ each of the wave packets delocalizes. Furthermore, owing to the absence of intra-wave-packet repulsive DDI, an increase of $g^*_d$ can only amplify localization and so the molecular dimer width decreases monotonically as a function of $g^*_d$, unlike the case of the soliton dimer. As a result, molecular dimers become only stiffer (i.e., present increasing excitation energies) for growing DDI.

In contrast, the elementary excitations of the soliton dimer present a more involved behavior that stems from the interplay between intra- and intersoliton DDI. We study the lowest-lying excitations by monitoring the real-time dynamics of the solitons which follows a small distortion of the ground-state solution in the form $\psi_j(x,t=0) = \psi_j^{(0)} e^{-i(k_j x + \beta_j x^2)}$, corresponding to a perturbation of the soliton positions and widths. Figure 5 (bottom) shows the result of the Fourier transform of the position $\langle z(t) \rangle$ of one of the two oscillating solitons and hence the frequency of the dimer lowest-lying excitation (this is verified additionally by inspecting the Fourier transforms of soliton width and density oscillations). For sufficiently small DDI, and so for small soliton widths, the lowest-lying excited mode of the dimer is associated exclusively to the motion of the center of mass of each soliton. In consequence, as $g^*_d$ grows, so does the energy of dimer excitations, resembling the case of molecular dimers. In contrast to the molecular dimers, however, after reaching a certain critical value of $g^*_d$, the soliton dimer becomes progressively softer (i.e., it exhibits decreasing excitation energies). This phenomenon arises since the soliton widths increase due to the repulsive intrasoliton DDI, and, as a result, the lowest-lying excitation becomes eventually an admixture of both position and width distortions. As discussed before, for a sufficiently large $g^*_d$ the dimer becomes eventually unstable against expansion.

Finally, we stress that soliton dimers may exist as well in the 3D regime defined in Sec. III, i.e., for $|g^*| > |g^*_c|$. As depicted in Fig. 2, the stability threshold against the soliton dimer collapse is basically the same as that for an individual soliton. Unlike the 1D case, in the 3D regime the width of a soliton is relatively small $l_z \approx l_\perp$, and so the binding potential between the two solitons, such as the one depicted in Fig. 4, becomes comparably deep as the pointlike approximation $E_0^D$. Moreover, for $|g^*| > |g^*_c|$ the soliton width never becomes large enough to cause the mixing of position and width excitations. As a result, in the 3D regime, for growing $g^*_d$ values the soliton dimer becomes only stiffer, up to the collapse threshold, similarly to the molecular dimers.

V. SOLITON TRIMERS

Interestingly, the DDI may lead to the formation of soliton molecules composed of more than two solitons, in particular soliton trimers (Fig. 6). We note that trimers (and even more involved complexes) have been predicted as well for individual polar molecules [20,21]. However, molecular trimers have been found to exist only in a rather narrow window of dipole
moment orientations with respect to the trap axis, in the very vicinity of the magic angle, such that intrasite repulsion is minimized and intersite attraction is maximized. In particular, molecular trimers are precluded if the dipole orientation is aligned along the trap axis. Furthermore, as noted in Sec. IV, the formation of molecular bound states is handicapped by the fact that the intersite interactions not only provide a binding between the molecules but are also indispensable for the localization of the individual molecular wave packets themselves. This contrasts with the soliton molecules case, where the existence of localized wave packets is supported by intrasoliton interactions. Consequently, as we discuss in this section, the interplay between inter- and intrasoliton interactions allows for stable soliton trimers for dipole moment orientations in which molecular trimers are absent.

In the following we consider for theoretical simplicity the case of dipoles oriented along the y axis (in the side-by-side configuration, alike in the soliton dimer) but with \( g_d < 0 \), which may be achieved by means of a rotating magnetic field or microwave dressing for polar molecules. Naturally, the results would be however qualitatively very similar to the case of dipoles oriented along the tubes, since both scenarios are characterized by repulsive intersite DDI and attractive intrasite DDI. Although the attractive intrasite interactions seem naively to involve soliton fusion in the bottom tube, and hence to preclude the existence of the soliton trimer, such a trimer stems actually from a nontrivial interplay between intertube repulsion and intratube attraction. Namely, the single soliton in the upper tube provides a repulsive potential barrier that prevents the fusion of the two mutually attracting solitons in the bottom tube, hence keeping the soliton trimer stable.

A major difference with respect to soliton dimers lies in the fact that now \( g_d^* < 0 \), and hence the intrasoliton interaction is attractive. In consequence, for growing \( |g_d^*| \) the individual solitons shrink and the trimer is not unstable against the expansion of the individual solitons but rather against their collapse, as the solitons become eventually 3D for a sufficiently large \( |g_d^*| \). As shown for the soliton dimer, the threshold for the collapse instability is basically given by the intrasoliton potential.

We have thus analyzed the stability of a soliton in a single quasi-1D trap for \( g_d < 0 \) (see Fig. 7), using the same 3D variational Gaussian ansatz as discussed in Sec. III. Naturally, soliton trimers may exist only within the stability region of individual solitons.

In the following we analyze the properties of trimers well within the 1D regime, i.e., far from the 3D collapse threshold, for which we can safely employ the 1D GPE [Eq. (5)]. In particular, after obtaining the ground state of the trimer configuration by means of the imaginary time evolution of these equations, we have computed the binding potential of the trimer \( E_T(r) \) (Fig. 8) as a function of the distance \( r \) between the solitons in the bottom tube (Fig. 6). Crucially, at an intermediate distance \( r_{\text{min}} \), \( E_T(r) \) shows a local minimum that offers the possibility of a soliton trimer. A pointlike approximation of the solitons leads to a binding potential

\[
E_T^0(r) = g_d N \left[ \frac{1}{r^2} + \frac{16(r^2 - 8\Delta^2)}{(r^2 + 4\Delta^2)^{3/2}} \right].
\]

resulting in an equilibrium position \( r_{\text{min}} = 7 \) kHz. Inset: potential-energy minimum \( \Delta = 512 \) nm, \( s = 13.3 E_R \), and \( \omega_L = 26.7 \) kHz. Naturally, soliton trimers may exist only within the stability region of individual solitons.

Note that unlike the soliton dimer, the soliton trimer is related to a local minimum of the energy functional. In particular, the global energy minimum occurs when the two solitons in the bottom tube fuse into a single soliton, which forms a tilted dimer with the soliton in the upper...
The trimer configuration of Fig. 6 is hence strictly speaking a metastable solution, which is separated from the fused solution by a potential barrier (Fig. 8). Macroscopic quantum tunneling through this barrier is, however, negligible, and hence the metastable solution may be considered for all practical purposes as stable (as we have confirmed in real-time evolution). The potential barrier disappears at a sufficiently small $|g^*_d|$, for which the soliton trimer abruptly becomes unstable against the solitons fusion (see Figs. 7 and 9).

Finally, as in the case of the soliton dimer, we have analyzed the elementary excitations of the soliton trimer. Since now $g^*_d < 0$, the solitons are always well localized. Hence, in contrast to the soliton dimers, the lowest-lying excitations are related solely to the solitons’ center-of-mass motion (without an excitation of the width of the solitons). We may thus define two different types of elementary excitations, characterized by an in-phase and an out-of-phase motion of the soliton pair in the bottom tube, respectively [Fig. 9 (bottom)]. In analogy to Sec. IV, we have probed these modes perturbing the soliton widths and positions of the trimer ground state and monitoring the subsequent real-time dynamics governed by Eq. (5). After Fourier transforming the soliton positions, we obtained the lowest-lying excitations as a function of $|g^*_d|$. The results for the two elementary excitations frequencies are depicted in Fig. 9 (bottom), which shows, in particular, that for all $|g^*_d|$ values the out-of-phase mode is always less energetic than the in-phase mode.

VI. CONCLUSIONS

In summary, intersite dipolar interactions support the formation of soliton molecules in a stack of quasi-1D tubes. The stability properties of quasi-1D solitons and intersite soliton molecules depend crucially on the interplay between dipolar and contact interactions and the competition between intrasite and intersite effects. In particular, two different quasi-1D soliton regimes are possible: 1D solitons, for which the intrasoliton DDI is always repulsive and which become eventually unstable against soliton delocalization, and 3D solitons, for which the DDI changes its character from repulsive to attractive for increasing dipole moment and which become eventually unstable against soliton collapse. We have shown that, in contrast to the case of dimers of individual polar molecules, the interplay between intrasoliton interactions and intersoliton DDI leads to a nontrivial behavior of the elementary excitations of soliton dimers. In the purely 1D regime the growing DDI renders the dimer stiffer up to a point, beyond which an increase of DDI softens the dimer due to the admixture between position and width excitations. Finally, we have demonstrated that soliton trimers may be constructed for attractive intrasite and repulsive intersite DDI due to a subtle interplay between intratube attraction and intertube repulsion. Interestingly, these trimers occur in a regime where trimers of individual polar molecules do not exist. The reported soliton molecules can be observed under realistic conditions within current experimental feasibilities. Moreover, we emphasize that the soliton binding mechanism described in this work can be straightforwardly generalized to engineer even more intricate soliton complexes comprising a larger number of solitons in more sites of an optical lattice.

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