Soliton Molecules In Dipolar Bose-Einstein Condensates

Kazimierz Lakomy,¹ Rejish Nath,²,³ and Luis Santos¹

¹Institut für Theoretische Physik, Leibniz Universität, Hannover, Appelstrasse 2, D-30167, Hannover, Germany
²Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, D-01187 Dresden, Germany
³IQOQI and Institute for Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria

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Dipolar interactions support the formation of inter-site soliton molecules in a stack of 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 1D soliton characterized by purely repulsive DDI and a 3D soliton for which a sufficiently large dipole moment renders the DDI attractive. Furthermore, we find that contrary to the case of dimers of polar molecules, the soliton dimers exhibit a nontrivial behavior of the elementary excitations that stems from the competition between on-site and inter-site 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 ultra-cold polar molecules [1–3], atoms with large magnetic dipole moment [4–7], and Rydberg atoms [8] opens new promising perspectives in the rapidly progressing research on dipolar quantum gases. Interestingly, the presence of long-range and anisotropic dipole-dipole interactions (DDI) essentially modifies the behavior of quantum gases leading to a wealth of a new physics [9, 10].

Dipolar effects are particularly relevant to what concerns the nonlinear properties of dipolar Bose-Einstein condensates (BECs). Crucially, whereas non-dipolar BECs present a local Kerr-like type of nonlinearity, the nonlinearity in dipolar BECs exhibits a nonlocal character, similar to that in plasmas [11], photoactive 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 inter-site hopping. While a non-dipolar gas in such a deep lattice may be considered as a system of mutually independent gases, nonlocal inter-site 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 inter-site dimers [18, 19], trimers [20, 21] and filaments [22, 23].

The inter-site 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, inter-site interactions may lead to a correlated modulational instability, in which a locked density modulation pattern is shared among non-overlapping 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, intra-soliton 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 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 article is structured as follows. Sec. 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 inter-soliton 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 section 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 2D optical lattice with sites located at $y_j = j \Delta$ (Fig. 1). The inter-tube potential barrier is considered sufficiently large to suppress any hopping. In each tube we assume a strong harmonic confinement of frequency $\omega_i$ in the $xy$ plane and no confinement along the $z$ direction. The atoms possess a magnetic dipole moment $\mu$ (the results are equally valid for electric dipoles, such as polar molecules) oriented along the $y$ axis, in the side-by-side configuration, by a sufficiently large external field. Introducing a wavefunction $\Psi_j (\mathbf{r})$ that describes an atomic cloud in a site $j$ holding $N$ atoms, the system of non-local coupled Gross-Pitaevskii equations (GPE) reads

$$ih \partial_t \Psi_j (\mathbf{r}) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + U_j (\mathbf{r}) + gN |\Psi_j (\mathbf{r})|^2 ight. \left. + \sum_{m=0}^{M-1} \int d\mathbf{r}' V_d (\mathbf{r} - \mathbf{r}') |\Psi_m (\mathbf{r}')|^2 \right] \Psi_j (\mathbf{r}, t).$$ (1)

Here, $U_j (\mathbf{r}) = \frac{1}{2} m \omega_i^2 (x^2 + (y - y_j)^2)$ and $V_d (\mathbf{r} - \mathbf{r}') = g_d N \left( 1 - 3 \cos^2 \theta \right) / |\mathbf{r} - \mathbf{r}'|^3$ is the dipole-dipole potential where $g_d = \mu_0 \mu^2/4\pi$ with $\mu_0$ being the vacuum permeability and $\theta$ the angle between the vectors joining two interacting particles and the direction of the dipole moment. The short-range interactions are characterized by $g = 4\pi a_{sc} \hbar^2 / m$ with $a_{sc}$ being the $s$-wave scattering length. In the following we consider attractive short-range interactions ($a_{sc} < 0$).

III. DIPOLAR SOLITON IN A SINGLE QUASI-1D TRAP

We discuss first the conditions of existence of a stable bright soliton in a single quasi-1D trap ($M = 1$). To this end we assume a 3D anisotropic Gaussian ansatz

$$\Psi_0 (\mathbf{r}) = \frac{1}{\pi^{3/4} (l_x l_y l_z)^{1/2}} \exp \left( -\frac{x^2}{2l_x^2} - \frac{y^2}{2l_y^2} - \frac{z^2}{2l_z^2} \right),$$ (2)

where $l_x$, $l_y$, and $l_z$ are the variational widths along $x$, $y$ and $z$ directions, respectively. Employing this ansatz into Eq. (1) we obtain the energy of the system

$$E(l_x, l_y, l_z) = \frac{\hbar^2}{4m} \sum_{i=x,y,z} \frac{1}{l_i^2} + \frac{\omega_i^2}{4} \sum_{i=x,y} l_i^2$$

$$+ \frac{N}{4\sqrt{2} \pi^{3/2} l_x l_y} \left( g + \frac{2}{3} g_d K \left( \frac{l_z}{l_x}, \frac{l_z}{l_y} \right) \right),$$ (3)

with the function

$$K(r_x, r_y) = \int_0^{2\pi} \frac{1}{0} d\varphi \int_0^1 du \left( 1 - u^2 \right) \left[ 2r_y^2 - (r_x^2 + 2r_y^2) \cos^2 \varphi \right] - u^2$$ (4)

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 non-zero values of the soliton widths. In Fig. 2 we present the universal stability diagram as a function of the dimensionless parameters $g^* = gN/2\pi \hbar \omega_y l_y^2$, and $g_d^* = g_d N/2\pi \hbar \omega_y l_y^2$.

Interestingly, two different soliton regimes may be found, which differ remarkably in their properties and
stability for growing \( g_d > 0 \). For sufficiently small \( |g^*| < |g_c^z| \), with \( |g_c^z| \approx 1 \), a soliton may be considered as purely 1D, i.e., \( l_x = l_y = l_z = \sqrt{\hbar/m\omega_z} \), whereas \( l_z \gg l_x \). For such soliton, the DDI remains repulsive for any \( g_d^z \). As a result, the soliton width \( l_z \) increases monotonically for growing \( g_d^z \), until diverging 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), \( |g^*|/g_c^z > 2\pi/3 \) (straight solid line in Fig. 1). On the contrary, for \( |g^*| > |g_c^z| \) the atomic cloud cannot be considered any more as 1D, since \( l_z \) becomes comparable with the transversal widths. As a result, a stable soliton solution occurs that clearly displays a 3D character. In this regime, the DDI interaction changes its character from repulsive to attractive at a finite \( g_d^z > 0 \) value, and hence for further growing \( g_d^z \) the soliton width decreases until the soliton becomes unstable against 3D collapse. Furthermore, we note that in the vicinity of \( |g_c^z| \), the stability diagram presents an interesting reentrant character as a function of \( g_d \), first expanding, then re-binding and finally collapsing (Fig. 3). Interestingly, contrary to the soliton-expansion transition, at which the soliton width smoothly diverges, the re-binding transition is first-order-like, since the soliton abruptly re-binds 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 wavefunctions factorize \( \Psi_j (r) = \phi^+_j (x, y) \psi_j (z) \), 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

\[
\begin{align*}
\hbar^2 \partial_z \psi_j (z) & = \left[ -\frac{\hbar^2}{2m} \partial^2_z + \frac{gN}{2\pi l_z^2} n_j (z) \\
& + \frac{g_d N}{3} \sum_{m=0}^{M-1} \int dk_z e^{ik_z z} \hat{n}_m (k_z) F_{m-j} (k_z) \psi_j (z) \right],
\end{align*}
\]

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

\[
F_{q} (k_z) = \frac{\int dk_2 dk_y}{\pi} \left( \frac{3k^2_y}{k^2_x + k^2_y + k^2_z} - 1 \right)
\times e^{-\frac{1}{2}(k^2_x+k^2_y)l_z^2 - i k_y q l_z}.
\]

For stable individual solitons the inter-site DDI may result for \( g_d > 0 \) in a binding of two solitons in different quasi-1D tubes into a soliton dimer (Fig. 4). This dimer resembles the case of the recently reported dimers of individual polar molecules. However, as discussed below, the interplay between intra-soliton interactions and inter-soliton interactions leads to a non-trivial effects in the physics of the soliton dimer, which do not occur in the case of molecular dimers due to the absence of on-site 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

\[
E_D (z_r) = \frac{g_d N}{3} \int dz \ n_1 (z - z_r) \int dk_z e^{ik_z z} \hat{n}_0 (k_z) F_1 (k_z).
\]

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

FIG. 4. (Color online) Inter-soliton binding potential for the case of the soliton dimer. The red dashed line represents the potential calculated within the point-like approximation \( E_D^p \). The blue solid line shows the actual potential computed numerically with Eq. (7). Here, we consider the case of \(^{52}\text{Cr}\) condensate \((\mu = 6 \mu_B, \text{with } \mu_B \text{ the Bohr magneton}), a_{\perp} = -7.1 a_0 \) (with \( a_0 \) the Bohr radius), \( N = 100 \), \( \Delta = 6 l_z = 512 \text{ nm} \), and the lattice potential depth \( s = 13.3 E_R \) (recoil energy). These parameters refer to \( \omega_z = 26.7 \text{ kHz} \) and \((g^*, g_d) = (-0.88, 0.45)\). The inset depicts schematically the soliton dimer arrangement.
We calculate $E_D(z_r)$ evolving Eq. (5) in imaginary time to obtain the ground state of the dimer $\psi_j^0(z)$ and then shifting the solitons to the distance $z_r$. Due to the anisotropy of the DDI the inter-soliton potential is maximally attractive for $z_r = 0$, becoming repulsive for large $z_r$ (Fig. 4). Naturally, the binding potential $E_D(z_r)$ calculated for actual soliton wave-packets is significantly weaker than that expected for point-like particles $E_D(z_r) = g_d N (z_r^2 - 2\Delta^2)/(z_r^2 + \Delta^2)^{3/2}$. 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). The binding would be of course 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 intra-soliton DDI, an increase of $g_d$ results in a broadening of the solitons, and eventually to the instability of the individual solitons against expansion. Note, however, that the attractive inter-soliton interactions, while providing the binding mechanism itself, induces a trapping of each soliton by its neighbor, which contributes to stabilization of each soliton against expansion. This 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.

The properties of the soliton dimer must be compared with those of inter-site dimers formed by individual polar molecules. In the latter case, the localization of each molecular wave-packet is solely due to the attractive inter-site 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 stiffer (i.e. present growing excitation energies) for growing DDI.

On the contrary, the lowest-lying excitation of the soliton dimer presents a more involved behavior due to the interplay between intra- and inter-soliton DDI. We study the lowest-lying excitations by monitoring the real-time evolution 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 their widths. Fig. 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 a small solitons 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 because the soliton widths increase due to the repulsive intra-soliton 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 $|g^*| > |g_d^*|$. As depicted in Fig. 2, the stability threshold against the soliton dimer collapse is basically the same as that for an individual soliton. Contrary to the 1D case, in the 3D regime the width of a soliton is relatively small $l_z \simeq l_\perp$ and so the binding potential between the two solitons,
such as the one depicted in Fig. 4, becomes comparably deeper, approaching the point-like approximation $E_D^0$. 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, similar to the case of molecular dimers.

V. SOLITON TRIMERS

Interestingly, the DDI may lead to the formation of soliton molecules comprising 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 intra-site repulsion is minimized and inter-site 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 inter-site interactions do 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 case, where the existence of localized wavepackets is supported by intra-soliton interactions. As a result, as we discuss in this section, the interplay between inter- and intra-soliton interactions allows for stable soliton trimers for dipole moment orientations in which molecular trimers are absent.

![FIG. 6. Scheme of the soliton trimer. The dipole moments are aligned in the head-to-tail configuration providing attractive intra-site and repulsive inter-site dipolar interactions. In our work we mimick this scheme with qualitatively equivalent arrangement of dipoles aligned along the $y$ axis (side-by-side configuration) but with $g^*_d < 0$ (see text).](image)

In the following we consider for theoretical simplicity the case of dipoles oriented along the $y$ axis (in the side-by-side configuration as that of the soliton dimer) but with $g_d < 0$. This may be achieved by means of a rotating magnetic field [36], or microwave dressing for polar molecules [37]. The results would be however qualitatively very similar to the case of dipoles oriented along the tubes, since both cases are characterized by repulsive inter-site DDI and attractive intra-site DDI. Although the attractive inter-site interactions seem naively to involve soliton fusion in the bottom tube, and hence to preclude the existence of the soliton trimer, such trimer results actually from a nontrivial interplay between inter-tube repulsion and intra-tube 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 intra-soliton interaction is attractive. As a result for growing $|g^*_d|$ the individual solitons shrink, i.e. the trimer is not unstable against the expansion of the individual solitons but rather against their collapse, since the solitons become eventually 3D for a sufficiently large $|g^*_d|$. As shown in the dimer case, the threshold for the collapse instability is basically given by the intra-soliton physics. We have hence 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 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 GPEs (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 $r_{min}$ $E_T(r)$ shows a local minimum that offers the possibility of a soliton trimer. A point-like approximation of the solitons would induce a binding

$$E_T(r) = g_d N \left[ \frac{1}{r^3} + \frac{16(r^2 - 8\Delta^2)}{(r^2 + 4\Delta^2)^{5/2}} \right],$$

resulting in an equilibrium position $r_{min}^0/\Delta \simeq 3.73$, independently of $g_d$. This approximation, however, departs significantly from the actual binding potential $E_T(r)$, proving again the relevance of the spatial extension of solitons. Specifically, as shown in Fig. 9 (top), the trimer size, understood as the actual equilibrium distance $r_{min}$, decreases with growing $|g_d^*|$ (whereas the binding energy increases). We also note that, as it may be expected, the soliton trimer is more loosely bound than the soliton dimer. For typical parameters of $^{52}$Cr condensate, which we employed for the Fig. 8, the binding energy is of the order of $10\text{Hz}$. We stress, however, that the binding will be certainly stronger in the case of more magnetic atoms (Dy, Er) or polar molecules.

Note that contrary to the dimer case, the soliton trimer is related with a local minimum of the energy functional. In particular, the global energy minimum results from the fusion of the solitons in the bottom tube into a single soliton, which forms a tilted dimer with the top soliton. 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 negligible, and hence the metastable solution may be considered for all practical purposes as stable (as we have checked in real-time evolution). The potential barrier dissappears at a sufficiently small $|g_d^*|$, at which the soliton trimer becomes abruptly unstable against soliton fusion (see Fig. 7 and Fig. 9).

Finally, as for the case of the soliton dimers, we have analyzed the lowest-lying excitations of the soliton trimer. Since now $g_d < 0$, the solitons are always well localized. Hence, contrary to the dimer case, 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 hence 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)). As in 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 given by Eq. (5). After Fourier transforming the soliton positions, we obtain the lowest-lying excitations as a function of $|g_d^*|$. The results of the two excitation frequencies are depicted in Fig. 9 (bottom), which shows that for all $|g_d^*|$ the out-of-phase mode is always less energetic than the in-phase
VI. CONCLUSIONS

In summary, inter-site dipolar interactions support the formation of soliton molecules in a stack of quasi-1D tubes. The stability properties of quasi-1D solitons and inter-site soliton molecules depend crucially on the interplay between dipolar and contact interactions, and the competition between intra-site and inter-site effects. In particular, two different quasi-1D soliton regimes are possible: 1D solitons for which the intra-soliton DDI is always repulsive and that become eventually unstable against soliton delocalization, and 3D solitons, for which the DDI changes its character from repulsive to attractive for growing DDI, and that become eventually unstable against soliton collapse. We have shown that, contrary to the case of dimers of individual polar molecules, the interplay between intra-soliton interactions and inter-soliton DDI leads to a non-trivial behavior of the lowest-lying excitations of soliton dimers. In the purely-1D regime a growing DDI render the dimer stiffer up to a maximum beyond which an increasing DDI softens the dimer due to the admixture between position and width excitations. Finally, we have shown that soliton trimers may be constructed for attractive intra-site and repulsive inter-site DDI due to a subtle interplay between intra-tube attraction and inter-tube repulsion. Interestingly, these trimers occur in a regime in which trimers of individual polar molecules are not possible. 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.

VII. ACKNOWLEDGEMENT

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