Formation of matter-wave soliton molecules

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\textbf{Abstract.} We propose an experiment for forming matter-wave soliton molecules. In the proposed setup, we show that if two solitons are initially prepared in phase and with a sufficiently small separation and relative velocity, a bound pair will always form. This is verified by direct numerical simulation of the Gross–Pitaevskii equation and by the derivation of the exact interaction energy of two solitons, which takes the form of a Morse potential. This interaction potential depends not only on the separation but also on the relative phase of the solitons and is essential for an analytical treatment of a host of other problems, such as the soliton gas and the Toda lattice of solitons.

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1. Introduction

Interactions between solitons have been the subject of intensive studies in the last few decades [1–3]. This was motivated both by the fundamental physics involved and by the prospects of important technological applications (see e.g. [4]). At the fundamental level, solitons show dual nature by not only behaving as classical particles but also exhibiting wave nature when they, for instance, scatter off each other. In particular, it was first pointed out, by Karpman and Solov’ev using perturbation theory [1], by Gordon using the exact two solitons solution [2] and by Anderson and Lisak employing a variational approach [3], that at large distances the force between two solitons decays exponentially with their separation and is proportional to the cosine of their phase difference. From the applications point of view, this interaction between solitons is actually a problem since it leads, when using optical solitons in fibers as data carriers, to the destruction of the information stored in a sequences of solitons.

The exciting possibility of forming the so-called soliton molecules gives yet another stimulus to the problem. Such molecules have indeed recently been realized experimentally with optical solitons by Stratmann et al, who also measured the relative phase of the two solitons and studied their binding mechanism [5]. Matter-wave soliton molecules have, however, not yet been created experimentally. Theoretically, soliton molecules have been studied previously in two-dimensional (2D) Bose–Einstein condensates without [6] and with [7] dipolar interactions. In the latter case an effective molecular soliton–soliton potential was found, which results from the dipolar nature of the condensate and interlayer effects. Experimentally, bright solitons and soliton trains were observed as the remnants of a collapsing condensate that was created by using a Feshbach resonance to switch the interaction from repulsive to attractive [8]. It was found that neighboring solitons repel each other in spite of the fact that the interatomic interactions are attractive. A variational calculation showed that the repulsive force is caused by a $\pi$ phase difference between the solitons [9], in agreement with known results for optical solitons [1–3]. The conditions in these experiments are, thus, not favorable for the formation of bound states of solitons. Instead, if the two solitons start with zero phase difference, they attract each other and may ultimately form a molecule. The analysis presented below shows that while this is indeed a necessary condition, it is not sufficient for soliton molecule formation. The initial separation and relative velocity need to be sufficiently small such that the interaction is not dramatically weakened by the exponential tail and the kinetic energy of the relative motion does not considerably exceed the soliton–soliton interaction energy.

An adjusted version of a recent experiment by Hulet [10] is suggested here as a possible experimental method for realizing soliton molecules in strongly elongated Bose–Einstein condensates. In the experiment of [10], see also [11] for the experimental setup, a trapped bright soliton was launched onto a potential barrier at the center of a harmonic trap. Here, partial transmission and reflection created two solitons, which then after half an oscillation in the trap recombine again into a single one. We will show, however, that a soliton molecule can be formed if both the harmonic trapping potential and the potential barrier are switched off at the time when the two solitons reach their classical turning points. This guarantees the relative velocity to be zero. Moreover, the two solitons are, then, also guaranteed to have zero relative phase, since they were created coherently from the same soliton. The separation between the solitons prepared in this way is controlled by the curvature of the harmonic trap. Thus, it appears that all the conditions for soliton molecule formation can be met in such an experimental setup. In the following, we show that this is indeed the case via direct numerical simulations.
of the Gross–Pitaevskii equation (GPE). This is then followed by an analytical analysis of the soliton–soliton interaction energy, which also confirms the feasibility of our proposal. Moreover, finding an analytic interaction potential for two solitons at an arbitrary separation is not only important for the present problem of forming soliton molecules, but may also lay the foundation for a host of other problems involving soliton interactions such as the soliton Toda lattice [12] and the soliton gas [13].

2. Soliton molecule formation

In this section, we present a simulation that reproduces the results of the experiment of [10], and put forward a new experiment that leads to the generation of matter-wave soliton molecules. The proposal for the new experiment is analyzed with the same simulation that reproduces the experiment of [10], to make sure that our proposal is realistic.

The evolution of solitons in the original experiment of [10], as well as in our modified proposal, can be described by the GPE

$$\left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar}{2m}\nabla^2 - \left(\frac{1}{2}m(\omega^2_\perp r^2 + \omega^2_z z^2) + V_{\text{ext}}(z)\right) + \frac{4\pi a \hbar^2}{m} |\Psi(x, t)|^2\right] \Psi(x, t) = 0,$$

(1)

where \(a\) is the s-wave scattering length, \(\omega_z\) and \(\omega_\perp\) are the axial and radial frequencies of the harmonic trapping potential, respectively, and \(V_{\text{ext}}(z)\) is the potential barrier located at the center of the harmonic trap. Since the role of this potential barrier is to split the soliton into two, the height and width of the barrier will be its important characteristics, while its shape will be less important, as the numerical simulations will show. Therefore, a square or a Gaussian shape can be taken. While in the experiment a Gaussian shape is employed, we take here, for numerical convenience, a square potential and comparison between the two choices is made below. For the strongly elongated \((\omega_\perp \gg \omega_z)\) trapping potential, an effective 1D GPE can be obtained by averaging over the radial degrees of freedom with \(\Psi(z, t) = \int dr 2\pi r \Psi(x, t)\) and replacing the scattering length according to \(a \rightarrow a/2\pi q_\perp^2\), where \(q_\perp\) is the equilibrium width of the wavefunction in the radial direction [9]. In dimensionless form, the effective 1D GPE takes the form

$$\left[i\frac{\partial}{\partial t} + \frac{1}{2}\frac{\partial^2}{\partial z^2} - \left(\frac{1}{2}\lambda^2 z^2 + V_{\text{ext}}(z)\right) + g |\Psi(z, t)|^2\right] \Psi(z, t) = 0,$$

(2)

where lengths are scaled to the transverse characteristic length \(a_\perp = \sqrt{\hbar/m\omega_\perp}\) of the harmonic potential, time to \(1/\omega_\perp\) and the wavefunction \(\Psi(z, t)\) to \(1/\sqrt{a_\perp}\). In these units, the strength of the interatomic interaction will be given by the ratio \(g = -2Naa_\perp/q_\perp^2\) and the strength of the trapping potential is given in terms of the ratio \(\lambda = \omega_z/\omega_\perp\). The wavefunction is normalized to unity, and hence the number of atoms \(N\) appears in \(g\).

In a typical experiment [8, 11], \(\omega_\perp \simeq 2\pi \times 200\text{Hz}, \omega_z \simeq 2\pi \times 5\text{Hz}, a \simeq -3a_0\), where \(a_0\) is the Bohr radius, and \(N \simeq 5000\). In this case, the unit of length is \(a_\perp = 3 \times 10^{-6}\text{m}\), and the unit of time is \(1/\omega_\perp = 0.8\text{ms}\). Following the experiment of [10, 11], we take the initial position of our soliton at 0.5 mm, which is about 167\(a_\perp\) from the center of the trap, and the height of the potential barrier \(V_{\text{ext}}/\hbar \simeq 1.2\text{kHz} \simeq 6\hbar \omega_\perp\). Taking into account these typical values and taking the transverse equilibrium width \(q_\perp\) to be equal to \(a_\perp\), the strength of the interatomic interaction will be approximately \(g \simeq 0.5\). The strength of the trapping potential will be \(\lambda^2 \simeq 6 \times 10^{-4}\hbar \omega_z\).

We can now show that equation (2) indeed accounts for the interesting recombination of the two returning solitons at the center, as can be seen in figure 1.
Figure 1. Spacio-temporal density plots for a single soliton splitting into two solitons by the potential barrier at the center of a harmonic trap. Upon returning to the trap center, the two solitons recombine into the original one. The parameters of the experiments of \[8, 10\] have been used, namely \(\omega_\perp \simeq 2\pi \times 200 \text{ Hz}, \omega_z \simeq 2\pi \times 5 \text{ Hz}, a \simeq -3a_0\) and \(N \simeq 5000\). Initial soliton parameters: amplitude \(= 0.8a_\perp\), position \(= 250a_\perp = 0.5 \text{ mm}\), initial speed \(= 4a_\perp \omega_\perp = 10 \text{ mm s}^{-1}\) and interaction strength \(g = 0.5\). The square barrier’s parameters: height \(= 0.75\bar{h} \omega_\perp\) and width \(= 0.5a_\perp = 1.5 \times 10^{-6} \text{ m}\).

To create soliton molecules with this experiment, we propose switching off both the trapping potential and the potential barrier precisely at the classical turning point of the two solitons (in figure 1 this takes place at \(t \simeq 130 \text{ ms}\)). At this point the relative speed of the two solitons vanishes, which represents one essential condition for creating the soliton molecule. It is then hoped that the overlap between the two solitons will be sufficient to initiate their attraction. It is clear, however, from figure 1 that at the classical turning point the separation between the two solitons is much larger than their widths, which diminishes the possibility of creating a soliton molecule. To overcome this problem, we launch the soliton from a distance closer to the trap center. This will result in a smaller separation between the two solitons at their classical turning point. In figure 2, we show one case where this is possible. In figure 2(a), the soliton splitting and recombination at the potential barrier is shown. In figure 2(b), the formation of a soliton molecule is shown as a result of switching off the potential, as described above. The periodic exchange of energy between the solitons and their center-of-mass oscillation are evidence of the creation of the soliton molecule, which will be more pronounced in the subsequent figures.

Several parameters affect the result of the above-described procedure for creating a soliton molecule. These comprise the strength of the trapping potential, the time scale for switching off the potentials, the initial width, speed and position of the soliton, the height and width of the potential barrier and the strength of the interatomic interaction. We present here a detailed investigation of the effect of some of these parameters. It turns out that soliton molecules can almost always be created when these parameters are changed, as long as the two solitons are set in an initial state of zero relative speed and small enough separation.

We start this detailed investigation by increasing the strength of the harmonic potential, which causes the two solitons to reach their classical turning point at a shorter time \(t_0\). To calculate \(t_0\), we Fourier transform the wave function and obtain the center-of-mass speed as
Figure 2. Spatio-temporal density plots for (a) the experiment of [10] and (b) our proposal for soliton molecule formation. In (a), a single soliton is split by the potential barrier into two solitons that, upon returning to the trap center, recombine into the original one. In (b), the harmonic trapping potential and the potential barrier, shown with the solid blue curve, are switched off at $t = 15.75$ when the two solitons reach the classical turning point. Parameters: (a) initial velocity $= -1.0$, amplitude $= 1.0$, position $= 5$, interaction strength $g = 1.0$ and harmonic trap strength $\lambda^2 = 0.0113$; (b) initial velocity $= -0.8$, amplitude $= 0.8$, position $= 5$, interaction strength $g = 1.0$ and harmonic trap strength $\lambda^2 = 0.0225$. The square barrier’s parameters: height $= 0.75$ and width $= 0.5$. All numbers are given in terms of scaling units as described above.

a function of time. A minimization procedure results in the time $t_0$ for which the speed is a minimum. In figure 3, we plot $t_0$ versus $\lambda^2$. We choose three points on this curve where we also simulate molecule formation, as shown in figure 4. The values of $t_0$ used to create the molecules of figure 4 are slightly larger than those of figure 3. This is merely because of the numerical inaccuracy in determining $t_0$ from the Fourier transformation. By increasing the strength of the harmonic potential and hence the initial speed, the amplitude of the transmitted soliton will be larger than the reflected one and hence the difference between the intensities of the two solitons will increase. It is known that the frequency of relative oscillation of the two solitons in a molecule is proportional to the difference in amplitude of the solitons (see also below). This explains the increase in the molecule’s frequency from figures 4(a) to 4(c).

To investigate the effect of the time scale $T$ of switching the external potentials off, we employ the following time-dependent potential:

$$V(z, t) = \frac{1}{2} \left[ 1 - \tanh\left( \frac{t - t_0}{T} \right) \right] V(z),$$

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Figure 3. Plot of time to reach the classical turning point, $t_0$, versus strength of the trapping potential, $\lambda^2$. The parameters used are $\omega_{\perp} \simeq 2\pi \times 200$ Hz, $a \simeq -3a_0$, $N \simeq 5000$. Initial soliton parameters: amplitude $= 0.8a_{\perp}$, position $5a_{\perp}$ and interaction strength $g = 1.0$. The square barrier’s parameters: height $= 0.75\hbar \omega_{\perp}$ and width $\sim 1.0a_{\perp}$. The unit of length is $a_{\perp} \simeq 17 \times 10^{-6}$ m and the unit of time is $5.0 \text{ ms}$. The three points correspond to subfigures of figure 4.

Figure 4. Spatio-temporal density plots for a single soliton splitting into two solitons by the potential barrier at the center of a harmonic trap. The parameters are the same as in figure 3. The values of $t_0$ and $\lambda$ used in these figures are indicated in figure 3.

where $V(z)$ is the sum of the trapping potential and the potential barrier. We start by switching the potentials off over a time scale much shorter than that of the soliton’s center-of-mass dynamics. To take a reference case, we consider figure 4(a) where $t_0 = 15.9$ and the potentials are switched off suddenly and $T$ is infinitely small. The period of center-of-mass oscillation is about $2t_0$. Repeating this simulation using the above time-dependent potential with $T = 0.01$ results in the molecule of figure 5(a), which is essentially identical to that of figure 4(a). Switching off the potentials rather slowly with $T = 0.1$, the molecule does not form, as shown in figure 5(b). For a molecule to form with $T = 0.1$, we had to change $t_0$ to a new value, namely $t_0 = 16.0$, as shown in figure 5(c). The conclusion is thus that the time scale for switching off the potentials is not a crucial factor in the formation of the molecule; the potentials can be switched off either rapidly or over a time scale comparable with the center-of-mass motion.

The initial speed of the soliton affects the ratio of the reflected to the transmitted soliton. This is shown in figure 6, where we plot the number of atoms in the transmitted soliton versus...
Figure 5. Spatio-temporal density plots for soliton molecule formation using different time scales to switch off the potentials. In (a), $T = 0.01$, $t_0 = 15.9$; in (b), $T = 0.1$, $t_0 = 15.9$; in (c), $T = 0.1$, $t_0 = 16.0$. The rest of the parameters are the same as in figure 3.

Figure 6. The number of atoms in the transmitted soliton, $N_1$, relative to the total number, $N$, versus the initial speed of the soliton, $v_0$. The parameters are the same as in figure 3(a). Filled square points correspond to figure 7 and the filled circle corresponds to figure 4(a).

the initial speed. We choose two points on this curve to simulate the molecule formation as shown in figure 7. The main effect of the initial speed is to determine the ratio of the number of atoms in one soliton to the other. In figure 7(a), the speed is high enough ($v_0 = -0.9$) such that the left soliton of the molecule is larger than the right one, as can be seen from the darkness of the density plot. The interesting case of figure 7(b) where the two solitons periodically coalesce is a result of choosing an initial speed ($v_0 = -0.6$) that results in almost two equal solitons.

Finally, the effect of the height and width of the potential barrier will be similar to that of the initial speed. For larger barrier height and width, the reflected soliton will be larger than the transmitted one, but a soliton molecule can always be formed once the right $t_0$ is chosen such that the two solitons start at rest and close enough together. For instance, we simulate the molecule formation using a Gaussian potential barrier rather than a square one. We take the same parameters as those of figure 3(a). It turns out that a slight adjustment of the barrier width and $t_0$ was needed. The barrier takes the form $V_{ext}(z) = V_0 \exp[-(x/(d_0/1.2))^2]$, where $V_0$ and
Figure 7. Spatio-temporal density plots for molecule formation using two values of the soliton’s initial speed. In (a), \( v_0 = -0.9 \), and in (b), \( v_0 = -0.6 \).

Figure 8. Spatio-temporal density plots for soliton molecule formation. This figure is similar to figure 4(a) but replacing the square barrier with a Gaussian barrier.

\( d_0 \) are the height and width of the square barrier, respectively. The factor 1.2 was introduced to adjust the width of the barrier. The turn-off of the potential was also adjusted to \( t_0 = 15.93 \) in comparison with \( t_0 = 15.90 \) for the square barrier. The result of this simulation is shown in figure 8, where it is clear that the shape of the barrier has no significant effect.

In another version of this experiment, one can also think of phase imprinting one of the two solitons once it reaches the classical turning point. In such an experiment, the phase of the cycle performed by the molecule is controlled. For instance, one can imprint a \( \pi \) phase difference, leading initially to an increase in the separation of the solitons. If their initial separation is small enough, however, they will ultimately return back and form the molecule since their relative phase will change from \( \pi \) to zero as they move away from each other and the force becomes attractive, as will be shown next. In figure 9, we show the result of such a simulation. The imprinted \( \pi \) phase on the right soliton resulted in an initial repulsion, but that did not hinder molecule formation. In comparison with the similar case of figure 3(a), the molecule here has a larger bond length.
3. Soliton–soliton interaction energy

As mentioned in the introduction, the interaction energy of two solitons depends on their separation and on their relative phase. It is also known that such an interaction may lead to the formation of a bound state of two solitons. The key point here is that dynamically the relative phase of two solitons changes as their separation changes. If two solitons that are initially in phase approach each other sufficiently slowly, their relative phase changes such that the force between them becomes repulsive. When the two solitons then move away from each other, the force becomes attractive again and the cycle completes itself. Thus, the manner in which the relative phase changes with the separation between the solitons is essential for understanding their binding properties. This fact is understood in the literature, but to the best of our knowledge has not yet been captured analytically in a single formula that accurately gives the interaction potential of the solitons for both short and large separations. Here, we arrive at this objective by deriving the exact dependence of the phase, and hence the interaction potential, on the soliton separation. In addition to being of importance by itself, this potential provides a convenient analytical understanding for the possibility of soliton molecule formation.

Using the inverse scattering method, the exact two-soliton solution of the homogeneous version of equation (2) is derived in [2]. In [14], a re-derivation puts the solution in terms of eight parameters, namely the two initial center-of-mass positions $z_{1,2}$ of the solitons, their center-of-mass velocities $v_{1,2}$, their phases $\Phi_{1,2}$ and their square amplitudes $n_{1,2}$. The separation between the solitons can then be extracted analytically, from which also the force follows in terms of these parameters. Here, we extend this formalism to derive the interaction energy and to show that it takes the form of a Morse potential.

For simplicity, the relative velocity is set to zero and the limit of nearly equal soliton densities $n_\pm = n_2 - n_1 \ll n_+ = n_2 + n_1$ is taken. The separation $\Delta(t)$ between the solitons and their relative phase $\Phi(t)$ can then be derived from the exact two-soliton solution and turns out

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*Figure 9.* Spatio-temporal density plots for soliton molecule formation. This figure is similar to figure 4(a) but with imprinting a $\pi$ phase on the reflected soliton at its classical turning point. The parameters used here are the same as those of figure 4(a) except for $t_0 = 15.55$. 

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to be given by
\[
\Delta(t) = \frac{4}{\alpha} \log \left[ \frac{\alpha (\alpha^2 + 2\alpha \beta \cos(\omega t + \Phi_0) + \beta^2)}{\beta \alpha^2 n^2} \right]
\]
and
\[
\Phi(t) = \tan^{-1} \left( \frac{\beta \sin(\omega t + \phi_0)}{\alpha + \beta \cos(\omega t + \phi_0)} \right) - \tan^{-1} \left( \frac{\alpha \sin(\omega t + \phi_0)}{\beta + \alpha \cos(\omega t + \phi_0)} \right),
\]
where \(\beta = \exp(\alpha x_0/4)\), \(\omega = \alpha g n_- / 8\) and \(\alpha = gn_+\). In addition, \(x_0\) and \(\phi_0\) are two constants that can be determined from the initial conditions \(\Delta(0) = \Delta_0\) and \(\Phi(0) = \Phi_0\). The equations of motion for \(\Delta\) and \(\Phi\) can now be obtained by differentiating twice with respect to \(t\). The resulting equations are simplified by inverting equations (4) and (5) to express \(\cos(\omega t + \phi_0)\) and \(\sin(\omega t + \phi_0)\) in terms of \(\Delta\) and \(\Phi\). Finally, we obtain in this manner
\[
\ddot{\Delta} = -\frac{\alpha^3}{8} e^{-(1/4)\alpha \Delta} \cos \Phi,
\]
\[
\ddot{\Phi} = \frac{\alpha^4}{32} e^{-(1/4)\alpha \Delta} \sin \Phi,
\]
which are identical to Gordon’s formulae [2]. Here, however, we also have obtained the exact solutions of these equations of motion, namely equations (4) and (5). In [16], equations (6) and (7) were also derived perturbatively and then rewritten into a single equation for the complex field \(Z = \alpha \Delta + i\Phi\), namely \(\dot{Z} = -(\alpha^4/32) \exp(-iZ)\), which as expected turns out to be integrable. However, this work is distinguished from that of [16] by the fact that we derive the equations of motion and their solution from the two-soliton exact solution of the GPE, whereas in the latter reference the equations were derived from a perturbative expansion of the corresponding Lagrangian. While in our case no condition is assumed about the separation between the solitons, the results of [16] were derived in the limit of large soliton separations. Furthermore, we derive here an explicit form for the soliton–soliton potential, as we show next.

Equations (4)–(7) allow us to obtain the force \(\ddot{\Delta}\) in terms of \(\Delta\) by solving equation (4) for \(\cos(\omega t + \phi_0)\) and to substitute the solution in equation (6). Integrating the resulting expression with respect to \(\Delta\) leads to the soliton–soliton potential energy \(V_{ss} = -\int \ddot{\Delta} d\Delta\):
\[
V_{ss} = \frac{(\alpha^2/4) \cos \Phi_0}{e^{(1/4)\alpha \Delta_0} - e^{(1/4)\alpha \Delta_{eq}}} \left( e^{-(1/2)\alpha(\Delta - \Delta_{eq})} - 2e^{-(1/4)\alpha(\Delta - \Delta_{eq})} \right),
\]
which has the form of a Morse potential with a minimum at \(\Delta_{eq}\) given by
\[
\Delta_{eq} = \Delta_0 + \frac{4}{\alpha} \log \left( \frac{\alpha^2 - 2\alpha \beta \cos \Phi_0 + \beta^2}{\alpha^2 + \beta^2} \right).
\]
Here, \(\beta = \beta(\Delta_0, \Phi_0)\) corresponds to the real solution of the initial conditions.

Equation (8) is, to the best of our knowledge, the first quantitative description of the interaction potential between two solitons that is valid for both long and short separations. The first term on the right-hand side corresponds to a repulsive force and the second part corresponds to an attractive force. The presence of these two parts of the soliton–soliton interaction is implicit in Gordon’s equations of motion, equations (6) and (7). The novelty of our result is in obtaining

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Figure 10. Interaction potential between two bright solitons in terms of their separation. The solid curve is obtained numerically from the exact two solitons solution of the GPE. The dashed curve corresponds to formula (8). Parameters: $n_- = 0.2, n_+ = 4.7, g = 0.5, \Phi_0 = 0$.

explicit exact solutions to these equations of motion, which allows us to eliminate the time dependence and thus to obtain the soliton–soliton potential in terms of the separation only.

Alternatively, the potential can be determined from the exact solution directly. To that end, the locations of the two solitons are calculated numerically from the density $|\Psi(z, t)|^2$, from which the soliton separation and the associated acceleration are computed. Integrating the resulting force numerically, we again obtain an interaction potential. In figure 10, we plot the interaction potential obtained by the two methods. It is clear from this figure that the numerics captures the main features of the potential in equation (8) apart from a slight change in the location of the equilibrium point and depth of the potential. The change is due to the fact that the difference of the center-of-mass positions is numerically difficult to define uniquely and is therefore not exactly equal to the parameter $\Delta$ in the exact solution when the two solitons are too close together and interference effects take place. The shape of this potential, specifically the existence of a global minimum, proves that a bound state of two solitons can be formed provided the initial separation and relative phase are such that the energy is negative.

Finally, we note that both the equilibrium point and depth of the potential depend on the initial conditions. For further clarification of this rather unusual situation, we plot in figure 11 the soliton separation $\Delta(t)$ and relative phase $\Phi(t)$ during one period of the molecule’s oscillation. It is clear that by increasing the initial separation, the equilibrium point around which the solitons oscillates also increases. Note that, for both cases, the phase changes from 0 to $\pi$ over half the period $\pi/\omega$ of the molecule’s oscillation, which means that the force changes from attractive to repulsive over the same period of time. On the other hand, the dynamics of $\Delta(t)$ depends on $\Delta_0$ since for larger $\Delta_0$ there is initially a smaller overlap between the solitons and thus they will approach each other more slowly. By the time the force has changed sign, the solitons of the molecule with larger $\Delta_0$ have a final separation that is larger than the one with smaller $\Delta_0$, but both now have to start moving away from each other, which amounts to different equilibrium points. We have also checked that the same conclusions are drawn directly from the exact solution of the GPE.
4. Other applications

Having an analytic formula for the interaction potential as a Morse potential, it is appealing to consider further applications. In particular, we can consider a classical gas of solitons interacting with the Morse potential in equation (8). Here, the thermodynamics is expected to be enriched by the dependence of the potential on the relative phase of the solitons.

The equation of state of such an imperfect gas can be derived by a virial expansion \( P/k_B T = \rho + B_2 \rho^2 + B_3 \rho^3 + \cdots \), where \( \rho \) is the number density and \( B_2 \) and \( B_3 \) are the second and third virial coefficients. The second virial coefficient is given in terms of the two-body partition function, which reduces to the following integration on the soliton–soliton potential:

\[
- \left( \frac{1}{2} \right) \int \left[ \exp \left( - \frac{V_{ss}}{k_B T} \right) - 1 \right] d\Delta.
\]

Due to the facts that \( V_{ss} \) depends on the initial conditions and in the partition function all configurations should be taken into account, an additional integral on all possible initial conditions should be performed. A simpler but equivalent approach is using the potential that corresponds to equation (6), namely \( V_{ss} = - (\alpha^2/2) \exp(-\alpha \Delta/4) \cos \Phi \), where \( \Phi \) is treated as an independent thermodynamic variable and the initial conditions are absent from the potential. In the limit of weak interactions \( \alpha \ll k_B T \), a simple expression can be derived, \( B_2 = -(\pi/8)\alpha^3/(k_B T)^2 \), which leads to the equation of state

\[
\frac{P}{k_B T} = \rho - \frac{\pi}{8} \frac{\alpha^3}{(k_B T)^2} \rho^2.
\]  

Exploring the possibility of a phase transition to a soliton liquid requires extending the virial expansion to the third virial coefficient, which involves three-body processes and hence requires knowledge of the three-soliton solution, which is beyond the scope of this paper.

As another interesting application, we briefly consider a Toda lattice of solitons, which was successfully used to model the dynamics of a train of \( N \) solitons in external potentials [15]. The
force on the \( j \)th soliton at position \( z_j \) will be given by

\[
\ddot{z}_j = F_{ss}(\Delta_{j+1}) - F_{ss}(\Delta_{j-1}),
\]

where \( \Delta_{j+1} = z_{j+1} - z_j \), \( \Delta_{j-1} = z_j - z_{j-1} \) and \( F_{ss} = -dV_{ss}/d\Delta \). The ground state of such a system will be a series of equidistant solitons with peak intensities alternating between two slightly different values. The value of \( n_- \) cannot be arbitrarily small since the nearest-neighbor separation between the solitons in the lattice diverges as \( \log n_- \) \[14\]. On the other hand, \( n_- \) should be small enough that the solitons are sufficiently separated and that the coalescence condition \( n_+ g = 1 \) is avoided \[14\]. In this configuration, the net force on any soliton will vanish and the lattice moves as a rigid object that can be considered as a ‘soliton of solitons’. Collective excitations and sound waves can be considered as low-energy excitations.

To investigate the collective modes of the Toda lattice of solitons, we linearize the equation of motion, equation (11), in small deviations from the equilibrium separation. Since the density alternates between two values, all pairs of neighboring solitons will have the same equilibrium separation \( \Delta_{eq} \). Small variations in the soliton’s position \( z_j \) around the equilibrium value \( j \Delta_{eq} \) are given by \( z_j = j \Delta_{eq} + u_j \), with \( u_j \ll \Delta_{eq} \). In terms of \( u_j \), equation (11) takes the form

\[
\ddot{u}_j = F_{ss}(\Delta_{eq} + u_{j+1} - u_j) - F_{ss}(\Delta_{eq} + u_j - u_{j-1}) .
\]

Expanding in powers of \( u_j \) up to the second order, this equation takes the form

\[
\ddot{u}_j = \omega_T^2 (u_{j+1} - 2u_j + u_{j-1}) ,
\]

where \( \omega_T^2 \) is the force constant given by

\[
\omega_T^2 = \frac{d}{d\Delta} V_{ss}(\Delta_{eq}) = \frac{(\alpha^4/32) \cos \Phi_0}{e^{(1/4)\alpha \Delta_{eq}} - e^{(1/4)\alpha \Delta_{eq}}} .
\]

The dispersion relation is obtained by substituting the periodic solution \( u_j = A e^{i(\Delta_{eq} - \omega t)} \), namely

\[
\omega(k) = 2 \omega_T |\sin(k \Delta_{eq}/2)| .
\]

The phase difference between solitons enters this relation through \( \Delta_{eq} \) and \( \omega_T^2 \). In the long-wavelength limit \( (k \ll 1/\Delta_{eq}) \), the expansion in small \( k \) gives the speed of sound

\[
v_{ph} = \partial \omega / \partial k = \omega_T \Delta_{eq}
\]

of the phonons of the Toda lattice.

In spite of the dependence of \( \omega_T^2 \) on \( \cos \Phi_0 \) in equation (14), \( \omega_T \) is real for all values of \( \Phi_0 \). Invoking equation (9) shows that for \( 0 \leq \Phi_0 \leq \pi/2 \), \( \Delta_{eq} \geq \Delta_0 \), while for \( \pi/2 \leq \Phi_0 \leq \pi \), \( \Delta_{eq} \leq \Delta_0 \). Thus, in both cases, \( \omega_T^2 \) > 0 and \( \omega_T \) is always real. Substituting \( \Delta_{eq} \) from equation (9) in (15), we obtain

\[
v_{ph} = \frac{1}{8} \sqrt{\frac{\alpha^2 (\alpha^2 + \beta^2)}{\beta}} \Delta_{eq} e^{-(1/8)\alpha \Delta_{eq}} .
\]

Substituting \( \Delta_{eq} \) and \( \beta \) from equations (4) and (9), we obtain

\[
v_{ph} = \frac{1}{8} \sqrt{\frac{4X}{X - 1}} \left[ \Delta_0 + 4 \alpha \log \left( \frac{1 - 2X}{1 - X} \right) \right] ,
\]

where \( X = (2\alpha^2/g^2 n_0^3) \exp(-\alpha \Delta_0/4) \cos \Phi_0 \). It should be noted here that the arguments of the square root and logarithm functions are always positive. This can be shown by noting
from equation (4) that \( \Delta_0 \) is bounded by \( \Delta_{\text{max}} = \frac{4}{\alpha} \log[\alpha(\alpha + \beta)^2/\beta g^2 n^2], \) where this expression is obtained by setting, in equation (4), \( \Delta(t) = \Delta_0 \) and \( \cos(\omega t + \Phi_0) = 1. \) Replacing \( \Delta_0 \) by \( \Delta_{\text{max}} \) in the expression for \( X, \) we obtain an expression for the maximum of \( X, \) namely \( X_{\text{max}} = [2\alpha\beta/(\alpha + \beta)] \cos \Phi_0. \) This shows that \( X_{\text{max}} \leq 1/2 \) for all \( \alpha \) and \( \beta, \) which proves our statement. For large initial soliton separation, the phonons’ speed reduces to

\[
v_{\text{ph}} = \frac{1}{8} g^2 n_+ n_- \Delta_0, \tag{19}\]

which is simply the natural frequency of the molecule \( \omega \) multiplied by its initial bond length.

5. Conclusions

In conclusion, we have shown that a molecule of two bright solitons can be realized in attractive Bose–Einstein condensates. This was demonstrated both by numerical simulations and by showing that the interaction potential between the two solitons is of molecular type and takes the form of a Morse potential. Applications of this potential to the problems of the soliton gas and the Toda lattice of solitons were pointed out.

Final further remarks on the feasibility of our experimental proposal are in order. Firstly, it has been shown in [17] that collisions of 3D bright Bose–Einstein solitons range from being elastic to completely destructive due to the onset of collapse during the interaction. The facts that in the experiments the confining potential is almost 1D and that stable solitons of a few thousand atoms per soliton were created, scattered by a potential barrier and recombined at the barrier again producing the original soliton suggest the 3D effects to be not affecting the stability of the solitons and their interaction. The successful simulation of the experiment of [10] using a 1D Gross–Pitaevskii is another proof of the validity of neglecting 3D effects. Secondly, in [18], it has been shown that quantum fluctuations affect the interaction between the solitons through modulating their relative phase. In the present situation, the two solitons are created coherently from a single soliton, and therefore, their relative phase is expected to be less random than in the case of these two references where solitons are created incoherently by the collapse of a repulsive condensate. It should be noted here that methods of controlling the relative phase between solitons were also considered in [19].

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