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Vibration spectrum of a two-soliton molecule in dipolar Bose–Einstein condensates

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A B S T R A C T

We study the vibration of soliton molecules in dipolar Bose–Einstein condensates by variational approach and numerical simulations of the nonlocal Gross–Pitaevskii equation. We employ the periodic variation of the strength of dipolar atomic interactions to excite oscillations of solitons near their equilibrium positions. When the parametric perturbation is sufficiently strong the molecule breaks up into individual solitons, like the dissociation of ordinary molecules. The waveform of the molecule and resonance frequency, predicted by the developed model, are confirmed by numerical simulations of the governing equation.

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1. Introduction

One of the remarkable properties of Bose–Einstein condensates (BEC) is that, they can support self-localized states, known as solitons, i.e. wave packets with particle like features. Solitons emerge from a fine balance between dispersive spreading of the wave packet and its self-focusing due to the nonlinearity of the medium. While experimental and theoretical studies of single solitons and soliton trains in BEC are reported in many publications (see e.g. review article [1] and book [2]), the interaction of solitons and formation of their bound states remain less explored.

In other areas of physics, such as fiber optics and fiber lasers, the subject of soliton molecules is developed much better. In particular, the existence and some properties of soliton molecules in dispersion-managed optical fibers has been investigated in [3–5]. The binding mechanism of fiber optic solitons was proposed in [6]. Averaged dynamics of soliton molecules in dispersion-managed fiber links, in the context of optical communications, was recently studied in [7]. A survey of soliton molecules in dissipative systems, such as mode-locked fiber lasers, can be found in a review article [8].

In some media the nonlinear response depends on the field intensity in a certain neighborhood of the given location. Over the recent years these so called *nonlocal nonlinear media* have become the subject of intensive research due to their relevance to many

fundamental and applied problems of modern physics. Among other phenomena, solitons in nonlocal optical media are investigated too, both theoretically and experimentally (for a recent review see [9]). The existence of mutual interaction of spatial optical solitons in nonlocal media and the possibility of formation of their bound states was reported in [10]. Interaction of dark solitons under competing nonlocal cubic and local quintic nonlinearities was investigated by means of a variational technique [11].

Nonlocal nonlinearity naturally arises in Bose–Einstein condensates due to the long range dipole–dipole interactions between atoms [12]. The existence of stable isotropic and anisotropic 2D solitons in dipolar BEC was reported, respectively, in [13] and [14]. The conditions for stability and some dynamical effects with solitons in 1D dipolar BEC were studied in [15–17].

Our objective in this work is the investigation of soliton interactions in dipolar BEC with a main emphasis on the vibrational spectrum of a two-soliton molecule. At first we develop the variational approximation (VA) [18,19], which allows to find the stationary shape of the soliton molecule in dipolar BEC. Then we introduce the ground state wave function, obtained by means of VA, as initial condition into the governing nonlocal Gross–Pitaevskii equation and periodically change the coefficient of nonlinearity. Such a parametric perturbation excites the internal modes of the soliton molecule, giving rise to resonant behavior at some specific frequencies. Spectral peaks on the vibration spectrum reveal much about the nature of soliton molecules. If the perturbation is sufficiently strong, the molecule can break up into individual non-interacting solitons, in a process which is similar to dissociation of ordinary molecules. It should be noted that molecular vibra-

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tions under external perturbations represent one of the efficient methods in exploring the driven chemical reactions [20]. In this context, the present study may be regarded as an attempt to apply the ideas from physical chemistry to the field of cold quantum gases. In the relevant experiments with BEC the coefficient of non-local nonlinearity, which depends on the strength of dipole–dipole interactions as $\sim d^2$, can be varied by exposing the condensate to external electric fields. In addition, spatially modulated polarizing external fields can induce atomic dipole moments, thereby enhancing the nonlocal effects in the condensate [21]. Also the time-dependent dipole–dipole interaction can be realized via precession of the direction of external field, for example by additional transversal magnetic field [22].

2. The model and variational approach

The governing equation of our model is the one-dimensional nonlocal Gross–Pitaevskii equation (GPE) which describes the evolution of the condensate with only dipole–dipole atomic interactions [23]

$$i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{2\alpha d^2}{l_\perp^3}\psi\int_{-\infty}^{+\infty}R(|x-\xi|)|\psi(\xi,t)|^2 d\xi = 0, \quad (1)$$

where $\psi(x,t)$ is the mean-field wave function of the condensate, normalized to the number of atoms $N = \int_{-\infty}^{\infty}|\psi|^2 dx$, d is the magnetic or electric dipole moment of the atoms with mass m, $l_\perp = \sqrt{\hbar/m\omega_\perp}$ is the harmonic oscillator length, $\omega_\perp$ is the frequency of transverse confinement for the condensate. The parameter α is connected to the angle ϕ, which dipoles form with respect to x direction. For dipoles, rapidly oscillating in the plane, perpendicular to the x axis, the angular coefficient can change from $\alpha = 1$ ($\phi = 0$) to $\alpha = -1/2$ ($\phi = \pi/2$). Eq. (1) can be reduced to dimensionless form via new variables $t \to \omega_\perp t$, $x \to x/l_\perp$, $\psi \to \sqrt{2|\alpha|a_d}\psi$, and $a_d = md^2/\hbar^2$.

$$i\frac{\partial\psi}{\partial t} + \frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + g(t)\psi\int_{-\infty}^{+\infty}R(|x-\xi|)|\psi(\xi,t)|^2 d\xi = 0, \quad (2)$$

where $g(t)$ is the time-dependent coefficient, responsible for the long-range dipolar atomic interactions. The time dependence can be realized via change of the angle ϕ between atomic dipoles and the x axis, by means of external electric or magnetic fields. For simplicity we excluded the contact interactions term $\sim 2\hbar\omega_\perp a_s|\psi|^2\psi$ from the governing equation. This is justified in experimental conditions when the atomic scattering length a_s is reduced to zero by means of a Feshbach resonance technique [24]. On the other hand, recently it was shown that Bose-condensed ^{164}Dy [25] and ^{168}Er [26] can reach strongly dipolar regime, for which the relative strength of the dipolar and contact interactions is $\varepsilon_{dd} = \mu_0\mu^2 m/12\pi\hbar^2 a_s > 1$, even without minimization of the atomic s-wave scattering length.

In further calculations we employ the analytically tractable Gaussian response function

$$R(x) = \frac{1}{\sqrt{2\pi}\,w}\exp\left(-\frac{x^2}{2w^2}\right), \quad (3)$$

which is normalized to one $\int_{-\infty}^{+\infty}R(x)dx = 1$. This response function is simple for analytical treatment and sufficient for understanding of the problem at hand. In fact $R(x)$ is qualitatively similar to the response function, obtained from rigorous calculations in [27]. As a trial function for the two-soliton molecule we use the first Gauss–Hermite function

$$\psi(x,t) = A(t)\cdot x\cdot\exp\left[-\frac{x^2}{2a(t)^2} + ib(t)x^2 + i\phi(t)\right], \quad (4)$$

with the norm $N = A^2 a^3\sqrt{\pi}/2$, which is a conserved quantity of the governing equation. So, in this setting the center-of-mass of the molecule does not change in time. Only the distance between solitons of the molecule is variable. In other words, each soliton can perform oscillations near its equilibrium position. The distance between center-of-mass positions of two solitons (separation, or bond length) is determined as $\Delta(t) = 4a(t)/\sqrt{\pi}$. It should be noted, that similar ansatz was employed in the context of antisymmetric solitons in dispersion-managed optical fibers [28,29].

Eq. (2) can be derived from the Lagrangian density

$$\mathcal{L} = \frac{i}{2}(\psi\psi_t^* - \psi^*\psi_t) + \frac{1}{2}|\psi_x|^2$$
$$- \frac{1}{2}g(t)|\psi(x,t)|^2\int_{-\infty}^{\infty}R(x-\xi)|\psi(\xi,t)|^2 d\xi, \quad (5)$$

where the subscript denotes derivative with respect to corresponding variable, i.e. $\psi_t = \partial\psi/\partial t$, $\psi_x = \partial\psi/\partial x$.

Now using the response function (3) and ansatz (4), we obtain the Lagrangian density (5). Subsequent integration over the space variable $L = \int\mathcal{L}dx$ yields the averaged Lagrangian

$$\frac{L}{N} = \frac{3}{2}a^2 b_t + \phi_t + \frac{3}{4a^2} + 3\,a^2 b^2$$
$$- \frac{g(t)N}{8\sqrt{2\pi}}\cdot\frac{3a^4 + 4a^2 w^2 + 4w^4}{(a^2+w^2)^{5/2}}. \quad (6)$$

The Euler–Lagrange equations $d/dt(\partial L/\partial v_t) - \partial L/\partial v = 0$ for variational parameters $v \to \phi, b, a$ yield the following system

$$N_t = 0, \quad a_t = 2\,a\,b,$$
$$b_t = \frac{1}{2a^4} - 2\,b^2 - \frac{g(t)N}{8\sqrt{2\pi}}\cdot\frac{a^4 + 4w^4}{(a^2+w^2)^{7/2}}. \quad (7)$$

The first equation in (7) is decoupled from others and states the conservation of the wave packet's norm. The equation for the width can be derived from the last two equations in (7)

$$a_{tt} = \frac{1}{a^3} - \frac{g(t)N}{4\sqrt{2\pi}}\cdot\frac{a(a^4 + 4w^4)}{(a^2+w^2)^{7/2}}. \quad (8)$$

This equation is similar to equation of motion for a unit mass particle in the anharmonic potential

$$a_{tt} = -\frac{\partial U}{\partial a}, \quad \text{with}$$
$$U(a) = \frac{1}{2a^2} - \frac{gN}{12\sqrt{2\pi}}\cdot\frac{3a^4 + 4a^2 w^2 + 4w^4}{(a^2+w^2)^{5/2}}. \quad (9)$$

The stationary state a_0 corresponding to the minimum of the potential well $\partial U/\partial a = 0$ gives the equilibrium separation between solitons $\Delta_0 = 4a_0/\sqrt{\pi}$, and the amplitude via the norm $A_0 = \sqrt{2N/(a_0^3\sqrt{\pi})}$. Therefore, the shape of the soliton molecule, given by Eq. (4) is determined by the variational approximation.

The weakly perturbed soliton molecule will perform oscillations with a frequency

$$\omega_0 = \left(\frac{3}{a_0^3} - \frac{g_0 N}{4\sqrt{2\pi}}\cdot\frac{2a_0^6 - 5a_0^4 w^2 + 24a_0^2 w^4 - 4w^6}{(a_0^2+w^2)^{9/2}}\right)^{1/2}. \quad (10)$$

Fig. 1 illustrates the potential $U(a)$ and shape of the two-soliton molecule.

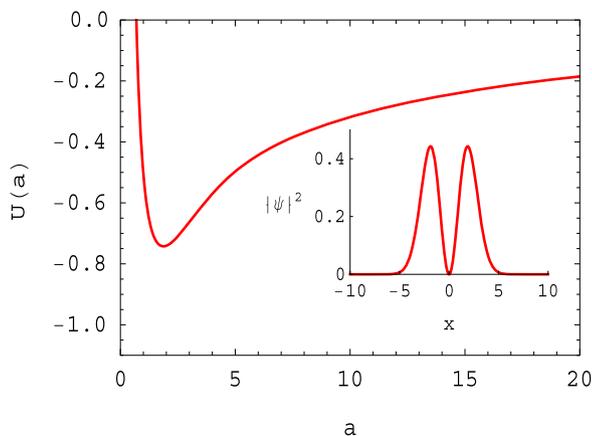**Fig. 1.** (Color online.) The shape of the anharmonic potential given by Eq. (9). The inset shows the ground state waveform of a two-soliton molecule, as predicted by VA for a Gaussian response function (3) with $w = 5$. The norm, width and amplitude of the molecule are $N = 2$, $a_0 = 1.87$, $A_0 = 0.59$, respectively. The coefficient of nonlocal nonlinearity is $g_0 = 20$.

To verify the accuracy of the developed approach, we introduce the VA predicted waveform for a two-soliton molecule into the GPE (2), and let the molecule to evolve for some period of time. The results are shown in Fig. 2. As is evident from this figure, the stationary state of the molecule is indeed well predicted by the VA. Periodic oscillations of solitons near equilibrium positions are observed, when they are set in motion toward each-other with a small velocity. The frequency and period of oscillations, predicted by VA $\omega_0 \simeq 0.5$, $T_0 = 2\pi/\omega_0 \simeq 12.6$ for $N = 2$ and $g_0 = 20$, are also confirmed by GPE simulations.

3. Response of the soliton molecule to parametric perturbation

Understanding the molecular vibrations can help to control chemical reactions, that is why it is an important subject in physical chemistry. Relevant phenomenon is the intramolecular vibrational energy transfer, which significantly affects the rate of some chemical reactions [30]. Our interest in exploring the vibration dynamics of soliton molecules in dipolar condensates is motivated, to some extent, by these analogies.

Vibrations of the soliton molecule can be induced by periodic or random variations of the coefficient of nonlinearity in the GPE (2). In relevant experiments this can be done by exposing the condensate to external electric field, which acts on the dipoles, by changing their strength or orientation in space. Since the coefficient of nonlocal nonlinearity depends of the dipole moments of atoms as $g \sim d^2$, the electric field leads to variation of this coefficient.
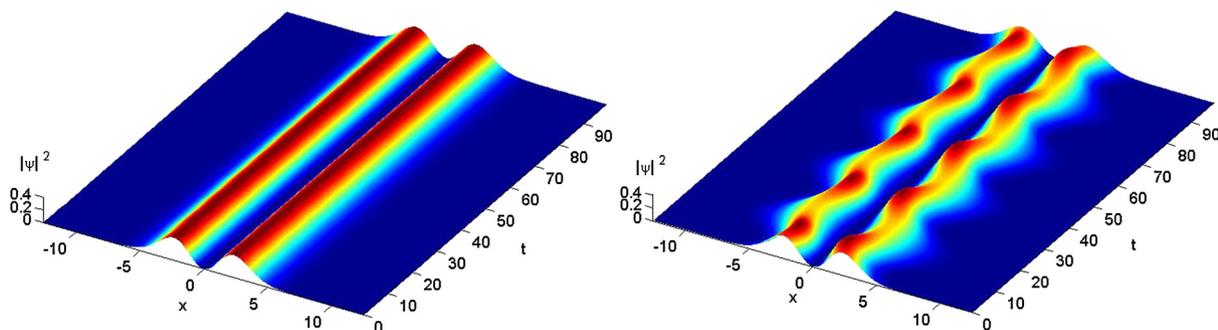
Below we present the vibration dynamics of a two-soliton molecule, based on numerical simulations of the VA Eq. (8) and the governing GPE (2). Ordinary differential equation (8) is solved by fourth-order Runge–Kutta procedure with adaptive step-size control [31]. Numerical solution of the GPE (2) is performed by split-step fast Fourier transform method [32], which was proved to be quite effective in solving similar problems in fiber optics and BEC. We have used 2048 Fourier modes in the integration domain of length $x \in [-6\pi, 6\pi]$, and the time step was $\delta t = 0.001$. To speed up the calculation of the integral term in the GPE we employ the convolution theorem. The accuracy of calculations was monitored by checking the conserved quantities of the GPE, such as the norm and field momentum. These quantities were conserved within relative error $\sim 10^{-3}$. Radiation of linear waves by the oscillating soliton molecule was not detected.

In the left panel of Fig. 3 we show the dynamics of center-of-mass positions of two solitons, forming the molecule, when the coefficient of nonlinearity is periodically varied in time at resonance frequency, which is predicted by VA. At initial stage of the evolution the amplitude of oscillations grows linearly, as is usual for ordinary resonance phenomenon. Later the amplitude of oscillations starts to decrease due to de-tuning from the resonance. This is a manifestation of the nonlinear resonance phenomenon, when the frequency of oscillations starts to depend on its amplitude [33]. Oscillations with growing and decreasing amplitude repeat as time progresses. Observed discrepancy between the VA and GPE is explained by the fact, that in GPE simulations internal vibrations of solitons interfere with their center-of-mass dynamics, while in the VA approach these phenomena are neglected. The amplitude vs. frequency curve, presented in the right panel of Fig. 3, characterizes the vibration spectrum of the two-soliton molecule. Strong peak at the main frequency and weaker peaks at harmonics corroborate with predictions of the VA and results of numerical simulations of the governing GPE.

4. Dissociation of the soliton molecule

Direct external forcing or parametric perturbations give rise to excitation of internal modes of the soliton molecule. In its simplest form the excitation shows up as vibration of solitons near their equilibrium positions. Few examples of small amplitude dynamics of the molecule were shown in the previous section. If the perturbation is sufficiently strong, the molecule can break-up into individual non-interacting solitons. This is analogue of the dissociation of ordinary molecules under perturbation [34].

In Fig. 4 we illustrate the process of dissociation of a two-soliton molecule under periodically varying nonlocal nonlinearity. As can be observed, the separation between solitons starts to oscillate with growing amplitude, and finally diverges at some time instance. The molecule breaks-up into two individual solitons, mov-
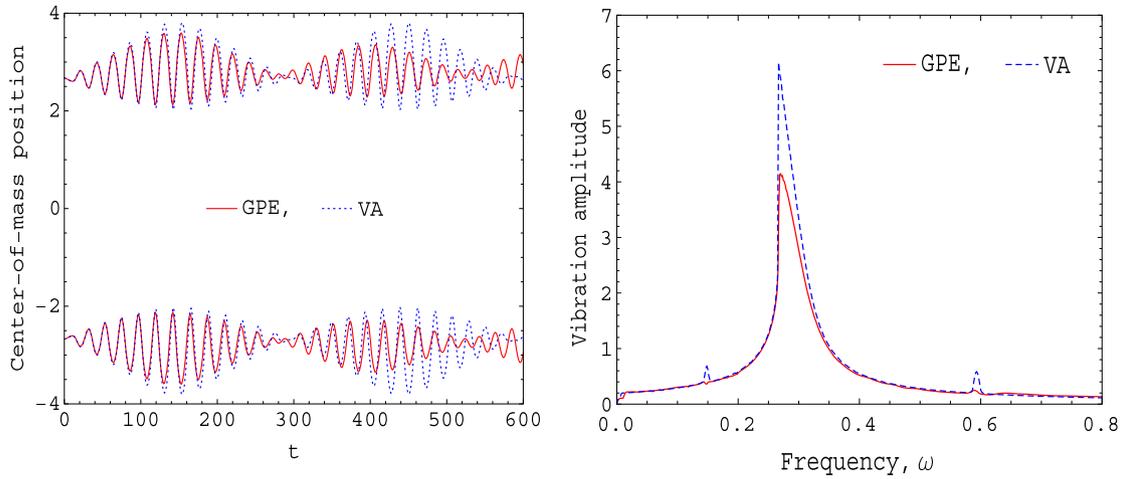

Fig. 2. (Color online.) Left panel: In stationary state of the molecule solitons stay at their equilibrium positions $x_0 = \pm 2a_0/\sqrt{\pi}$ and do not show any dynamics. Right panel: If solitons are set in motion by assigning some velocity towards each-other, they oscillate near equilibrium positions. The initial state corresponds to a two-soliton molecule, shown in the inset of Fig. 1. The initial velocity $a_t(0) = 2a_0 b_0$ is assigned via the chirp parameter $b_0 = -0.05$ in Eq. (4).

Fig. 3. (Color online.) Left panel: Periodic variation of the coefficient of nonlocal nonlinearity $g(t) = g_0 \cdot (1 + \epsilon \sin(\omega \cdot t))$ with a small amplitude $\epsilon = 0.01$ and $g_0 = 10$ at a resonance frequency $\omega = 0.297$, gives rise to vibration of solitons near their equilibrium positions. At initial stage the amplitude of oscillations increases linearly, as inherent to usual resonance phenomenon, and then decreases again due to de-tuning from the resonance. There is the manifestation of the phenomenon of nonlinear resonance. Right panel: The amplitude of molecule's vibrations as a function of frequency at $\epsilon = 0.05$. The main resonance and second harmonic are evident at specific frequencies, as predicted by VA (blue dashed line) and confirmed by numerical simulations of the GPE (2) (red solid line). Parameters are the same as in Fig. 1.
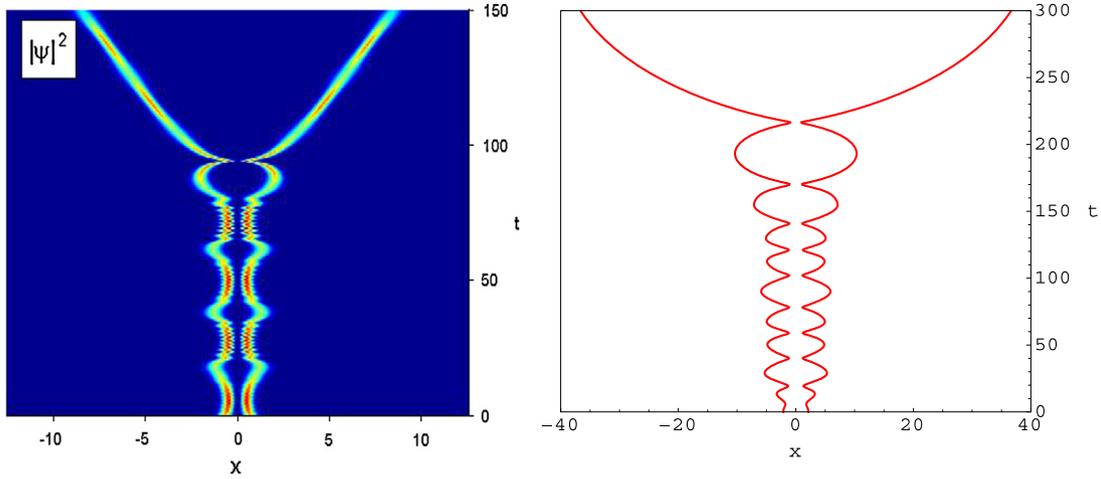

Fig. 4. (Color online.) Left panel: Dissociation of the two-soliton molecule under periodic variation of the coefficient of nonlocal nonlinearity $g(t) = g_0(1 + \epsilon \sin(\omega t))$ at a resonance frequency $\omega = 0.51$ for $g_0 = 20$, $\epsilon = 0.4$, according to numerical simulation of the GPE (2). Right panel: The same process according to VA Eq. (8), which is in qualitative agreement with the result of GPE simulation. Current positions of two solitons are determined from Eq. (8) as $x(t) = \pm 2a(t)/\sqrt{\pi}$.

ing apart with some velocity. Although the qualitative agreement between the result of numerical GPE simulations and corresponding prediction of VA is evident, the break-up times are notably different. This discrepancy can be explained by the fact that VA does not take into regard the interaction between the dynamics of the molecule and internal vibrations of individual solitons.

In the limit of strong non-locality, when the waist of the response function is greater than the spatial extent of the soliton molecule ($w \gg a$), the main equation of the VA model (8) can be reduced to the following form

$$a_{tt} = \frac{1}{a^3} - \frac{g(t)N}{\sqrt{2\pi}\, w^3} a. \tag{11}$$

For $g(t) = g_0 + g_1 \sin(\Omega t)$ we have the equation

$$a_{tt} + f(t)a = \frac{1}{a^3}, \tag{12}$$

where

$$f(t) = \omega_0^2(1 + \epsilon \sin(\Omega t)), \quad \omega_0^2 = \frac{g_0 N}{\sqrt{2\pi}\, w^3}, \quad \epsilon = \frac{g_1}{g_0}.$$

Eq. (11) has the form of the Ermakov–Pinney equation, which arises in a variety of contexts [35–37]. The main feature of Eq. (11) is that its general solution

$$a(t) = \sqrt{\alpha(t)^2 + \frac{1}{W}\beta(t)^2} \tag{13}$$

can be presented in terms of the linearly independent solutions $\alpha(t)$, $\beta(t)$ of the Mathieu equation

$$v_{tt} + f(t)v = 0, \tag{14}$$

and W is the constant Wronskian $W = \alpha \beta_t - \alpha_t \beta$. The Ermakov–Pinney equation inherits the instability features of the associated Eq. (14), which is parametrically unstable for

$$|\Omega - 2\omega_0| = \frac{\epsilon \omega_0}{2}. \tag{15}$$

Numerical simulations, presented in this work, are performed using the parameters of the ^{164}Dy condensate [25], whose atoms have a largest permanent magnetic dipole moment $\mu = 10\mu_B$ in the ground state. Strong radial confinement with a frequency $\omega_\perp = 2\pi \times 60$ Hz provides quasi-one dimensionality of the system.

Corresponding radial harmonic oscillator length is $l_\perp = \sqrt{\hbar/m\omega_\perp} \simeq$ 1 µm. The axial confinement for the condensate in the attractive regime, although present in the initial stage of its preparation, later can be removed to allow the soliton freely move along the x axis. Characteristic length of dipolar interactions is estimated from $a_{dd} = \mu_0\mu^2 m/(12\pi\hbar^2) \simeq 7 \times 10^{-9}$ m, where $\mu_0 = 12.57$ N/A^2 permeability of vacuum, $\mu = 10\mu_B = 9.274 \times 10^{-23}$ A m^2 and $m = 164$ amu $= 2.72 \times 10^{-25}$ kg are the magnetic moment and mass of the ^{164}Dy atom, respectively. For this set of parameters the two-soliton molecule with dimensionless norm $N = 2$ and waist of the response function $w = 5$, will contain $\sim 5 \times 10^3$ atoms. This number is compatible with the total number of condensed atoms $\sim 15 \times 10^3$ produced in the experiment [25].

5. Conclusions

Bright solitons in dipolar Bose–Einstein condensates can form stable bound states, known as soliton molecules. In this work we have studied the small amplitude dynamics of a two-soliton molecule by analytical and numerical methods. The analytical approach, based on the variational approximation, allows to find the stationary shape of the soliton molecule. The model also predicts, that interaction potential between two anti-phase bright solitons in dipolar BEC has a molecular type property. Specifically, solitons attract each-other at long distances and repel at short distances. At a distance between solitons, where attractive and repulsive forces come to balance, the molecule stays in its stationary state. The internal modes of the soliton molecule can be excited by periodic variation of the strength of dipole–dipole atomic interactions in the condensate. In the simplest case excitation of the molecule shows up as vibration of solitons near their equilibrium positions. In numerical experiments the spectrum of molecule's vibrations has been obtained by measuring the largest and smallest separation between two oscillating solitons at a given frequency of the perturbation, in a wide frequency domain. If the perturbation is sufficiently strong, the molecule can break up into individual non-interacting solitons, which is an analogue of the dissociation of ordinary molecules. Comparison between the results of numerical simulations of the GPE and predictions of the variational approximation shows a good qualitative agreement.

Acknowledgements

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