

Master in Photonics

MASTER THESIS WORK

**PROPAGATION OF COLLECTIVE MODES
IN NON-OVERLAPPING DIPOLAR
BOSE-EINSTEIN CONDENSATES**

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Propagation of collective modes in non-overlapping dipolar Bose-Einstein Condensates

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Abstract. The aim of this project consists of studying long-range effects of the dipolar interaction between non-overlapping dipolar Bose-Einstein Condensates when several excitations are applied on one of them. Although the natural frame for the theoretical analysis is the Quantum Mechanics frame, a classical approach is suggested. The coupled-pendulum model is applied for double and triple-well configurations, and dipolar and quadrupolar excitations are compared in the cases of dipolar and non-dipolar Bose-Einstein Condensates.

Keywords: Bose-Einstein Condensate, Dipolar interaction, Excitation, Long-range

1. Introduction

The so-called Bose-Einstein Condensation is a quantum phase transition. It can be found in bosonic systems below a critical temperature that is characteristic of the system. When a system suffers Bose-Einstein Condensation, all the particles occupy the same single-particle ground state. For instance, one of the systems that holds this kind of transitions are ultracold quantum bosonic gases. When the particles possess dipolar momentum, the condensate is called a dipolar Bose-Einstein Condensate.

Since the first experimental realization of a dipolar Bose-Einstein Condensate of Chromium [1] and Dysprosium [2] atoms, there has been growing interest in atomic and molecular dipolar gases [3] due to the long-range and anisotropic nature of such interaction. The investigation on this kind of interaction is expecting to give rise to important new features not only at microscopic level, but at macroscopic level as well. A central issue in the phenomena produced by the dipole moment of the particles is to understand the mechanism of the expansion and propagation of collective modes which have been already experimentally observed in magnetic dipolar atomic gases [4]. The development of new experimental techniques focused on the realization of molecular gases with large electric polar moment, where the dipolar effects are particularly strong, has led to the hope that challenging new frontiers in this area of research can be opened. However, the research in dipolar gases has tended to focus mostly on the study of

the anisotropic effects of the dipolar interaction [3, 5], rather than on the long-range ones, where there are only few proposals: cat states in triple-well potentials [6, 7] and propagation of center-of-mass modes studied by means of a variational method [8, 9].

The aim of the present work is to study the propagation of dipolar and quadrupolar modes induced by the long-range nature of the dipolar interaction by solving the full 3D time-dependent Gross-Pitaevskii equation (TDGPE). We consider two dipolar Bose-Einstein condensates (dBECs) harmonically trapped in a double-well configuration such that the overlap between the two clouds is negligible as well as the corresponding tunneling effect. The only effective force acting between the two BECs is the one produced by the long-range behaviour of the dipolar interaction.

In order to solve the Gross-Pitaevskii equation we use two different numerical methods: the Imaginary Time Step Method for the statics and Hammings method for the dynamics. As a test, we study the propagation of center-of-mass (dipolar) modes, and our results are in agreement with the ones obtained within the variational method [8, 9]. Then, we investigate the propagation of other excitations (monopolar and quadrupolar modes), that is, the appearance and the shift of new characteristic frequencies. Finally, we also propose a coupled-pendulum model that yields a qualitative description of the problem. As an extension, we test our model in a triple-well configuration, comparing the results to the case of the double-well configuration, and finding out that the classical model gives a qualitative description of the dipolar coupling.

2. Dipolar interaction in BECs and double-well configuration

Bose-Einstein condensates can be described in the mean-field framework by the Gross-Pitaevskii equation, which looks like a non-linear Schrödinger equation, provided a large number of particles, a dilute system and only s -wave scattering interaction [10]. The time-dependent Gross-Pitaevskii equation (TDGPE) is:

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\vec{r}) + g|\Psi(\vec{r}, t)|^2 \right] \Psi(\vec{r}, t), \quad (1)$$

where $\Psi(\vec{r}, t)$ is the wavefunction of the condensate, which is normalized to the number of particles $N = \int |\Psi(\vec{r}, t)|^2 d\vec{r}$, m is the mass of the bosons, $V_{ext}(\vec{r})$ is the trapping potential and $g = 4\pi\hbar^2 a/m$ is the coupling constant that contains information about the contact interaction, being a the s -wave scattering length. Nevertheless, when dipolar effects are considerable, Eq.(1) must be modified to take into account the dipolar interaction:

$$V_D(|\vec{r} - \vec{r}'|, \theta) = d^2 \frac{1 - 3 \cos^2 \theta}{|\vec{r} - \vec{r}'|^3}. \quad (2)$$

Here $\vec{d} = \sqrt{\mu_0/4\pi} \vec{\mu}$ is the dipole moment and θ is the angle between \vec{d} and the relative position between two dipoles $\vec{r} - \vec{r}'$. All the atoms are assumed to have the same dipole moment, both in magnitude and vector orientation. We can see from (2) that the dipolar interaction is anisotropic and long-range, since it decays as $1/r^3$. Therefore, the

condensates will need to be close enough in order to analyze the long-range properties of the interaction.

The dipolar interaction term is added in the TDGPE in the following way:

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\vec{r}) + g|\Psi(\vec{r}, t)|^2 + d^2 \int d\vec{r}' |\Psi(\vec{r}', t)|^2 \frac{1 - 3 \cos \theta}{|\vec{r} - \vec{r}'|^3} \right] \Psi(\vec{r}, t). \quad (3)$$

Once all the two-body interactions are included in the equation, the trapping potential can be selected to reach the more suitable configuration that will enhance the effects we want to study. Here, we consider a double-well trap with a large enough barrier height in order to avoid the tunneling of particles:

$$V_{ext}(x, y, z) = \frac{1}{2} m [\omega_0^2 (y^2 + z^2) + \omega_x^2 \min((x + x_c)^2, (x - x_c)^2)]. \quad (4)$$

In our system, $m = 52$ uma, the number of particles is $N = 5000$ (2500 bosons each BEC) and $\omega_x = 1500 \times 2\pi$ Hz $\gg \omega_0 = 50 \times 2\pi$ Hz, thus, each dBEC has a pancake-shaped geometry (Fig. 1). The parameter $2x_c$ controls the distance between the two dBECs, we have chosen $2x_c = 3\mu m$. Finally, the dipole moments are oriented in the x -direction. The purpose of this choice is to ensure more stability in our condensate [3]. When the Gross-Pitaevskii equation does not have a stationary solution for a set of given parameters, the iteration procedure does not converge. This can be a signature of the system collapse. Experimentally, it is interpreted as the phenomena where inelastic collisions between particles start to play a serious role, and the condensate becomes broken. Cigar-shape geometry stimulates collapse and other dipole moment orientations would decrease dipolar effects.

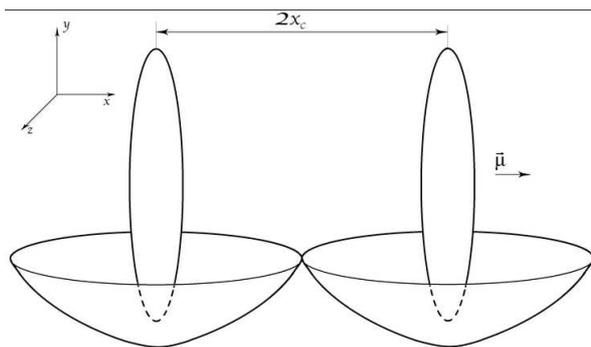


Figure 1. Illustration of the double-well configuration. The dipole moments are oriented in the x -direction, perpendicular to the pancake-shaped dBECs.

3. Dipolar drag effect

One of the nicest effects that one can realise in these configurations is the dipolar drag effect. When one of the condensates is excited (i.e. we give some velocity to the center of

mass), although there is no tunneling between both condensates, the other condensate starts to move due to the long-range effects of the dipolar interaction. Dipolar drag is one of the so called propagation of collective modes, produced by the long-range nature of the dipolar interaction. It has been already studied in electron gases, under the name of Coulomb drag [11, 12].

3.1. The coupled-pendulum model

Before presenting the numerical simulations, a qualitative description of the propagation of a collective mode between two non-overlapping dBECs can be found in the frame of classical mechanics [8]. We consider the classical analogy of two-coupled pendulums, where the natural oscillation frequency of each pendulum corresponds to the frequency of the excited mode, and the coupling string α corresponds to the dipolar coupling. The two natural modes of oscillation are:

$$\omega_{in} = \omega_0 \quad (5)$$

$$\omega_{out} = \omega_0 \sqrt{1 + 2\alpha/\omega_0^2}, \quad (6)$$

which are the *in-phase mode* and the *out-of-phase mode*, respectively. In the dipolar drag effect when the center-of-mass mode is excited, ω_{in} is the frequency of the trap in the direction of the initial displacement (Kohn's theorem).

The previous result can be generalized to n coupled pendulums. The eigenvalues of the problem are:

$$\omega_{ev} = \omega_0 \sqrt{1 + (2 + \gamma)\alpha/\omega_0^2}. \quad (7)$$

And the parameter γ can be found by solving the following equation [13]:

$$(1 + \gamma)^2 \xi(\gamma, n - 2) - 2(1 + \gamma) \xi(\gamma, n - 3) + \xi(\gamma, n - 4) = 0, \quad (8)$$

where

$$\xi(\gamma, n) = (-1)^n \frac{\sinh((n + 1)\Omega(\gamma))}{\sinh \Omega(\gamma)}, \quad \text{with } \Omega(\gamma) = \text{arccosh}\left(-\frac{\gamma}{2}\right). \quad (9)$$

The parameter α , depends on the dipole moment d , the distance between the two condensates $2x_c$ and their density gradient. Whereas the first two parameters are easily tunable, the latter is more difficult to control (in spite of the fact that it can be changed by varying all the parameters). Therefore, these two parameters and the frequency of the excited mode will detune the shift of the *out-of-phase mode* frequency ω_{out} [8].

3.2. Numerical results

In order to observe this effect we have to consider the following:

- The perturbation must be in a transversal direction of the pancake-shaped dBEC, because the confinement in the longitudinal direction (ω_x) is so tight that leads to a small frequency shift (6).

- The dipole orientation shall be in the x -direction, otherwise, the dipolar interaction favors the interaction between the particles of the same condensate rather than the coupling with the other condensate.
- The scattering length a has to be small to ensure that the dBEC is dominated by the dipolar interaction. In this work, $a = 0.001 a_B$, where $a_B = 5.2918 \cdot 10^{-11}$ m is the Bohr radius. It is important to remind that experimentally the scattering length can be tuned by means of Feshbach resonances: by applying a magnetic field, for certain values, the scattering length suffers a resonant behaviour, taking values that go over $-\infty$ to $+\infty$, giving us the possibility to carelessly tune a in our simulations.

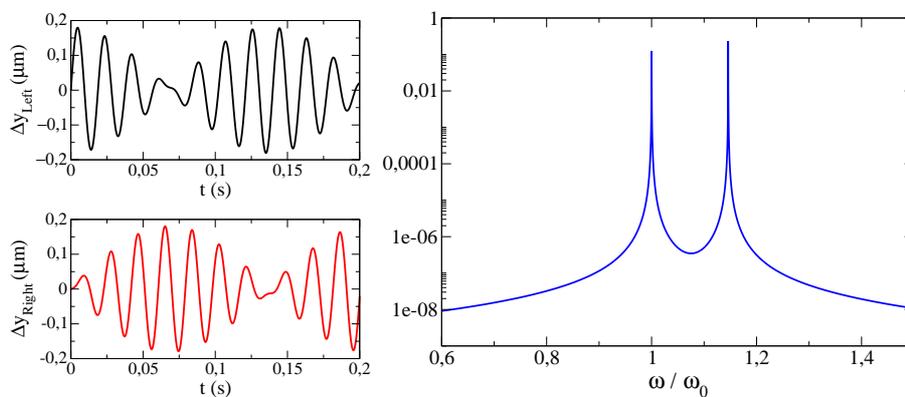


Figure 2. Left: Displacements of the centers of mass of the left (above) and right (below) condensate with the value of $d/\mu_B = 10$, where $\mu_B = 9.274 \cdot 10^{-24}$ J/T is the Bohr magneton. Right: Fourier transform (logarithmic scale) of the displacement of the center of mass of both condensates. The first peak corresponds to $\omega_0 = 50 \text{ Hz} \times 2\pi = 314.16 \text{ Hz}$, whereas the second one is $\omega_{out} = \omega_0 \sqrt{1 + 2\alpha/\omega_0^2}$. The strength is plotted in arbitrary units.

The numerical process can be resumed by three steps:

- (i) By using the Imaginary time step method, we find the stationary solution to reach the ground state of the system, which has the form $\Psi(\vec{r}, t) = \Psi_{GS}(\vec{r}) \exp(-i\mu t/\hbar)$, where μ is the chemical potential.
- (ii) Then, we add a momentum to the wavefunction of the left condensate displacing it out of its ground state, with the transformation (in the region $x < 0$):

$$\Psi(\vec{r}, 0) \rightarrow \Psi_{GS}(\vec{r}) e^{i\lambda y}, \quad (10)$$

where λ quantifies the magnitude of the perturbation. We remind that the kick must be in a transversal direction of the pancake, where the BEC is less confined.

- (iii) The excited new wavefunction is evolved in time by solving Eq.(3) using the Hamming's method (predictor-modifier-corrector).

In Fig. 2 we show the displacements of the centers of mass of both condensates and the corresponding Fourier analysis. One can see that the right dBEC starts to oscillate

due to the dipolar coupling. The beating of the oscillations comes from the presence of the two normal modes of the coupled system. The frequencies are obtained by Fourier analysis, the lower frequency corresponds to the *in-phase mode* (5) and the second peak is the *out-of-phase mode* which is slightly shifted from the excitation frequency ω_0 (6).

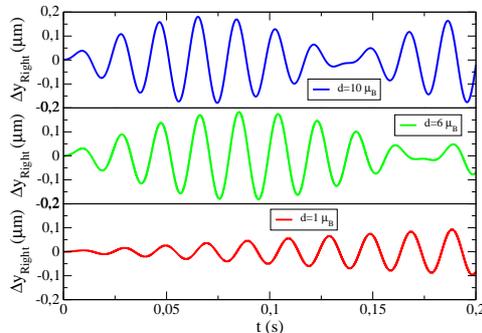


Figure 3. Displacement of the center of mass of the condensate of the right for different dipole moments. From top to bottom, $d = 10 \mu_B$, $d = 6 \mu_B$ and $d = 1 \mu_B$.

In Fig. 3, we show the displacement of the center of mass of the right dBEC for different values of d : the frequency shift is larger and the time response is smaller when the dipole moment increases. We have used the values: $d/\mu_B = 1; 6$ and 10 .

4. Beyond dipolar excitations

As an extension, we have studied the propagation of other collective excitations in the same system (for $d = 10\mu_B$), in particular, the monopolar excitation (breathing mode) and quadrupolar ones ($2x^2 - y^2 - z^2$, yz , xy).

In order to know the frequency of the collective mode for a single dBEC, one can use the following equations obtained for contact interaction [10, 14]:

$$\omega^2(m = 0) = \omega_0^2 \left(2 + \frac{3}{2}\beta^2 \mp \frac{1}{2}\sqrt{9\beta^4 - 16\beta^2 + 16} \right) \quad (11)$$

$$\omega^2(m = \pm l) = l\omega_0^2 \quad (12)$$

$$\omega^2(m = \pm(l - 1)) = (l - 1)\omega_0^2 + \omega_x^2, \quad (13)$$

where $\beta = \omega_x/\omega_0$ is the anisotropy of the BEC (in our case $\beta = 30$), $l = 1$ for center-of-mass modes, and $l = 2$ for quadrupolar ones. The case $m = 0$ refers the monopolar mode, which has to be dealt separately. Since we consider a pancake-shaped condensate with large β , we will see that not all these frequencies will be excited in our simulations neither even all these modes are totally decoupled.

For a dBEC the frequencies of the collective modes are slightly shifted with respect to the contact interacting ones (11-13)

4.1. Monopolar excitations

As regards the monopolar excitation, when $\beta \gg 1$, from (11) there are two frequencies with $m = 0$:

$$\omega_1 = \sqrt{10/3} \omega_0 \approx 1.83 \omega_0 \quad (14)$$

$$\omega_2 = \sqrt{3} \omega_x. \quad (15)$$

Although these results have been obtained for contact interaction, in presence of dipolar interaction, the values are slightly shifted [3, 4]. To quantify this shift, we have studied the monopolar response of a single dBEC with $\beta = 30$, by solving the TDGPE and we have found $\omega_1 = 1.9 \omega_0$, which is slightly shifted from the purely contact interacting value (14).

Now we study the propagation of the monopolar excitation between two non-overlapping dBECs. The perturbation corresponding to the monopolar excitation (breathing mode) is the following one (only applied on the left condensate):

$$\Psi(\vec{r}, 0) \rightarrow \Psi_{GS}(\vec{r}) e^{i\lambda(x^2+y^2+z^2)}. \quad (16)$$

Evolving now this wavefunction in time by solving the TDGPE, we find similar results to the dipolar drag case, but with different frequencies (Fig. 4). In other words, only the low-lying energy frequency (ω_1) and its corresponding shifted frequency are excited. In comparison with the dipolar drag effect, the magnitude of the shift in both cases is similar. Therefore, we see one frequency at $\omega = 1.9 \omega_0$ and its corresponding shifted frequency, showing that the coupled-pendulum model can be extended also for monopolar modes.

4.2. Quadrupolar excitations

The frequencies corresponding to quadrupolar excitations in a pure contact interacting BEC are (12,13):

$$\omega_1 = \sqrt{2} \omega_0 \quad (17)$$

$$\omega_2 = \omega_x. \quad (18)$$

Three kind of quadrupolar excitations are implemented in the perturbation of the wavefunction, $2x^2 - y^2 - z^2$ (also known as quadrupolar), xy and yz respectively:

$$\Psi(\vec{r}, 0) \rightarrow \Psi_{GS}(\vec{r}) e^{i\lambda(2x^2-y^2-z^2)} \quad (19)$$

$$\Psi(\vec{r}, 0) \rightarrow \Psi_{GS}(\vec{r}) e^{i\lambda xy} \quad (20)$$

$$\Psi(\vec{r}, 0) \rightarrow \Psi_{GS}(\vec{r}) e^{i\lambda yz}. \quad (21)$$

Looking at the results of the time evolution (Fig. 4), those of the $2x^2 - y^2 - z^2$ excitation leads to a surprise, owing to the fact that it is shockingly similar to the results obtained for monopolar excitations. The reason for this similarity is that in a pancake

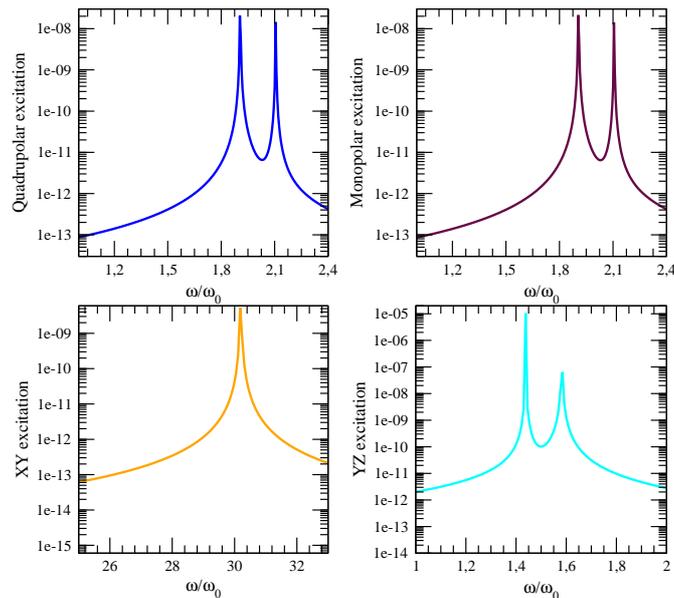


Figure 4. Fourier transform of the monopolar and quadrupolar responses ($2x^2 - y^2 - z^2$, xy and yz). The strength is in logarithmic scale and arbitrary units.

geometry, with large β , the quadrupolar excitation degenerates to the monopolar one because the x -component of the perturbation gets almost inhibited due to the strong confinement. The frequencies obtained are the same for both cases.

In contrast, it is not the case for the xy and yz excitation, as can be seen in Fig.4. The former excites only the $\omega_2 = \omega_x$ frequency, whereas the latter excites $\omega_1 = 1.45\omega_0$, and a second shifted frequency. The responsible of these differences is the kind of excitation. The xy excitation only has one term, which depends on x . It means that the relevant frequency in the trap will be ω_x . However, since the dBEC is tightly confined in the x -direction, the corresponding shift due to the dipolar coupling cannot be resolved.

As regards the yz excitation, since the perturbation does not affect the x -direction, the frequency excited will be that of lower energy. In the numerical results we obtain one peak in the spectrum at $\omega_1 = 1.45\omega_0$, and, in addition, a second frequency due to the dipolar interaction will appear in this case because the frequency of the trap in the transversal direction is small.

By symmetry and geometry, xz excitation is analogous to the xy excitation, and $y^2 - z^2$ will be also analogous to the yz excitation. In a pancake geometry, one can recover one or the other simply rotating the coordinate system.

5. Dipolar drag effect in a triple-well configuration

Let us extend the dipolar drag effect to the case, now, of a triple-well trap. Some studies have been carried out in triple-well configurations related with dipolar effects [15], phase diagrams [6] or symmetry breaking [7]. In the classical analogy of three

coupled-pendulums (7-9), the eigenvalues of the problem are:

$$\omega_{in} = \omega_0 \quad (22)$$

$$\omega_{out,1} = \omega_0 \sqrt{1 + \alpha/\omega_0^2} \quad (23)$$

$$\omega_{out,2} = \omega_0 \sqrt{1 + 3\alpha/\omega_0^2}. \quad (24)$$

Although there are three eigenmodes, it is possible to excite only two frequencies by choosing the appropriate initial conditions. If we perturb only the condensate of the center, looking to the eigenvectors of the problem, only the two frequencies that preserve the symmetry of the system, ω_{in} and $\omega_{out,2}$, will appear in the movement of the center of mass (the other frequency corresponds to a non-symmetric mode).

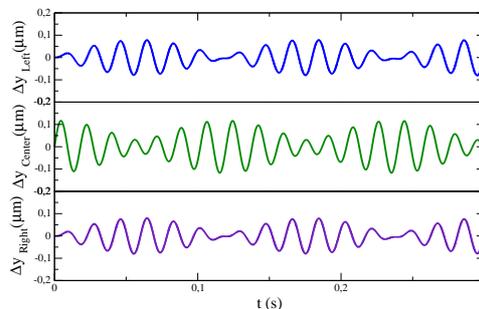


Figure 5. Displacements of the centers of mass of the three different condensates in the triple-well configuration, when we perturb only the condensate of the center. From top to bottom, condensate of the left, center and right.

In Fig. 5, we present the numerical results obtained by solving the TDGPE exciting only the center-of-mass mode of the centered dBEC. As expected, only two frequencies are involved in the movement of the three non-overlapping dBECs. We have obtained the corresponding frequencies by Fourier analysis and have compared them with the case of only two dBECs:

$$\frac{(\omega_{out,2}^2 - \omega_0^2)_{3well}}{(\omega_{out}^2 - \omega_0^2)_{2well}} \approx 1.6. \quad (25)$$

It is very close to the value of the ratio 1.5 obtained in the classical analogy. This means that the classical coupled-pendulum model yields a qualitative description of the dipolar coupling between few non-overlapping dBECs. Another remarkable fact is that, indeed, the magnitude of the shift is increased for three condensates compared with the case of two.

In Fig. 6, we show the displacements of the centers of mass when only the left condensate is perturbed. All three frequencies appear in the movement, and, as a consequence, the displacements of the centers of mass have a more complex behaviour.

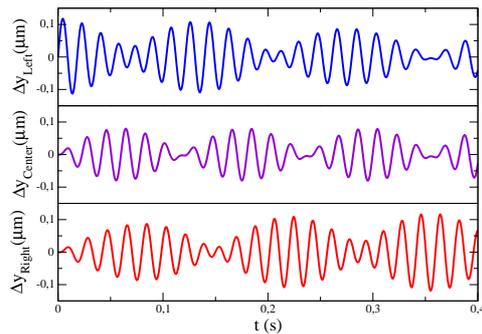


Figure 6. Displacements of the centers of mass of the three condensates in a triplewell configuration when we excite only the condensate of the left. From top to bottom, condensate of the left, center and right.

6. Summary and conclusions

In the present work, the full 3D-TDGPE has been numerically solved to study the long-range character of the dipolar interaction. We have investigated the propagation of collective modes, such as dipolar and quadrupolar excitations, between non-overlapping pancake-shaped dBECs. A classical coupled-pendulum model has been proposed.

We have analyzed the effect of different parameters in the propagation of the excitations. The dipole moment enhances the dipolar effects, whereas the enlargement of the scattering length and the distance between condensates leads the system to be dominated by the contact interaction which hides the desired long range effects.

New lines of research can be opened by studying dipolar coupling in other configurations: different dipole orientations or in cigar-shaped dBECs. Long-range effects of the dipolar interaction can be studied also beyond mean-field framework.

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