Mean-field description of dipolar bosons in triple-well potentials

D Peter\textsuperscript{1,2}, K Pawłowski\textsuperscript{1,3}, T Pfa\textsuperscript{1} and K Rzażewski\textsuperscript{1,3,4}

\textsuperscript{1} 5. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany
\textsuperscript{2} Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany
\textsuperscript{3} Center for Theoretical Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland
\textsuperscript{4} Faculty of Mathematics and Sciences, Cardinal Stefan Wyszyński University, ul. Dewajtis 5, 01-815, Warsaw, Poland

E-mail: peter@itp3.uni-stuttgart.de

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Abstract

We investigate the ground-state properties of a polarized dipolar Bose–Einstein condensate trapped in a triple-well potential. By solving the dipolar Gross–Pitaevskii equation numerically for different geometries we identify states which reveal the non-local character of the interaction. Depending on the strength of the contact and dipolar interaction we depict the stable and unstable regions in parameter space.

1. Introduction

The physics of cold atoms in optical lattices is an active field of research in both experiment and theory [1–5]. Interaction between the atoms and tunnelling across the lattice is easily controlled using Feshbach resonances and by tuning the intensity of the external lasers, respectively. Already in one of the first experimental realizations of the system a quantum phase transition between a Mott insulator and a superfluid has been shown [3]. Together with the ultra-precise spatial resolution [6, 7], this system is a good candidate for quantum simulators [8] or, in the far future, even an element of a new generation of computers [9].

The search for new phases is ongoing and dipolar interactions present additional possibilities [10–12]. The major feature of the dipolar interaction is its long-range character. Thus, the new phases are expected to reveal inter-site effects even in the case of suppressed tunnelling. The first indication of such a phenomenon has already been shown in the dynamical properties of a Bose–Einstein condensation of very weakly interacting \textsuperscript{39}K [13] and in the study of the stability of \textsuperscript{52}Cr, loaded in a 1D optical lattice [14]. Furthermore, the anisotropy of the dipolar interaction allows us to control both inter- and on-site interactions by choosing the appropriate geometry of the lattice sites with respect to the polarization direction of the dipoles [15]. The easiest model systems consist of a few linked wells. In particular, the double-well system has received a lot of attention [16, 17]. As the entanglement between the two macroscopically occupied modes has been demonstrated, it may be considered as an extension of a qubit [18, 19]. On the other hand, many interesting effects, including Josephson oscillations and quantum self-trapping, were observed in the frame of the mean-field approximation [20].

In a recent discussion, the triple-well potential, loaded with a dipolar gas, was studied [21]. An extended Bose–Hubbard model is used to describe the system, as in most related references concerning optical lattices [10, 22, 23]. This model assumes fixed, occupation-independent parameters. For increasing particle numbers and interaction strength, this approximation is less reliable. Due to the interaction, the on-site spatial distribution of the atoms shrinks in the case of an attractive gas and broadens if the interactions are repulsive. The most dramatic case occurs for a dipolar gas when the number of atoms or the strength of interaction is above a critical value. The sample collapses and then explodes in a so-called Bose–Nova [24]. As the shape of the atomic cloud changes with the interaction, the parameters of the Bose–Hubbard model cannot be uniquely defined. In this paper, we study the triple-well case using a mean-field approach. Within this picture, the ground states for different geometries and interaction strength are discussed. We consider experimentally relevant parameters, especially for magnetic dipolar gases like Cr or Dy.
The paper is organized as follows. In section 2, we describe both the Bose–Hubbard model and the mean-field approach for a dipolar gas in an external triple-well potential, which is modelled by overlapping Gaussian wells. We discuss the limitations of the Bose–Hubbard approach and then switch to the mean-field picture. An important new aspect arises. Depending on the geometry and the interaction parameters, the ground-state solution may be unstable. In section 3, we present a phase diagram for two specifically chosen geometries. The ground-state solution may be unstable. In section 3, we present a phase diagram for two specifically chosen geometries. The remaining part of parameter space and contact-interacting origin whereas the inter-site couplings $U_1, U_2$ only depend on the dipolar interaction, as the density–density overlap is negligible. For point-like, tightly localized wavefunctions $\phi$, the inter-site couplings satisfy $U_2 = U_1/2^3$ as the dipolar interaction falls off like $r^{-3}$. The resulting forms, however, are also valid for extended wavefunctions and $U_2 = U_1/\alpha$ with $4 \leq \alpha \leq 8$.

In the special case of $J = 0$ the model can be solved analytically and four distinct phases appear [21]. We quickly review them here to compare with our results. For $U_0 > 0$ and $U_1/|U_0| \leq 8/15$ as well as for $U_0 < 0$ and $U_1/|U_0| < -8$, the phase A is present with

$$n_1 = n_3 = \left\lfloor \frac{8(U_0 - U_1)}{24U_0 - 31U_1}N \right\rfloor$$

where $\lfloor \cdot \rfloor$ denotes the integer part. The other three phases are described by a single fixed ground state. Phase B appears for $U_0 > 0$ and $8/15 < U_1/|U_0| < 8$ and is characterized by the ground state $n_1 = n_2 = N/2$. For $U_0 > 0$ and $U_1/|U_0| > 8$, as well as for $U_0 < 0$ and $U_1/|U_0| > -1$, phase C is present where all particles are occupying a single well. The central well is favoured if (weak) tunnelling is present and thus we describe this phase by $n_2 = N$. The remaining part of parameter space $U_0 < 0$, $-8 < U_1/|U_0| < -1$ is filled with phase D, having two degenerate states with $n_1 = n_2 = N/2$ or $n_1 = n_3 = N/2$.

2. System and model

We consider a Bose–Einstein condensate consisting of $N$ dipolar particles with a dipole moment $d$ which may be of either electric or magnetic origin. A strong external field is orienting the dipoles such that they all point in the same direction. The particles are subject to an external potential $V(r)$ with three (nearly) equivalent minima, see figure 1(a), which is modelled by three overlapping Gaussian wells:

$$V(r) = -V_0 \sum_{x=0,1,2} \exp \left(-\frac{2x^2}{w_x^2} - \frac{2y^2}{w_y^2} - \frac{2(z-s-1)^2}{w_z^2}\right).$$

The parameter $V_0$ determines the centre depth of the individual wells and the widths $w_i$ parametrize the geometry of a single well (size in each direction). The spacing between the wells is given by $l$. A potential like this can be created by means of Gaussian laser beams [21].

The particles are interacting via contact and dipolar interactions. The contact interaction is fully characterized by the scattering length $a$. The dipolar interaction between polarized dipoles at positions $r_1, r_2$ is given by

$$V_{dd}(r_1, r_2) = C_{dd} \left(\frac{1 - 3 \cos^2(\vartheta)}{r^3}\right),$$

where $r = |r| = |r_1 - r_2|$ is the inter-particle distance and $\vartheta$ is the angle between $r$ and the dipole moment $d$. The factor $C_{dd}$ is equal to $d^2/\mu_0/4\pi$ for magnetic, and $d^2/4\pi\epsilon_0$ for electric dipoles. In analogy to the scattering length one introduces the length scale $a_{dd} = mC_{dd}/3\hbar^2$, characterizing the strength of the dipolar interaction [25].

Throughout this work, we are using a dimensionless system by measuring all lengths in units of the spacing $l$, all energies in units of $\hbar^2/m l^2$ and time in units of $m l^2/\hbar$ ($m$ is the mass of the dipolar particles). We will keep the same notation for quantities with and without units, though.

2.1. Extended Bose–Hubbard model

Following the discussion in [21], we outline how a Bose–Hubbard model can be derived for the dipolar triple-well system. First we assume that the three minima of the potential are well separated, such that the on-site wavefunctions $\phi_i(r)$ for each site may be described by a single function: $\phi_i = \phi(r-r_i)$, with $r_i$ being the centre of the $i$th well. The field operator $\hat{\Psi}(r) = \sum_{i=1}^{N} \hat{a}_i \phi_i(r)$ can then be written in terms of the annihilation operators $\hat{a}_i$ at site $i$. Interpreting these operators as annihilating a particle at site $i$ is correct as long as the potential is deep enough such that the overlap between the wavefunctions of two adjacent sites is small. The Hamiltonian is then expressed in Bose–Hubbard form as

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U_0}{2} \sum_{i=1}^{N} \hat{n}_i (\hat{n}_i - 1) + U_1 (\hat{n}_1 \hat{n}_2 + \hat{n}_2 \hat{n}_3 + \hat{n}_3 \hat{n}_1),$$

where the number operators are defined as $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ and $(i, j)$ sums over neighbouring sites. The hopping rate is given by

$$J = - \int d^3r \phi_i^\dagger(r) \left(-\frac{1}{2} \nabla^2 + V(r)\right) \phi_{i+1}(r)$$

and the interaction is parametrized by the three parameters

$$U_k = \int d^3r \int d^3r' |\phi_i(r)|^2 |\phi_{i+1}(r')|^2 (4\pi a \delta(r-r'))$$

$$+ V_{dd}(r-r').$$

The on-site interaction $U_0$ includes parts of both dipolar and contact-interacting origin whereas the inter-site couplings $U_1, U_2$ only depend on the dipolar interaction, as the density–density overlap is negligible. For point-like, tightly localized wavefunctions $\phi$, the inter-site couplings satisfy $U_2 = U_1/2^3$ as the dipolar interaction falls off like $r^{-3}$. The following results, however, are also valid for extended wavefunctions and $U_2 = U_1/\alpha$ with $4 \leq \alpha \leq 8$.

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2.2. Restrictions of the Bose–Hubbard model

There are two main issues with the Bose–Hubbard approach that we will address in this section. Both restrictions arise from the assumption that a ground-state wavefunction $\phi$ exists which does not depend on the number of particles and the interaction strength.

The Bose–Hubbard method intrinsically leads to a stable ground-state solution as this is a premise of the model. This assumption, however, does not hold true in general for interacting quantum gases. As we would like to describe both repulsive and attractive interactions, this problem is of relevance in our system. The stability issue will be discussed in section 2.4.
The second assumption is that the parameters \( J \) and \( U_0 \), which are calculated by means of the single-particle wavefunction \( \phi \), are constant for all particle numbers \( N \). This approximation is certainly good for small particle numbers and small values of \( a/a_{ho} \). We demonstrate, however, that it is not well suited in our case.

For simplicity, we consider a purely contact-interacting Bose–Einstein condensate of \( N \) particles in a spherically symmetric harmonic well with frequency \( \omega \). We calculate the interaction energy as a function of \( a/a_{ho}N \), where \( a_{ho} = \sqrt{\hbar/m\omega} \) is the harmonic oscillator length. The Bose–Hubbard approach suggests a quadratic scaling \( E_{\text{int}} = U_0/2N(N-1) \) with the number of particles.

For \( a/a_{ho}N \ll 1 \), this relation is a valid approximation, see figure 2. However, we have in mind a system of at least 100 atoms with a typical scattering length of \( a \approx 5 \) nm and traps with a width of \( a_{ho} \approx 500 \) nm. The resulting factor of \( a/a_{ho}N \approx 1 \) is just in the crossover region of the diagram. For this value, the interaction energy calculated by the quadratic term is already 35% off, compared to the numerical simulation. The extension to dipolar interacting gases is further increasing the problem. Inter-site repulsion or attraction can lead to changes of the neighbouring on-site wavefunctions.

2.3. Mean-field approach

For reasons being apparent now, we will use an alternative approach and describe the system in a mean-field picture. We stress that this approach requires, contrarily to the Bose–Hubbard model, that the particle number \( N \gg 1 \). The Gross–Pitaevskii equation for our system is given by [26]

\[
\frac{\hbar}{2} \frac{\partial}{\partial t} \Psi(r, t) = \left[ -\frac{1}{2} \nabla^2 + V(r) + 4\pi a(N-1)|\Psi|^2 + \Phi_{dd}(r, t) \right] \Psi(r, t),
\]

where we have introduced the condensate wavefunction \( \Psi(r, t) \) which we normalize to unity. The dipolar interactions are included by the mean-field potential

\[
\Phi_{dd}(r, t) = 3a_{dd}N \int d^3r' \frac{1 - 3 \cos^2(\vartheta)}{|r - r'|^3} |\Psi(r', t)|^2.
\]

We find the ground state of equation (7) by imaginary time evolution on a 3D grid [27]. The dipolar interaction part is efficiently computed in momentum space by means of fast Fourier transformations, as the mean-field potential \( \Phi_{dd} \) has the form of a convolution.

Although both the Bose–Hubbard Hamiltonian and the Gross–Pitaevskii equation are derived from the same multi-particle Hamiltonian in second quantized form there is no direct link between the two models. This implies that there can be no relation between \( a, a_{dd}, N \) and the Bose–Hubbard parameters \( U_0, U_1 \) since the latter depend on \( \Psi \) which is not fixed in the mean-field approach.

Figure 1. (a) Cut of the triple-well potential along the symmetry axis. It is modelled by three overlapping Gaussians of width \( w \). (b) Repulsive and (c) attractive configuration of the dipoles.

Figure 2. Interaction energy of a contact-interacting gas in a harmonic trap, compared to the energy term \( U_0/2 \cdot N(N-1) \) of the Bose–Hubbard model. The quadratic scaling is only reasonable for \( a/a_{ho} \ll 1 \). The strongly interacting regime is well described by the Thomas–Fermi approximation.

\[
E_{\text{int}} / U_0/2N(N-1) \times 10^2 \times a/a_{ho}N^{-1}
\]

- Bose–Hubbard scaling
- Thomas–Fermi approximation
- Numerical simulation

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2.4. Stability

Dipolar quantum gases have a complex stability behaviour [25] which leads to some peculiariities when treating them numerically. Typically, a critical scattering length $a_{\text{crit}}$ can be defined, which depends on the geometry of the external potential and the strength of the dipolar interaction [25].

For all scattering lengths $a < a_{\text{crit}}$ the system is unstable and no ground state can be found. The crossing of the stability threshold leads to a collapse of the condensate wavefunction which can easily be identified in the simulation. The collapse in a single harmonic trap has been studied in detail [25]. Above the critical value of the scattering length, a stable solution can be found for any $a > a_{\text{crit}}$.

As we are going to trace out the stability threshold of the triple-well configuration we need to assure that the simulation is not crossing any unstable regions during the imaginary time evolution. We proceed as follows. The simulation is set up with an initial Gaussian wavefunction which spreads over all wells. The spreading is such that the width in the $z$-direction is equal to the spacing between the wells to assure a certain fraction of particles in each well. We stress that the final state does not depend on the chosen initial wavefunction. The Gaussian can even be placed asymmetrically over one of the outer wells and the imaginary time evolution still yields the same (symmetric) ground state.

In the first sequence of imaginary time evolution all interactions are set to zero ($a = a_{\text{dd}} = 0$) and we reach the ground state for the non-interacting case, see figure 3 for $a_{\text{dd}} = 0$. This is our starting point to reach any point in the parameter space. The diagrams in figures 4 and 5 are scanned line by line from right to left. We start at a high scattering length $a$ with $a_{\text{dd}}$ still set to zero to assure that we are in the stable region. After the ground state for the contact-interacting case is reached we select the final value of $a_{\text{dd}}$ and probe one horizontal line in the diagram by subsequent runs of imaginary time evolution while decreasing $a$ until the wavefunction collapses to basically one grid point. At this point, the simulation has reached the critical scattering length $a_{\text{crit}}$.

2.5. Geometry

Performing the numerical simulations, we have to choose a fixed geometry and strength for the external potential, like the widths of a single well in all spacial directions $w_x, w_y, w_z$ and the depth of the potential $V_0$. We reduce the parameter space by choosing reasonable values for the parameters, having symmetries as well as physical limitations in mind.

The width in the $z$-direction is restricted, as the different wells are not clearly distinct for $w_z \gg 1/2$ (remember that we are measuring lengths in units of the spacing between two wells). Oppositely, for $w_z \ll 1/2$ the tunnelling is too low to reach the ground state of the system with imaginary time evolution (or in an experiment). In the simulations, we will therefore set $w_z$ to a value of $1/2$. We ask for two conditions to fix the values for the two remaining widths $w_x$ and $w_y$. As we focus especially on inter-site effects, changing the polarization direction (from an attractive inter-site coupling to a repulsive one) should not change the on-site effects\(^5\). To satisfy this requirement, the width in one of the directions perpendicular to $z$ has to be equal to $w_z$. Without loss of generality, we define $x$ to be the polarization direction for the ‘repulsive geometry’ ($z$ for the ‘attractive’ case). Therefore, we need to set $w_x = w_y$.

The second condition concerns the stability. To see a large variety of states we want the stability of a single well to be higher than in the spherical case (lower critical scattering length $a_{\text{crit}}$ for the same $a_{\text{dd}}$). To fulfill this, the remaining width $w_y$ has to be larger than the other two [28]. This leads us to cigar-shaped traps which are placed side by side, as shown in figures 1(b) and (c). We fix the trap aspect ratio to a value of $\omega_z/\omega_x = 1/8$ as this turns out to be a reasonable value for an experiment, too. We stress that simulations with different aspect ratios $\alpha_z/\alpha_x < 1$ do not show a qualitatively different behaviour.

For the depth of the potential there are also certain limitations. If $V_0$ is too low, the potential is not able to trap the particles. If it is too large, the tunnelling rate is suppressed (see above). It turns out that $V_0 = 80$ is a reasonable value which allows for a large diversity of ground states. Again, additional simulations show that the behaviour is not sensitive to the precise value of this parameter, even quantitatively.

2.6. Interaction

We simulate the dimensionless Gross–Pitaevskii equation (7). As all parameters of the external potential are fixed, there are only two free quantities. These are the values of the contact and dipolar interaction strength given by the dimensionless products $aN$ and $a_{\text{dd}}N$. Note that it is not necessary to change the number of particles $N$ independently. In the following, we will present simulations where we change both $aN$ and $a_{\text{dd}}N$ to scan the remaining parameter space. Note also that in our dimensionless units the values of $a$ and $a_{\text{dd}}$ depend on the spacing between two lattice sites.

3. Results

To analyse the structure of the states we plot the ratio $n = (n_1 + n_3)/N$ in analogy to [21]. In the simulation, we calculate the occupation numbers $n_i$ by integrating the density $n(r)$ over the volume of the $i$th well. We have divided the whole volume of the simulation into three parts such that $\sum n_i = N$.

As we have a finite tunnelling rate due to the finite potential depth and spacing, the states found with the mean-field calculations are always symmetric ($n_1 = n_3$) with respect to the central well. The two asymmetric states in the D phase found in the Bose–Hubbard approach are only present for tunnelling $J = 0$. For $J > 0$, the symmetric and anti-symmetric combination of both states split in energy and yield a symmetric density distribution.

Let us first discuss the non-interacting ground state of the triple-well system. In a simple 3-mode approach we can

\(^5\) There might be changes in the on-site energy due to second-order effects: if the changed inter-site coupling leads to a different shape of the on-site wavefunction. Strictly speaking, this condition can only be fulfilled for a single well.
Figure 3. Purely dipolar states for $a = 0$ and different values of $a_{dd}N$ in the repulsive case. Particles move to the outer wells as the dipolar inter-site repulsion grows.

Figure 4. The quantity $n = (n_1 + n_3)/N$ is plotted for the geometry with repulsive inter-site interactions, see figure 1(b). (a) Black coloured areas indicate regions of instability where no ground state could be found. For the purely contact-interacting case ($a_{dd} = 0$, $a > 0$), we find an equally populated state with $n_1 = n_3 = n_2$ for $a = -2N/3$ (white). (b) Horizontal cuts through the phase diagram on the left are shown for different values of $a_{dd}N$, as indicated by the labels. The behaviour changes qualitatively around the threshold value $a_{dd}N \approx 0.3$. Note that only a narrow region of the phase diagram is shown in the cuts.

use localized wavefunctions $\Psi_i = \sqrt{n_i/N}\phi_i$, centred at the $i$th well, as defined in section 2.1. If the ground-state energy of a single well is $E_0$ and the overlap integral for neighbouring wells is $J$, we have to diagonalize

$$H = \begin{pmatrix} E_0 & -J & 0 \\ -J & E_0 & -J \\ 0 & -J & E_0 \end{pmatrix},$$

from which we immediately find the ground state $(1/2, 1/\sqrt{2}, 1/2)$ with occupation numbers $n_2 = N/2$ and $n_1 = n_3 = N/4$, giving a ratio of $n = 1/2$. Close to the origin of the diagrams in figure 4 we find indeed states with $n \approx 1/2$ (see also figure 3 for $a_{dd}N = 0$). Note that the non-interacting ground state in the Bose–Hubbard model for $U_k = 0$ is given by

$$\left(\hat{a}_1^+/\sqrt{2} + \hat{a}_2^+ + \hat{a}_3^+/\sqrt{2}\right)^N(000)$$

which also yields $\langle n_2 \rangle = N/2$ and $\langle n_1 \rangle = \langle n_3 \rangle = N/4$.

Adding a repulsive contact interaction leads to a flattening of the density profile in the sense that we expect to have a uniform distribution $n_1 = n_2 = n_3 = N/3$ (or a ratio of $n = 2/3$) for large scattering lengths. For $a_{dd} = 0$, we observe states with $0 \leq n \leq 2/3$. Every state with a ratio $n > 2/3$ is thus a clear indication of the dipolar inter-site effects.

3.1. Repulsive inter-site interactions

Figure 4 shows an overview of the states found by imaginary time evolution for the geometry with repulsive inter-site interactions. We find the whole spectrum $0 < n < 1$. Once $n$ approaches the value of 0 or 1, the states become unstable. In particular, we observe ground states with a ratio of $n > 2/3$, implying that there are fewer particles in the middle well than in the outer ones ($n_2 < n_1 = n_3$), a clear indication of the inter-site repulsion. States with $n \approx 0$ appear even in the purely contact-interacting case for $a_{dd}N = 0$, see figure 4(b), and are therefore less suited to demonstrate the long-range nature of the interaction. The on-site attraction for negative $a$ is enough to concentrate the atoms in the central well until the condensate finally collapses for $aN \approx -0.055$.

Figure 4(b) also reveals that a threshold value exists at $a_{dd}N \approx 0.3$ with a sudden change of behaviour. For dipolar interactions weaker than this critical value, the ratio $n$ is always lower than $2/3$. This region is dominated by the on-site interactions. For decreasing contact interaction the ratio smoothly approaches $n \approx 0$ and finally collapses. Contrarily, for an interaction strength larger than $a_{dd}N \approx 0.3$, the ratio $n$ increases when lowering the scattering length until it finally reaches $n \approx 1$ and collapses. The behaviour of the border, separating stable from unstable regions, is also different below and above the threshold. Below, the instability is triggered by
in both parts are solely caused by inter-site effects. A flipped repulsive case (upper part) and the attractive case (lower part, instabilities, states with Black colour again indicates unstable regions. Close to the geometry with attractive inter-site interactions, see figure 1(c). The system gets more stable for higher values of $a$. Figure 5. (a) The quantity $n = (n_1 + n_2)/N$ is plotted for the geometry with attractive inter-site interactions, see figure 1(c). Black colour again indicates unstable regions. Close to the instability, states with $n \approx 0.5$ form which resemble the non-interacting ground state. (b) Combined plot which shows the repulsive case (upper part) and the attractive case (lower part, flipped $a$ axis). Both situations match exactly if $a_{dd} = 0$ but also for larger $a_{dd}$ the plot combines to a consistent picture. Differences in both parts are solely caused by inter-site effects.

a collapse in the middle well as it holds most of the particles. The system gets more stable for higher values of $a_{dd}N$ (critical scattering length decreases with growing dipolar interaction). Above the threshold, the instability is caused by the particle flow to the outer wells which finally leads to a collapse in either the left or the right well. This is a clear signature of the inter-site effects. In this regime, the system gets less stable for growing dipolar strength ($a_{crit}$ increases for growing dipolar interaction). We remark that the threshold value is not depending on the aspect ratio of the single wells but changes with the depth of the potential.

3.2. Attractive inter-site energy

Figure 5(a) shows an overview of the states for the geometry with attractive inter-site interactions. We can immediately see that the inter-site attraction is destabilizing the system as it has a larger $a_{crit}$ for most values of $a_{dd}$. We observe the whole spectrum of ratios $n$ between the equally populated state with $n = 2/3$ and $n = 0$. Approaching the value of $n = 0$, the states become unstable. In this situation, the collapse is again initiated in the middle well. As we do not observe any states with $n$ outside the range $0 \leq n \leq 2/3$, the attractive geometry is not suited to demonstrate the inter-site effects doubtlessly.

3.3. Combined picture

Figure 5(b) shows a combined plot of both cases (repulsive and attractive inter-site interaction). For $a_{dd} = 0$, both situations are identical. Differences in the upper and lower parts are solely caused by inter-site effects, as the geometry of the triple-well potential was designed in such a way (the on-site energy does not change when rotating the polarization direction).

We now compare our findings to the results of the Bose–Hubbard approach. Within the mean-field theory and our numerical simulations we observe the counterparts of all states of phase A, as well as states close to those of the phases B and C. For phase D with its two degenerate states $n_1 = n_2 = N/2$ and $n_2 = n_3 = N/2$, the comparison is a bit subtle. The mean ratio of both states is $n = 1/2$, which can be seen in the simulations. However, these states are related to the non-interacting state which also has $n = 1/2$. The mean-field approach is unable to distinguish both cases and finds only the symmetric states.

As we do not observe extended regions in the phase diagram with $n = 0$ or $n = 1$, we conclude that the regions which correspond to the phases B, C and D are unstable; an aspect which is not observable in the Bose–Hubbard approach. We remark, however, that the presented theory is only valid for large particle numbers. For small samples with few particles, the Bose–Hubbard approach is well justified and stable phases should appear.

Even in the absence of extended phases, the clear indication of inter-site effects is still visible. In particular, the ground states with $n > 2/3$ above the threshold value at $a_{dd}N \approx 0.3$ do not appear for purely contact-interacting condensates and should therefore be considered as a strong evidence for dipolar inter-site interactions.

Finally, we justify the range of values used for the parameters $aN$ and $a_{dd}N$. We recall that the unit of length we use is the spacing between two wells. We adopt the suggested experimental parameters of $[21]$ where a spacing of $l = 1.7 \mu m$ is used. For 2000 $^{52}$Cr atoms with a dipolar length of $a_{dd} \approx 0.79$ nm, the (dimensionless) value of $a_{dd}N \approx 0.93$ has the right order of magnitude. The scattering length $a \approx 5.8$ nm leads to the dimensionless value $aN \approx 6.8$. This value, however, can be tuned precisely by means of a Feshbach resonance $[29]$, thus allowing for the detection of the interesting states close to the border of instability. Smaller samples of atoms could still provide the necessary dipolar interaction strength when using different species like Dy with a dipolar length of $a_{dd} \approx 7.1$ nm $[30]$.

4. Conclusions

In this paper, we studied the properties of a dipolar quantum gas, loaded into a triple-well potential. Using the numerical solution of the non-local Gross–Pitaevskii equation, the phase diagram of the system has been obtained. In particular, we identified the range of parameters where the ground states reveal strong inter-site effects and we traced out the instable regions in the phase diagram. We find that ultra-cold gases of atoms with a high magnetic moment, like Cr or Dy, are suited to demonstrate these features. The presented ground states were compared to the results of the dipolar Bose–Hubbard model.

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