Localization–delocalization transition of dipolar bosons in a four-well potential

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Abstract

We study interacting dipolar atomic bosons in a four-well potential within a ring geometry and outline how a four-site Bose–Hubbard (BH) model including next–nearest–neighbor interaction terms can be derived for the above four-well system. We analyze the ground state of dipolar bosons by varying the strength of the (effective) interaction between particles in next–nearest-neighbor wells. We perform this analysis both numerically and analytically by reformulating the dipolar-boson model within the continuous variable picture applied in Buonsante et al (2011 Phys. Rev. A 84 061601(R)). By using this approach we show that when the (effective) next-nearest-neighbor interaction crosses a precise value of the on-site interaction, the ground state exhibits a change from the uniform state (pertaining to the delocalization regime) to a macroscopic two-pulse state, with strongly localized bosons (localization regime). These predictions are confirmed by the results obtained by diagonalizing numerically the four-site extended BH Hamiltonian.

Keywords: ultracold gases, trapped gases, interacting dipolar bosonic gases

1. Introduction

Dipolar quantum gases [1] confined in a multiple-well geometry are attracting growing attention [2–11] due to the considerably rich scenario of novel properties and effects that emerges from the interplay of anisotropic dipole–dipole (dd) interactions (coupling the magnetic/electric moments of dipolar bosons) with two-boson contact interactions and the interwell boson tunneling.

In this class of systems, special interest has been focused in the last decade on the simple model where bosons are trapped by a triple-well potential. This system, effectively described by a three-site extended Bose–Hubbard (EBH) model, combines the effect of long-range dipolar interactions [12, 13] with the nontrivial, highly nonlinear dynamics of BH models [14–16]. Note that the description by means of the BH model for bosons in multi-well systems is reliable within certain conditions on the number of particles and the strength of the dipolar interaction which has to not dominate the contact interaction [8, 9].

More specifically, in the presence of the open-chain geometry, the BH triple well has made evident the non-local character of dipolar interactions within the Josephson-like dynamics [6] (in the supplemental material of the latter reference, Lahaye and co-workers have considered a four-site square system to discuss the realization of interferometric arrangements) and the possibility to induce macroscopic interwell coherence independent from the tunneling parameter [7]. This system has revealed as well a complex ground-state phase diagram where unstable regimes can be controlled through the dipolar and contact interactions [8]. However, it is worth observing that this is true as long as the s-wave scattering length (which characterizes the contact interaction) is larger than a critical value depending on the geometry of the external potential and the strength of the dipolar interaction [10].

By adopting instead the ring geometry (closed chain with periodic boundary conditions) one finds that, in addition to translational invariant vortex-like states [17, 18] arising when the system includes only contact interactions, the presence of
dipolar interactions shows the formation of different density-wave states [11] and the possibility to observe the transition between them. Recently, the ground-state phase diagram of the closed BH triple well has been explored to show the influence of the possible anisotropy of dipolar interactions [12] while the coherent control of boson tunneling through dipolar interactions has been studied in the presence of high-frequency time-periodic local potentials [13]. In the recent paper [19] the ground-state properties of dipolar bosons trapped in a three-well potential have been investigated when the on-site interaction $U_0$ and the dipolar interaction $U_1$ are varied. The ring geometry assumed for this model has been used to show its complete equivalence with the symmetric three-site BH model. The nice result was that the term representing dipolar interactions can be absorbed in the on-site interaction term of the equivalent BH model whose strength has the form $U = U_0 - U_1$. This equivalence has allowed one to exploit the considerable amount of information about the low-energy properties of BH model to investigate the three-well dipolar model. In particular, by varying $U_0$ and $U_1$, the ground state of dipolar bosons has been found to involve dramatic changes of their space distribution which, within the equivalent BH picture, are caused by the change of the on-site interaction from attractive ($U < 0$) to repulsive ($U > 0$). The corresponding entanglement properties have been explored.

In this work, we consider interacting dipolar bosons at zero temperature confined in a four-well potential forming an equilateral triangle. The microscopic dynamics of this system is still described by a four-site EBH Hamiltonian which includes hopping processes through the amplitude $J$, and the on-site interactions through $U_0$. The novel aspect is that the presence of the fourth well totally changes the symmetry properties of the dipolar model due to the further coupling between non-adjacent sites. Then, in addition to the nearest-neighbor interaction $V_1$, the model includes the diagonal interaction $V_2$ between non-adjacent sites. We show that the use of the boson-number conservation leads to an equivalent EBH where removing nearest-neighbor interactions not only causes a new effective onsite interaction $U$, as in the three-site case, but also determines the occurrence of a new effective interaction $U_1 = V_1 - V_2$ between non-adjacent sites. Such interactions dramatically change the properties of the ground state.

To explore the new scenario we resort to the semi-quantum approach applied in several papers (see, e.g., [20–23]) which reduces the Schrödinger problem of many-boson models to a diagonalizable form. A ‘dual’ version of this method is also known which has been developed for spin models and applied to two-mode bosonic systems [24]. In the sequel, we refer to this method as the continuous variable picture (CVP). The latter allows one to derive a suitable set of equations describing the boson populations of low-energy states and to exploit their solution to reconstruct the low-energy eigenstates of the system. This diagonalization scheme has been successfully applied to highlight the inner mechanism governing the localization–delocalization transition characterizing the BH models with attractive interaction [23, 25]. Very recently, Li and Das Sarma have studied this kind of transition in a four site BH model in the presence of artificial magnetic fields [26].

Within the CVP framework the ground-state structure is predicted to exhibit a change when $U_1$ becomes larger than $U_0/2$. The regime characterized by the uniform-boson distribution (delocalization regime) transforms into a non-uniform distribution (localization regime) where the ground state features the almost complete boson-localization in two non-adjacent wells. The so predicted delocalization–localization transition is corroborated by the results deriving from the numerical diagonalization of the four-site BH Hamiltonian. Thanks to the numerical approach one observes that the delocalization regime corresponds to a Fock state with the bosons equally shared among the four wells. The localization regime corresponds, instead, to a symmetric superposition of two Fock states each one characterized by non-adjacent wells occupied by half of the total boson-population. It is interesting to observe that the emergence of the two-pulse state as ground state allows us to establish an immediate link with the mechanism responsible for the occurrence of the checkerboard-insulator in optical lattices (that, actually, can be regarded as multi-well systems) [27].

2. The model Hamiltonian

The model describing $N$ dipolar interacting bosons trapped by a potential $V_i(r)$ can be derived from the bosonic-field Hamiltonian

$$
\hat{H} = \int d^3r \hat{\Psi}^\dagger(r) H_0 \hat{\Psi}(r) + \frac{1}{2} \int d^3r d^3r' \hat{\Psi}^\dagger(r) \hat{\Phi}^\dagger(r') V(r-r') \hat{\Phi}(r') \hat{\Psi}(r),
$$

where $\hat{\Psi}(r)$ is the bosonic field, $H_0 = p^2/(2m) + V_i(r)$, $p = -i\hbar \nabla$, and $m$ is the boson mass. The trapping potential

$$
V_i(r) = \frac{m}{2} \omega_i^2 z_i^2 - V_0 \sum_{i=1}^4 \exp \left( -\frac{2(\vec{r}^2 - \vec{r}_i^2)}{w^2} \right),
$$

characterized by the trapping frequency $\omega_z$ in the axial direction, represents the superposition of a strong harmonic confinement along axis $z$ with $L$ (planar) potential wells placed at the equidistant sites $\vec{r}_i$ of a ring lattice. Width $w$ parametrizes the geometry of each well providing the size of each of these in the $x$–$y$ plane. In the presence of four potential wells the lattice is a square with side $\sqrt{2}L$ and vertices $\vec{r}_i = (\ell, 0) = -\vec{r}_\ell$ and $\vec{r}_0 = (0, \ell) = -\vec{r}_\ell$, $V_0$ is the depth of each well. The bosonic field $\hat{\Psi}(r)$ can be expanded in terms of the annihilation operators $\hat{a}_k$

$$
\hat{\Psi}(r) = \sum_{k=1}^4 \phi_k(r) \hat{a}_k,
$$

obeying the standard bosonic commutators $[\hat{a}_k, \hat{a}_l^\dagger] = \delta_{kl}$. Owing to the form of the trapping potential, single-particle
wave functions $\phi_k(r)$ exhibit a factorized form

$$\phi_k(r) = g(z)w_k(\vec{r} - \vec{r}_k)$$  \hspace{1cm} (4)

in which $g(z)$ represents the ground-state wave function of harmonic potential $(m\omega^2/2)z^2$, and the planar wave function $w_k(\vec{r} - \vec{r}_k)$ ($\vec{r}_k$ is the center of the $k$th well) describes the localization at the $k$th well.

Note that we are assuming that the planar part of the potential $V_k$ is strong enough compared to other energies (the interaction energies in particular) such that the on-site wave functions $w_k(\vec{r})$ ($k = 1, \ldots, 4$) are fixed, being independent on the number of bosons in each well. We shall work under the hypothesis that the four minima of the $x-y$ potential are well separated. In such a way, the on-site wave function $w_k(\vec{r})$ may be described by a single function $w_k = w_k(\vec{r} - \vec{r}_k)$, where $\vec{r}_k$ is the center of the $k$th well. The condition $w \ll \ell$ (remember that $w$ is the width of each Gaussian in the $x-y$ potential of equation (2)) entails that bosons are strongly localized in the proximity of sites $\vec{r}_k$ in the $x-y$ plane. The functions $w_k(\vec{r} - \vec{r}_k)$ and $w_i(\vec{r} - \vec{r}_i)$ are orthogonal for $i \neq k$ so that one easily proves the orthonormality condition

$$\int d^3r \phi^*_k(r)\phi_i(r) = \delta_{ki}.$$  

Potential $V(r - r') = g \delta^3(r - r') + V_{dd}(r - r')$, describing boson–boson interactions, is the sum of a short-range $g$-dependent contact potential (with $g = 4\pi\hbar^2a_s/m$ and $a_s$ the interatomic s-wave scattering length) and of a long-range dd potential

$$V_{dd}(r - r') = \frac{1 - 3 \cos^2 \theta}{|r - r'|^3}.$$  \hspace{1cm} (5)

The coupling of dipoles through the relevant magnetic moment $\mu$ (electric moment $d$) is embodied in $\gamma = \mu_0\mu^2/4\pi$ ($\gamma = d^2/4\pi\varepsilon_0$) in which $\mu_0$ ($\varepsilon_0$) is the vacuum magnetic susceptibility (vacuum dielectric constant). The relative position of the particles is given by the vector $r - r'$. For external (electric or magnetic) fields large enough the boson dipoles are aligned along the same direction, so that the angle is the average between the vector $r - r'$ and the dipole orientation.

### 2.1. Four-well dipolar-boson model

By assuming symmetric wells and neglecting the next-nearest-neighbor hopping, the resulting dipolar-boson model is described by the four-site EBB Hamiltonian

$$\hat{H} = \hat{H}_1 - J \sum_{i=1}^{4} \left( \hat{a}_i^\dagger \hat{a}_{i+1} + h.c. \right).$$  \hspace{1cm} (6)

where $J$ is the hopping amplitude, $\hat{a}_{i+1} = \hat{a}_i$ due to the ring geometry, and the interaction Hamiltonian

$$\hat{H}_1 = \frac{U_0}{2} \sum_{i=1}^{4} \left[ \hat{n}_i (\hat{n}_i - 1) + V_f \hat{n}_i \hat{n}_{i+1} \right] + V_2 (\hat{n}_i \hat{n}_3 + \hat{n}_2 \hat{n}_4),$$  \hspace{1cm} (7)

in addition to the standard boson–boson interaction $U_0$, includes the terms depending on $V_f (V_2)$ which describe dipolar interactions between nearest (next-nearest) neighbors. In the square-ring geometry and for point-like, tightly localized wavefunctions $\psi_k$, one has $V_2 = V_f/(2\sqrt{2})$ since the dd interaction falls off like $r^{-3}$. In $\hat{H}$, the local number operator $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ counts the number of particles in the $i$th well of the ring.

The three macroscopic parameters $J$, $U_0$ and $V_1$ are defined as follows. The hopping amplitude is given by

$$J = -\int d^3r \phi^*_k(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_k(r) \right] \phi_i(r),$$  \hspace{1cm} (8)

where $k$ and $l$ ($k \neq l$) are two nearest-neighbor sites, while the on-site interaction $U_0$ combines the contributions of short-range and dd interactions [6]

$$U_0 = g \int d^3r \left| \phi_k(r) \right|^4 + \frac{\gamma}{2} \int d^3r \int d^3r' \left| \phi_k(r) \right|^2 V_{dd}(r - r') \left| \phi_l(r') \right|^2.$$  \hspace{1cm} (9)

We write the nearest-neighbor interaction amplitude $V_1$ in the form

$$V_1 = \frac{\gamma}{2} \int d^3r \int d^3r' \left| \phi_k(r) \right|^2 V_{dd}(r - r') \left| \phi_l(r') \right|^2,$$  \hspace{1cm} (10)

(with $k$ and $l$ [$k \neq l$] being two nearest-neighbor sites) since the main contribution is due to the dipolar potential $V_{dd}$ [6]. The comparison with the three-site EBB model, describing dipolar bosons trapped in three wells, shows how the presence of more than three wells induces significant changes in the interaction processes. In the triple-well case, the relevant Hamiltonian reads

$$\hat{H}_3 = -J \left[ \hat{a}_1^\dagger \hat{a}_2 + \hat{a}_1^\dagger \hat{a}_3 + \hat{a}_2^\dagger \hat{a}_3 + \hat{a}_2^\dagger \hat{a}_1 + \hat{a}_3^\dagger \hat{a}_1 + \hat{a}_3^\dagger \hat{a}_2 \right] + \frac{U_0}{2} \sum_{i=1}^{3} \hat{n}_i (\hat{n}_i - 1) + U_f \sum_{i=1}^{3} \hat{n}_i \hat{n}_{i+1}.$$  \hspace{1cm} (11)

Thanks to the equality

$$\hat{N}^2 = \sum_{i=1}^{3} \hat{n}_i^2 + 2 \sum_{i=1}^{3} \hat{n}_i \hat{n}_{i+1},$$

where $\hat{N} = \hat{n}_1 + \hat{n}_2 + \hat{n}_3$, is such that $[\hat{H}_3, \hat{N}] = 0$, the Hamiltonian $\hat{H}_3$ reduces to the simpler three-site BH model (the so-called BH trimer)

$$\hat{H}_3 = -J \left[ \hat{a}_1^\dagger \hat{a}_2 + \hat{a}_1^\dagger \hat{a}_3 + \hat{a}_2^\dagger \hat{a}_3 + \hat{a}_2^\dagger \hat{a}_1 + \hat{a}_3^\dagger \hat{a}_1 + \hat{a}_3^\dagger \hat{a}_2 \right] + \frac{U_0}{2} \sum_{i=1}^{3} \hat{n}_i (\hat{n}_i - 1) + U_f \hat{N} (\hat{N} - 1).$$  \hspace{1cm} (12)

In the latter formula, $U \equiv U_0 - U_f$ shows that the nearest-neighbor (dipolar) interactions have been absorbed by the effective on-site interaction $U$ while $U_f$ only appears in the constant term $U_f \hat{N} (\hat{N} - 1)/2$. Based on this result, the ground-state structure of $\hat{H}_3$ has been thoroughly investigated in [19] by exploiting the well-known properties of the BH-trimer ground state both in the attractive ($U < 0$) and repulsive ($U > 0$) interaction regime.
The application of the same scheme to the four-well dipolar model, where
\[
\hat{N}^2 = \sum_{i=1}^{4} \hat{n}_i^2 + \sum_{i \neq j} \hat{n}_i \hat{n}_j,
\]
shows that, in addition to \(2(\hat{n}_1 \hat{n}_2 + \hat{n}_2 \hat{n}_3 + \hat{n}_3 \hat{n}_4 + \hat{n}_4 \hat{n}_1)\), the nonlocal term depending on \(\hat{n}_1 \hat{n}_3 \) now includes the contribution \(2(\hat{n}_1 \hat{n}_3 + \hat{n}_2 \hat{n}_4)\) involving the coupling of non-adjacent operators \(\hat{n}_i\). This leads to recast model (6) into the form
\[
\hat{H} = C(\hat{N}) - J \sum_{i=1}^{4} (\hat{\alpha}_i \hat{\alpha}_{i+1} + \text{h.c.}) - \frac{U}{2} \sum_{i=1}^{4} \hat{n}_i (\hat{n}_i - 1) - U (\hat{n}_1 \hat{n}_3 + \hat{n}_2 \hat{n}_4),
\]
where \(U = U_0 - V_1\) and \(C(\hat{N}) = V_1 \hat{N}(\hat{N} - 1)/2\), characterized by the effective coupling \(U_0 = V_1 - V_2 = V_1(1 - 1/\sqrt{8})\) between next nearest-neighbor sites. Then the new form of Hamiltonian (6) is that of the four-site BH model where the effective on-site interaction parameter is once more \(U = U_0 - V_1\) but, unlike the case of dipolar bosons in three-well potential, a new interaction term modify the spectral properties of the model with respect to the case of the BH Hamiltonian.

### 3. The four-well dipolar-boson model within the CVP

The CVP is obtained by observing that physical quantities depending on the local boson populations \(n_i\) can be equivalently described in terms of densities \(x_i = n_i/N\). For \(N\) large enough, the latter can be seen as continuous variables. This assumption leads to reformulate in terms of densities \(x_i\) both Fock states and, accordingly, the action of bosonic operators on such states. After setting \(n_1, n_2, \ldots, n_L \equiv |x_1, x_2, \ldots, x_L\rangle\) and observing that creation (destruction) processes \(n_i \rightarrow n_i + 1 \ (n_i \rightarrow n_i - 1)\) entail that
\[
|\ldots, x_i, \ldots \rangle \rightarrow |\ldots, x_i \pm \epsilon, \ldots \rangle, \quad \epsilon = 1/N,
\]
one determines the effect of the action of Hamiltonian \(\hat{H}\) on a generic quadratic state \(|\Psi\rangle = \sum_{\vec{n}} \Psi(\vec{n}) |\vec{n}\rangle\), where \(|\vec{n}\rangle = |n_1, n_2, \ldots, n_L\rangle\). The corresponding calculations describing the essence of this approach are discussed in the appendix. Within the new formalism the eigenvalue problem \(\hat{H}|\Psi\rangle = E|\Psi\rangle\) for the BH Hamiltonian
\[
\hat{H} = U_0 \sum_{i=1}^{L} \hat{n}_i (\hat{n}_i - 1) - J \sum_{i<j} A_{ij} \hat{\alpha}_i \hat{\alpha}_j,
\]
takes the CVP form [23]
\[
[-D + V]|\psi_E(\vec{x})\rangle = \hat{E}|\psi_E(\vec{x})\rangle, \quad \hat{E} = \frac{E}{N^2 |U|},
\]
including the generalized Laplacian
\[
D = \sum_{i<j} \frac{\epsilon^2}{2} A_{ij} (\partial_x - \partial_y) \sqrt{x_i x_j} (\partial_x - \partial_y),
\]
with \(\tau = J/(N|U|)\), and the effective potential
\[
V = \frac{\sigma}{2} \sum_{r=1}^{L} x_r (x_r - \epsilon) - 2\tau \sum_{r=1}^{L} \sqrt{x_r x_{r+1}},
\]
where \(\sigma = U/|U|\) assumes the value \(\sigma = +1 \ (\sigma = -1)\) in the presence of an effective on-site repulsive (attractive) interaction \(U > 0 \ (U < 0)\).

The solutions \(\psi_E(\vec{x})\) to this problem (and the relevant eigenvalues \(E\)) are found by observing that it can be reduced to a multidimensional harmonic-oscillator problem in the proximity of the extremal points of \(V\). The essential information concerning the ground-state configuration is thus obtained by imposing the stationarity condition of \(V\). In the following, we use this condition to determine the ground state of model (6) and its dependence on the model parameters.

#### 3.1. Bosonic-population equations characterizing the ground state

The application of the CVP to the four-well dipolar-boson model (6) yields the new eigenvalue equation
\[
\hat{H}|\psi_E(\vec{x})\rangle = \hat{E}|\psi_E(\vec{x})\rangle, \quad \hat{E} = \frac{E}{N^2 |U|},
\]
where the effective Hamiltonian \(\hat{H}\) contains the generalized Laplacian \(D\) defined on the squared ring
\[
D = \tau \sum_{r=1}^{4} (\partial_{x_r} - \partial_y) \sqrt{x_r x_{r+1}} (\partial_{x_{r+1}} - \partial_y),
\]
and the potential
\[
V = \frac{\sigma}{2} \sum_{r=1}^{4} x_r (x_r - \epsilon) - U_1 (x_1 x_3 + x_2 x_4) - 2\tau \sum_{r=1}^{4} \sqrt{x_r x_{r+1}},
\]
in which \(U_1 = U_0/|U|\) and \(\sigma = 1\) owing to the conservation of the total boson number \(N\). At this point, we observe that due to ring geometry \(x_{r+1} \equiv x_r\) and for \(N\) large enough the parameter \(\epsilon\) is sufficiently small. We can thus write a more useful version of \(V\) which underlines its symmetric character under exchanges of boson populations, that is
\[
V = \frac{\sigma}{2} \left( x_1^2 + x_2^2 + x_3^2 + x_4^2 - U_1 (x_1 x_3 + x_2 x_4) - 2\tau \left( \sqrt{x_1^2 + x_3^2} + \sqrt{x_2^2 + x_4^2} \right) \right).
\]

In general, two main regimes (the repulsive and attractive ones) can be identified by considering the interplay between parameters \(U_0\) and \(U_1\) occurring in the effective potential \(V\) or, equivalently, in Hamiltonian \(\hat{H}\). For a given \(U_0\), one has
\[
0 < U_1 < U_0 \rightarrow \sigma = +1, \quad 0 < u_1 < \infty, \quad (17)
\]
\[
U_0 < U_1 \rightarrow \sigma = -1, \quad \infty > u_1 > 1. \quad (18)
\]

The derivation of the equations for variables \(x_i\) discussed
below shows how the first case actually splits into two independent, significantly different, regimes.

To derive the equations for the \( x_i \) one must consider the constraint \( 1 = x_1 + x_2 + x_3 + x_4 \), implying that one of the coordinates \( x_i \) can be seen as a dependent variable. By assuming, for example, \( x_4 = 1 - (x_1 + x_2 + x_3) \), the equations \( \partial V/\partial x_i = 0 \) with \( i = 1, 2, 3 \) gives

\[
\sigma(x_1 - x_4) - u_1(x_3 - x_2) - \frac{\tau}{\sqrt{x_1 + \sqrt{x_2}} + \sqrt{x_3 + \sqrt{x_4}}} = 0,
\]

\[
\frac{\sigma + u_1)(x_2 - x_4)}{\sqrt{x_2 + \sqrt{x_4}}} = 0,
\]

\[
\sigma(x_3 - x_4) - u_1(x_1 - x_2) - \frac{\tau}{\sqrt{x_2 + \sqrt{x_4}}} + \frac{\sqrt{x_1 + \sqrt{x_3}}}{\sqrt{x_4}} = 0,
\]

determining the configurations \( (x_1, x_2, x_3, x_4) \) for which the stationarity condition of \( V \) is realized. Since densities \( x_i \) describe the bosonic populations (BP), we will refer to such equations as the BP equations. In general, such equations can be shown [23] to describe different weakly-excited states in the absence of dipolar interaction.

3.2. Solutions of the BP equations

A large amount of information can be extracted from the reduced BP equations. By rewriting equation (20) in the form

\[
\Delta_{24} [(\sigma + u_1)(\sqrt{x_2 + \sqrt{x_4}}) + \frac{2\tau\sqrt{x_1}}{\sqrt{x_2 + \sqrt{x_4}}} = 0,
\]

with \( \Delta_{24} = \sqrt{x_2} - \sqrt{x_4} \), one easily identifies the solution \( x_2 = x_4 \) entailing that the equation (19) becomes

\[
(x_1 - x_2) \left[ (\sigma - u_1) + \frac{2\tau}{\sqrt{x_1} + \sqrt{x_2}} \right] = 0.
\]

Such equations show that three different regimes characterize the low-energy scenario relevant to \( V \) and, more in general, to the four-well dipolar model. For \( U_i < U_0 \) (corresponding to \( \sigma = +1 \)) one has two cases

\[
0 < U_i < U_0/2 \quad (\iff u_1 < 1),
\]

\[
U_0/2 < U_i < U_0 \quad (\iff u_1 > 1),
\]

in addition to the case

\[
U_0 < U_i < \infty \quad (\iff u_1 > 1),
\]

where \( \sigma = -1 \). Note that, in the proximity of \( U_0 \) (namely, in the limit \( U_1 \to (U_0)^+ \)), parameter \( u_1 \) can assume arbitrarily large values.

Apart from \( x_4 = x_2 \) and \( x_2 = x_1 \), equations (21) and (22) do not provide further solutions for \( \sigma = +1 \) and \( u_1 < 1 \) in that the factors contained in the squared brackets is always positive. Summarizing, solution \( x_1 = x_3 = x_2 = x_4 \) is the unique solution for \( 0 < U_i < U_0/2 \). This is the ultraweak dipolar-interaction regime.

A more structured solution is obtained from equation (22) in the interval \( U_0/2 < U_i < U_0 \), where, in addition to \( \sigma = +1 \), the inequality \( u_1 > 1 \) holds. From equation (22) one gets

\[
x_{12} = \frac{4\tau^2}{(u_1 - 1)^2},
\]

which, combined with the constraint \( 1 = 2(x_1 + x_2) \), gives

\[
x_1 = \frac{1}{4}\left[ 1 \pm \sqrt{1 - f} \right],
\]

\[
x_2 = \frac{1}{4}\left[ 1 \mp \sqrt{1 - f} \right].
\]

with

\[
f = \frac{64\tau^2}{(u_1 - 1)^2} = \frac{64J^2}{N^2(2U_1 - U_2)^2},
\]

in the interval \( 0 \leq \tau \leq |u_1 - 1|/8 \). Then, by observing that \( x_1 = x_3 \) and \( x_4 = x_2 \), the configuration of the system appears to be completely determined. The range of \( J \) where these solutions are defined depends on \( U_0 \) and \( U_1 \). In view of definitions \( u_1 = U_1/|U_0 - U_1| \) and \( \tau = J/(N|U_1|) \), after rewriting the latter inequality for \( \tau \) in the form

\[
J/N < |U_1| - |U_0 - U_1||/8,
\]

one finds that for \( U_1 \to U_0/2 \) the range of \( J/N \) tends to zero while, for \( U_1 \to (U_0)^+ \), the range is \( J/N < U_0/8 \). This case represents the weak dipolar-interaction regime.
A third case is found for $U_l > U_0$ entailing $\sigma = -1$. equations (21) and (22) take the form

$$\Delta_{s+1} \left[ (u_1 - 1) (\sqrt{\xi_2} + \sqrt{\xi_4}) + \frac{2 \sqrt{\xi_1}}{\sqrt{x_1} \sqrt{x_2}} \right] = 0,$$

(26)

respectively,

$$(x_1 - x_2) \left[ \frac{2 \sqrt{\xi_1}}{\sqrt{x_1} \sqrt{x_2}} - (1 + u_1) \right] = 0.$$  (27)

Since $u_1 > 1$, the first equation is solved once more by $x_2 = x_4$ while the second one is solved either by

$$x_1 = x_2 \quad \text{(uniform solution)}$$

or by setting

$$\frac{2 \sqrt{\xi_1}}{1 + u_1} = \frac{\sqrt{\xi_1}}{\sqrt{x_2}}.$$

One immediately gets the relevant solutions given by

$$x_1 = \frac{1}{4} \left[ 1 + \sqrt{1 - g} \right], \quad x_2 = \frac{1}{4} \left[ 1 + \sqrt{1 - g} \right].$$  (28)

with

$$g = \frac{64 \tau^2}{(u_1 + 1)^2} = \frac{64 \tau^2}{N^2 (2U_l - U_0)^2},$$  (29)

where the range of $\tau$ is determined by $0 \leq \tau \leq (u_1 + 1)/8$.  

Note that $g \equiv f$ given by equation (24).  The inequality defining the upper bound can be rewritten in the more explicit form

$$J \leq N (2U_l - U_0)/8$$

showing that $J \leq NU_0/8$ for $U_l \rightarrow U_l^*$, and $T \leq NU_0/8$ for a generic, arbitrarily large $U_l > U_0$.  This case represents the strong dipolar-interaction regime.

### 3.3. The low-energy scenario

In the CVP form (15) of the dipolar-boson model the energy of the system in the proximity of minimum-energy configurations is described by potential (16). The comparison of the energies corresponding to the BP configurations analyzed in the previous section reveals the change of structure of the minimum when the parameter $U_l$ is varied with respect to $U_0$.

Numerical calculations confirm that both the uniform solution and solution (23) represent minimum-energy configurations in the corresponding regimes.

The energy of the uniform solution $x_i = 1/4$ with $i = 1, 2, 3, 4$ obtained from (16) is easily found to be

$$V_0 = \frac{\sigma - u_1}{8} - 2 \tau, \quad \tau = \frac{J}{N|U|}.$$  

This represents the ground-state energy for $U_l < U_0/2$, namely, when $u_1 < 1$ and $\sigma = +1$ (ultraweak dipolar interaction).

In the subsequent interval $U_0/2 < U_l < U_0$, where $\sigma = +1$ but $u_1 > 1$, the new solutions (23) and (24) have been found in addition to the uniform solution. Since $x_1 = x_3$ and $x_2 = x_4$

$$V = \left( 1 - u_1 \right) \left( x_1^2 + x_2^2 \right) - 8 \tau \sqrt{x_1} \sqrt{x_2}$$

giving the minimum-energy formula

$$V_0^* - \frac{1 + u_1}{4} = \frac{8 \tau^2}{1 + u_1},$$

where the variable $\tau$ is defined by $0 \leq \tau \leq (u_1 - 1)/8$. By observing that inequality $\tau \leq (|1 - u_1|)/8$ defines the range of $\tau$, the two energies are found to coincide for $\tau = (|1 - u_1|)/8$, consistently with the fact that, in this case, the solution described by (23) and (24) reduce to the uniform solution. For $U_l \rightarrow (U_l/2)^*$ one has $u_1 \rightarrow 1^+$ which, owing to $\tau \leq (|1 - u_1|)/8$, implies that $\tau \rightarrow 0$. As expected, in this limit one obtains that $V_0 = 0 = V_0^*$. Going to the opposite extreme $U_l \rightarrow U_l^*$ one easily checks that

$$V_0^* = -\frac{|1 - u_1|}{4} - \frac{8 \tau^2}{|1 - u_1|} < V_0 = -\frac{|u_1 - 1|}{8} - 2 \tau.$$  

By observing that inequality $\tau \leq (|1 - u_1|)/8$ now becomes $\tau \leq NU_0/8$, the condition $V_0^* = V_0$ is reached for $J = NU_0/8$. Note that the diverging factor $1/J|U|$ in the previous expressions is in fact irrelevant since the effective energies are defined by $N^2|U| \times V_0$ (see the energy eigenvalue in (15)).

The transition from the regime $0 \leq U_l < U_0/2$ to the one with $U_0/2 < U_l < U_0$ thus entails the change of the ground-state structure, which from the uniform-boson distribution relevant to $x_i = 1/4$ transforms into a non-uniform distribution with two separated peaks such that either $x_1 = x_3 < x_2 = x_4$ or $x_2 = x_4 < x_1 = x_3$.

For $U_l \geq U_0^*$ (strong dipolar-iteration regime) one has $\sigma = -1$ and $1 < u_1 < \infty$ for any $U_l$. As a consequence, potential (16) takes the form

$$V = \left( 1 + u_1 \right) \left( x_1^2 + x_2^2 \right) - 8 \tau \sqrt{x_1} \sqrt{x_2},$$

giving the minimum-energy formula

$$V_0^* = -\frac{1 + u_1}{4} - \frac{8 \tau^2}{1 + u_1},$$

when the $x_i$ corresponding to solution (28) are substituted. Since

$$1 + u_1 = \ldots = \frac{2U_l - U_0}{|U|}, \quad |1 - u_1| = \ldots = \frac{2U_l - U_0}{|U|},$$

in the interval $U_0/2 \leq U_l \leq U_0$ and $U_l \geq U_0^*$, respectively, then $1 + u_1$ and $|1 - u_1|$ describe the same function of $U_l$. Hence, $V_0^*$ simply represents the continuation of $V_0$ in the upper interval $U_l \geq U_0$ with $V_0^* = V_0$ for $U_l \rightarrow U_0$. Once more, one easily checks that

$$V_0^* = -\frac{1 + u_1}{4} - \frac{8 \tau^2}{1 + u_1} < V_0 = -\frac{|u_1 - 1|}{8} - 2 \tau,$$

for essentially any value of $u_1$ where $V_0$ is the uniform-
solution energy corresponding to the choice \( \sigma = -1 \). Note that solution (28) is defined provided \( \tau \leq 1 + u |1| / 8 \) is satisfied (the value \( \tau \equiv (1 + n_1) / 8 \) is the unique case for which \( V^0 = V_0 \). Not surprisingly, this inequality reproduces the more explicit one \( J/N \leq (2U_1 - U_0)/(8|U|) \) already found for solution (23). For \( U_1 \to (U_0)^+ \) one has \( J \leq NU_0/8 \) while for \( U_1 > U_0 \) one has \( J \leq NU_1/4 \).

The fact that \( V^0 = V_0 \) for \( J/N \equiv (2U_1 - U_0)/(8|U|) \) suggests that when the previous inequality is violated the minimum energy becomes that described by the uniform solution. This circumstance is confirmed by the fact that both solutions (23) and (28) reproduce the uniform solution whenever \( \tau \) tends to its extreme permitted value.

Concluding this analysis shows that, rather counterintuitively, the crucial change in the ground-state structure takes place when \( U_1 \) crosses \( U_0/2 \) (transition from the ultra-weak-interaction to the weak-interaction regime) while the change of the effective dipolar interaction \( U = U_1 - U_0 \) from repulsive \( (U > 0 \to \sigma = +1) \) to attractive \( (U < 0 \to \sigma = -1) \) is completely irrelevant. The emerging ground state significantly differs from that of the dipolar-boson model in a triple well. In the latter case the transition from the weakly-attractive regime, characterized by the uniform solution (full boson delocalization), to the strongly-attractive regime \( (U_1 \gg U_0) \) shows that the ground state becomes a symmetric superposition of three macroscopic states each one describing the almost complete localization of bosons in one of the three wells (Schrödinger-cat state)

\[ |E_0 \rangle \approx \frac{1}{\sqrt{3}} (|N, 0, 0, 0 \rangle + |0, N, 0, 0 \rangle + |0, 0, N, 0 \rangle). \]

Such a state manifestly reflects the equivalence of the three-well dipolar-boson system with the attractive BH trimer. The ground state significantly differs from that of the dipolar-boson model in a triple well. In the latter case the transition from the weakly-attractive regime, characterized by the uniform solution (full boson delocalization), to the strongly-attractive regime \( (U_1 \gg U_0) \) shows that the ground state becomes a symmetric superposition

\[ |E_0 \rangle \approx \frac{1}{\sqrt{2}} (|N/2, 0, N/2, 0 \rangle + |0, N/2, 0, N/2 \rangle) \]

the second Fock state corresponding to the equivalent configuration \( x_1 \approx x_3 \approx 0 \) and \( x_2 = x_4 \approx 1/2 \). Even for \( U_1 \gg U_0 \), states involving the full localization of bosons in one of the four wells \( (|N, 0, 0, 0 \rangle, |0, N, 0, 0 \rangle, \ldots) \) are in no way involved in the ground state. The latter in turn reflects the crucial role played by the term \( U_1(n_{13} + n_{24}) \) of Hamiltonian (13).

4. Dipolar-boson ground state

The ground state of the Hamiltonian (6) can be written in the form of superposition of different Fock states which, due to the conservation of total boson number \( N \), reads

\[ |\Psi \rangle = \sum_{n_1=0}^{N} \sum_{n_2=0}^{N-n_1} \sum_{n_3=0}^{n_2} c_{n_1,n_2,n_3} |n_1, n_2, n_3 \rangle, \quad (30) \]

where we have omitted the occupation number of the fourth well \( n_4 = N - (n_1 + n_2 + n_3) \).

Different ground states \( |\Psi \rangle \) are sustained by the Hamiltonian (13) (that is fully equivalent to the Hamiltonian (6), as shown in section 2) depending on the relative magnitude of the parameters \( U_1 \) and \( U_0 \). To show how this causes changes in the ground-state structure, we have studied the probabilities \( |c_{n_1,n_2,n_3}|^2 \) on varying of \( U_1 \) in suitable ranges of values (see the discussion below) by keeping fixed both \( J \) and \( U_0 \). The results of this analysis, performed for a total boson number \( N = 32 \), are shown in figure 1 (where, for convenience of representation, we report only \( |c_{n_1,n_2,n_3}|^2 \gtrsim 1 \times 10^{-5} \)). Moreover, in figures 1 and 2 we assume \( U_0 \) as the energy scale \( (U_0 = 1) \). Let us give a look to plots of figure 1 starting from the top panels. Here \( 0 < U_1 < U_0/2 \). This corresponds to the ultraweak dipolar-interaction regime. By inspecting these distributions, two things can be clearly observed. As a first, \( |c_{n_1,n_2,n_3}|^2 \) attains its maximum value for \( n_1 = n_2 = n_3 = 8 \) that is equivalent, in the CVP language, to \( x_1 = x_2 = x_3 = x_4 \); the uniform solution. The second observation is that increasing \( U_1 \) has the effect to produce a progressive depletion of state \( (8^8, 8, 8) \), with \( |N/4, N/4, N/4, N/4 \rangle \) remaining the maximally populated state, thus confirming the predictions of the CVP approach.

The bottom panels of figure 1, instead, represent what happens in the weak dipolar-interaction regime characterized by \( U_0/2 < U_1 < U_0 \). We have chosen the values of \( U_1 \) in accordance with the analysis of the previous section so that to satisfy the inequality (25). We have studied, in other words, the ground state corresponding to the parameter values in the (lower) shaded area of figure 2. The panel corresponding to \( U_1 = 0.50251 \) reveals that a transition occurs in the ground state: the bosons populate with the highest probability the states \( |0, 16, 0 \rangle \) and \( |16, 0, 16 \rangle \) (i.e. the states \( |0, N/2, 0, N/2 \rangle \) and \( |N/2, 0, N/2, 0 \rangle \), respectively) that, in the CVP fashion, correspond to \( x_1 = x_3 = x_4 \).

The ground state of the Hamiltonian (6) is therefore a symmetric superposition of the states \( |0, N/2, 0, N/2 \rangle \) and \( |N/2, 0, N/2, 0 \rangle \). This result corroborates the CVP studies that predict a change in the ground-state structure from the uniform state to a macroscopic two-pulse state when \( U_1 \) crosses \( U_0/2 \). By further increasing \( U_1 \) the above superposition is still the ground state and the \( |c|^2 \) pertaining to \( |0, 16, 0 \rangle \) and \( |16, 0, 16 \rangle \) become larger, as it can be seen from the fifth and sixth panels corresponding to \( U_1 = 0.5030 \) and \( U_1 = 0.5038 \), respectively.

As a conclusive remark, we note that the CVP-predicted localization–delocalization transition is captured by numerics in wider terms. In fact, we have found numerically the ground-state of the four-site BH Hamiltonian (6) with \( N = 32 \) in correspondence to \( J = 0.03 \) (top panels of figure 3) and \( J = 0.035 \) (middle panels of figure 3), and \( J = 0.04 \) (bottom
panels of figure 3). From these plots, one can clearly see the change experienced by the ground-state when the boundary \(U_{20} \) is crossed, like so expected from CVP. As for figure 1, also in this case, the second panel of each \(J\)-fixed pair has been obtained by choosing the Hamiltonian parameters so that the inequality (25) is satisfied.\

5. Conclusions

We have considered a system of interacting dipolar bosons confined by a four-well potential with a ring geometry. The microscopic dynamics of this system are ruled by a four-site BH model including interactions between bosons in next-nearest–neighbor wells. We have studied the ground state of the four-well realization of the BH Hamiltonian by varying the amplitude \(U_{1}\) of the (effective) interaction of next-near–nearest wells. We have attacked the problem from two sides, i.e. both analytically and numerically. From the analytical point of view we have reformulated the dipolar-boson model within the framework of the CVP. By exploiting this approach we have shown that the ground-state structure exhibits a dramatic change when the amplitude \(U_{1}\) becomes larger than a precise fractional value of the on-site interaction \(U_{0}\). More precisely, \(U_{1} > U_{0}/2\) signs the delocalization–localization transition. In the delocalization regime, the ground state is uniform (equally shared bosons among the four wells), while in the localization one, the system is a macroscopic two-pulse state where the bosons are strongly localized. These CVP results are corroborated by those obtained from the numerical diagonalization of the four-site BH Hamiltonian. Indeed, within this approach it can be clearly observed that in the delocalization regime the ground state is uniform (equally shared bosons among the four wells), while in the localization one, the system is a macroscopic two-pulse state where the bosons are strongly localized. These CVP results are corroborated by those obtained from the numerical diagonalization of the four-site BH Hamiltonian. 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the four sites. This result, in addition to validate the approach based on the CVP to the low-energy states of many-bosons systems, shows the considerable influence of the number of wells on the ground-state structure and prompts further study on dipolar bosons trapped in a ring lattice involving $L > 4$ potential wells.

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Appendix. Application of the CVP

The action of the hopping-term operators on a generic quantum state $|\Psi\rangle = \sum_{\ell} \psi^{\ell} (\ell) |\ell\rangle$ where $|\ell\rangle$ represents the Fock state $|n_1, n_2, \ldots, n_L\rangle$, yields

$$\hat{a}_{x}^\dagger \hat{a}_{x'}^\dagger |\Psi\rangle = \sum_{x}^{\star} \psi (x) N \sqrt{x_{x'} \epsilon} \left| x_{x'} + \epsilon \right| \ldots, x_{x'},$$

where $\psi(x) \equiv \psi(x_1, x_2, \ldots, x_L)$ has replaced $\Psi (\ell)$.

In this scheme, the key approximation amounts to assume that only the first and second-order contributions must be considered in the Taylor expansion in $\epsilon$ of the function $\psi (\ldots, x_r + \epsilon, \ldots, x_s - \epsilon, \ldots) \sqrt{x_r + \epsilon} \sqrt{x_s - \epsilon}$ occurring in $\hat{a}_{x}^\dagger \hat{a}_{x'}^\dagger |\Psi\rangle$.

Figure 3. Horizontal axis: kets $|n_1, n_2, n_3\rangle$ (the fourth well occupation being $n_4 = N - (n_1 + n_2 + n_3)$). Vertical axis: the squared modulus of ground-state coefficients $|c_{n_1,n_2,n_3}|^2$. Here: $U_0 = 1$ and $N = 32$. Top panels ($J = 0.03$): $U_1 = 0.499$ (left); $U_1 = 0.50438$ (right). Middle panels ($J = 0.035$): $U_1 = 0.499$ (left); $U_1 = 0.5038$ (right). Bottom panels ($J = 0.04$): $U_1 = 0.499$ (left); $U_1 = 0.5051$ (right).
This gives
\[ \hat{a}_r^\dagger a_r \ket{\Psi} = N \sum_{s,r} \sqrt{x_r x_s} \psi(x) e^{\sqrt{x_r x_s} \left( \frac{\partial \psi}{\partial x_r} - \frac{\partial \psi}{\partial x_s} \right)} \]
\[ + \sqrt{x_r x_s} \frac{\psi(x)}{2x_r} e^\frac{e^2}{2\sqrt{x_r x_s}} \]
\[ \times \left( \frac{\partial^2 \psi}{\partial x_r^2} + \frac{\partial^2 \psi}{\partial x_s^2} - 2 \frac{\partial^3 \psi}{\partial x_r \partial x_s} \right) \]
\[ + \frac{\psi(x)}{8x_r^2} + \frac{1}{2x_r} \left( \frac{\partial \psi}{\partial x_r} - \frac{\partial \psi}{\partial x_s} \right) \]
\[ + ... \]
\[ ... \]
\[ \ket{\hat{\ell}}. \]

Then, the action of the typical hopping term of BH Hamiltonians \( \sum_{s,r} A_{sr} \hat{a}_r^\dagger a_r \) on a generic state \( \ket{\Psi} \) can be shown to be represented by
\[ \sum_{s,r} A_{sr} \hat{a}_r^\dagger a_r \ket{\Psi} = \frac{N}{2} \sum_{\hat{s}} \left( \sum_{s,r} A_{sr} \psi(\hat{s}) \right) \]
\[ \times \left[ 2 \sqrt{x_r x_s} + \frac{e^2 x_r + x_s}{2} \right] \]
\[ \times \left( \frac{\partial^2 \psi}{\partial x_r^2} + \frac{\partial^2 \psi}{\partial x_s^2} - 2 \frac{\partial^3 \psi}{\partial x_r \partial x_s} \right) \]
\[ + e^2 A_{sr} \left( \delta_{sr} - \delta_{sr} \right) \sqrt{x_r x_s} \left( \frac{\partial \psi}{\partial x_r} - \frac{\partial \psi}{\partial x_s} \right) \]
In such formulas \( A_{sr} \) represents the adjacency matrix. The latter is, in general, zero except for nearest-neighbor sites for which \( A_{sr} = 1 \). To complete the description of this scheme, one must consider the action of terms such as \( \sum_i \hat{a}_i^\dagger \) on \( \ket{\Psi} \). This is easily found to be
\[ \sum_i \hat{a}_i^\dagger \ket{\Psi} = N^{-1} \sum_i \hat{a}_i^\dagger \psi(\hat{s}) \ket{\hat{s}}. \]

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