

Realizing multiband states with ultracold dipolar quantum simulators

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The manipulation of dipolar interactions within ultracold molecular ensembles represents a pivotal advancement in experimental physics, aiming at the emulation of quantum phenomena unattainable through mere contact interactions. Our study uncovers regimes of multiband occupation which allow to probe more realistic, complex long-range interacting lattice models with ultracold dipolar simulators. By mapping out experimentally relevant ranges of potential depths, interaction strengths, particle fillings, and geometric configurations, we calculate the agreement between the state prepared in the quantum simulator and a target lattice state. We do so by separately calculating numerically exact many-body wave functions in the continuous space and single- or multiband lattice representations, and building their many-body state overlaps. Our findings reveal that for shallow lattices and stronger interactions above half filling, multiband population increases, resulting in fundamentally different ground states than the ones observed in simple lowest-band descriptions, e.g., striped vs checkerboard states. A wide range of probed parameter regimes in its turn provides a systematic and quantitative blueprint for realizing multiband states with two-dimensional quantum simulators employing ultracold dipolar molecules.

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Introduction. Ultracold atomic and molecular systems have emerged as fundamental tools for exploring quantum physics and simulating complex many-body phenomena [1–11]. The ability to control and manipulate magnetic atoms [12–15] and dipolar molecules [16–22] has dramatically broadened the spectrum of quantum systems we can study, particularly those governed by long-range interactions. For example, by transferring the population of molecules to their rovibrational ground state using the STIRAP technique, their large electric dipole moments can be aligned using an external electric field, which significantly enhances their interaction strengths. This has led to many breakthroughs, including the creation of molecular dipolar Bose-Einstein condensates [23], supersolid phases [24–36], and quantum magnets [37–39].

By using counterpropagating laser beams and incorporating flat-bottom traps, optical lattices with hard-wall boundaries and depths of up to $10E_R$ can be achieved [40–43]. When integrated with these optical lattices, dipolar systems allow for the simulation of long-range Hamiltonians akin to those in condensed matter and high-energy physics, unveiling unique behaviors not seen in traditional systems with short-range interactions. This progress in experimental capabilities is matched by theoretical advancements, enhancing

our understanding of quantum systems' properties and uncovering novel phenomena such as new quantum and spin liquid phases, altered phase transition behaviors, and modified dynamics and entanglement spread [44–47].

A particularly exciting development is constructing complex extensions of prototypical lattice models such as the Bose-Hubbard model (BHM) [48–50], a cornerstone in the study of strongly correlated physics [51–71]. While research has largely focused on the BHM's adaptation to long-range interactions [72–76] and the new quantum phases that emerge from them [77–82], the potential of dipolar simulators to explore multiband models has received less attention. This is particularly intriguing in two-dimensional (2D) geometries, where the enhanced control over interaction anisotropy, interaction strength tunability, and geometric frustration allows for the exploration of rich phase diagrams featuring topologically ordered phases such as quantum Hall states, quantum spin liquids, and unconventional superfluids enhanced by the long-range nature of the interactions.

In our study, we precisely identify the conditions—spanning potential depths, interaction strengths, particle fillings, and geometric configurations—under which these 2D multiband models can be realized. We provide a detailed comparison of the physics observed in experimental setups to that in the corresponding lattice models, assessing their congruence through ground-state energies, density distributions, and many-body wave function fidelities. Our findings show that in shallow lattices with strong interactions above half filling, higher bands are quickly populated. The higher-band participation has stark effects on the density configuration observed. This discrepancy is especially pronounced in incommensurate geometries with nearly degenerate ground states that are a key element of many 2D systems. Our work thus highlights

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the potential to simulate more intricate 2D multiband lattice models with ultracold dipolar systems toward applications in exotic 2D physics. It also offers insights for future experimental designs and a roadmap for evaluating dipolar quantum simulators' accuracy.

Physical scenario. We consider repulsive-interacting dipolar bosons of mass m in a 2D optical lattice

$$A(\mathbf{x}) = \frac{A_0}{E_R} \left[\sin^2 \left(\frac{\pi x}{L_0} + \phi_x \right) + \sin^2 \left(\frac{\pi y}{L_0} + \phi_y \right) \right], \quad (1)$$

where L_0 is the distance between two neighboring minima (unit of length) and E_R is the recoil energy of the optical lattice (unit of energy). The optical lattice has hard-wall boundaries that restrict the number of minima to exactly S_x in the x direction and S_y in the y direction ($S_i \in \mathbb{N}$), thereby recreating a lattice with $S_x \times S_y$ sites. The phases ϕ_x and ϕ_y are used to center the lattice around the origin depending on the number of sites [83]. For the dipole-dipole interactions (DDI), we assume a strong transverse harmonic confinement which suppresses the divergence [84–88] and yields the regularized form

$$\mathcal{U}_V(\mathbf{x} - \mathbf{x}') = \frac{VL_0^3}{E_R(|\mathbf{x} - \mathbf{x}'|^3 + \alpha)}, \quad (2)$$

where $\alpha = 0.05$ and V denotes the bare DDI strength between two bosons at unit distance. To limit multiple occupation of each site to $<1\%$, we add very strong contact repulsions shaped as a narrow Gaussian $\mathcal{U}_G(\mathbf{x}, \mathbf{x}')$ [89]. The full system is thus governed by the Hamiltonian

$$\begin{aligned} \mathcal{H}_{\text{cont}} = & \int d\mathbf{x} \hat{\Psi}^\dagger(\mathbf{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 + A(\mathbf{x}) \right] \hat{\Psi}(\mathbf{x}) \\ & + \frac{1}{2} \int d\mathbf{x} \int d\mathbf{x}' \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}^\dagger(\mathbf{x}') W(\mathbf{x}, \mathbf{x}') \hat{\Psi}(\mathbf{x}') \hat{\Psi}(\mathbf{x}). \end{aligned} \quad (3)$$

Here $\hat{\Psi}^\dagger(\mathbf{x})$ annihilates (creates) a boson at position $\mathbf{x}$ and $W(\mathbf{x}, \mathbf{x}') = \mathcal{U}_V(\mathbf{x}, \mathbf{x}') + \mathcal{U}_G(\mathbf{x}, \mathbf{x}')$

To benchmark the validity of the 2D dipolar quantum simulator, we systematically map out its ground state properties in terms of three experimentally crucial parameters: (i) the depth of the optical lattice potential A_0 , which we vary from $5E_R$ to $10E_R$, (ii) the DDI strength V , which we vary in the regime of $1E_R$ to $10E_R$, and (iii) different geometries (varying S_x and S_y independently) and number of particles N , which allows us to probe a wide parameter space of filling fractions $\nu = N/(S_x \times S_y)$ up to $\nu = 0.67$.

Methods. To model the experimental setup, we solve the many-body Schrödinger equation directly for the continuous-space Hamiltonian (3) by employing the multiconfigurational time-dependent Hartree method for bosons (MCTDH-B) [90–93], implemented by the MCTDH-X software [94–98], which recasts the many-body wave function into a superposition of M single-particle functions called orbitals. MCTDH-X can obtain the many-body ground state by optimizing both the coefficients and the orbitals [97]. This is done by solving a coupled set of equations of motion derived from the time-dependent variational principle in imaginary time [97]. The accuracy of the many-body calculations is determined by

the number of orbitals. As $M \rightarrow \infty$, the method becomes exact [90], but in practice the correct physics can be obtained for much smaller values of M , as demonstrated in the Supplemental Material [89]. MCTDH-X allows us to obtain the continuous-space many-body wave function $|\Psi\rangle_C$ and observables derived from it, such as the total energy of the system E and the particle density $\rho_C(\mathbf{x})$ (see the Supplemental Material [89] for details). For a sufficiently deep optical lattice, the continuous-space system should map onto a BHM via a tight-binding approximation where the field operators are rewritten in terms of maximally localized Wannier functions $\hat{\Psi}^{(\dagger)}(\mathbf{x}) = \sum_{\alpha} w_{\alpha}^{(*)}(\mathbf{x}) \hat{b}_{\alpha}^{(\dagger)}$. The Wannier functions are typically obtained by applying a unitary transformation to Bloch states, followed by an optimization process that minimizes their spread [99–104]. Since in our case the lattice is finite, the Wannier functions are instead built as a superposition of a particle in box potential wave functions [89,105]. Each Wannier function is centered at a specific site j . Rewriting the continuous-space Hamiltonian with Wannier functions yields the lattice Hamiltonian

$$\mathcal{H}_{\text{DBH}} = - \sum_{\alpha, \beta} J_{\alpha\beta} \hat{b}_{\alpha}^{\dagger} \hat{b}_{\beta} + \sum_{\alpha, \beta, \gamma, \delta} V_{\alpha\beta\gamma\delta} \hat{b}_{\alpha}^{\dagger} \hat{b}_{\beta}^{\dagger} \hat{b}_{\gamma} \hat{b}_{\delta}. \quad (4)$$

Here $\hat{b}_{\alpha}^{(\dagger)}$ denotes bosonic operators for band σ of site j summarized in a unique index $\alpha = (j, \sigma)$. The lattice model encapsulates tunneling processes between different sites and intra- or interband density-density interactions, with couplings $J_{\alpha\beta}$ and $V_{\alpha\beta\gamma\delta}$ obtained from Wannier function overlaps (see the Supplemental Material [89]).

Long-range interactions in closed geometries can quickly lead to higher-band populations. To discern this, we consider dipolar BHM in the lowest-band approximation (1BDBH) and the “one-and-a-half band” approximation (1.5BDBH), where one band is used in one spatial direction and two bands are employed in the other. To obtain the ground state of the lattice Hamiltonian we perform exact diagonalization with the QuSpin Python library [106–108]. We then use the Wannier function basis to reconstruct continuous-space versions $|\Psi_{1/1.5\text{BDBH}}\rangle$ with corresponding density $\rho_{1/1.5\text{BDBH}}(\mathbf{x})$. The continuous-space many-body wave function is projected onto the Wannier function basis $|\Psi_{C \rightarrow 1/1.5\text{BDBH}}\rangle$. This allows us to compute many-body fidelities $|\langle \Psi_{C \rightarrow 1/1.5\text{BDBH}} | \Psi_{1/1.5\text{BDBH}} \rangle|^2$, i.e., a number between zero and one which quantifies the agreement between continuous-space and lattice descriptions (for further details see the Supplemental Material [89]).

Results. We begin by considering systems described by $M = S$ orbitals and Wannier functions (lowest band), respectively. Figure 1 delineates a comprehensive portrayal of fidelity across a spectrum of variables including optical lattice depth, DDI intensity, and filling fractions. Each graphical representation is derived from a distinct combination of lattice dimensions $S_x \times S_y$ and configurations (3×3 , 3×4 , 4×4 , or 5×5) in conjunction with a range of particle numbers ($N = 3$ to $N = 6$) (see the Supplemental Material [89]). Such diversity facilitates the formulation of overarching conclusions concerning the continuum-lattice mapping paradigm. Predominantly, Fig. 1 exhibits a tendency where fidelity diminishes for shallower lattices (lower A_0) and intensified DDIs (higher V).

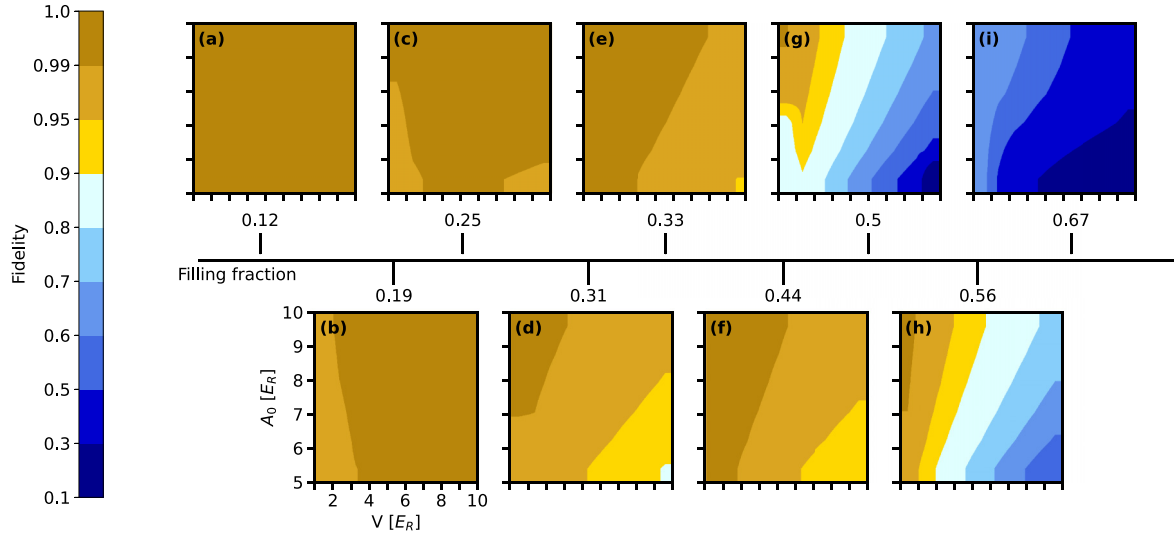


FIG. 1. Fidelity of 2D dipolar quantum simulators and 1BDBH model in different parameter regimes. (a)–(i) Many-body fidelity as a measure for the transition of a single- to multiband dipolar Bose-Hubbard model quantum simulator, for varying lattice depth A_0 , interaction strength V , and filling fraction ν . The labels of (b) apply to all panels.

The first observation is in accordance with general expectations that the tight-binding mapping is less precise for shallower lattices, since the interband gap is generally proportional to A_0 . The second observation unveils a fascinating aspect linked to the extended reach of DDIs. As V is increased, so is the interaction energy and more and more coupling terms between distant sites have to be accounted for in the lattice picture. This encompasses not merely single-band density-density interactions, but also density-assisted tunneling terms across sites and bands, culminating in a larger projection of the continuous-space ground state onto excited lattice bands. Consequently, the fidelity of the state of the continuous-space Hamiltonian with the single-band lattice state is reduced, a phenomenon consistent with prior studies in 1D setups [71].

The increasing discrepancy between continuous-space and lattice calculations in the low A_0 /high V regimes is also corroborated by comparing the energy of the corresponding ground states, summarized in Fig. 2 (for a comprehensive plot of all filling fractions, see the Supplemental Material [89]). In accordance with the variational principle, the

continuous-space ground state energy is always lower than the lattice one, highlighting how the lattice Hamiltonian is an approximation of the continuous-space one. Moreover, as with the fidelity, the difference in energy increases with stronger interactions and shallower lattices, suggesting an increased population of higher bands.

While A_0 and V significantly influence the amount of higher-band contribution, the filling fraction ν is the most important factor. Figure 1 shows that up to $\nu = 0.25$, the lowest-band dominates the physics with above 99% fidelity across most scenarios. For slightly larger filling fractions up to 0.44, the fidelity remains very high in most regions and only drops to around 90% at low lattice depths ($A_0 \lesssim 6E_R$) and/or very strong interactions ($V \gtrsim 7E_R$). However, filling fractions above 0.5 see a rapid decline in the fidelity to values below 50%. Interestingly, this can even occur for deep lattices with $A = 10E_R$. The reason for this decrease should again be attributed to a sharp increase in the interaction energy—this time by cramming more particles—which grants them the ability to overcome the band gap and excite states in higher bands, thereby reducing the lowest-band population. The dipolar quantum simulator at high densities is thus definitely breaking out of the lowest-band picture.

To quantify the contributions from higher bands, in Fig. 3 we present detailed comparisons between the 1BDBH and the 1.5BDBH models for the 3×3 geometry. In simpler 1BDBH calculations, as previously seen, the fidelity drops monotonically for decreasing A_0 and increasing V . Higher filling states with $N = 5$ and $N = 6$ exhibit the most striking fidelity drop, with low points of 51% and 14%, respectively. However, by including additional bands, accuracy improves for all scenarios. This improvement is most notable for $N = 6$ ($\nu = 0.67$), where the two models predict completely different states as can be seen in the insets of Fig. 3(d): the ground state of the 1BDBH model exhibits a checkerboard pattern, while the one of the 1.5BDBH is instead in a striped configuration. This illustrates two key points: Approximating the dipolar quantum simulator with lowest-band models can lead

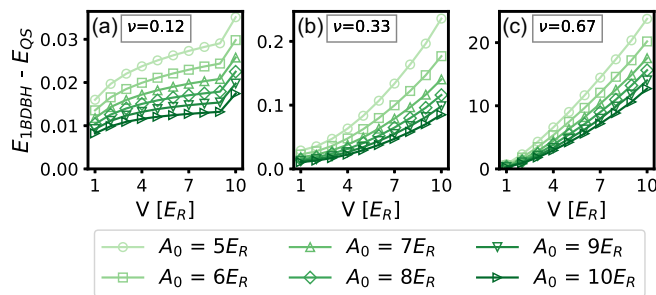


FIG. 2. Energetics of the dipolar quantum simulator: (a)–(c) Difference in the ground state energy between the 1BDBH model (E_{1BDBH}) and the continuous-space quantum simulator (E_{QS}), as the filling fraction ν increases.

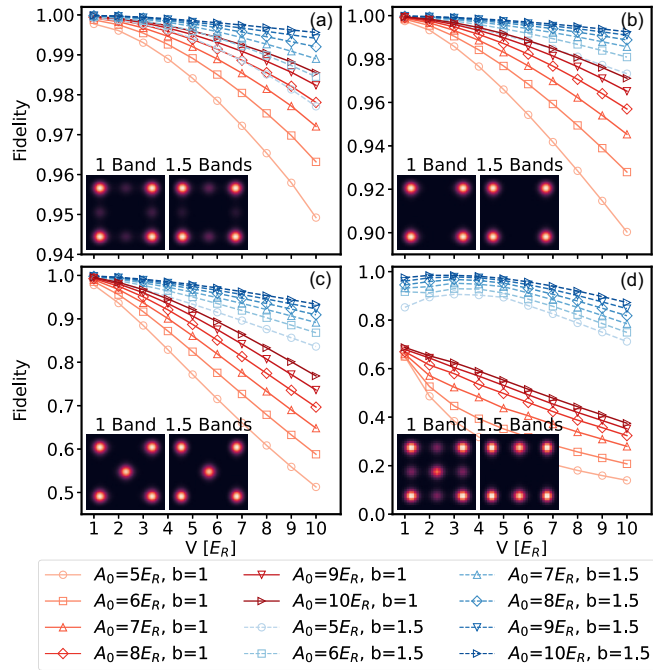


FIG. 3. Improvement of the quantum simulator accuracy for the higher-band model. Many-body fidelity between continuous-space and 1-band or 1.5-band lattice model in a 3×3 geometry as a function of A_0 and V for (a) $\nu = 0.33$, (b) $\nu = 0.44$, (c) $\nu = 0.56$, (d) $\nu = 0.67$. The insets show the particle density of the single- and 1.5-band dipolar BHM for the values of $A_0 = 5E_R$, $V = 10E_R$.

to significant errors in high-density situations. Conversely, the setup is already equipped to handle richer, higher band models without extra adjustments.

Another key factor that affects the properties of the ground state in the quantum simulator is system geometry. Depending on particle number and lattice geometry, strong repulsion may make the particle ordering incommensurate. This can lead to spontaneous lattice symmetry breaking which generates quasidegenerate ground states. Two examples of lattice quasidegeneracies are shown in Fig. 4(a), quantified as the relative gap between the ground state and the first excited state at the four extremal values in our (V, A_0) -parameter range (for the rest of the geometries, see the Supplemental Material [89]). Two types of states where V has opposite effects (stabilizing vs destabilizing) can be identified. The first type consists of geometries that can accommodate the ground state in the most symmetric configuration in the localized limit [e.g., four isolated particles in the corners and none in the center as in Fig. 4(b)]. These states preserve all discrete symmetries of the lattices, such as C_4 rotations, reflections, and inversions, which makes them very stable as confirmed by a large gap to excited states. The second type, instead, encompasses geometries with incommensurability, e.g., $N = 3, 5 \times 5$ lattice shown in Fig. 4(c). For these states, localizing forces such as lattice potential and repulsions clash with the available minima provided by the lattice symmetries. In milder cases, this favors a more delocalized ground state which does accommodate the symmetries but can be easily excited to similar states of quasidegenerate energies. In more severe cases (e.g., $N = 6, 3 \times 3$ and 3×4 lattices), a total breaking of rotational

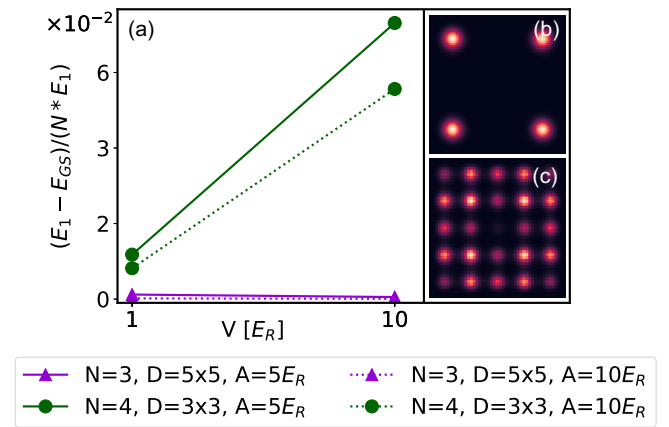


FIG. 4. Effect of lattice depth and dipolar interaction strength on incommensurability. (a) Relative energy differences per particle (N) between the first excited state (E_1) and the ground state (E_{GS}) in the 1BDBH model. Insets: particle density of (b) a commensurable state with $N = 4$, $D = 3 \times 3$, $A_0 = 10E_R$, $V = 10E_R$ and (c) an incommensurable state for $N = 3$, $D = 5 \times 5$, $A_0 = 5E_R$, $V = 1E_R$.

symmetries occurs, leading to a ground state partitioned into multiply degenerate sectors, e.g., two opposite checkerboard patterns, a feature known in extended BH models for states above half filling [109–111]. These results demonstrate that DDI not only offer an experimental platform to realize multi-band models, but in conjunction with different 2D geometries can also produce ground-state (quasi)degeneracies that are important ingredients to achieve exotic quantum states, i.e., with topological features. This is a feature exclusive to quantum simulators in 2D and higher dimensions.

Discussion and outlook. We have presented a comprehensive analysis of the accuracy of 2D dipolar quantum simulators by performing quantitative comparisons between continuous-space models of experimental setups and effective lattice models in a wide range of relevant lattice depths, interaction strengths, and filling fractions. Our study highlights that ultracold dipolar systems can be a very powerful instrument to reach regimes of multiband occupation and thereby probe more realistic, complex long-range interacting lattice models in 2D. The population of higher bands can drastically alter ground-state properties, e.g., turning a checkerboard phase into a striped one. In general, regimes of high interaction strengths, shallow lattices, and high fillings should generate the richest multiband physics. While highly symmetric states could be simulated with greater accuracy, incommensurability effects unique to 2D landscapes emerge from the competition between spatial geometry and localizing interactions and potentials, and can drastically alter spectral features. As a consequence, quasidegenerate ground states can arise, which can be completely modified by the presence of higher-band contributions. These findings should be useful for the simulation of 2D models whose unconventional physics emerge from degenerate states, like Hall systems, flat-band systems, or frustrated magnets. They could even prompt the question of whether lowest-band descriptions are sufficient to encompass the most exotic physics of lattice models systems, for instance in solid state settings, which interact via

even longer ranged couplings such as unscreened or weakly screened Coulomb forces, e.g., in low-dimensional or thin-film systems. Our results showcase the enormous possibilities offered by ultracold dipolar quantum simulators to reproduce these multiband lattice models.

Our study, based on a rigorous, quantitative comparison between lattice and continuous-space descriptions, should provide a reliable blueprint for the correct realization of long-ranged quantum simulators. While we have focused on repulsive interactions in two dimensions, we expect a rich physics to arise for attractive regimes and different spatial geometries, too. This is particularly important in light of discoveries of interesting new phases in attractive dipolar BHM models such as exotic quantum liquids [47,82,112] and self-bound quasicrystalline order [113]. In particular, a key question to address will be the treatment of singularities

arising for DDIs at zero distance, which can occur in continuous space but are truncated by the lattice formulation. Our approach of quantitatively comparing continuous-space and lattice descriptions by calculating many-body overlaps should shed light on those issues.

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