Unveiling Emergent Crystal Orders of Incommensurate Dipolar Bosons in One-Dimensional Lattices using Full Distribution Functions

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We explore the ground-states of a few dipolar bosons in optical lattices with incommensurate filling. The competition of kinetic, potential, and interaction energies leads to the emergence of a variety of crystal state orders with characteristic one- and two-body densities. We probe their transitions and construct the emergent state diagram as a function of the dipolar interaction strength and the lattice depth. We demonstrate that the crystal state orders can be observed using the full distribution functions of the particle number which we extract from simulated single-shot images.

The experimental realization of stable Bose-Einstein condensates (BECs) of dipolar atoms [1–6] and molecules [5, 6] provides new perspectives to study the phase transitions in correlated quantum systems [7, 8]. The dipole-dipole interactions are of anisotropic and long-range nature causing a plethora of new phenomena absent in conventional BEC, e.g., directional elongation [9–11] and geometric stabilization [9, 10, 12–14]. The lower dimensionality results in additional physical features: p-wave superfluidity [15, 16], Luttinger-liquid-like behavior [17–20] and anisotropy in curved geometries [21–23].

Trapped atoms in optical lattices serve as quantum simulators for condensed matter systems [24–34], exploiting the precise experimental tunability of these quantum systems. Even few-particle systems have been experimentally studied providing a bottom-up access to many-body physics [35–37]. The interplay between anisotropic long-range interaction and contact interaction in dipolar bosons results in the emergence of new phases: Besides the usual superfluid and Mott-Insulator phases, a density wave phase (DW) [38, 39], characterized by an alternate filling of lattice sites and a supersolid phase [40–44], with coexistent DW structure and superfluidity, and more exotic phases such as a Haldane insulating phases [39, 45], checkerboard phases [38, 46] and Mott solids [47] were predicted. Dipolar atoms with strong interactions feature a crystal state (CS) [17, 21, 22, 48–50, 52, 53].

In this letter, we investigate the plethora of crystal orders that emerge in one-dimensional lattices incommensurately filled with dipolar bosons and put forward protocols to detect them experimentally. Crystal states with different orders emerge for different strengths of the dipolar interaction, due to a competition between kinetic, potential, and dipolar interaction energies. We demonstrate that all the emergent crystal orderings can be identified using the full distribution functions of the position-dependent particle number operator extracted from absorption or single-shot images. We study a few dipolar atoms in a one-dimensional optical lattice and determine the ground-state properties numerically with MCTDHB [59, 60] implemented in the MCTDH-X software [61–63]. Arbitrarily strong interacting systems can be investigated with MCTDHB [64–71] allowing us to explore the full range of interaction strengths and observe two distinct crystal orders. We specify two observables to characterize these distinct orders of the crystal state and compute the state diagram, i.e., the finite-size analog of the phase diagram in the thermodynamic limit. We establish experimental protocols for the detection of the state diagram based on the full distribution function, the variance, and a binning analysis of single-shot images [52, 72–74].

We consider polarized, dipolar bosons in a quasi-one-dimensional lattice potential, $V_{d} = V \sin^2(\kappa x)$, with a depth $V$ and a wave-vector $\kappa$. A tight transversal confinement with a characteristic length $a_{1}$ prevents an excitation into the transverse direction and ensures the quasi-one-dimensionality of the system. The interaction is purely dipolar, $V_{\text{int}}(x_{i} - x_{j}) = g_{d}/|x_{i} - x_{j}|^3$; the dipolar interaction strength, $g_{d}$, is $g_{d} = d_{d}^2/4\pi\varepsilon_0$ for electric dipoles and $g_{d} = d_{m}^2\mu_{0}/4\pi$ for magnetic dipoles, $d_{m}$ is the dipole moment, $\varepsilon_0$ the vacuum permittivity, and $\mu_{0}$ the vacuum permeability [75]. For large separations, $|x_{i} - x_{j}| \gg a_{1}$, we recover the far-field dipole-dipole interaction $\sim 1/r^3$ and for small separations, $|x_{i} - x_{j}| \ll a_{1}$, the transversal confinement introduces a short-scale cutoff $\alpha \approx a_{1}^{-3}$ [49, 76, 77]. We make all quantities dimensionless by expressing them in terms of the lattice recoil energy for particles of mass $M$, $E_{R} = \hbar^2\kappa^2/2M$. In this work, we set the cutoff $\alpha = 0.05$ which corresponds to an aspect ratio $\gamma = 25.6$ and consider $N = 8$ bosons. We impose hard-wall boundary conditions to restrict our lattice to $S = 5$ sites. Our setup can be generalized for larger ensembles.

We analyze possible orderings in the crystal state with the density $\rho(x) = \langle \Psi^\dagger(x) \Psi(x) \rangle$ as a function of the interaction strength $g_{d}$ [Fig. 1(a)]. For $g_{d} = 0$, we obtain a pure superfluid state ($SF$). As $g_{d}$ increases,
FIG. 1. (a) One-body density $\rho(x)$ as a function of dipolar interaction strength $g_d$ for a lattice depth $V = 8$. For small interactions $g_d \lesssim 0.8$, in the $SMI$ state, the density exhibits a five-fold structure. As $g_d$ increases, the density develops a twofold splitting in the doubly-occupied central three wells displaying the onset of $SMI \rightarrow KCS$ transition. For even larger $g_d$, the density distribution transitions to a pattern with alternating single and double occupations. This signifies the $DW$ transition and formation of $DWCS$ state. See Supplementary Information (SI) [88], Sec. S1 for the momentum space one-body density. (b) Natural occupations (plotted cumulatively) as a function of interaction strength $g_d$. For small $g_d$, the $SF$ fraction results in the dominance of $\lambda_1$. With increasing $g_d$, the fragmentation increases as several $\lambda_{<1}$ become significant. Beyond the $SMI \rightarrow KCS$ transition, the system is maximally fragmented with $M = 8$ orbitals populated almost equally. Both $x$-axis in logscale.

the incommensurate setup implies the absence of a pure Mott-Insulator state ($MI$) since a $SF$ coexists with the $MI$ [78]. This coexistence of $MI$ and $SF$ (henceforth $SMI$) is seen in the structure of $\rho(x)$: the two outer wells have a smaller population than the central wells; $N = 5$ atoms in a $MI$ state coexist with $N = 3$ bosons in the $SF$ fraction. The $SF$ localizes in the central wells because this minimizes the kinetic energy in our setup with hard wall boundaries.

The crystal transition occurs at $g_d \approx 1$: due to repulsive dipolar interactions, the bosons avoid each other and minimize their overlap to save interaction energy. The one-body density [Fig. 1(a)] exhibits a splitting of the density in the doubly occupied central wells — a signature of onset of the crystal transition. In terms of bosons occupation per site, the crystal state is ordered as $1, [11], [11], [11], 1$. Here, a two-hump density in doubly-occupied lattice sites in the crystal state is represented as $[11]$. Since the double occupation of the three central wells is a result of the kinetic energy term in the Hamiltonian, we term this state “kinetic crystal state” ($KCS$).

Upon a further increase of the interaction strength $g_d$, the repulsive tail of the long-range dipolar interaction overcomes the kinetic energy and makes the double occupation of adjacent sites energetically unfavorable [Fig. 1(a)]: instead of nearest neighbors, next-nearest neighbors are doubly occupied in a density-wave-ordered structure at $g_d \gtrsim 3$. For our setup, a pure density-wave-order would have the occupations $2, 1, 2, 1, 2$. Due to the strong dipolar interaction, the bosons density in doubly occupied sites is spatially split and a density-wave crystal state ($DWCS$) with occupations $[11], [11], [11], [11]$ is obtained. The $KCS$ and the $DWCS$ are among possible crystal orders and hence subsets of a general crystal state $CS$. Here, and henceforth, we use the label $CS$ for a crystal state in either the $KCS$ or the $DWCS$ arrangement.

For very large values of the interaction $g_d > 15$, the long-range interactions overwhelm the lattice potential [SI [88], Sec. S2]. Consequently, the $DWCS$ gradually transmutes to an equispaced crystal state where the bosons are not localized around the potential minima anymore (not shown). See SI [88], Sec. S3 for other possible crystal orders at different particle numbers and lattice sizes.

The various crystal arrangements of the atoms with respect to the lattice can be obtained from a purely classical model [SI [88], Sec. S3]. However, the many-body calculations we present are necessary to capture the quantum properties of the crystal state: many modes do contribute to the quantum field of the crystal state (cf. Fig. 1) and thus its properties can be assessed only through the analysis of a realistic model of the many-body wavefunction. Moreover, the classical description does not contain a $SF$ or $MI$ state so the transition from a non-crystal to a crystal order cannot be obtained from a classical model.

To unveil the mechanisms underlying the localization and coherence in the emergent states, we now discuss the two-body density $\hat{\rho}_2(x_1, x_2) = \langle \Psi | \hat{\Psi}(x_1) \hat{\Psi}(x_2) | \Psi \rangle$ for characteristic values of $g_d$ (Fig. 2). Unlike the particle arrangement corresponding to the one-body density [Fig. 1(a)], our analysis of the two-body density exhibits true quantum many-body properties of the crystal state: the two-body densities in Fig. 2(b)–(d) — unlike for classical, semi-classical, and mean-field models — cannot be represented as a product of one-body densities.

For small interaction strength in the $SF$ ($g_d = 0.0005$) the maxima of $\rho^{(2)}$ are nearly uniformly distributed where both arguments $x_1$ and $x_2$ are in the vicinity of a minimum of the lattice potential [Fig. 2(a)]. For a larger interaction, $g_d \approx 0.1$, a partial depletion along the diagonal of $\rho^{(2)} (x_1 \approx x_2)$ occurs. This depletion results from the formation of an $MI$ that coexists with a $SF$ fraction [Fig. 2(b)]. At even stronger interactions, $g_d = 1.5$, the bosons in the doubly-occupied central wells crystallize forming the $KCS$. Here the diagonal of $\rho^{(2)}$ is completely depleted, $\rho^{(2)} \approx 0$ for $x_1 \approx x_2$: a correlation hole is formed, the probability of detecting two bosons at same position ($x_1 = x_2$) becomes negligible. The split maxima in the three central wells result from the on-site
interaction-driven splitting $2 \rightarrow 11$. For $g_d \approx 6$, the system is in the DWCS [Fig. 2(d)]. A split inter-site structure of the two-body density $\hat{\rho}^{(2)}$ is now present for every odd site of the lattice potential. The diagonal depletion is larger compared to the KCS [compare Fig. 2(c) and (d)] for $x_1 \approx x_2$. The non-uniform distribution of the maxima of $\rho^{(2)}$ clearly signals the DWCS.

When the interactions increase even further, the DWCS – to minimize the interaction energy – transforms into a crystal state (not shown) where the distribution of the maxima in both $\rho(x)$ and $\rho^{(2)}(x_1, x_2)$ becomes equispaced and independent of the underlying lattice potential. This crystal state for very strong interactions ($g_d \gtrsim 15$) is different from the SMI, the KCS, and the DWCS, since the distribution of maxima of the densities is not dictated by the minima of the lattice potential.

The transition from the SMI to the KCS and the DWCS depends also on the lattice depth $V$. To address the role of the lattice depth $V$ and the interaction strength $g_d$, we construct the state diagram of the system as a function of $g_d$ and $V$. The SMI $\rightarrow$ CS transition can be determined from a state order-parameter constructed from eigenvalues of the one-body reduced density matrix (RDM) as defined in Ref. [52]. The first order RDM is defined as

$$\hat{\rho}^{(1)}(x, x') = \langle \Psi | \hat{\Psi}^\dagger (x) \hat{\Psi} (x') | \Psi \rangle = \sum_i \lambda_i \varphi_i^*(x) \varphi_i(x'). \quad (1)$$

By diagonalizing $\hat{\rho}^{(1)}$, the eigenvalues $\lambda_i$ (natural occupations) and eigenfunctions $\varphi_i(x)$ (natural orbitals) are obtained. The values $\lambda_i$ determine the degree of condensation or fragmentation of a state. If a single natural occupation is macroscopic ($\lambda_1 \approx N$), the system is condensed [79] and if multiple $\lambda_i$s are macroscopic, the system is fragmented [80, 81].

The natural occupations are shown as a function of the interaction strength in Fig. 1(c). For small interactions, $0 < g_d < 0.002$, the system is in a condensed SF and a single natural orbital is macroscopically occupied ($\lambda_1 \approx N$). With increasing interactions $0.002 < g_d < 2$, the system fragments and multiple natural orbitals have a macroscopic occupation. The occupations change gradually as the interactions increase and for $g_d \gtrsim 2$ the crystal state is reached and $m = N$ natural orbitals are (almost) equally populated [Fig. 1(b)]. The equal importance of the natural orbitals is a hallmark of the many-body features of the crystal state; it implies that the density matrices of higher order, $\hat{\rho}^{(p)} (p > 1)$ are not representable as products of first-order density matrices $\hat{\rho}^{(1)}$.

Thus the determination of quantities such as the phase diagram and the full distribution function of the atom number operator (see below) require a many-body model and cannot be achieved through the classical model we present in the SI [88], Sec. S2.

We now define the crystal state order-parameter $\Delta$, (see Ref. [52])

$$\Delta = \sum_k \left( \frac{\lambda_k}{N} \right)^2, \quad (2)$$

where $\lambda_k$ is the $k$th natural occupation. The maximal value, $\Delta = 1$, is obtained for the SF, while the CS is identified by the minimum value, $\Delta = \frac{1}{N}$. Hence, for the $N = 8$ system at hand $\Delta \rightarrow 0.125$ characterizes the CS transition. Fig. 3(a) shows the plot of $\Delta$ as a function of $g_d$ and $V$ clearly displaying the transition from the SMI state to the CS state.

For small interactions $g_d$ and a shallow lattice depth $V$, the bosons are fully condensed into a SF and $\Delta \approx 1$. With increasing $g_d$ and/or $V$, the SMI forms; fragmentation and – consequently – a reduction in the value of $\Delta$. Further increase of $g_d > 1$ decreases $\Delta$ gradually towards its minimum value $\Delta = 0.125$ for all values of $V$ marking the onset of the KCS. When $\Delta$ reaches its minimum, the maximally (eightfold) fragmented CS is reached; the orderings of the CS that we analyze in the following are the KCS or the DWCS. Importantly, by analyzing $\Delta$ alone, the KCS $\rightarrow$ DWCS transition cannot be identified.

To identify the KCS $\rightarrow$ DWCS, we use the population imbalance of even and odd sites defined as

$$\Theta = \frac{1}{N} \sum_{o,e} \langle n_o \rangle - \langle n_e \rangle, \quad (3)$$

where $o$ and $e$ label odd and even lattice sites, respectively, and $\langle n_o \rangle$ and $\langle n_e \rangle$ their respective population. The
FIG. 3. Characterization and detection of the KCS and the DWCS. (a) Crystal order parameter $\Delta$ as a function of interaction strength $g_d$ and lattice depth $V$. The maximum $\Delta = 1$ correspond to the completely condensed SF. The SMI is revealed by intermediate values of $\Delta$. The minimum value of $\Delta = \frac{1}{2} = 0.125$ corresponds to a CS thereby characterizing its formation. The $SMI \rightarrow KCS$ transition boundary is indicated by the continuous line ($\Delta = 0.2$) while the $KCS \rightarrow DWCS$ obtained from $\Theta$ [Panel (b)] is indicated by the dashed line. (b) Imbalance parameter $\Theta$ as a function of $g_d$ and $V$. Both SMI and KCS correspond to low values of $\Theta$. The transition to the maximum value of $\Theta$ indicates the $KCS \rightarrow DWCS$ transition. The continuous line displays the transition boundary ($\Theta = 3$) while the dashed line shows the $SMI \rightarrow KCS$ transition obtained from $\Delta$ [Panel (a)]. (c–e) Full distribution functions $P_n(x)$ as a function of the interaction strength $g_d$ for a barrier height of $V = 8$ evaluated from 10000 single-shot images. The structure in the probability to find zero particles $P_0(x)$ and one particle $P_1(x)$ resembles that of the one-body density [compare Fig. 1(a)]. The vanishing of $P_2(x)$, the probability of finding two particles at $x$, clearly exhibits the transition to the CS. At large interactions, $g_d \gtrsim 6$, $P_0(x)$ and $P_1(x)$ exhibit a density wave pattern. This pattern along with vanishing $P_2(x)$ reveals the DWCS state. See SI [88], Sec. S4 for the complementary full distribution functions in momentum space. All x-axis in logscale.

even-odd imbalance $\Theta$ is maximal for the density mod-
ulation corresponding to the DWCS state. Fig. 3(b) shows $\Theta$ as a function of $g_d$ and $V$ to characterize the KCS → DWCS transition. The small imbalance for small values of $g_d$ results from the localization of the atoms in the central wells. For larger $g_d$, $\Theta$ becomes small since the SMI possesses a uniform density.

As $g_d$ increases further, an increase to maximum even-
odd imbalance indicates the KCS → DWCS transition. The $KCS \rightarrow DWCS$ transition shows a stronger dependence on $V$ compared to $SMI \rightarrow KCS$ transition. A shallower lattice potential favors the $KCS \rightarrow DWCS$ transition at lower $g_d$ while deeper lattices require larger $g_d$ for the transition, Fig. 3(b).

We now discuss an experimental protocol to detect all the emergent states and thereby the state diagram presented above using standard imaging [82–86]. These so-called single-shot measurements correspond to a projective measurement of the wavefunction. Ideally, the images contain an instantaneous snapshot of the position of all $N$ particles distributed according to the $N$-particle probability distribution $|\Psi|^2$. Here, we compute a set of single-shot simulations from our MCTDHB-groundstate wavefunctions [72–74, 87] and evaluate the full distribution functions of the particle number, i.e., we quantify the probability $P_n(x)$ to detect $n$ particles at positions $x$ [Fig. 3(c–e)].

In the delocalized $SMI$ several particles can be de-
tected in the same site with a significant probability: $P_n(x)$ are nonzero for $n \leq 2$. When the KCS is reached at $g_d \approx 1$, the bosons become completely separated and localized resulting in $P_{n \geq 2}(x) \approx 0$. The transition from the SMI via the KCS to the DWCS with increasing interaction strength $g_d$ is characterized unequivocally through the analysis of the full distribution functions $P_0(x), P_1(x)$ and $P_2(x)$. While $P_0$ and $P_1$ exhibit the distribution patterns of the KCS and the DWCS, $P_2 \approx 0$ signals the bosons complete isolation in crystal states. The results of Fig. 3(c–e) show a good agreement with the ones of Fig. 1(a) and Fig. 3(a–b), demonstrating the $KCS$ and $DWCS$ transition for the same values of $g_d$.

The simultaneous presence of density-wave order in $P_{0/1}$ and isolation, $P_{n \geq 2} \approx 0$, can thus experimentally identify the KCS and the DWCS (See SI [88], Sec. S4 for $P_{n \geq 3} \approx 0$).

An alternative experimental protocol using the variance of single-shot measurements to quantify the order parameter $\Delta$ [52, 73] intertwined with a binning of them to quantify the even-odd-imbalance $\Theta$ is described in the SI [88], Sec. S5.

We have thus proposed two viable experimental proto-
cols to detect the state diagram of dipolar bosons in lat-
tices with incommensurate filling, the crystal state tran-
sition, and the plethora of emergent crystal orders.

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In general, the dipole-dipole interaction potential in 1D also includes a contact (Dirac delta) term owing to the transverse confinement that can be safely neglected for strong interaction strengths [52].
This Supplementary Information discusses the one-body momentum density in Sec. S1, the kinetic, potential, and interaction energies in Sec. S2, illustrates complementary possible crystal orders for different lattice sizes and particle numbers with a classical model in Sec. S3, as well as the higher-order distribution functions of the particle number operator in real space, $P_{n>2}(x)$, and the full distribution functions of the particle number operator in momentum space in Sec. S4. An alternate detection protocol for the phase diagram [Fig. 3(a–b) of the main text] using the variance of single-shot images intertwined with a binning analysis is demonstrated in Sec. S5.

**S1. ONE-BODY MOMENTUM DENSITY**

Here, we analyze the one-particle momentum density for the same parameters as in Fig. 1 of the main text to assess the spatial coherence of the state, see Fig. S1.

For small to moderate interaction strengths ($g_d \lesssim 0.8$), the density exhibits a central momentum peak surrounded by a delocalized background distribution or small-amplitude peaks in a stripe-like topology. The amplitude and the width of the central peak reduce when the interaction strength $g_d$ increases. The presence of a localized central peak indicates the presence of the delocalized SF fraction that coexists with the localized MI state which in turn is responsible for the delocalized background distribution. When the transition to the crystal state occurs at $g_d \approx 1$, the momentum distribution completely loses the stripe-like topology forming a uniformly delocalized distribution: the crystal state is characterized by strong spatial confinement and decoherence, i.e., a vanishing superfluid fraction.

**S2. ENERGY**

The emergence of distinct quantum phases in dipolar interacting ultracold bosons is a result of the interplay between the interaction, kinetic, and potential energies. In this section we discuss this interplay of energies for the same system as shown in the main text, i.e., $N = 8$, $V = 8$, $S = 5$, as a function of the interaction strength, see Fig. S2.

The kinetic and potential energy clearly dominate over the interaction energy at small to intermediate interaction strength $g_d \lesssim 0.3$. This dominance is responsible for the formation of the SF and SMI states. The KCS state forms in the region, where the interaction energy and the potential energy are comparable, but smaller than
FIG. S2. The kinetic, potential, and interaction energies, $E_K$, $E_P$, and $E_I$, respectively, as a function of interaction strength $g_d$ for $N = 8$, $V = 8$, and $S = 5$. While the kinetic and potential energy $E_K + E_P$ dominate for small to intermediate interactions, the interaction energy $E_I$ clearly dominates for large $g_d$.

the potential energy, i.e., $E_K \approx E_I < E_P$ in Fig. S2 for $g_d \in [0.3, 2]$. For larger interaction energies the KCS order becomes energetically unfavorable and the DWCS state emerges. This DWCS state gradually melts as the interactions increase; when the interaction energy $E_I$ eventually dominates over the kinetic and potential energies, $E_I > E_P > E_K$, a “pure” crystal state CS is formed.

S3. POSSIBLE CRYSTAL STATES

In this section, we investigate a complementary model of classical dipolar particles in a lattice in order to highlight that there are several possible ways that dipolar particles may arrange their positions in a lattice as a function of the strength of the dipolar interactions between them.

The energy of classical dipoles in a lattice is given as

$$E_{\text{class}}(x_1, \ldots, x_N) = \sum_{i=1}^{N} V_{\text{el}}(x_i) + \sum_{i<j} V_{\text{int}}(x_i - x_j). \tag{1}$$

Here, $x_k$ is the position of the $k$-th particle, $V_{\text{el}}(x) = V\sin^2(kx)$ is the lattice potential energy, and $V_{\text{int}} = \frac{g_d}{|x_i - x_j|^{3+\alpha}}$ is the dipolar interaction between particles $i$ and $j$. As in the main text, we use $\alpha = 0.05$.

Since we consider the ground state of classical particles (at rest), there’s no kinetic energy contribution. Consequently, the kinetic crystal state (KCS) observed in the main text for quantum particles, is not present in our classical results below. However, we are able to demonstrate that the density-wave crystal state (DWCS) is a generic feature for classical dipolar particles in lattices of different sizes and different filling factors.

A. Classical model verification

We now discuss the results for the positions of classical dipolar particles obtained from minimizing the energy in Eq. (1). To verify the classical model, we begin our investigation with the same configuration, $N = 8$ particles in $S = 5$ sites, as discussed in the main text. In Fig. S3, we show the positions $x_1, \ldots, x_8$ that minimize $E_{\text{class}}$ as a function of the interaction for three values of the lattice depth, $V = 5, 8$ and $V = 15$.

The positions of classical dipoles in a lattice, due to the absence of kinetic do not feature a kinetic crystal state like the one observed for the quantum particles in the main text. However, the DWCS is obtained also in the classical model with the same ordering of particles ([11], 1, [11], 1, [11]) similarly to the quantum case in the main text. We infer that we can use our classical model to investigate the possible DWCS orders – also for other configurations of the number of particles $N$ and the number of lattice sites $S$. 
FIG. S4. Classical crystal orders for different incommensurate fillings. The (classical) position of the atoms $x$ as a function of the interaction strength $g_d$ is plotted for various atom numbers, $N = 8, 13, 18$, keeping the same $S = 5$ lattice size. The different fillings display different DWCS configurations $\ldots$, $[11], [1], [11], [1]$ in (a), $[111], [11], [111], [11], [111]$ in (b), and $[1111], [111], [1111], [111], [1111]$ in (c) as well as the transition from the DWCS to the CS state.

B. Density-wave crystal states for different filling factors

We now discuss the density-wave crystal states that we obtain from our classical model, Eq. (1), for the same number of lattice sites as in the main text, $S = 5$, but for different incommensurate filling factors, see Fig. S4.

The DWCS states with orders $[11], [1], [11], [1]$ and $[111], [11], [111], [11], [111]$ and $[1111], [111], [1111], [111], [1111]$ are observed for $N = 8$ and $N = 13$ and $N = 18$ particles in $S = 5$ wells in Fig. S4 panels (a), (b), and (c), respectively. Note that, for a larger particle number, the transition from a DWCS to a CS occurs for lower values of interaction $g_d$. This is because interaction energy per site grows faster compared to the potential and kinetic energies as a function of particle number at a fixed value of $g_d$.

C. Density-wave crystal states for different lattice sizes

We now discuss the density-wave crystal states that we obtain from our classical model, Eq. (1), for larger lattice sizes than in the main text ($S = 7, 9$), but for a similar incommensurate filling factor, see Fig. S5.

It is clearly seen that the DWCS with the configuration $\ldots$, $[11], 1, [11], 1, [11], \ldots$ prevails also for the case of lattices with a larger number of sites.

In summary, we find that there is a rich variety of density-wave crystal states of dipolar particles, already in the classical model that we investigated here. This underlines the importance of the experimental protocols that we put forward to detect these states in quantum systems.

S4. FULL DISTRIBUTION FUNCTIONS IN MOMENTUM SPACE $P_n(k)$ AND IN REAL SPACE FOR LARGER $P_{n>2}$

A. Full distribution functions in momentum space

In Fig. S6, we show the probability $P_n(k)$ to find $n$ particles with momentum $k$ for the same parameters as in Fig. (3)(c–e) of the main text. $P_0(k)$ and $P_1(k)$ shows identical distribution with the momentum density [Fig. 1(b)] of the main text but with opposite signs. Increasing $n$ shows a distinct narrowing of the distribution. For higher-order distributions $P_{n>2}(k)$, the maximum probability is centered at $k = 0$ but falls off sharply and the background is strongly reduced. We remark here, that the total number of events in the plots for $P_2(k)$ and, especially, for $P_{n>6}(k)$ is extremely small; thus the probability to find 5 or more particles at the same momentum is extreme small. For $P_6(k)$ the maximum count is $\mathcal{O}(10)$ and for $P_8(k)$ it is $\mathcal{O}(1)$ out of $N \times N_{\text{shots}} = 8 \times 10000 = 80000$. 

FIG. S6. Full distribution functions $P_n(k)$ in momentum space for the same parameters as in Fig. (3)(c–e) of the main text.

B. Higher order distribution functions in real space $P_{n>2}(x)$

In Fig. S7(a–b), we show the probability $P_n(x)$ to find $n$ particles at position $x$ for the same parameters as in Fig. (3)(c–e) of the main text for $P_{n>2}(x)$. Unlike that of the momentum space, the $x$-space probability becomes zero for $P_{n>2}(x)$. There is a very small region where $P_3(x) \neq 0$. $P_{n\geq 4}(x) = 0$ for all $x$.

S5. DETECTION OF THE CRYSTAL DENSITY WAVE FROM THE VARIANCE AND IMBALANCE IN SINGLE-SHOT IMAGES

Alternative to the analysis of the full distribution functions as shown in the main text, the emergent phases and the phase diagram for the one-dimensional lattices, incommensurately filled with dipolar bosonic atoms, can also be experimentally detected using the single-shot variance in combination with the single-shot expectation of the imbalance parameter $\Theta$ (Eq. (3) in the main text).

To characterize the transition from the $SMI$ state to the $CS$, we use the variance $\mathcal{V}$ of simulated single-shot measurements in position space i.e. deviations of each single-shot measurement from the mean-value of many single-shot samples (see Refs. [1, 2] for the mathematical definition of $\mathcal{V}$).

The variance strongly depends on the degree of localization, i.e., on how much the positions of the bosons fluctuate from image to image [1]. For increasing localization, the variance decreases. Since the $CS$ corresponds to a maximal localization of the system, $\mathcal{V}$ attains its minimum for the $CS$. Fig. S7(c) displays the variance $\mathcal{V}$ as a function of position $x$ for $V = 8$. A clear reduction of the variance $\mathcal{V}(x)$ is seen with interaction $g_d$ as the system transition from the $SMI$ to the $CS$. The variance integrated over space $\mathcal{V}$ hence can be used to determine the $CS$ transition experimentally.

Fig. S8(a) displays the variance $\mathcal{V}$ as a function of $g_d$ and $V$.

The $SF$ state is maximally delocalized, thus having a maximum value of $\mathcal{V}$. With increasing interactions, the $SMI$ state is reached and the partial localization of the bosons at the lattice sites leads to a decrease of $\mathcal{V}$. When the $CS$ is reached at large values of $g_d$, the bosons are completely localized. The vanishing overlap between the bosons forces $\mathcal{V}$ towards its minimum in the $CS$. The results of Fig. S8(a) are in good agreement with the ones of Fig. 3(a) of the main text, predicting the transition to the $CS$ state for the similar values of $g_d$ and $V$. The variance of single-shot images can thus be used to experimentally determine accurately the transition to the crystal state.

In order to detect the transition to the $CDW$ state, we evaluate the population imbalance parameter $\Theta$, Eq. (3) of the main text, by binning the single-shot samples: we count for each single-shot the number of atoms detected.
FIG. S8. Determining the CS and the DW transitions using single-shot simulations. (a) Variance of single-shots in real-space $V(g_d, V)$ as a function of $g_d$ and $V$. Every data point corresponds to variance $V$ computed from 10000 single-shot samples. $V$ is maximum for SF decreasing for SMI and reaches a minimum for CS. The distinct transition to minimum $V$ clearly displays the CS transition. (b) Imbalance obtained from binning single-shot simulation $\vartheta$. The distinct transition to high $\vartheta$ demonstrates the experimental detection of the DW transition.

The value of $\vartheta$ as a function of $g_d$ and $V$ is shown in Fig. S8(b). The transition to the DW state is clearly visible in the value of the $\vartheta$: the state diagram of the even-odd imbalance parameter $\Theta$ [Fig. 3(b) of the main text] closely resembles the behavior of the imbalance parameter $\vartheta$ obtained from the binning of single-shot measurements [Fig. S8(b)]. Our simulations of single-shot measurements correspond to the experimental imaging process. We have thus demonstrated a viable experimental protocol to detect both, the crystal state and the crystal density wave transitions and, therefore, a protocol to determine the state diagram of lattices that are incommensurately filled with dipolar bosons.

[1] B. Chatterjee and A. U. J. Lode, Phys. Rev. A 98, 053624 (2018).

[2] A. U. J Lode and C. Bruder, Phys. Rev. Lett. 118, 013603 (2017).