Superstripes and quasicrystals in bosonic systems with hard-soft corona interactions

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The search for spontaneous pattern formation in equilibrium phases with genuine quantum properties is a leading direction of current research. In this paper, we investigate the effect of quantum fluctuations—zero-point motion and exchange interactions—on the phases of an ensemble of bosonic particles with isotropic hard-soft corona interactions. We perform extensive path-integral Monte Carlo simulations to determine their ground-state properties. A rich phase diagram, parametrized by the density of particles and the interaction strength of the soft-corona potential, reveals supersolid stripes, kagome, and triangular crystals in the low-density regime. In the high-density limit, we observe patterns with 12-fold rotational symmetry compatible with periodic approximants of quasicrystalline phases. We characterize these quantum phases by computing the superfluid density and the bond-orientational order parameter. Finally, we highlight the qualitative and quantitative differences of our findings with the classical equilibrium phases for the same parameter regimes.

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I. INTRODUCTION

The emergence of self-organized patterns from an initially disordered phase is a central subject of investigation in several branches of physics, both in the classical and in the quantum regime [1–7]. Different physical processes, both in and out of equilibrium, may display a spontaneous formation of structures described by appropriate symmetries, order parameters, or topological indices.

A central direction of research is the investigation of complex correlated phases arising from tunable two-body interaction potentials. Long-range interactions decaying as a power law with variable exponents and signs [8] are a natural framework for probing quantum droplets [9–14], stripe phases [15], hexatic or smectic crystalline phases, and recently even supersolids [16–18]. Theoretical proposals demonstrated the possibility of observing quasicrystal patterns in BECs [19,20]. Importantly, recent experiments realized two-dimensional (2D) quasicrystalline lattices [21,22], paving the way to Bose glass phases [23–25]. Likewise, finite-range potentials with single or multiple intrinsic length scales became relevant due to their experimental implementation in cavities [26], Rydberg-dressed atoms [27,28], ultra-long-range Rydberg molecules [29–32], and spin-orbit coupled Bose-Einstein condensates [33]. A common phenomenon in such systems is clustering [34–37], which results from the joint effect of a two-body interaction regular at the origin and sufficiently high densities [20,38–41]. In the opposite case of singular interparticle interactions where clustering is forbidden, one usually expects well-known (super)fluid and insulating crystalline phases. However, the effects of quantum fluctuations in systems with hard-core and multiple length-scale potentials have yet remained unexplored.

In this paper, we investigate how the zero-point motion affects the phases of 2D bosonic systems in the presence of paradigmatic microscopic hard-soft corona interactions in the zero-temperature limit. We highlight the differences with the classical equilibrium phases mapping the quantum phase diagram for a wide range of densities and interactions. We analyze the (anisotropic) superfluid properties of the system at an intermediate value of the density between the fluid and the triangular crystal phase. In addition, upon increasing the density to the maximum packing fraction, we show that patterns with 12-fold rotational symmetry can be stabilized when setting the length scale of the interparticle interaction to specific values. Notably, we emphasize the qualitative structural, and quantitative differences of our results in the quantum system with the equilibrium phases derived from classical simulations.

II. MODEL

The Hamiltonian describing a 2D system composed of \(N\) identical bosons of mass \(m\) is

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_{r_i}^2 + \sum_{i<j}^{N} V(r_{ij}).
\]

The circularly symmetric interparticle hard-soft corona potential has the form

\[
V(r_{ij}) = \begin{cases} 
+\infty, & r_{ij} < \sigma_0, \\
\hbar^2 \varepsilon / m \sigma_0^2, & \sigma_0 \leq r_{ij} < \sigma_1, \\
0, & r_{ij} > \sigma_1.
\end{cases}
\]

In Eq. (2) \(r_{ij}\) is the radial distance between the particles located at \(r_i\) and \(r_j\), respectively. It is convenient to scale...
random tiling. Centroids of the worldlines and the corresponding
obtained upon initializing the simulation with a square-triangle
shots for the same control parameters
classical (left) and quantum (right) simulation equilibrium snap-
the 12-fold quasicrystal, where 12 main peaks are clearly visible.

\[ \varepsilon \]

The quantum regime is discussed in Fig. 3.

The soft-disk potential, in which \( \sigma_0 \) is absent, displays an
even richer physics in the quantum regime \( [41,46] \). Indeed,
pair potentials with a negative Fourier component favor the
formation of particle clusters, which can, in turn, crystallize to
form a so-called cluster crystal. At high particle densities, well
described by mean-field calculations, one finds modulated su-
perfluid states with broken translational symmetry in the form
of density waves \([47]\). Most interestingly, at low densities one
observes the emergence of defect-induced supersolid phases
in the vicinity of commensurate solid phases, as conjectured
by Andreev, Lifschitz \([48]\), and Chester \([49]\).

III. METHODS

We carried out PIMC simulations to determine the equilib-
rium properties of Hamiltonian \((1)\), hence attaining its exact
ground state in the limit \( T \to 0 \). Simulations have been per-
formed in the canonical ensemble with the number of particles
\( N \) in the range \( 100–400 \). We employ the worm algorithm
in continuous space to access genuine quantum macroscopic
observables such as the superfluid fraction \([50–52]\).

An essential ingredient of the PIMC algorithm is the esti-
mate of the many-body density matrix at high temperature.
To accurately account for the hard-soft corona interaction we
first perform a pair-product approximation and then separate
the contribution of the hard core and the soft core of the
interaction in Eq. \((2)\) into the pair action

\[
u_p(\rho(r, r', \beta)) = -\log\left( \frac{\rho(r, r', \beta)}{\rho_0(r, r', \beta)} \right) = u_{pHC} + u_{pSC} \quad (3)
\]

In Eq. \((3)\), \( \rho(r, r', \beta) \) is the pair-density matrix in the center-
of-mass frame interacting through Eq. \((2)\), and \( \rho_0(r, r', \beta) \)
is the density matrix for noninteracting particles. Here, \( r \)
\( (r') \) is the relative position of the pair of particles before
(after) the evolution in imaginary time. The exact numerical
calculation of the full pair-density matrix, while possible in
principle, suffers from the strong oscillatory behavior of high
angular momentum partial waves. We overcome this issue by
evaluating \( u_{pHC} \) via the well-known Cao-Berne equation for
the hard-core potential in two dimensions \([53,54]\). Then, we
calculate the contribution \( u_{pSC} \) of the soft-corona interaction
semiclassically within a WKB approach (see Supplemental
Material \([55]\) for the details of the implementation of the
algorithm, including Refs. \([56–57]\) therein).

The results in the quantum regime are compared in Fig. 1(c)
with the classical equilibrium phases. The latter are
obtained by employing a Monte Carlo algorithm based on
classical annealing methods \([57]\). In several cases we observe
distinct phases in the two regimes, confirming the relevance
of quantum fluctuations at low temperatures.
FIG. 2. High-density structural transition for an ensemble of boltzmannons interacting via the potential in Eq. (2) with \( \varepsilon = 9 \) when initializing the system from a triangular (black), SQRT (dark green), and a sigma phase (light green). (a) Energy per particle as a function of the scaled density \( \rho \sigma^2 \) for a system of \( N = 224 \) (triangular), \( N = 237 \) (SQRT), and \( N = 200 \) (sigma phase) particles at temperature \( T = 0.5 \hbar^2/m \sigma_0^2 \). At low density \( \rho \sigma^2 < 0.78 \) the ground state is a triangular lattice. At high density, the system is in the sigma phase. At \( \rho \sigma^2 > 0.78 \) the ground state is a triangular lattice. The transition between the two phases takes place around \( 0.78 < \rho \sigma^2 < 0.95 \) (gray region). The dashed lines show the position of the double tangent of the Maxwell construction. Insets: Snapshots of the boltzmannons interacting via the potential in Eq. (2) with \( \varepsilon = 9 \). (b) BO order parameter \( \chi_v \), of the ground state computed from Eq. (4) as a function of the scaled density across the transition with \( v = 6 \) (black) and \( v = 12 \) (green).

IV. RESULTS

To investigate the emergence of nontrivial crystalline phases we examine the Fourier intensity of the density of particles \( \rho(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) \) and the pair correlation function \( g(r) \) [6]. In addition, we introduce the bond-orientational order parameter (BOO) \( \chi_v \), which accounts for the local ordering of pairs of particles,

\[
\chi_v = \left( \sum_{b_j} \frac{1}{N_{b_j}^{(1)}} e^{i \delta_b} \right)^2.
\] (4)

In Eq. (4) \( N_{b_j}^{(1)} \) is the number of nearest-neighbor bonds of the \( j \)th particle, and \( \delta_b \) is the angle between a reference axis and the bond segment. The average is performed over all particles \( i \) belonging to the same time slice \( n \tau \) [see Fig. 1(a)]. We compute the respective dominant modes \( v \), for example, \( v = 6 \) in hexatic phases and the triangular crystal and \( v = 12 \) for a 12-fold rotational symmetry.

In Fig. 2 we discuss the high-density limit phase diagram for \( \sigma_1/\sigma_0 = 1.95 \) and \( \varepsilon = 9 \). In this regime, PIMC trajectories are only affected by zero-point motion fluctuations and it is reasonable to label those worldlines as boltzmannons rather than bosons. We refer to boltzmannons when particles are regarded as distinguishable, i.e., excluding particle exchanges [60,68,69].

Upon increasing \( \rho \sigma^2 \), we observe that a triangular lattice does not spontaneously turn into a dodecagonal quasicrystal, but a structural transition into a sigma phase is energetically favorable. It is known that a sigma phase consists of a periodic pattern that approximates the dodecagonal quasicrystalline phase [35,70]. Figure 1(b) depicts a square-triangle random tiling with prototiles given by triangles and squares (SQRT) [71] in agreement with previous classical simulations [65,66,66,72,73]. We compute the energy per particle for a wide range of densities and identify a wide coexistence region for \( 0.78 \lesssim \rho \sigma^2 \lesssim 0.95 \) via a Maxwell double-tangent construction. We confirm our results reducing the temperature to values well below the average kinetic energy per particle. The calculation of the BOO supports our observation of the transition from a triangular lattice at low densities into a 12-fold symmetric pattern. Differently from the classical case, BOO does not saturate to unitary values due to the zero-point motion.

In Fig. 3 we show the phase diagram of the system in the limit \( T \to 0 \) and taking the ratio \( \sigma_1/\sigma_0 = 2.5 \) for a wide range of \( \varepsilon \) and intermediate densities \( \rho \sigma^2 \). For small values of \( \varepsilon \) the ground state behaves as a usual superfluid (blue region) in agreement with the properties of a liquid with pure hard-core interactions (\( \varepsilon = 0 \)) [42,74]. Increasing the density, the system undergoes a transition from a superfluid to a
triangular crystal (gray region) around $\sigma_0^2 \rho \approx 0.32$. The light gray region in between represents a coexistence phase. In the triangular crystal, the worldlines are entirely localized. For the pair interaction of Eq. (2), clustering of bosons that takes place for a pure soft-disk interaction is prohibited for parameters considered in Fig. 3.

By increasing the density $\rho \sigma_0^2$ we observe a sequence of phases breaking continuous translational symmetry into different patterns. At $\rho \sigma_0^2 \approx 0.075$ we first have a transition superfluid to solid, followed by a reentrant transition solid to superfluid. Then, at $\rho \sigma_0^2 \approx 0.2$ the system enters into a stripe phase (red). A notable feature is that this is driven entirely by quantum fluctuations. A direct comparison for $(\varepsilon, \rho \sigma_0^2) = (7.0, 0.23)$ between the classical and the quantum phases proves that the delocalization of the worldlines stabilizes the stripe configuration, whereas the corresponding classical equilibrium phase is a disordered one. The snapshot of the configuration in the classical case and the centroids of worldlines in the quantum one are respectively shown in Fig. 1(c). To corroborate this statement we computed the average kinetic energy of the stripe phase to be $E_{\text{kin}}/k_B T \approx 42$, much larger than thermal fluctuations. The potential energy contributions in the two cases are instead comparable.

Within the central part of the lobe the system reorganizes into a labyrinth phase (orange) [67,75]. Upon further increasing $\rho \sigma_0^2$ the labyrinth phase is replaced by a kagome lattice (violet). Finally, for $\rho \sigma_0^2 \approx 0.35$, we encounter a phase coexistence phase region and again a triangular crystal for larger densities.

In order to fully account for the bosonic nature of the system, we include particle exchanges to calculate the superfluid fractions along the line with $\varepsilon = 8$ in Fig. 3. The superfluid fraction $f_S$ is computed via the winding number estimator

$$f_S^{(i)} = \frac{m}{\hbar^2} \frac{L_i^2}{N} \langle W_i^2 \rangle,$$

where $\langle \cdots \rangle$ denotes the thermal average of the winding number operator $W_i$ along the direction $L_i$ with the index $i = x, y$ [76,77]. The total superfluid fraction $f_S$ of the system is given by the trace of this tensor divided by the number of spatial dimensions of the system. The results are shown in Fig. 4 where we plot the superfluid fraction for different values of the scaled density $\rho \sigma_0^2$. Simultaneously, we extract the histogram of the permutations $P(L)$ involving $L$-bosons [55].

We find an insulating behavior for the triangular crystal at both low ($\rho \sigma_0^2 = 0.1$) and high densities ($\rho \sigma_0^2 = 0.45$), and the kagome crystal [Fig. 4(c)], which display vanishing superfluidity. For the latter we observe quasilocal exchanges with few particles, i.e., up to $L \approx 10$. Notably, stripes [Fig. 4(a)] display a supersolid character. Along the direction of the stripe we have $f_S^{(1)} = 0.71(7)$, and a finite, nonzero signal, perpendicular to them, $f_S^{(2)} = 0.35(6)$. Finally, coexistence phases at intermediate densities also display a finite $f_S$.

V. DISCUSSION AND CONCLUSIONS

We analyzed the properties of the phases of an ensemble of bosonic particles interacting via hard-soft corona potentials in the quantum degenerate regime. We demonstrated that the phases display qualitative and quantitative differences from the classical case, especially regarding the structural properties. For instance, intricate pattern formations such as stripe phases are stabilized by quantum fluctuations and concurrently exhibit supersolid behavior. Extensions of this work include the detailed analysis of the high-density and high-interaction limit of the phase diagram to investigate the (two-step) transition from the liquid and the kagome phase to the triangular lattice [43,78]. Another interesting line concerns the study of the Berezinskii-Kosterlitz-Thouless (BKT) transition from a superfluid to normal fluid at intermediate densities both in the liquid and the stripe phase, which might be relevant for the implementation of this model in experimental platforms such as Rydberg systems, cavities, or dipolar systems [19,79–82]. The interaction potential of Eq. (2) can be implemented, e.g., via microwave shielding techniques for the hard-core barrier [30–32], combined with a dressing scheme for the soft corona whose strength can be controlled via magnetic or optical Feshbach resonances through the coupling to ultra-long-range Rydberg molecular states [29,83].

Finally, we mention that our model is studied within a pure 2D setup in the absence of external confinement along the horizontal plane. It is to be expected that the introduction of trapping along any direction (possibly anisotropic) would change qualitatively the stability of fragile patterns such as the quasicrystalline phase [84]. These results pave the ground for general classifications of interaction potentials and phases...
with (quasi-)long-range orientational order, the identification of the order of phase transitions for a wide interval of densities, and interactions in the quantum regime.

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