Auxiliary-Field Monte Carlo Method to Tackle Strong Interactions and Frustration in Lattice Bosons

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We introduce a new numerical technique, the bosonic auxiliary-field Monte Carlo method, which allows us to calculate the thermal properties of large lattice-boson systems within a systematically improvable semiclassical approach, and which is virtually applicable to any bosonic model. Our method amounts to a decomposition of the lattice into clusters, and to an ansatz for the density matrix of the system in the form of a cluster-separable state—with nonentangled, yet classically correlated clusters. This approximation eliminates any sign problem, and can be systematically improved upon by using clusters of growing size. Extrapolation in the cluster size allows us to reproduce numerically exact results for the superfluid transition of hard-core bosons on the square lattice, and to provide a solid quantitative prediction for the superfluid and chiral transition of hardcore bosons on the frustrated triangular lattice.

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Introduction.—Models of strongly correlated bosons on a lattice (or lattice-boson field theories) play a central role in the description of quantum many-body systems, encompassing the whole of quantum magnetism (due to exact spin-boson mappings) [1,2] and including superconducting networks [3] and ultracold bosons in optical lattices [4,5] to cite some relevant examples. Large-scale numerical approaches, particularly those based on quantum Monte Carlo (QMC) calculations [6,7], have been instrumental in the understanding of the equilibrium properties of quantum magnets and strongly correlated bosons (see Refs. [8,9] for some recent examples). Nonetheless, the presence of frustrated couplings in the magnetic Hamiltonians, or, more generally, of gauge fields in the lattice-boson Hamiltonians, leads inevitably to a well-known sign problem for the worldline QMC approach [10]. Overcoming this limitation is an urgent problem, when considering the significant progress in the experimental study of bosonic frustration with quantum magnets [1,2] or ultracold atoms in artificial gauge fields [11,12]. Promising strategies in this direction, applicable to frustrated $S = 1/2$ spin models in their thermal disordered phase, are offered by diagrammatic Monte Carlo calculations [13–15] and numerical linked-cluster expansion [16,17].

In the face of the significant hurdles to simulate bosonic frustration, a valuable guiding principle to attack lattice bosonic field theories is to capture salient traits of their physics using states that are weakly entangled in real space. This principle is at the basis of the two most common approaches to interacting bosons: (i) Gutzwiller mean-field (MF) theory [5,18,19], used to predict phase diagrams of strongly correlated bosons, despite the fact that it eliminates any form of correlation and entanglement between spatial building blocks (single sites or clusters thereof); (ii) and c-field (CF) theory [20,21], which accounts at most for weak quantum effects, describing only regimes which have a classical analog, but nonetheless incorporate fluctuations when supplemented with stochastic treatments such as Monte Carlo calculations. Recently, we have shown [22] that quantum many-body systems at finite temperature exhibit a strong spatial separation between quantum coherent fluctuations—whose wavelengths are upper-bounded by a quantum coherence length $\xi_Q(T)$ that is finite as long as $T > 0$—and thermal fluctuations, whose wavelengths can be arbitrarily large upon approaching a critical point. In particular, degrees of freedom separated by a distance larger than ξ_Q are nearly separable: hence, the system admits a description in terms of states that possess short-range entanglement only, but which can exhibit classical correlations of arbitrary range. Clearly, one would need the complementary strengths of MF theory and CF theory to acquire a satisfactory description.

This Letter introduces a new, semiclassical numerical method—the bosonic auxiliary-field Monte Carlo (bAFMC) method—which is precisely designed to exploit the separation of scales between quantum and classical fluctuations at finite temperature. bAFMC breaks a lattice boson or spin system into clusters that are treated exactly, and which are further coupled via a fluctuating classical auxiliary field (AF) mediating classical correlations. Quantum fluctuations are faithfully described up to the length scale of a cluster, while a Monte Carlo treatment of the AF allows us to account for the thermal fluctuations at all length scales. The cluster decomposition introduces, therefore, an artificial cutoff in the wavelengths of quantum fluctuations, that can be removed via an extrapolation of the

results to infinite cluster size. We validate our approach, showing that it can reproduce quantitatively the thermodynamics (including critical phenomena and broken symmetry phases) of strongly interacting lattice-boson problems, as exemplified by the Berezhinskii-Kosterlitz-Thouless (BKT) transition of hard-core bosons on a square lattice, and we further apply it to reconstruct the multiple phase transitions of hard-core bosons on the frustrated (or π-flux) triangular lattice.

Model Hamiltonian and path-integral treatment.—For the sake of concreteness, we shall focus on the case of the Bose-Hubbard model with arbitrary hopping terms

$$\hat{\mathcal{H}} = \sum_{i<j} \hat{h}_{ij} + \sum_i \hat{g}_i \tag{1}$$

where $\hat{h}_{ij} = -J_{ij}\hat{b}_i^\dagger \hat{b}_j + \text{H.c.}$ and $\hat{g}_i = U/2(\hat{b}_i^+)^2\hat{b}_i^2 - \mu\hat{b}_i^\dagger\hat{b}_i$. Here $\hat{b}_i$, $\hat{b}_i^\dagger$ are bosonic operators, and the indices i and j run on the sites of a d-dimensional lattice. In the most general case the matrix J_{ij} is Hermitian, and its complex matrix elements describe the presence of a gauge field. While motivated by the field of cold atoms [4,5,12] this model is also of immediate relevance to (frustrated) quantum magnetism when taking the limit $U \to \infty$, which produces a quantum $S = 1/2$ XY model [23].

Our approach starts by decomposing the lattice into clusters (see Fig. 1), implying a decomposition of the hopping matrix as $J_{ij} = \mathcal{J}_{ij} + \mathcal{L}_{ij}$, where $\mathcal{J}_{ij}$ is the matrix of the *intercluster* couplings, while $\mathcal{L}_{ij}$ contains only the *intracluster* couplings. The path-integral treatment of the Bose-Hubbard model [25] allows us to decouple the various clusters via a Hubbard-Stratonovich (HS) transformation, introducing an imaginary-time-dependent, complex auxiliary field $\Phi_i(\tau)$, which is defined on the sets $\mathcal{C}_c$ of "boundary" sites i of the clusters (labeled by the c index), satisfying the condition that $\mathcal{J}_{ij} \neq 0$ for some j. This leads then to the following form for the partition function (see Supplemental Material—containing Refs. [26,27]—for an explicit derivation [28]):

$$\mathcal{Z} = \int \mathcal{D}[\Phi_i(\tau)] \exp(-S[\Phi_i(\tau)]) \prod_c \mathcal{Z}_c[\{\Phi_{i\in\mathcal{C}_c}(\tau)\}], \tag{2}$$

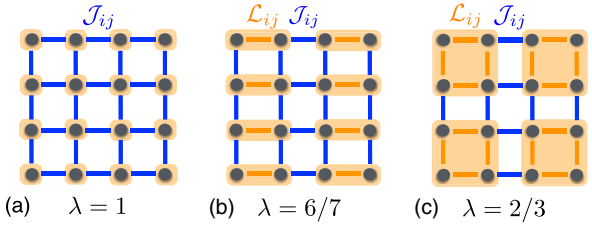

FIG. 1. Cluster decompositions of the square lattice with nearest-neighbor hoppings. Orange-shaded areas identify the clusters, with intracluster bonds $\mathcal{L}_{ij}$ marked in orange; the intercluster bonds $\mathcal{J}_{ij}$ are instead marked in blue. The λ parameter is the surface-to-bulk ratio of the cluster (see text).

where $S[\Phi_i(\tau)] = \int d\tau \sum_{ij} \Phi_i^*(\tau)(\tilde{\mathcal{J}}^{-1})_{ij}\Phi_j(\tau)$ is the action involving exclusively the auxiliary fields, while

$$\mathcal{Z}_c[\Phi_{i\in\mathcal{C}_c}(\tau)] = \text{Tr}[T_\tau e^{-\int d\tau \hat{\mathcal{H}}_c(\{\Phi_i(\tau),\Phi_i^*(\tau)\})}] \tag{3}$$

is the effective partition function of a single cluster: here T_τ is the imaginary-time ordering operator, and $\hat{\mathcal{H}}_c(\{\Phi_i(\tau), \Phi_i^*(\tau)\}) = \sum_{i,j\in c}\hat{h}_{ij} - \sum_{i\in\mathcal{C}_c}(\Phi_i(\tau)\hat{b}_i^\dagger + \Phi_i^*(\tau)\hat{b}_i) + \sum_{i\in c}(\hat{g}_i + K\hat{n}_i)$ is the effective single-cluster Hamiltonian, including the intracluster hopping, the coupling to the auxiliary field, and the local diagonal terms. Moreover, we have introduced the shifted matrix $\tilde{\mathcal{J}}_{ij} = \mathcal{J}_{ij} + K\delta_{ij}$, with $K = (1+\epsilon)|\Lambda_{\min}|$ and $\Lambda_{\min}$ the minimal (negative) eigenvalue of $\mathcal{J}$. An $\epsilon > 0$ assures the positive definiteness of $\tilde{\mathcal{J}}$, as required by the HS transformation. The shift K is then compensated by a complementary shift in the chemical potential appearing in $\hat{\mathcal{H}}_c$ [29].

Quantum mean-field approximation and auxiliary-field Monte Carlo method.—The expression Eq. (2) for the partition function (widely used as a basis of the field-theoretical treatment [25,30]) is exact, but impractical for a Monte Carlo sampling, since the single-cluster partition functions $\mathcal{Z}_c$ are generally complex objects, leading to a sign problem [31]. To cast the AF formulation of the partition function into a practical tool for numerics, an approximation is in order. A most natural one—turning $\mathcal{Z}_c$ into a positive real number—is to treat the AF as a *classical* complex field, namely, $\Phi_i(\tau) = \Psi_i$ independent of τ. Such an approximation amounts to decoupling clusters in their imaginary-time fluctuations: as discussed in Refs. [22,24], this is equivalent to decoupling their quantum fluctuations via a so-called cluster *quantum* mean-field (cQMF) approximation (namely, a MF approximation restricted to quantum fluctuations only). This corresponds to casting the density matrix $\hat{\rho}$ of the system (such that $\mathcal{Z} = \text{Tr}\hat{\rho}$) into the form

$$\hat{\rho} \approx \hat{\rho}_{\text{cQMF}} = \int \mathcal{D}[\Psi]P[\Psi] \otimes_c \hat{\rho}_c(\{\Psi_{i\in\mathcal{C}_c}, \Psi^*_{i\in\mathcal{C}_c}\}), \tag{4}$$

where $\mathcal{D}[\Psi] = \prod_{i\in\mathcal{C}}(d\Psi_i d\Psi_i^*/2\pi i)$ is the AF metric, $P[\Psi] = (\det X)^{-1}\exp[-\beta\sum_{ij}\Psi_i^* X_{ij}\Psi_j]$ and $\hat{\rho}_c = \exp[-\beta\hat{\mathcal{H}}_c(\{\Psi_i, \Psi_i^*\})]$. We have introduced the symbol $X = \tilde{\mathcal{J}}^{-1}$. Equation (4) is easily recognizable as a *separable* form for the density matrix [32], in which entanglement between clusters is absent; Eq. (4) actually expresses a strong form of separability, called Hamiltonian separability [22], which implies absence of entanglement *and* quantum correlations, while still describing classical correlations (according to the definition of Ref. [32]).

The partition function descending from the cQMF approximation, $\mathcal{Z} \approx \text{Tr}(\hat{\rho}_{\text{cQMF}})$, describes then an effective classical field theory for the AF, governed by the action

$$S_{\text{eff}}[\Psi] = \beta \sum_{ij} \Psi_i^* X_{ij} \Psi_j - \sum_c \log \mathcal{Z}_c[\{\Psi_{i\in\mathcal{C}_c}\}]. \quad (5)$$

This effective classical field theory results from integrating quantum fluctuations with wavelengths upper bounded by the linear size of the clusters, l_c. In the spirit of real-space renormalization group transformations, this latter scale can be seen as a moving cutoff, setting the boundary between the fully quantum and the effective classical description of the system. By sending l_c to infinity we recover the exact description of the system: as shown in Ref. [24], a quantitative extrapolation of the cQMF results towards the exact description can be achieved as a power law in the bulk-to-boundary ratio $\lambda = N_{\text{ext}}/(N_{\text{int}} + N_{\text{ext}})$, where N_{int} is the number of internal bonds to each cluster, while N_{ext} is the number of bonds connecting the cluster to the outside. The introduction of a cutoff scale for quantum fluctuations and entanglement is fundamentally justified at finite temperature by the finiteness of the quantum coherence length ξ_Q [22], beyond which two degrees of freedom can be considered as essentially (Hamiltonian) separable. The quality of the cQMF approximation is therefore controlled by the ratio between the two length scales l_c and ξ_Q [24]. Finally, it can be shown [28] that a *saddle-point* approximation to the effective action, Eq. (5), reproduces cluster MF (cMF) theory (albeit with modified couplings and chemical potential). Hence, the cQMF approximation is a clear improvement over cMF theory via the inclusion of intercluster classical correlations.

The bAFMC approach consists in solving numerically the effective classical field theory, described by the action $S_{\text{eff}}[\Psi]$, via Monte-Carlo sampling (see the Supplemental Material [28] for a detailed discussion). At zero temperature the saddle-point approximation to the classical auxiliary field becomes exact, so that in this limit the bAFMC approach reduces to a modified cMF theory [28]. Yet the finite-temperature behavior is captured by bAFMC beyond any mean-field description. Indeed the effective action S_{eff} (supplemented with a judicious cluster decomposition) possesses all the symmetries of the original Hamiltonian that are relevant to the expected critical phenomena [33], and it preserves the short-ranged nature of the original couplings [28]. Therefore, unlike in any mean-field approach, a Monte Carlo sampling of the fluctuations governed by $S_{\text{eff}}[\Psi]$ shall reproduce the correct nature of phase transitions or extended critical phases that one may expect in the original system.

Hard-core bosons on the square lattice.—As a first validation stage, we test the bAFMC approach in the case of hard-core bosons on the square lattice at half filling, corresponding to the quantum $S = 1/2$ XY model on the same lattice. The Hamiltonian is obtained as a limiting case of Eq. (1) with $U \to \infty$, $\mu = 0$, and $J_{ij} = J$ for i, j nearest neighbors on the square lattice, and zero otherwise. We introduce the reduced temperature $t = k_B T/J$. This

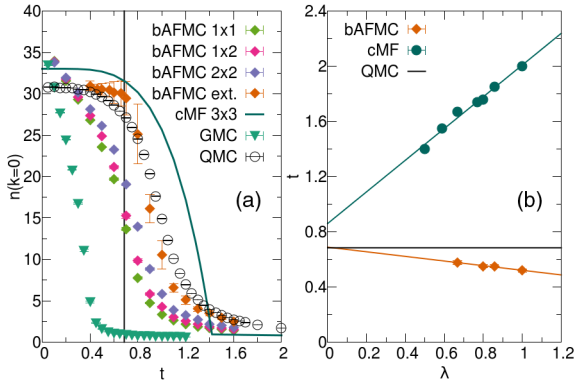

FIG. 2. (a) Comparison of exact QMC, bAFMC (for various cluster sizes, plus extrapolation), GMC, and cMF results for $n(k = 0)$ of hardcore bosons on a 12×12 lattice. (b) Cluster scaling of the BKT transition temperature from bAFMC, compared to the critical temperature from cMF; solid lines are linear fits, whose extrapolated $\lambda \to 0$ value is to be compared with the QMC value $t = 0.6854$ [34] (solid horizontal line).

Hamiltonian features a BKT transition at $t_{\text{BKT}} \approx 0.6854$ (estimated via QMC) [34], and an extended critical phase for $t < t_{\text{BKT}}$, which are both inaccessible to mean-field treatments. Moreover, the hardcore limit, while numerically favorable due to the restricted dimensions of the local Hilbert space, is the farthest possible from the classical limit of bosonic theories, and therefore possibly the hardest to describe quantitatively within a semiclassical setting.

Figure 2(a) shows the temperature dependence of the $k = 0$ peak in the momentum distribution, $n(k = 0) = \sum_{ij} \langle \hat{b}_i^\dagger \hat{b}_j \rangle / L^2$ for a lattice of size $L = 12$, as obtained via different methods: (i) Numerically exact QMC [35]; (ii) the cMF approach based on a 3×3 cluster [19]; (iii) the semiclassical approach of Ref. [36] [here dubbed the Gutzwiller Monte Carlo method (GMC)], which amounts to a Monte Carlo sampling of different Gutzwiller mean-field wave functions $|\Psi\rangle = \otimes_i |\psi_i\rangle$ weighted by the Boltzmann weight $e^{-\beta \langle \Psi | \hat{\mathcal{H}} | \Psi \rangle}$; and (iv) the bAFMC approach based on clusters of growing size from 1×1 up to 2×2. The latter two approaches have the common aspect of reducing to cMF theory at zero temperature (albeit a modified one in the case of bAFMC [28]). The cMF predicts an unphysical true condensation transition for a $2d$ system, whose temperature grossly overestimates the BKT temperature, and even an extrapolation in the size of the cluster turns out to be problematic (see below); on the opposite front, the GMC approach, while capturing correctly the BKT physics [36], significantly underestimates the transition, without offering any viable (e.g., cluster-based) strategy for further improvement. The bAFMC results, on the other hand, are the closest ones to the QMC method of the three approximation schemes considered here: even though the considered cluster decompositions give results which remain relatively far from the exact ones, a clear trend towards

the exact values is observed upon increasing the cluster size; an explicit QMC calculation shows that $\xi_Q < 1$ for $t \gtrsim 0.25$ [28], so that our largest clusters exceed this length. In particular, a systematic linear extrapolation in the λ coefficient can be made which reproduces quite closely the exact results—the linear form is justified by the boundary chemical potential shift, producing a linear effect in λ on the thermodynamics of single clusters. The residual discrepancy is a limitation of the very basic linear extrapolation scheme (imposed by the limited number of cluster sizes we considered), and it can still be systematically improved upon. Most importantly, irrespective of the cluster size all effective classical theories produced by the bAFMC approach possess a genuine BKT transition, whose critical temperature can be estimated from the expected critical scaling $n(k=0) \sim L^{7/4}$ (here, for system sizes $L = 12, 24$, and 36 [28]). The BKT temperatures so extracted are then plotted as a function of the λ parameter in Fig. 2(b): a simple linear extrapolation towards $\lambda = 0$ produces the estimate $t_{\mathrm{BKT}}(\lambda = 0) = 0.69(2)$, in very good agreement with the QMC estimate. A similar extrapolation of the critical temperature for the cMF condensation transition does *not* converge towards the QMC estimate, suggesting that, even within a cluster approach, the MF transition cannot be reliably used as an estimate of the quasicondensation transition of $2d$ hard-core bosons.

Hardcore bosons on the triangular lattice.—Having validated the bAFMC for hard-core bosons on the square lattice, we move on to apply it to an open problem of strongly correlated bosons in the presence of a frustrating gauge field, namely, the case of hard-core bosons on a triangular lattice (TL) at half filling with a π-flux [or Eq. (1) $J_{ij} = -J$ for nearest-neighbor sites, and other parameters as for the square lattice], corresponding to the antiferromagnetic $S = 1/2$ XY model on the same lattice. The ground state of the model displays three-sublattice long-range order, which entails the ordering of both the spin variables (bosonic phases) as well as of the spin chirality (bosonic plaquette current) $\kappa_\triangle = \sum (i\hat{b}_i^\dagger \hat{b}_j + \mathrm{H.c.})$, where the sum runs over oriented ij pairs on the elementary triangular plaquette. In the classical spin ($S \to \infty$) limit a broad consensus exists [37] about the existence of two thermal phase transitions: a lower-temperature BKT transition at T_{BKT} with quasicondensation at finite momentum on the corners of the Brillouin zone [$\pm \boldsymbol{Q} = \pm(4\pi/3, 0)$ and equivalent wave vectors], and a higher temperature *chiral* transition at T_c associated with the appearance of a vortex lattice: the latter is characterized by a divergence of the chirality structure factor $S_\kappa = L^{-2} \sum_{\triangle,\triangle'} \langle \kappa_\triangle \kappa_{\triangle'} \rangle$. Chiral ordering on the triangular lattice has been recently observed by cold-gas experiments in the bosonic classical limit (large occupancy with weak interactions) [38,39].

Our bAFMC investigation of the frustrated TL focused on three different cluster shapes: single site, triangular, and rhombic [see Fig. 3(a)]. The temperature dependence of the momentum distribution peak $n(\boldsymbol{Q})$ [shown in Fig. 3(a)] as well as that of the chirality structure factor S_κ (see Ref. [28]) are observed to depend rather weakly on the cluster shape around the BKT and chiral transitions: this is a clear signature that the range of quantum correlations in the thermal critical regime is strongly suppressed by frustration with respect to the case of the unfrustrated square lattice. Correspondingly, the estimates of the critical temperatures T_{BKT} and T_c extracted from finite-size scaling show a rather weak dependence on the λ parameter [see Fig. 3(b)], which gives further confidence in their extrapolation to $\lambda \to 0$. The separation between T_{BKT} and T_c increases when λ decreases, and their extrapolated values [$T_{\mathrm{BKT}}(\lambda = 0) = 0.272(7)$, $T_c(\lambda = 0) = 0.290(4)$] exhibit a sizable relative separation of 6%, to be compared with the separation of 2% in the classical spin limit [37]. This shows that quantum effects can strongly increase the delicate spin-chirality decoupling observed in classical frustrated magnets, making it potentially observable with state-of-the-art experiments on cold-atom quantum simulators [40].

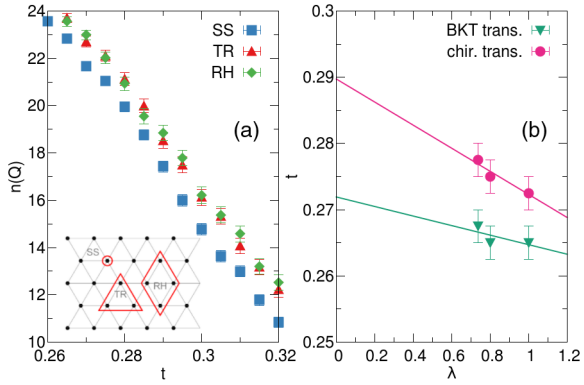

FIG. 3. (a) Momentum distribution peak $n(\boldsymbol{Q})$ of hard-core bosons on the 12×12 frustrated triangular lattice from bAFMC on different cluster sizes (pictured in the inset). (b) Cluster scaling of the BKT and chiral transition temperatures; solid lines are linear fits.

Conclusions.—We have introduced a new numerical approach (the bosonic auxiliary-field Monte Carlo method) based on a semiclassical approximation to the partition function, which eliminates any sign problem at the expense of the truncation of long-range quantum correlations beyond a given cutoff, set by a cluster decomposition of the lattice. This approximation is well controlled due the generically short-ranged nature of quantum correlations at finite temperature, and, most importantly, it can be systematically improved by moving the cutoff to larger length scales. Our approach positions itself among the methods which are limited by entanglement and quantum correlations—such as tensor-network Ansätze, including the density-matrix renormalization group [42]: while the success of the latter is mostly based on the weakness of entanglement in the ground state of physical Hamiltonians of interest, the success of our method exploits for the first

time the weak entanglement and quantum correlations present in *thermal* states. Access to larger clusters than the ones used here could be easily granted by the use of Lanczos reconstruction of the low-lying spectrum [43] (when treating sufficiently low temperatures) or by the recently proposed reconstruction of an effective auxiliary-field Hamiltonian from a limited sample of configurations [44]. The wide applicability of our approach to bosonic systems makes it a very suitable candidate to investigate prominent models of frustration, which are of central interest to quantum magnetism and quantum simulation with ultracold atoms.

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which is not well controlled in the $S = 1/2$ limit, and which may systematically underestimate quantum effects and, hence, overestimate the critical temperatures.

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