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Frustrated Extended Bose-Hubbard Model and Deconfined Quantum Critical Points with Optical Lattices at the Antimagic Wavelength

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The study of geometrically frustrated many-body quantum systems is of central importance to uncover novel quantum mechanical effects. We design a scheme where ultracold bosons trapped in a one-dimensional state-dependent optical lattice are modeled by a frustrated Bose-Hubbard Hamiltonian. A derivation of the Hamiltonian parameters based on Cesium atoms, further show large tunability of contact and nearest-neighbor interactions. For pure contact repulsion, we discover the presence of two phases peculiar to frustrated quantum magnets: the bond-order-wave insulator with broken inversion symmetry and a chiral superfluid. When the nearest-neighbor repulsion becomes sizable, a further density-wave insulator with broken translational symmetry can appear. We show that the phase transition between the two spontaneously symmetry-broken phases is continuous, thus representing a one-dimensional deconfined quantum critical point not captured by the Landau-Ginzburg-Wilson symmetry-breaking paradigm. Our results provide a solid ground to unveil the novel quantum physics induced by the interplay of nonlocal interactions, geometrical frustration, and quantum fluctuations.

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Introduction.—Geometrically frustrated many-body quantum systems [1,2] represent a fruitful research field where a plethora of novel phases of matter has been unveiled. Paradigmatic examples are different topological insulators [3–6] and superconductors [7,8], spin liquids [9–11], and valence bond solids [12–14]. Nevertheless, because of the deep complexity generated by competing interactions, frustration, and quantum fluctuations, various scenarios are still poorly understood. In this respect, numerical studies are highly demanding and often affected by finite size effects [15]. At the same time, possible sample imperfections and limited detection probes narrow the efficiency of solid-state experimental platforms [16,17].

The tunability and control offered by quantum simulation experiments based on ultracold atoms in optical lattices [18] provide a promising alternative for understanding the behavior of a large variety of physical systems [19]. However, theoretical proposals to engineer ultracold frustrated synthetic materials are mainly based on direct implementations of specific geometries [20–24] and alternative approaches are scarce [25–27]. Moreover, experimental realizations of frustrated quantum systems relying on optical lattice engineering successfully achieved weakly interacting [28–31], classical [32–34], or kinetically frustrated [35–39] regimes. Noticeably, these experiments investigated configurations with purely local couplings, while realizations of geometrically frustrated systems with beyond-contact interactions have not yet been achieved.

Interactions with an extended range are a key ingredient to create spontaneous-symmetry-broken (SSB) states of matter with broken translational symmetry. The occurrence of these phases in various physical systems [40–42] has sparked significant experimental interest leading to their observation in atomic frustration-free atom-cavity [43,44] setups, continuum- [45–47], and lattice-dipolar [48] systems, as well as in out-of-equilibrium configurations [49,50]. While Rydberg atoms in optical tweezer arrays allow engineering long-range couplings also in frustrated geometries [51,52] and polar molecules in optical lattices represent a promising platform in this direction [53], their effectiveness remains limited to the study of spin-$1/2$ systems. In this respect, proposals to investigate Hamiltonians with an enlarged Hilbert space, where beyond-contact repulsion and geometric frustration strongly compete are absent.

As illustrated schematically in Fig. 1, we design a realistic experimental setup, where a frustrated extended BoseHubbard Hamiltonian is realized using an atomic mixture in a one-dimensional (1D) lattice at the antimagic wavelength [25,54,55]. At this wavelength, the two

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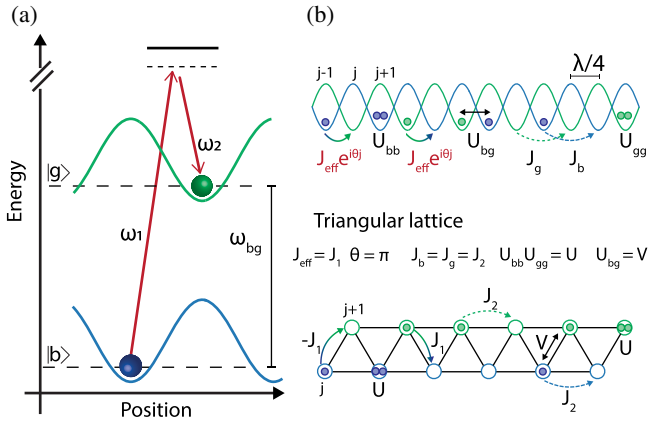

FIG. 1. Experimental scheme to realize Eq. (1). (a) State-dependent optical lattice at the antimagic wavelength λ. Because of the opposite polarizability, both states experience a trapping potential with opposite strength. Raman-assisted tunneling between neighboring sites is induced using a two-photon Raman transition between states $|b\rangle$ and $|g\rangle$ for $\omega_{bg} = \omega_1 - \omega_2$ the energy difference between the two states on neighboring lattice sites. (b) The state-dependent lattice can be seen as two shifted sublattices with an effective lattice spacing of $\lambda/4$ (for a retroreflected configuration), intra- and interspecies tunneling $J_b, J_g/J_{\text{eff}}e^{\iota\theta j}$, and interaction $U_{bb}, U_{gg}/U_{bg}$ (upper panel). (c) Choosing $J_b = J_g = J_2$, $J_{\text{eff}} = J_1$, $\theta = \pi$, $U_{bb} = U_{gg} = U$, and $U_{bg} = V$ this scheme is modeled by the frustrated extended Bose-Hubbard model defined in Eq. (2).

different components experience the same polarizability with opposite signs, generating an opposite potential for each of the components. While this technique can be employed with several atomic species [56–62] with minimal heating, we provide specific values for an implementation with Cesium atoms. Here, convenient inter- and intraspecies Feshbach resonances [63] enable the engineering of frustrated quantum systems with tunable contact and nearest-neighbor (NN) interactions without requiring large electric or magnetic dipole moments. Remarkably, in the presence of only local repulsion we recover the phases predicted to occur in frustrated triangular quantum magnets [64–69]. The latter include chiral superfluidity (CSF) and a site-inversion SSB bond-ordered-wave (BOW) insulator. When the NN repulsion is turned on, the BOW phase is destabilized in favor of a translational SSB insulator, namely, a density wave (DW). By performing variational-uniform-matrix-product-states (VUMPS) calculations [70,71], we find the transition between the two SSB insulators (DW-BOW) to be continuous and thus going beyond the Landau–Ginzburg-Wilson symmetry-breaking paradigm [72,73], which would instead predict a discontinuous first-order phase transition. As pioneering works demonstrated [74–76], quantum fluctuations can indeed give rise to second-order continuous phase transitions between different ordered SSB phases where the gap vanishes in one specific point: the deconfined quantum critical point (DQCP). Because of their deep quantum nature combined with possible exotic properties like fractional excitations and emergent gauge fields, an exceptional theoretical effort has unveiled the presence of DQCPs in a large variety of 2D spin [77–88] and fermionic [89–92] models as well as in 3D [93,94], 1D [95–100], and 0D [101] two-level systems. Moreover, unique evidence of their possible existence has been provided in recent solid-state experiments [102–105]. Here, we prove that DQCPs can be accurately investigated with ultracold atoms in an optical lattice.

Frustrated extended Bose-Hubbard (FEBH).—As shown in Fig. 1(a), we consider a two-component Bose gas trapped in a 1D state-dependent optical lattice with L sites. The two atomic species, hereafter defined as $|b\rangle$ and $|g\rangle$, experience opposite polarizability and, because of the antimagic wavelength condition, remain localized in two sublattices formed, respectively, by the intensity maxima and minima of the periodic potential. This configuration thus mimics an effective discrete geometry with $\tilde{L} = 2L$ sites and lattice spacing $\lambda/4$ (for retroreflected lattices), see Fig. 1(b). Since the two sublattices have by definition the same depth, the $|b\rangle$ and $|g\rangle$ bosons experience the same direct hopping amplitude $J_b = J_g = J$. On the other hand, intra- U_{bb}, U_{gg} and interspecies U_{bg} interactions are potentially different and tunable. Furthermore, tunable Raman-assisted tunneling processes $J_{\text{eff}}e^{\iota\theta j}$ connect consecutive sites of different sublattices; as a consequence, one tunneling event is accompanied by converting one internal state into the other [Fig. 1(a)] and j is the $\tilde{L}$-lattice site index. Here J_{eff} and θ are given by the intensity and wave vector of the Raman coupling [106,107]. This setup is accurately modeled by the Hamiltonian

$$H = -\sum_j \left[J(a_j^\dagger a_{j+2} + \text{H.c.}) + J_{\text{eff}} e^{\iota\theta j}(a_j^\dagger a_{j+1} + \text{H.c.}) \right] + \sum_j \left[\frac{U_{bb}}{2} n_{2j-1}(n_{2j-1} - 1) + \frac{U_{gg}}{2} n_{2j}(n_{2j} - 1) \right] + U_{bg} \sum_i n_i n_{i+1}, \tag{1}$$

where $a_j^\dagger / a_j$ is a bosonic creation or annihilation operator. To provide a more concrete implementation, we focus on two internal states of cesium $|b\rangle \equiv |F = 3, m_F = 3\rangle$ and $|g\rangle \equiv |F = 3, m_F = 2\rangle$, where the interactions are tunable [108]. A further essential aspect of the proposed configuration is its reliance on adiabatic state preparation. For instance, it is possible to prepare an initial state with N bosons in the $|b\rangle$ state forming a Mott insulator with $N = N_b = L$. By subsequently introducing $J_{\text{eff}}e^{\iota\theta j}$, it becomes possible to populate the $|g\rangle$ state and therefore reach the regime of half-filling $\bar{n} = N/\tilde{L} = 0.5$, with $N = N_b + N_g$, which is particularly suitable to explore

SSB phases [48]. Finally, an adiabatic lowering of the lattice depth gives rise to a finite direct tunneling J.

As a specific example, we fix $U_{gg} = U_{bb} = U$ and $\theta = \pi$ so that, after renaming $J = J_2$, $J_{\text{eff}} = J_1$, and $U_{bg} = V$, Eq. (1) becomes

$$H_{\text{FEBH}} = -\sum_j \Big[J_2(a_j^\dagger a_{j+2} + \text{H.c.}) + J_1(-1)^j (a_j^\dagger a_{j+1} + \text{H.c.}) \Big] + \frac{U}{2}\sum_j n_j(n_j - 1) + V\sum_j n_j n_{j+1}, \quad (2)$$

with $J_1, J_2 > 0$. As shown in Fig. 1(b), Eq. (2) describes a frustrated extended Bose-Hubbard model in a triangular ladder at half filling, where the staggered nature of J_1 gives rise to the effective geometrical frustration and U (V) accounts for the contact (NN) interaction. Although various versions and regimes of similar models have been theoretically studied [123–131], configurations with staggered NN tunneling both with and without NN interaction have not been investigated.

Effective frustrated quantum magnet.—We begin our analysis by considering the $V = 0$ case. As shown in Fig. 2(a), in this regime H_{FEBH} hosts three different phases. For weak frustration, namely, for small J_2/J_1, we detect a gapless superfluid (SF), captured by the quasi long-range-order (LRO) of the correlator defined as

$$g^1(|i-j|) = \langle b_i^\dagger b_j \rangle, \quad (3)$$

see Fig. 2(b). On the other hand, $g^1(|i-j|)$ vanishes exponentially for strong enough U and larger J_2/J_1. This behavior signals the appearance of a gapped phase [132] which, as shown in Fig. 2(c), is characterized by a finite value of the local order parameter [133]

$$\Delta B = \frac{1}{L}\sum_j \langle B_j + B_{j+1} \rangle, \quad (4)$$

where $B_j = (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j)$. Specifically, $\Delta B \neq 0$ demonstrates the presence of a dimerized BOW phase with broken site-inversion symmetry. A notable observation is that this lattice dimerization bears a striking resemblance to the Peierls instability [134]. In particular, while in real materials the effective dimerization is generated by the electron-phonon coupling, here it is induced by the combination of finite interaction, quantum fluctuation, and geometrical frustration. It is further relevant to mention that the symmetry-protected topological nature of 1D [109] and 2D [135] BOW phases have been recently discovered. In the strongly frustrated regime of large J_2/J_1, the BOW gives way to a new gapless state where $g^1(|i-j|)$ exhibits

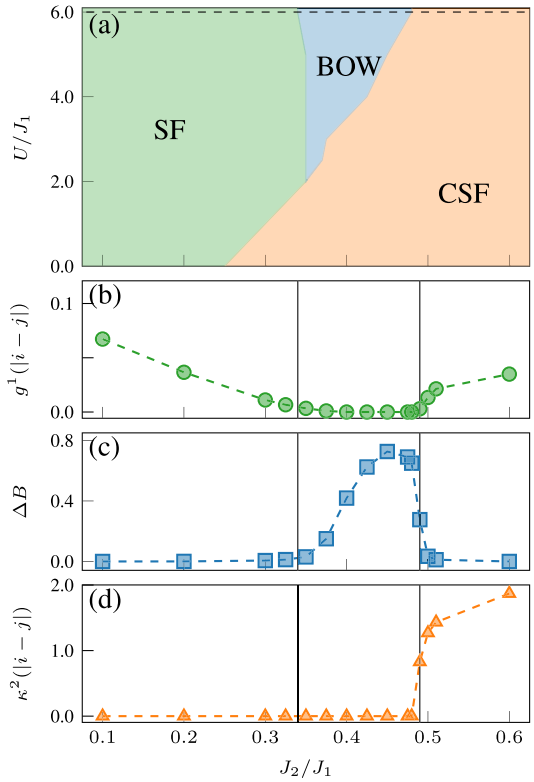

FIG. 2. (a) Phase diagram of H_{FEBH} Eq. (2) as a function of J_2/J_1 and U/J_1, showing the superfluid, bond-order-wave, and chiral superfluid phases; (b) superfluid correlator $g^1(|i-j|)$ for $|i-j| = 100$; (c) bond-order-wave order parameter ΔB; (d) chiral superfluid correlator $\kappa^2(|i-j|)$ for $|i-j| = 100$. The vertical continuous lines in (b)–(d) are the estimated transition points for $U/J_1 = 6$ [dashed line in (a)]. All the figures refer to the configuration where the total density $\bar{n} = 0.5$ and the NN repulsion $V = 0$. The VUMPS simulation have been performed by using a bond dimension $\chi = 400$.

quasi LRO. The findings in Fig. 2(d) illustrate that this regime can be classified as a CSF captured by the LRO of the correlator defined as

$$\kappa^2(|i-j|) = \langle \kappa_i \kappa_j \rangle, \quad (5)$$

where $\kappa_j = -(\imath/2)(b_j^\dagger b_{j+1} - b_{j+1}^\dagger b_j)$ is the vector chiral order parameter [125,126]. This point shows this CSF to be characterized by alternated finite currents between NN sites, thus resembling an effective vortex-antivortex antiferromagnetic crystal with staggered loop currents around each effective triangular plaquette. As shown in Refs. [65,66], the three phases discussed above appear in the phase diagram of triangular Heisenberg Hamiltonians, which are believed to accurately model specific frustrated quantum magnets [64,67–69]. We confirm this strong analogy by considering the limit of infinite contact repulsion $U = \infty$, where Eq. (2) maps exactly onto a magnetic frustrated Heisenberg model [108]. Although

Eqs. (4) and (5) may suggest that detecting CSF and BOW phases requires demanding protocols to extract hopping amplitudes, we propose in [108] an alternative scheme. Here, the CSF can be revealed through measurements of the momentum distribution, while the BOW can be detected through a string correlator that only requires local density measurements. Our scheme thus presents itself as a valuable and alternative method for studying and comprehending frustrated quantum magnets.

Deconfined quantum critical points.—The scattering properties of Cs atoms also make it possible to engineer sizable nonlocal repulsion in the range $V/U < 0.3$, see Ref. [108]. In order to be able to reach relatively large values of V, we fix $U/J_1 = 6$ [see the dashed line in Fig. 2(a)] and we concentrate on the regime of weak and intermediate frustration [136]. Our VUMPS analysis in Fig. 3(a) finds the SF stable with respect to the addition of moderate V. On the contrary, for a gradual increase of the NN repulsion the system undergoes a phase transition from the BOW to a different SSB insulator identified by the local order parameter

$$\delta N = \frac{1}{L}\sum_j (-1)^j (n_j - \bar{n}). \tag{6}$$

A finite δN, which can be accurately probed through quantum gas microscopy [137], reflects the spatial alternation between empty and singly occupied sites, revealing the appearance of a DW characterized by broken translational symmetry. Phase transitions between two gapped SSB phases are usually described by the Landau–Ginzburg-Wilson theory [72,73]. The latter predicts the existence of a first-order transition where the gap never vanishes and it exhibits a discontinuity between two finite values. Interestingly, configurations deep in quantum regimes can deviate from this paradigm. Quantum fluctuations can indeed give rise to continuous phase transitions between different SSB states, where the gap vanishes only at a single point: the deconfined quantum critical point [74,75]. The numerical detection of DQCPs is highly challenging. On the one hand, their complete characterization requires algorithms directly mimicking the thermodynamic limit and, on the other hand, the diverging correlation length ξ occurring at criticality requires a specific entanglement scaling [138]. In this respect, VUMPS are particularly suitable. This advantage stems from the fact that the variational optimization is performed on a unit cell directly in the thermodynamic limit. In this way it is possible to avoid the slower and nonmonotonous convergence to the variational optimum [71] peculiar to algorithms involving a gradual growth of the system size. Thanks to this technique, our results in Figs. 3(b)–3(d) clearly demonstrate the BOW-DW transition to be continuous and therefore the presence of 1D DQCPs. Specifically, we find that ΔB and δN vanish continuously exactly at the same V/J_1, see Fig. 3(b). In order to rule out the presence of a weakly first-order phase transition, we extract the correlation length ξ [139]. Within a matrix-product-state (MPS) formalism, ξ must not depend on the bond dimension χ in the presence of a finite gap. On the other hand, a χ-dependence in the form of a cusp should be observed only at the critical point [96,97,100]. Figure 3(c) accurately confirms this behavior. In the inset of Fig. 3(c) we further extract the central charge c through the relation $S = c\log[\xi(\chi)]/6$, where for MPS around a critical point it is proven that $\xi(\chi) \sim \chi^{\kappa}$ with $\kappa/6 = [c(\sqrt{12/c}+1)]^{-1}$ [138]. Conformal field theories rigorously demonstrate that the extracted $c = 1$ implies indeed the presence of a critical regime which, in this case, is further characterized by an emergent $U(1)$ symmetry. In order to enforce our results, we calculate the decay of the correlations functions

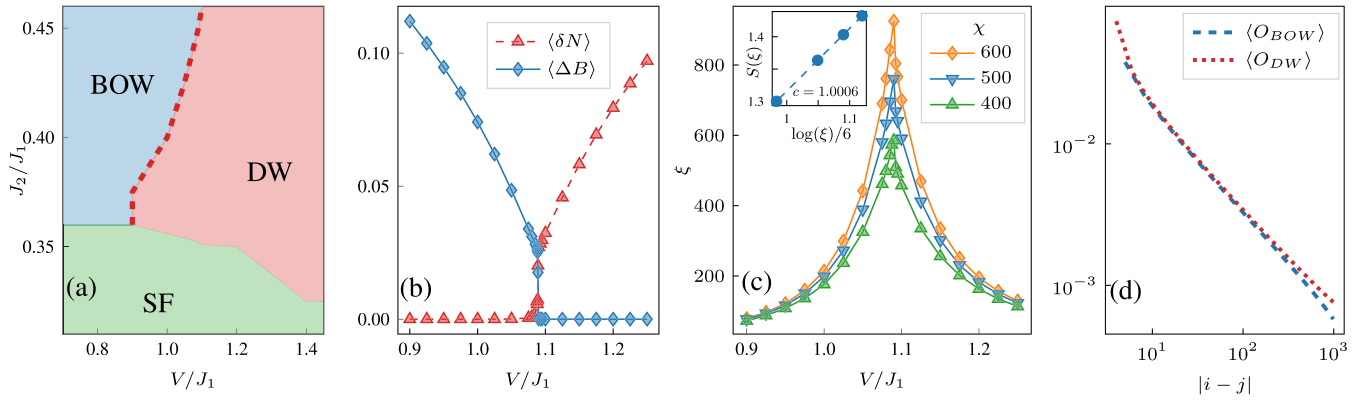

FIG. 3. Effect of the NN repulsion V in the Hamiltonian (2). For all the panels, we fix $U/J_1 = 6$ and $\bar{n} = 0.5$. (a) Phase diagram of H_{EFBH} in the $V/J_1 - J_2/J_1$ plane, using $\chi = 400$. (b) ΔB and δN as a function of V/J_1 for $J_2/J_1 = 0.45$ and $\chi = 600$. (c) The correlation length ξ as a function of V/J_1 for different bond-dimension χ and fixed $J_2/J_1 = 0.45$. Inset: scaling of the entanglement entropy $S(\xi)$ as a function of ξ at the critical point for bond dimensions $\chi = 400$, 500, 600 showing the extrapolated central charge $c = 1$. (d) Decay of O_{DW} and O_{BOW} at the critical point for fixed $J_2/J_1 = 0.45$.

$$O_{\mathrm{BOW}}(|i-j|) = \langle (B_i + B_{i+1})(B_j + B_{j+1}) \rangle, \quad (7)$$

$$O_{\mathrm{DW}}(|i-j|) = \langle (n_i - \bar{n})(n_j - \bar{n}) \rangle. \quad (8)$$

Here, we expect LRO of $O_{\mathrm{BOW}}/O_{\mathrm{DW}}$ uniquely in the BOW/DW phase while both should vanish algebraically at criticality. Figure 3(d) precisely shows the expected power-law decay. This point, that we have been able to demonstrate thanks to the fact that VUMPS mimic the thermodynamic limit, unambiguously proves the critical nature of this transition point. Finally, we point out that, as imposed in DQCPs [96], the two correlation functions clearly vanish in the thermodynamic limit with the same exponent.

Conclusions.—We designed an experimental scheme based on two-component bosonic atoms in an optical lattice at the antimagic wavelength. We modeled this setup through a single-band frustrated extended Bose-Hubbard model where contact and nearest-neighbor interactions, geometrical frustration and quantum fluctuation strongly compete. For contact interaction only, we demonstrated that states of matter peculiar to frustrated quantum magnets, namely, chiral superfluids and spontaneously symmetry-broken bond-order-wave insulators, can be created and accurately probed. For strong nearest-neighbor repulsion, a new spontaneously-symmetry-broken density wave insulator occurs. We proved that the phase transition between the two spontaneously symmetry-broken phases is continuous, thus representing an elusive quantum mechanical effect: one-dimensional deconfined quantum critical points not captured by the Landau–Ginzburg-Wilson symmetry-breaking paradigm.

From an experimental perspective, our findings offer an alternative approach to engineer beyond-contact interactions with two crucial advantages. First, it allows us to naturally incorporate the effect of geometrical frustration by means of an adiabatic state preparation and therefore to realistically explore deep quantum regimes. Second, it does not require the use of particles with strong magnetic or electric dipole moment. From the theory perspective, we performed an advanced numerical analysis of an unexplored version of the paradigmatic Bose-Hubbard Hamiltonian. This has revealed its richness of intriguing quantum mechanical effects. Specifically, on one side this model is able to mimic triangular frustrated quantum magnets and, on the other, it represents an example of a soft-core bosonic system exhibiting deconfined-quantum-critical points. Our work provides valuable insights and opens up new avenues for studying and comprehending strongly interacting frustrated quantum systems.

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