Fractionalized Fermionic Quantum Criticality in Spin-Orbital Mott Insulators

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We study transitions between topological phases featuring emergent fractionalized excitations in two-dimensional models for Mott insulators with spin and orbital degrees of freedom. The models realize fermionic quantum critical points in fractionalized Gross-Neveu* universality classes in $(2+1)$ dimensions. They are characterized by the same set of critical exponents as their ordinary Gross-Neveu counterparts, but feature a different energy spectrum, reflecting the nontrivial topology of the adjacent phases. We exemplify this in a square-lattice model, for which an exact mapping to a t-V model of spinless fermions allows us to make use of large-scale numerical results, as well as in a honeycomb-lattice model, for which we employ ϵ-expansion and large-N methods to estimate the critical behavior. Our results are potentially relevant for Mott insulators with d^1 electronic configurations and strong spin-orbit coupling, or for twisted bilayer structures of Kitaev materials.

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Topology has been established as an organizing principle for states of matter beyond the Landau paradigm of symmetry breaking. Significant progress has been made in systematically understanding symmetry-protected topological (SPT) phases [1,2], in particular in one dimension [3–7], the study of their phase transitions [8–10], and the nature of the respective critical points [11,12]. In contrast to these short-range entangled SPT states, universal properties of phases with intrinsic topological order are less well understood. Their long-range entanglement structure leads to highly unconventional features, such as emergent deconfined gauge fields and fractionalized excitations [13].

While conventional phase transitions can be understood by analyzing the fluctuations of a local order parameter in a Landau-Ginzburg-Wilson framework, the absence of such an order parameter in topological phases raises fundamental questions: What kind of (continuous) transitions involving topological phases are possible, and what are the universal properties of these unconventional quantum critical points [16]? Typically, systems hosting topological order involve strong interactions, so that only few controlled analytical studies and numerical results of the corresponding transitions are available, and are mostly limited to toy models [17]. An important example is given by a model of hard-core bosons, which has been shown to feature a fractionalized quantum critical point in the $(2+1)$-dimensional XY* universality class [18]. This unconventional universality class differs from the ordinary XY universality as a consequence of the topological degeneracy and the fact that only states with even numbers of fractionalized particles are allowed in the spectrum. Similarly, fractionalized counterparts of the ordinary Ising and $\mathrm{O}(N)$ universality classes have been discussed [19,20]. An effective model that realizes a related transition in the presence of gapless fermions has also been proposed [21]. However, although a number of topological phases are characterized by emergent fermionic excitations [22–26], a microscopic model that exhibits a fractionalized version of a fermionic quantum critical point appears as yet unknown.

In this Letter, we construct two such examples. Specifically, we show that in spin-orbital models featuring emergent gapless Majorana excitations coupled to a $\mathbb{Z}_2$ gauge field, there are continuous quantum phase transitions across which a global $\mathbb{Z}_2$ or SO(3) spin rotation symmetry is spontaneously broken and (a subset of) the Majorana fermions become gapped out. These fractionalized quantum critical points fall into fermionic Gross-Neveu* universality classes in $(2+1)$ dimensions, the nontopological counterparts of which have aroused significant interest lately in the context of interacting Dirac fermion systems [27].

Model construction.—Our starting points are spin-orbital implementations [28–32] of the bond-dependent Kitaev exchange interaction [23], which belong to a family of exactly soluble generalized Kitaev models recently introduced [33]. These models have quantum spin-orbital-liquid ground states with static gapped $\mathbb{Z}_2$-vortex excitations and ν_M itinerant gapless Majorana fermions hopping on the square (ν_M even) or honeycomb (ν_M odd) lattices. Adding three-body interactions induces chiral next-nearest-neighbor hopping of the Majorana fermions and opens up a topologically nontrivial band gap with Chern number $C = \nu_M$, giving rise to the sixteen anyon theories as classified in Kitaev's sixteenfold way [23].

We exploit the fact that these spin-orbital Kitaev models allow for simple antiferromagnetic Heisenberg (and Ising, respectively) spin interactions, which leave the vortex excitations static. Considering Mott insulators with orbital degeneracy and sizable bond-dependent exchanges, such perturbations are expected to be present in the respective material-specific Kugel-Khomskii [34,35] models. Adding the perturbations spoils the exact solubility, but the $\mathbb{Z}_2$ fluxes carried by the vortices remain good quantum numbers, such that resulting transitions are driven purely by interactions among the itinerant Majorana fermions. This allows us to find controlled theoretical descriptions based on the fermionic parton construction of the unperturbed model, and to use already available high-precision numerical results and established analytical techniques to study the resulting problems of interacting Dirac fermions.

Gross-Neveu transitions*.—For the $\nu_M = 2$ spin-orbital model on the square lattice with an Ising perturbation, we find an exact mapping to an interacting fermion-hopping problem on the π-flux lattice. This fermionic model has been studied before using large-scale quantum Monte Carlo simulations [36–39], allowing us to determine the phase diagram to high accuracy. Translating these results back to the spin-orbital model reveals the existence of a fractionalized fermionic quantum critical point in the Gross-Neveu-$\mathbb{Z}_2{}^*$ universality class, separating a gapless $\mathbb{Z}_2$-symmetric spin-orbital liquid from a partially ordered and fully gapped phase with Ising antiferromagnetic order in the spin sector, see Fig. 1(a). We furthermore show that the $\nu_M = 3$ spin-orbital model on the honeycomb lattice with a Heisenberg perturbation in the spin sector features a similar fermionic quantum critical point between a gapless SO(3)-symmetric spin-orbital liquid and a partially ordered and partially gapped phase, in which the SO(3) symmetry is spontaneously broken, Fig. 1(b). The corresponding universality class, dubbed Gross-Neveu-SO$(3)^*$, is a fractionalized version of a new member of the Gross-Neveu family, and we determine its critical behavior below.

Similar to the fractionalized bosonic transitions [20], the Gross-Neveu* universality classes are characterized by a spectrum that reflects the topological degeneracy of the adjacent phases and the additional constraints on the physical states [40]. However, here the order parameters are composite operators consisting of pairs of fractionalized particles and are therefore gauge invariant, and numerically and experimentally accessible. This means that not only the correlation-length exponents ν, but also the order-parameter anomalous dimensions η_ϕ in the Gross-Neveu and Gross-Neveu* universality classes coincide, in contrast to the bosonic situation [18]. We emphasize that this is not the case for the fermionic anomalous dimension η_ψ, which has a physical meaning only in the ordinary Gross-Neveu universality classes. Further, the change of the number

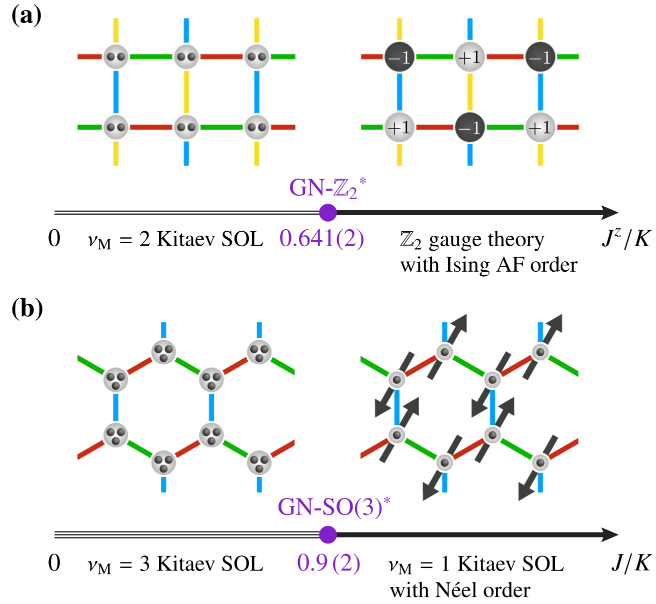

FIG. 1. (a) Adding a sufficiently strong antiferromagnetic Ising spin interaction to the $\nu_M = 2$ Kitaev spin-orbital liquid (SOL) on the square lattice gives rise to Ising antiferromagnetic order in the spin sector, with the remaining degrees of freedom described in terms of a $\mathbb{Z}_2$ gauge theory. The continuous transition at $J_c^z/K = 0.641(2)$ is in the Gross-Neveu-$\mathbb{Z}_2{}^*$ universality class. (b) The honeycomb-lattice model features a Gross-Neveu-SO$(3)^*$ quantum critical point at $J_c/K = 0.9(2)$ between the $\nu_M = 3$ Kitaev SOL and a $\nu_M = 1$ Kitaev SOL with Néel order in the spin sector.

of gapless Majorana fermions at the transition can be understood as a signature of distinct topological orders in the two adjacent phases [51]. Lastly, at elevated temperatures, additional nontrivial physics can be expected as a consequence of thermal flux excitations [52].

Ising order on the square lattice.—The $\nu_M = 2$ spin-orbital liquid is described by a Hamiltonian on the square lattice with a two-site unit cell and a biquadratic XY-spin and Kitaev-type-orbital interaction,

$$\mathcal{H}_K^{(2)} = -K \sum_{\langle ij \rangle_\gamma} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \otimes \tau_i^\gamma \tau_j^\gamma, \qquad K > 0, \quad (1)$$

where the Pauli matrices (σ^x, σ^y) $[(\tau^\gamma) = (\tau^x, \tau^y, \tau^z, \mathbb{1})]$ act on spin (orbital) degrees of freedom, and $\langle ij \rangle_\gamma$, $\gamma = 1, \ldots, 4$, denote the four inequivalent bonds in the unit cell. Representing the spin-orbital degrees of freedom using Majorana fermions [40], Eq. (1) can be mapped to a problem of two dispersing Majorana fermions c^x, c^y in the background of a $\mathbb{Z}_2$ gauge field [23,33], $\mathcal{H}_K^{(2)} \mapsto K \sum_{\langle ij \rangle} i u_{ij} (c_i^x c_j^x + c_i^y c_j^y)$, with $i \in A$, $j \in B$ sublattice. Importantly, Eq. (1) possesses an extensive number of conserved quantities given by the two (symmetry-inequivalent) plaquette operators $W_p^{(2)} = \sigma_k^z \sigma_n^z \otimes \tau_i^x \tau_j^y \tau_k^x \tau_n^y$ and $W_{p'}^{(2)} = \sigma_k^z \sigma_n^z \otimes \tau_k^y \tau_l^x \tau_m^y \tau_n^x$, which correspond to elementary

Wilson loop operators for the gauge field u_{ij} and thus constrain fluxes as excitations of the gauge field to be *static*. By Lieb's theorem [53], the ground-state flux configuration is given by $W_p^{(2)} = W_{p'}^{(2)} = -1$ for all p, p'.

We now add to $\mathcal{H}_K^{(2)}$ an antiferromagnetic Ising spin interaction of the form

$$\mathcal{H}_{J^z}^{(2)} = J^z \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \otimes \mathbb{1}_i \mathbb{1}_j, \qquad J^z > 0. \tag{2}$$

Importantly, from $[\mathcal{H}_{J^z}^{(2)}, W_p^{(2)}] = [\mathcal{H}_{J^z}^{(2)}, W_{p'}^{(2)}] = 0$ it follows that $\mathbb{Z}_2$ gauge fluxes remain static in the full system $\mathcal{H}^{(2)} = \mathcal{H}_K^{(2)} + \mathcal{H}_{J^z}^{(2)}$. Note that the exact solubility is spoiled at finite J^z, since upon mapping to Majorana fermions, the Ising term introduces short-range interactions, $\mathcal{H}_{J^z}^{(2)} \mapsto -J^z \sum_{\langle ij \rangle} c_i^x c_i^y c_j^x c_j^y$. Using complex fermions $f_j = (c_j^x + i c_j^y)/2$, the problem maps to

$$\mathcal{H}^{(2)} \mapsto \sum_{\langle ij \rangle} \left[2K u_{ij} (f_i^\dagger f_j + f_j^\dagger f_i) + 4J^z \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right) \right], \tag{3}$$

where $n_j = f_j^\dagger f_j$ is the fermion density operator and we have further performed a gauge transformation $f_j \mapsto -i f_j$ for $j \in B$. Note that the SO(2) spin rotation symmetry now corresponds to a global $U(1)$ phase rotation symmetry. Lieb's theorem remains applicable for finite J^z [53,54], and thus the ground-state flux sector of $\mathcal{H}^{(2)}$ describes a tight-binding model of spinless fermions on the π-flux lattice with hopping parameter $t \equiv 2K$ and nearest-neighbor repulsion $V \equiv 4J^z$ at half filling. In the noninteracting limit $J^z \ll K$, the spectrum features two Dirac nodes at the Fermi level, describing a Dirac semimetal phase in the fermionic model and a quantum paramagnet in the original theory. In the strong-coupling limit $J^z \gg K$, the system favors a charge-density-wave (CDW) state, in which the $\mathbb{Z}_2$ order parameter $\rho = (n_{i,A} - n_{j,B})/2$, where $n_{i,A}$ ($n_{j,B}$) refers to the fermion density on the A (B) sublattice, acquires a finite expectation value. In the spin-orbital basis, the CDW state corresponds to Ising antiferromagnetic order in the spin sector, $\langle \rho \rangle = \frac{1}{4} \langle \sigma_{i,A}^z - \sigma_{j,B}^z \rangle \neq 0$, while the orbital degrees of freedom feature a $\mathbb{Z}_2$ gauge structure [40]. Because Dirac fermions are stable against weak perturbations, we expect the order-disorder transition to occur at finite J^z/K. In fact, the fermionic model on the π-flux lattice has been studied before using large-scale quantum Monte Carlo simulations [36–38], which show a single continuous transition at $J_c^z = 0.641(2)K$ [39], characterized by the critical exponents $\eta_\phi = 0.51(3)$, $1/\nu = 1.12(1)$, and dynamical exponent $z = 1$. The quantum critical point in the fermionic model falls into the $(2+1)$-dimensional Gross-Neveu-$\mathbb{Z}_2$ universality, which has been excessively investigated in recent years [55–75]. Consequently, the transition in the spin-orbital model falls into the Gross-Neveu-$\mathbb{Z}_2{}^*$ universality class and is characterized by the same universal exponents.

Néel antiferromagnet on the honeycomb lattice.—On the honeycomb lattice, a spin-orbital liquid can be stabilized in a model with a biquadratic Heisenberg-spin and Kitaev-orbital interaction [29,33],

$$\mathcal{H}_K^{(3)} = -K \sum_{\langle ij \rangle_\gamma} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\gamma \tau_j^\gamma, \qquad K > 0, \tag{4}$$

where now $\langle ij \rangle_\gamma$, $\gamma = 1, 2, 3$, refer to the three inequivalent bonds in the two-site unit cell and $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$. As before, the spin-orbital operators can be represented by Majorana fermions, leading to a problem of three dispersing Majorana fermions $c_i = (c_i^x, c_i^y, c_i^z)^\top$ coupled to a $\mathbb{Z}_2$ gauge field u_{ij}, $\mathcal{H}_K^{(3)} \mapsto K \sum_{\langle ij \rangle} i u_{ij} c_i^\top c_j$. The gauge field is static as a result of the conservation of the flux operators $W_p^{(3)} = \mathbb{1} \otimes \tau_i^x \tau_j^y \tau_k^z \tau_l^x \tau_m^y \tau_n^z$. The ground state of $\mathcal{H}_K^{(3)}$ lies in the flux-free sector $W_p^{(3)} = +1$ for all p [53], and the three Majorana fermions lead to a well-defined spectrum on one-half of the lattice's Brillouin zone, featuring one complex Dirac node per Majorana flavor. Note that $\mathcal{H}_K^{(3)}$ possesses a global symmetry under SO(3) spin rotations, which in the fermionic representation corresponds to a flavor rotation.

We now add an antiferromagnetic Heisenberg interaction among only the spin degrees of freedom of the form

$$\mathcal{H}_J^{(3)} = J \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j, \qquad J > 0. \tag{5}$$

Crucially, the flux operators remain static since $[\mathcal{H}_J^{(3)}, W_p^{(3)}] = 0$. Such a spin-only Heisenberg interaction occurs generically in spin-orbital systems due to orbital-diagonal superexchange interactions [35,76]. Mapping $\mathcal{H}_J^{(3)}$ to the Majorana representation yields $\mathcal{H}_J^{(3)} \mapsto (J/4) \sum_{\langle ij \rangle} (c_i^\top \vec{L} c_i) \cdot (c_j^\top \vec{L} c_j)$, with the SO(3) generators $L_{\beta\gamma}^\alpha = -i\epsilon^{\alpha\beta\gamma}$ in the fundamental representation, revealing that $\mathcal{H}_J^{(3)}$ again maps to short-range interactions.

For $J \ll K$, the ground state of $\mathcal{H}^{(3)} = \mathcal{H}_K^{(3)} + \mathcal{H}_J^{(3)}$ is a semimetal with three flavors of gapless Dirac excitations, corresponding to the $\nu_M = 3$ spin-orbital liquid. For $J \gg K$, we expect the vector order parameter $\vec{n} = (c_{i,A}^\top \vec{L} c_{i,A} - c_{j,B}^\top \vec{L} c_{j,B})/4$ to acquire a finite expectation value, e.g., $\langle \vec{n} \rangle \propto \hat{z}$ without loss of generality. This breaks the SO(3) symmetry to a residual $\mathrm{SO}(2) \times \mathbb{Z}_2$ symmetry and gaps out two of the three Majoranas. However, since L^z has a zero eigenvalue, the third Majorana mode remains gapless in the ordered phase. In the spin-orbital basis, we have $\langle \vec{n} \rangle = \langle \vec{\sigma}_{i,A} - \vec{\sigma}_{j,B} \rangle / 2$. The symmetry-broken phase thus corresponds to Néel antiferromagnetic order in the spin sector. This phase can also be understood within a simple mean-field decoupling $\vec{\sigma}_i \simeq \langle\vec{\sigma}_i\rangle$ in the spin-orbital formulation of the model, yielding

$$\mathcal{H}_K^{(3)} + \mathcal{H}_J^{(3)} \simeq K|\langle\vec{n}\rangle|^2 \sum_{\langle ij\rangle_\gamma} \tau_i^\gamma \tau_j^\gamma - \frac{3N_{\mathrm{uc}}J}{2}|\langle\vec{n}\rangle|^2, \quad (6)$$

where N_{uc} is the number of unit cells. For large $J \gg K$, the spins order antiferromagnetically. The remaining orbital degrees of freedom are described by the $\nu_M = 1$ Kitaev honeycomb model with an effective antiferromagnetic Kitaev coupling $K|\langle\vec{n}\rangle|^2$.

To investigate the model at finite J/K, we employ Majorana mean-field theory. We decouple into onsite fields $\langle\vec{\sigma}_i\rangle = \langle c_i^\top \vec{L} c_i\rangle/2$, transforming as vectors under SO(3), and singlet bond variables $\chi_{ij} = \langle i c_i^\top c_j\rangle/3$. In the limiting cases for weak and strong interactions, the ground state is flux free [53]. Assuming that this property holds also at intermediate values of J/K, and restricting ourselves to isotropic and translation-invariant mean fields, we can solve the self-consistency equations iteratively [40]. At $J_c \approx 0.6K$, we find a direct continuous transition from the $\nu_M = 3$ spin-orbital liquid to the Néel-ordered phase with a single gapless itinerant Majorana fermion, corresponding to $\nu_M = 1$. We note that the true J_c/K should be expected to be larger than the mean-field result, as quantum fluctuations tend to destabilize the antiferromagnetic order [77,78].

To validate the qualitative mean-field picture more quantitatively, we perform infinite density renormalization group (iDMRG) simulations [79–81] for the spin-orbital model $\mathcal{H}^{(3)}$. The results for the Néel spin-order parameter and the ground-state expectation value of the plaquette operator $W_p^{(3)}$ are shown in Fig. 2. For the full range of J/K, the ground state stays in the zero-flux sector with $W_p^{(3)} = 1$. Furthermore, the Néel spin-order parameter shows a direct continuous transition from the paramagnetic $\nu_M = 3$ spin-orbital liquid to the Néel spin-ordered state at $J_c \approx 0.9K$. The critical coupling is larger than in the mean-field approximation, as expected.

Gross-Neveu-SO(3)* criticality.—Using a gradient expansion of the Majorana lattice model, we derive a continuum field theory describing the quantum critical point in the lowest flux sector. To this end, we fix the gauge $u_{ij} = +1$ for $i \in A$, $j \in B$ sublattice and introduce continuum complex fermion fields $\psi_s^\alpha(\mathbf{x})$ with sublattice index $s = A$, B and flavor index $\alpha = x, y, z$ by expanding the lattice Majorana fermions $c_{i,s}^\alpha = \psi_s^\alpha(\mathbf{x})e^{i\mathbf{K}\cdot\mathbf{x}} + \mathrm{H.c.}$ about the single Dirac point $\mathbf{K}$. Upon a Hubbard-Stratonovich decoupling of the resulting four-fermion term $[\bar\psi(\mathbb{1}_2 \otimes \vec{L})\psi]^2 \mapsto \frac{1}{2}\vec{\varphi}^2 - \vec{\varphi}\cdot\bar\psi(\mathbb{1}_2\otimes\vec{L})\psi$, with $\psi \equiv (\psi_A^x, \psi_A^y, \psi_A^z, \psi_B^x, \psi_B^y, \psi_B^z)^\top$, $\bar\psi \equiv \psi^\dagger(\sigma^z \otimes \mathbb{1}_3)$, and $\vec{\varphi}$ the continuum Néel order parameter field, we obtain the Euclidean action

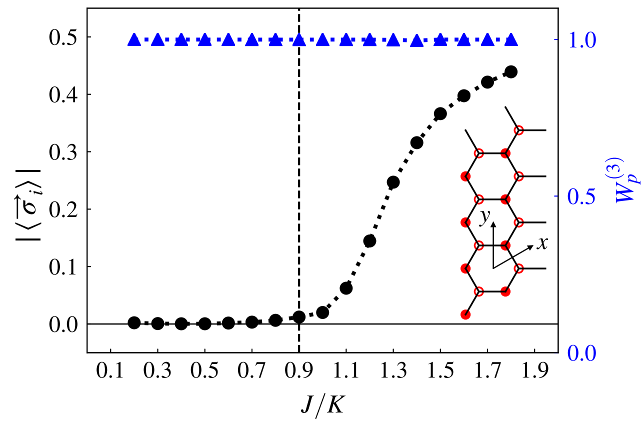

FIG. 2. The Néel spin-order parameter (black dots) and the ground-state expectation value of the plaquette operator $W_p^{(3)}$ (blue triangles) as a function of J/K in the spin-orbital model $\mathcal{H}^{(3)}$ from iDMRG calculations performed on an infinite cylinder with circumference of $L_y = 4$ unit cells. The iDMRG uses two unit cells along the x direction as its translationally invariant building block and the bond dimension is $\chi = 1000$.

$$\mathcal{S} = \int d^2\mathbf{x}d\tau\Big[\bar\psi\gamma^\mu\partial_\mu\psi + g\vec{\varphi}\cdot\bar\psi(\mathbb{1}_2\otimes\vec{L})\psi + \frac{1}{2}\vec{\varphi}(-\partial_\mu^2 + m^2)\vec{\varphi} + \lambda(\vec{\varphi}\cdot\vec{\varphi})^2\Big]. \quad (7)$$

Here, $(\gamma^\mu) = (\sigma^z, \sigma^x, \sigma^y) \otimes \mathbb{1}_3, \mu = 0, 1, 2,$ corresponds to a six-dimensional representation of the Clifford algebra, the Pauli matrices $\vec{\sigma}$ [SO(3) generators $\vec{L}$] act on the sublattice (flavor) indices, and we have allowed for dynamics and the symmetry-allowed quartic self-interaction of the order parameter. The theory describes three flavors of two-component Dirac fermions coupled to a vector order parameter that transforms in the fundamental representation of SO(3), corresponding to spin 1. The boson mass m^2 can be used to tune through the SO(3)-symmetry-breaking transition. For $m^2 > 0$, the order parameter $\vec{\varphi}$ is gapped and can be integrated out, corresponding to the paramagnetic spin-orbital-liquid phase characterized by three gapless Dirac fermions. For $m^2 < 0$, the minimum of the potential occurs at finite $\vec{\varphi}$, indicating spontaneous SO(3) symmetry breaking and an interaction-induced band gap for two out of the three fermions, with the third one remaining gapless, corresponding to the Néel-spin-ordered phase.

The existence of a quantum critical point at vanishing renormalized mass $m^2 = 0$ can be shown using a standard ϵ expansion about the upper critical space-time dimension of four. The flow equations admit an infrared stable fixed point at $g_*^2 > 0$ and $\lambda_* > 0$ that is characterized by a set of universal exponents [40]. Extrapolating the one-loop results to $\epsilon = 1$, we obtain the estimates $\eta_\phi \approx 0.33$ and $1/\nu \approx 1.1$. The remaining exponents α, β, γ, and δ can then be obtained by means of the usual hyperscaling relations

[82], and the dynamical critical exponent is $z = 1$. For completeness, we also quote the fermion anomalous dimension, which is accessible in the ordinary Gross-Neveu-SO(3) universality class only, reading $\eta_\psi \approx 0.17$. Note that this Gross-Neveu-SO(3) critical point defines a new universality class different from those of the Gross-Neveu-SU(2) (= chiral Heisenberg) model [56,63,83–91], in which case the fermion mass term transforms in the fundamental representation of SU(2), corresponding to spin $1/2$, and the spectrum in the ordered phase is fully gapped.

Upon generalizing the theory to N flavors of Dirac fermions coupled to an SO(3) vector order parameter, the critical properties can alternatively be computed within a $1/N$ expansion in fixed dimension. Extrapolating the leading-order results [40] to the physical $N = 3$, we obtain the estimates $\eta_\phi \approx 0.32$, $\eta_\psi \approx 0.14$, and $1/\nu \approx 0.5$. While the anomalous dimensions agree with the ϵ-expansion results within ∼5% accuracy, the agreement in the case of $1/\nu$ is significantly less favorable. This may be due to a sizable $1/N^2$ correction to this observable, similar to the situation in the Gross-Neveu-SU(2) model [85].

Discussion.—We have studied novel transitions between topological phases with concomitant symmetry breaking by making use of unbiased numerical results and controlled analytical approaches. The quantum critical points that we have discovered feature gapless Majorana fermions coupled to gapped $\mathbb{Z}_2$ gauge fields as well as gauge-invariant order-parameter bosons, and fall into a previously unknown family of fractionalized fermionic universality classes. They represent controlled instances of the larger class of unconventional quantum phase transitions that are characterized by fractionalized excitations, which includes deconfined quantum critical points between different conventionally ordered phases [92–96], between conventional and deconfined phases [21,97–100], as well as between different deconfined phases [101–103]. The models studied in this work belong to the latter class, with the deconfined modes at the critical point being in a one-to-one correspondence with the deconfined elementary excitations of the adjacent phases.

Our findings call for more detailed theoretical investigations of the Gross-Neveu* criticalities, in particular in the SO(3) case, for which currently only leading-order estimates are available. It would also be interesting to study the universal finite-size spectra, e.g., on the torus [19,20,74,104].

Our results may be relevant for $4d^1$ or $5d^1$ Mott insulators [76,105,106]. For instance, α-$ZrCl_3$ realizes strongly bond-dependent interactions in analogy to the d^5 Kitaev materials [107], and has been proposed as a candidate for an SU(4)-symmetric spin-orbital liquid on the honeycomb lattice [108]. Similarly, in double perovskite systems, strong spin-orbit coupling can lead to $j_{\mathrm{eff}} = 3/2$ multiplets subject to bond-dependent exchange interactions [109]. In particular, absence of ordering down to low temperatures has been observed in Ba_2YMoO_6, and Kitaev-type spin-orbital liquids have been proposed as candidate ground states [110]. In the above materials, resonant inelastic x-ray scattering and neutron scattering can separately probe spin and spin-orbital excitations, allowing to resolve potential partial order that we find in our models. Kugel-Khomskii-type models with anisotropic exchange interactions have also been proposed to describe correlated insulating phases in twisted bilayers [76,111–113]. In this regard, it may be of interest to consider twisted bilayer configurations of Kitaev materials, such as α-$RuCl_3$ [114,115].

In real materials, additional perturbations that generate fluctuations of the gauge field are present. When their magnitudes become of the order of the (unperturbed) flux gap, further transitions that might lead to confinement of the fractionalized particles can occur. The study of such transitions represents another interesting direction for future research.

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[1] X. Chen, Z.-C. Gu, Z.-X. Liu, and X.-G. Wen, Phys. Rev. B **87**, 155114 (2013).
[2] T. Senthil, Annu. Rev. Condens. Matter Phys. **6**, 299 (2015).
[3] F. Pollmann, A. M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B **81**, 064439 (2010).
[4] X. Chen, Z.-C. Gu, and X.-G. Wen, Phys. Rev. B **83**, 035107 (2011).
[5] N. Schuch, D. Pérez-García, and I. Cirac, Phys. Rev. B **84**, 165139 (2011).
[6] A. M. Turner, F. Pollmann, and E. Berg, Phys. Rev. B **83**, 075102 (2011).
[7] L. Fidkowski and A. Kitaev, Phys. Rev. B **83**, 075103 (2011).
[8] T. Grover and A. Vishwanath, Phys. Rev. B **87**, 045129 (2013).
[9] Y.-M. Lu and D.-H. Lee, Phys. Rev. B **89**, 195143 (2014).
[10] K. Slagle, Y.-Z. You, and C. Xu, Phys. Rev. B **91**, 115121 (2015).
[11] R. Verresen, R. Moessner, and F. Pollmann, Phys. Rev. B **96**, 165124 (2017).
[12] Y. Q. Qin, Y.-Y. He, Y.-Z. You, Z.-Y. Lu, A. Sen, A. W. Sandvik, C. Xu, and Z. Y. Meng, Phys. Rev. X **7**, 031052 (2017).

[13] Here, we refer to a phase as being topological if its low-energy excitations belong to superselection sectors that are invariant under the action of local operators [14,15]. This notion thus also includes gapless $\mathbb{Z}_2$ and $U(1)$ spin liquids.
[14] P. Bonderson and C. Nayak, Phys. Rev. B **87**, 195451 (2013).
[15] S. Sachdev, Rep. Prog. Phys. **82**, 014001 (2019).
[16] C. Xu, Int. J. Mod. Phys. B **26**, 1230007 (2012).
[17] M. Vojta, Rep. Prog. Phys. **81**, 064501 (2018).
[18] S. V. Isakov, R. G. Melko, and M. B. Hastings, Science **335**, 193 (2012).
[19] S. Whitsitt and S. Sachdev, Phys. Rev. B **94**, 085134 (2016).
[20] M. Schuler, S. Whitsitt, L.-P. Henry, S. Sachdev, and A. M. Läuchli, Phys. Rev. Lett. **117**, 210401 (2016).
[21] S. Gazit, F. F. Assaad, S. Sachdev, A. Vishwanath, and C. Wang, Proc. Natl. Acad. Sci. U.S.A. **115**, E6987 (2018).
[22] W. Rantner and X.-G. Wen, Phys. Rev. Lett. **86**, 3871 (2001).
[23] A. Kitaev, Ann. Phys. (Ansterdam) **321**, 2 (2006).
[24] T. Senthil, Phys. Rev. B **78**, 045109 (2008).
[25] Y.-C. He, M. P. Zaletel, M. Oshikawa, and F. Pollmann, Phys. Rev. X **7**, 031020 (2017).
[26] X.-Y. Song, C. Wang, A. Vishwanath, and Y.-C. He, Nat. Commun. **10**, 4254 (2019).
[27] R. Boyack, H. Yerzhakov, and J. Maciejko, arXiv:2004.09414.
[28] H. Yao, S.-C. Zhang, and S. A. Kivelson, Phys. Rev. Lett. **102**, 217202 (2009).
[29] H. Yao and D.-H. Lee, Phys. Rev. Lett. **107**, 087205 (2011).
[30] R. Nakai, S. Ryu, and A. Furusaki, Phys. Rev. B **85**, 155119 (2012).
[31] V. S. de Carvalho, H. Freire, E. Miranda, and R. G. Pereira, Phys. Rev. B **98**, 155105 (2018).
[32] W. M. H. Natori and J. Knolle, Phys. Rev. Lett. **125**, 067201 (2020).
[33] S. Chulliparambil, U. F. P. Seifert, M. Vojta, L. Janssen, and H.-H. Tu, Phys. Rev. B **102**, 201111(R) (2020).
[34] D. I. Khomskiĭ and K. I. Kugel', Phys. Status Solidi B **79**, 441 (1977).
[35] K. I. Kugel' and D. I. Khomskiĭ, Sov. Phys. Usp. **25**, 231 (1982).
[36] L. Wang, P. Corboz, and M. Troyer, New J. Phys. **16**, 103008 (2014).
[37] Z.-X. Li, Y.-F. Jiang, and H. Yao, New J. Phys. **17**, 085003 (2015).
[38] E. Huffman and S. Chandrasekharan, Phys. Rev. D **96**, 114502 (2017).
[39] E. Huffman and S. Chandrasekharan, Phys. Rev. D **101**, 074501 (2020).
[40] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.125.257202 for details of (a) the predicted spectral structure of the Gross-Neveu* universality classes, (b) the Majorana representation of the spin-orbital operators, (c) the strong-coupling limits of the models, (d) the Majorana mean-field theory, (e) the ϵ, and (f) the large-N calculations, which additionally includes Refs. [41–50].
[41] J. L. Cardy, J. Phys. A **18**, L757 (1985).
[42] S. Trebst, P. Werner, M. Troyer, K. Shtengel, and C. Nayak, Phys. Rev. Lett. **98**, 070602 (2007).
[43] I. F. Herbut, V. Juričić, and B. Roy, Phys. Rev. B **79**, 085116 (2009).
[44] A. M. Tsvelik, Phys. Rev. Lett. **69**, 2142 (1992).
[45] S. Chulliparambil, L. Janssen, M. Vojta, H.-H. Tu, and U. F. P. Seifert, arXiv:2010.14511.
[46] B. S. Shastry and D. Sen, Phys. Rev. B **55**, 2988 (1997).
[47] A. N. Vasil'ev, Y. M. Pis'mak, and Y. R. Khonkonen, Theor. Math. Phys. **46**, 104 (1981).
[48] J. A. Gracey, Int. J. Mod. Phys. A **06**, 395 (1991).
[49] J. A. Gracey, Int. J. Mod. Phys. A **33**, 1830032 (2018).
[50] R. Boyack, A. Rayyan, and J. Maciejko, Phys. Rev. B **99**, 195135 (2019).
[51] We may take the viewpoint that the two respective phases connected by the transition have parent gapped topologically ordered phases obtained by opening a topologically nontrivial gap for each itinerant Majorana fermion. The topological data of the two respective low-energy anyon theories of the gapped topological phases as classified in Kitaev's sixteenfold way [23] is then found to differ.
[52] J. Nasu, M. Udagawa, and Y. Motome, Phys. Rev. B **92**, 115122 (2015).
[53] E. H. Lieb, Phys. Rev. Lett. **73**, 2158 (1994).
[54] N. Macris and B. Nachtergaele, J. Stat. Phys. **85**, 745 (1996).
[55] L. N. Mihaila, N. Zerf, B. Ihrig, I. F. Herbut, and M. M. Scherer, Phys. Rev. B **96**, 165133 (2017).
[56] N. Zerf, L. N. Mihaila, P. Marquard, I. F. Herbut, and M. M. Scherer, Phys. Rev. D **96**, 096010 (2017).
[57] B. Ihrig, L. N. Mihaila, and M. M. Scherer, Phys. Rev. B **98**, 125109 (2018).
[58] J. A. Gracey, T. Luthe, and Y. Schröder, Phys. Rev. D **94**, 125028 (2016).
[59] J. A. Gracey, Phys. Rev. D **96**, 065015 (2017).
[60] L. Iliesiu, F. Kos, D. Poland, S. S. Pufu, D. Simmons-Duffin, and R. Yacoby, J. High Energy Phys. 03 (2016) 120.
[61] L. Iliesiu, F. Kos, D. Poland, S. S. Pufu, and D. Simmons-Duffin, J. High Energy Phys. 01 (2018) 36.
[62] J. Braun, H. Gies, and D. D. Scherer, Phys. Rev. D **83**, 085012 (2011).
[63] L. Janssen and I. F. Herbut, Phys. Rev. B **89**, 205403 (2014).
[64] G. P. Vacca and L. Zambelli, Phys. Rev. D **91**, 125003 (2015).
[65] B. Knorr, Phys. Rev. B **94**, 245102 (2016).
[66] H. Gies, T. Hellwig, A. Wipf, and O. Zanusso, J. High Energy Phys. 12 (2017) 132.
[67] L. Dabelow, H. Gies, and B. Knorr, Phys. Rev. D **99**, 125019 (2019).
[68] S. Chandrasekharan and A. Li, Phys. Rev. D **88**, 021701 (R) (2013).
[69] L. Wang, M. Iazzi, P. Corboz, and M. Troyer, Phys. Rev. B **91**, 235151 (2015).
[70] L. Wang, Y.-H. Liu, and M. Troyer, Phys. Rev. B **93**, 155117 (2016).
[71] S. Hesselmann and S. Wessel, Phys. Rev. B **93**, 155157 (2016).

[72] Y.-Y. He, X. Y. Xu, K. Sun, F. F. Assaad, Z. Y. Meng, and Z.-Y. Lu, Phys. Rev. B **97**, 081110(R) (2018).
[73] C. Chen, X. Y. Xu, Z. Y. Meng, and M. Hohenadler, Phys. Rev. Lett. **122**, 077601 (2019).
[74] M. Schuler, S. Hesselmann, S. Whitsitt, T. C. Lang, S. Wessel, and A. M. Läuchli, arXiv:1907.05373.
[75] Y. Liu, W. Wang, K. Sun, and Z. Y. Meng, Phys. Rev. B **101**, 064308 (2020).
[76] W. M. H. Natori, R. Nutakki, R. G. Pereira, and E. C. Andrade, Phys. Rev. B **100**, 205131 (2019).
[77] S. Sorella and E. Tosatti, Europhys. Lett. **19**, 699 (1992).
[78] F. F. Assaad and I. F. Herbut, Phys. Rev. X **3**, 031010 (2013).
[79] U. Schollwöck, Ann. Phys. (Amsterdam) **326**, 96 (2011).
[80] J. Hauschild and F. Pollmann, SciPost Phys. Lect. Notes 5 (2018).
[81] X.-Y. Dong and D. N. Sheng, Phys. Rev. B **102**, 121102(R) (2020).
[82] I. Herbut, *A Modern Approach to Critical Phenomena* (Cambridge University Press, Cambridge, England, 2007).
[83] B. Rosenstein, H.-L. Yu, and A. Kovner, Phys. Lett. B **314**, 381 (1993).
[84] I. F. Herbut, V. Juričić, and O. Vafek, Phys. Rev. B **80**, 075432 (2009).
[85] J. A. Gracey, Phys. Rev. D **97**, 105009 (2018).
[86] B. Knorr, Phys. Rev. B **97**, 075129 (2018).
[87] F. Parisen Toldin, M. Hohenadler, F. F. Assaad, and I. F. Herbut, Phys. Rev. B **91**, 165108 (2015).
[88] Y. Otsuka, S. Yunoki, and S. Sorella, Phys. Rev. X **6**, 011029 (2016).
[89] P. Buividovich, D. Smith, M. Ulybyshev, and L. von Smekal, Phys. Rev. B **98**, 235129 (2018).
[90] T. C. Lang and A. M. Läuchli, Phys. Rev. Lett. **123**, 137602 (2019).
[91] Y. Liu, Z. Wang, T. Sato, M. Hohenadler, C. Wang, W. Guo, and F. F. Assaad, Nat. Commun. **10**, 2658 (2019).
[92] T. Senthil, L. Balents, S. Sachdev, A. Vishwanath, and M. P. A. Fisher, Phys. Rev. B **70**, 144407 (2004).
[93] A. Nahum, J. T. Chalker, P. Serna, M. Ortuño, and A. M. Somoza, Phys. Rev. X **5**, 041048 (2015).
[94] H. Shao, W. Guo, and A. W. Sandvik, Science **352**, 213 (2016).
[95] C. Wang, A. Nahum, M. A. Metlitski, C. Xu, and T. Senthil, Phys. Rev. X **7**, 031051 (2017).
[96] T. Sato, M. Hohenadler, and F. F. Assaad, Phys. Rev. Lett. **119**, 197203 (2017).
[97] P. Ghaemi and T. Senthil, Phys. Rev. B **73**, 054415 (2006).
[98] F. F. Assaad and T. Grover, Phys. Rev. X **6**, 041049 (2016).
[99] L. Janssen, W. Wang, M. M. Scherer, Z. Y. Meng, and X. Y. Xu, Phys. Rev. B **101**, 235118 (2020).
[100] Y.-H. Zhang and S. Sachdev, Phys. Rev. B **102**, 155124 (2020).
[101] M. A. Metlitski, D. F. Mross, S. Sachdev, and T. Senthil, Phys. Rev. B **91**, 115111 (2015).
[102] L. Janssen and Y.-C. He, Phys. Rev. B **96**, 205113 (2017).
[103] R. Boyack, C.-H. Lin, N. Zerf, A. Rayyan, and J. Maciejko, Phys. Rev. B **98**, 035137 (2018).
[104] S. Whitsitt, M. Schuler, L.-P. Henry, A. M. Läuchli, and S. Sachdev, Phys. Rev. B **96**, 035142 (2017).
[105] G. Chen, R. Pereira, and L. Balents, Phys. Rev. B **82**, 174440 (2010).
[106] W. M. H. Natori, M. Daghofer, and R. G. Pereira, Phys. Rev. B **96**, 125109 (2017).
[107] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009).
[108] M. G. Yamada, M. Oshikawa, and G. Jackeli, Phys. Rev. Lett. **121**, 097201 (2018).
[109] J. Romhányi, L. Balents, and G. Jackeli, Phys. Rev. Lett. **118**, 217202 (2017).
[110] W. M. H. Natori, E. C. Andrade, E. Miranda, and R. G. Pereira, Phys. Rev. Lett. **117**, 017204 (2016).
[111] C. Xu and L. Balents, Phys. Rev. Lett. **121**, 087001 (2018).
[112] T. Kariyado and A. Vishwanath, Phys. Rev. Research **1**, 033076 (2019).
[113] L. Xian, M. Claassen, D. Kiese, M. M. Scherer, S. Trebst, D. M. Kennes, and A. Rubio, arXiv:2004.02964.
[114] S. Trebst, arXiv:1701.07056.
[115] L. Janssen and M. Vojta, J. Phys. Condens. Matter **31**, 423002 (2019).