Letter

Quantum Monte Carlo for gauge fields and matter without the fermion determinant

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Ab initio Monte Carlo simulations of strongly interacting fermionic systems are plagued by the fermion sign problem, making the nonperturbative study of many interesting regimes of dense quantum matter, or of theories of odd numbers of fermion flavors, challenging. Moreover, typical fermion algorithms require the computation (or sampling) of the fermion determinant. We focus instead on the meron cluster algorithm, which can solve the fermion sign problem in a class of models without involving the determinant. We develop and benchmark new meron algorithms to simulate fermions coupled to $\mathbb{Z}_2$ and $U(1)$ gauge fields in the presence of appropriate four-fermi interactions. Such algorithms can be used to uncover potential exotic properties of matter, particularly relevant for quantum simulator experiments. We demonstrate the emergence of the Gauss' law at low temperatures for a $U(1)$ model in $(1+1)$D.

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Introduction. Microscopic models involving fermions that strongly interact with each other, either directly or mediated via gauge fields, are essential ingredients of many theories in condensed matter and particle physics [1–3]. From the Hubbard model describing the physics of correlated fermions, to the quantum Hall effect and high-temperature superconductivity, fermions subjected to various interactions have been studied both perturbatively and nonperturbatively [4,5]. Fermions constitute the matter component of all microscopic theories of particle physics (as leptons in electromagnetic and weak interactions, as quarks in strong interactions) and interact with gauge fields (the photon, the $W^{\pm}, Z$, and the gluons, respectively) [6]. Gauge fields are also becoming increasingly important to condensed matter systems, from frustrated magnetism to theories of deconfined quantum criticality [7].

While quantum Monte Carlo (QMC) methods are robust for nonperturbative studies of the aforementioned systems, they are also vulnerable to the sign problem [8]. QMC methods work by performing importance sampling of fermion and gauge field configurations that make up the partition function. Since fermions anticommute, their sign problem can be straightforwardly understood when the configurations considered are worldlines: whenever fermions exchange positions an odd number of times, the configuration weight acquires another negative sign factor, leading to huge cancellations in the summation, accompanied by an exponential increase of noise [9].

A large family of QMC methods deal with the fermion sign problem using determinants: they introduce auxiliary bosonic fields and integrate out the fermions, or expand the partition function, $\mathcal{Z}$, as powers of the Hamiltonian (or parts of the Hamiltonian) and get fermion determinants for the resulting terms [10,11]. Because these methods result in weights that are the sums of many worldline configurations, they can be used more generically to simulate the largest classes of sign-problem-free Hamiltonians, with auxiliary field QMC as the most widely applicable method [12–20]. Determinantal methods in general scale with either the spatial lattice volume, or the spacetime lattice volume, which in terms of imaginary time β and spatial lattice dimension N goes either as $O(\beta^3 N^3)$ or $O(\beta N^3)$, depending on the method [21–26]. While this polynomial scaling is much better than the exponential scaling from a straightforward exact diagonalization, it is much worse than the linear scaling achievable for spin systems, where worldline-based methods can simulate systems orders of magnitude larger than typical simulable fermionic systems [27–32].

An alternative approach—well utilized in the lattice quantum chromodynamics community—is the hybrid Monte Carlo technique [33–35], which computes the fermion determinant stochastically, and theoretically scales linearly rather than cubicly with the spatial volume. For systems of massless fermions and thus zero modes in $\mathcal{Z}$, however, the method can run into complexities and the scaling significantly worsens, closer to the cubic

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scaling of before [36]. More recently, it has been applied to problems in condensed matter with some promising optimizations [37–39].

It is however possible to develop worldline-based algorithms for fermionic Hamiltonians [40–43]. Meron cluster methods [44], so named due to the presence of *merons* (half-instantons) in the first model for which they were developed to simulate [the 2D $O(3)$ sigma model with $\theta = \pi$], can be used to solve sign problems in four-fermion Hamiltonians for certain parameter regimes, as well as for free fermions with a chemical potential [45]. Because these methods sample worldlines, computing the weights scales linearly with the volume of the system, and negative terms in the partition function are taken care of by avoiding *merons*—this is what distinguishes them from bosonic simulations. The relative simplicity of these methods, with each weight corresponding to a worldline configuration and the lack of stabilization issues that can arise in determinantal methods [11], as well as the favorable scaling of the weight computations, makes them an attractive choice for simulation when applicable. Correspondingly, exciting opportunities open up when new interesting physical models are found which can be simulated using this method [46–48].

Recently, there has been intense experimental development to study the physics of confinement and quantum spin liquids [49–55] using tools of quantum simulation and computation. The microscopic models used to capture the physics involve fermions interacting with (Abelian) gauge fields. In this Letter, we develop meron cluster algorithms for a class of experimentally relevant models [56,57], enabling a robust elucidation of their phase diagrams. We also introduce new classes of $\mathbb{Z}_2$ and $U(1)$ multiflavored gauge-fermion theories, which might be realized in cold-atom setups and also be further studied using Monte Carlo techniques. Notably, the $U(1)$ family of these models seems to be one of the few families that falls outside the class of models known to be simulable by auxiliary-field methods, as are [23,58,59]. Moreover, the worldline nature of the method makes it easily employed to study the corresponding phases in these theories in higher spatial dimensions, and the resulting physically relevant configurations are promising inputs for machine learning algorithms.

Models. We start with the half-filled t-V model—a spinless fermionic Hamiltonian involving only the most local interactions,

$$H = \sum_{\langle xy \rangle} \left[-\frac{t}{2}(c_x^\dagger c_y + c_y^\dagger c_x) + V\left(n_x - \frac{1}{2}\right)\left(n_y - \frac{1}{2}\right)\right]. \quad (1)$$

Here $\langle xy \rangle$ are the nearest neighbor site pairs, $c^\dagger, c$ are the creation and annihilation operators, respectively, and the repulsive interaction V is given in terms of the number operator $n = c^\dagger c$. It is simulable by meron clusters for $V \geq 2t$ [45,48]. In this Letter, we extend the meron cluster method to physically interesting Hamiltonians involving gauge fields, which are lower-dimensional versions of quantum electrodynamics [60,61]. The $\mathbb{Z}_2$- and $U(1)$-gauge symmetric families are given by

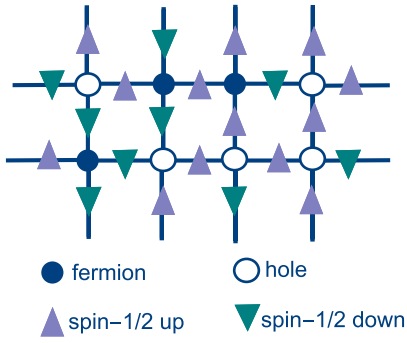


FIG. 1. Example fermion occupations and bond variables for the theories on a square spatial lattice with $N_f = 1$.

$$H_{N_f}^{(g)} = -\sum_{\langle xy \rangle} \prod_{f=1}^{N_f} \left(H_{\langle xy \rangle, f}^{(g)} + H_{\langle xy \rangle, f}^{(g),\mathrm{des}} \right). \quad (2)$$

The label $g \in \{U(1), \mathbb{Z}_2\}$ is the gauge symmetry, with

$$\begin{aligned} H_{\langle xy \rangle, f}^{\mathbb{Z}_2} &= t\left(c_{x,f}^\dagger s_{xy,f}^1 c_{y,f} + c_{y,f}^\dagger s_{xy,f}^1 c_{x,f} \right), \\ H_{\langle xy \rangle, f}^{U(1)} &= t\left(c_{x,f}^\dagger s_{xy,f}^+ c_{y,f} + c_{y,f}^\dagger s_{xy,f}^- c_{x,f} \right). \end{aligned} \quad (3)$$

The hopping of spinless fermions between the nearest neighbors $\langle xy \rangle$ are now governed by the presence of gauge fields, represented by spin-1/2 operators, s_{xy}^k, on the bond. Figure 1 illustrates the model degrees of freedom. Then $H_{\langle xy \rangle, f}^{(g),\mathrm{des}}$ is a designer term [62] that makes the models simulable by the meron algorithm,

$$\begin{aligned} H_{\langle xy \rangle, f}^{\mathbb{Z}_2,\mathrm{des}} &= -2t\left(n_{x,f} - \frac{1}{2}\right)\left(n_{y,f} - \frac{1}{2}\right) + \frac{t}{2}, \\ H_{\langle xy \rangle, f}^{U(1),\mathrm{des}} &= -t\left(n_{x,f} - \frac{1}{2}\right)\left(n_{y,f} - \frac{1}{2}\right) \\ &\quad - t s_{xy,f}^3 (n_{y,f} - n_{x,f}) + \frac{t}{4}. \end{aligned} \quad (4)$$

These terms serve a similar role as the $V = 2t$ term in the meron cluster algorithm applied to the t-V model [45], and similarly an additional particle-hole symmetric $V \geq 0$ term can be added to the models here in a sign-problem-free way. In the $\mathbb{Z}_2$ gauge theory, the gauge field $s^1 = \sigma^1/2$ couples to fermions, and the local $\mathbb{Z}_2$ symmetry is manifest via the commutation $[Q_x, H^{\mathbb{Z}_2}] = 0$, where $Q_x = (-1)^{\sum_f n_{x,f}} \prod_{f,\hat{\alpha}} s_{x,x+\hat{\alpha},f}^3 s_{x-\hat{\alpha},x,f}^3$, $\hat{\alpha}$ are the unit vectors in a d-dimensional square lattice. For the $U(1)$

theory, the unitary operator $V_{U(1)}$, which commutes with $H^{U(1)}$ is given by $V_{U(1)} = \prod_x e^{i\theta_x G_x}$, with $G_x = \sum_f [n_{x,f} - \sum_{\hat{\alpha}} (s^3_{x,x+\hat{\alpha},f} - s^3_{x-\hat{\alpha},x,f}) + ((-1)^x - 1)/2]$. In the terminology of gauge fields, our microscopic models are *quantum link models* [63], which realize the continuous gauge invariance using finite-dimensional quantum degrees of freedom. The identification with usual gauge field operators is $U_{xy,f} = s^+_{xy,f}, U^\dagger_{xy,f} = s^-_{xy,f}, E = s^3_{xy,f}$. We note that a straightforward application of the meron idea necessitates the introduction of an equivalent *flavor* index for gauge links as fermion flavors. Naively, the total Gauss law can be expressed through a product ($\mathbb{Z}_2$) or sum [$U(1)$] of the Gauss law of individual flavors degrees of freedom, and the resulting theories have $\mathbb{Z}_2^{\otimes N_f}$ and $U(1)^{\otimes N_f}$ gauge symmetry. However, flavored gauge interactions can also be turned on in the $U(1)$ model (as explained in the Supplemental Material [64]),

$$H^{U(1)}_{N_f=2} \to H^{U(1)}_{N_f=2} + J \sum_{\langle xy \rangle} s^3_{xy,1} s^3_{xy,2}, \tag{5}$$

or through a Hubbard-U interaction for both $\mathbb{Z}_2$ and $U(1)$-symmetric models [48]. These additions directly cause ordering for either the gauge field or the fermions, and the coupling between them leads to the interesting question of how the other particles are affected by this ordering. In similar contexts, interesting simultaneous phase transitions of both the fermions and gauge fields have been found [47,61,65–69] or conjectured [70,71].

Algorithm. The algorithm is best understood through the worldline configurations for the models defined in Eqs. (2) to (4) in the occupation number basis for the fermions and the electric flux (spin-z) basis for the gauge links. The partition function in $(1+1)$D is

$$\begin{aligned} \mathcal{Z} &= \mathrm{Tr}(e^{-\beta H}), \\ &= \sum_{\{s,n\}} \langle s_1, n_1 | e^{-\epsilon H_e} | s_{2N_t}, n_{2N_t} \rangle \langle s_{2N_t}, n_{2N_t} | \\ &\quad \times e^{-\epsilon H_o} \ldots e^{-\epsilon H_e} | s_2, n_2 \rangle \langle s_2, n_2 | e^{-\epsilon H_o} | s_1, n_1 \rangle, \end{aligned} \tag{6}$$

where $H = H_e + H_o$, and H_e (H_o) consists of Hamiltonian terms that correspond to even (odd) links. This Trotterized approximation, is a sum of terms over discrete time slices $1, \ldots, 2N_t$, each with locally defined electric flux and fermion occupation numbers. All terms within H_e and H_o commute with each other (there are straightforward generalizations for higher dimensions) [72]. Each of the terms in Eq. (6) is a worldline configuration, and the rules for allowable worldline configurations apply consistently to all models within each of the symmetry families. Figures 2(a)–2(c) give examples of such configurations for the t-V model as simulated by meron clusters.

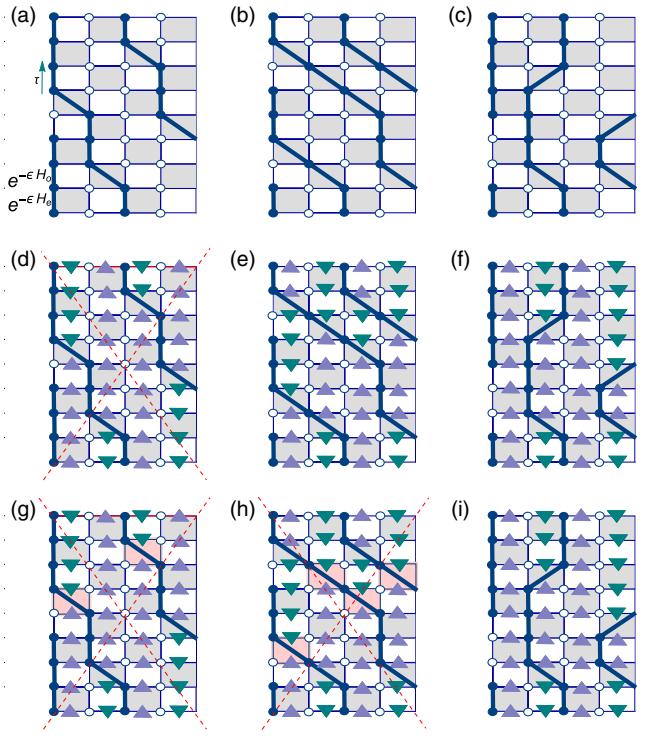


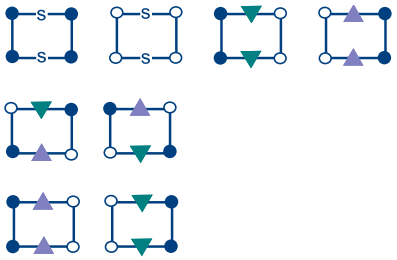
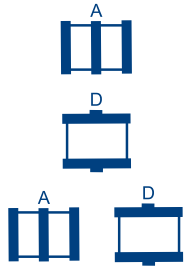
FIG. 2. Worldlines for the t-V model are in (a)–(c), the $\mathbb{Z}_2$ theory in (d)–(f), and the $U(1)$ theory in (g)–(i). Image (a) shows the imaginary time direction and the $(1+1)$D trotterization, which is the same for all images. Filled circles are sites occupied by fermions, and empty circles are holes. Figures in the second two rows also have link variables because they correspond to gauge theories: the upward triangles correspond to spin $+1/2$ and the downward triangles correspond to spin $-1/2$. While the fermionic worldlines are the same in each column, some configurations that are allowed for the t-V model have zero weight for the $\mathbb{Z}_2$ and $U(1)$ theories. These are crossed out, and zero-weight plaquettes are shaded red.

In the $\mathbb{Z}_2$ case, for each time slice a fermion has the option of hopping to an unoccupied nearest neighbor site of the same flavor. The hop flips the flux on the bond between the sites of the same flavor index—this is the result of the s^1_{xy} operator. Figures 2(d)–2(f) gives example configurations for the $N_f = 1$ version of this model. Due to the trace condition, odd winding numbers are ruled out because these would cause mismatch between the spins in the initial and the final state.

The possible worldline configurations for the $U(1)$ case are even more restrictive than the $\mathbb{Z}_2$ case. The s^+_{xy} and s^-_{xy} operators allow the hopping for a given flavor of fermion only in one direction or the other for each bond, depending on the orientation of the same flavored flux on the bond. Figures 2(g)–2(i) illustrates an example configuration and restrictions for the single flavor version of the $U(1)$ model. In $(1+1)$D, it is clear that all allowed configurations must have zero winding number.

The worldline configurations are a tool to obtain meron cluster configurations by introducing appropriate breakups,

TABLE I. Plaquettes and breakups for the $U(1)$-symmetric Hamiltonian. The middle cluster lines in the A breakups and binding lines in the D breakups distinguishes them from the original meron cluster breakups.

Plaquettes	Breakups
	

which decompose the terms in Eq. (6) into further constituents. In considering the allowed worldline configurations given in Fig. 2 for the $U(1)$ theory, for example, each of the active plaquettes in each time slice (shaded in gray) must be one of the plaquettes given in Table I. The plaquettes in each row share the same weight, computed using $\langle s_b, n_b | e^{-\epsilon H_b} | s_b', n_b' \rangle$, from Eq. (6), where b is a nearest neighbor bond, $b = \{x, y\}$. The corresponding breakup cell for each row gives allowable breakups: if all fermion occupations/spins are flipped along any one of the lines, the resulting plaquette also exists in this table. From the table, we see two such breakups are defined, A and D. Although these breakups resemble those from the original meron algorithm, in our case the breakups involve the link variables as well—either as additional lines for the A breakups, or as binding lines extending outward from the horizontal D breakup lines. This is a key difference for the gauge extension of the algorithm. By computing the matrix elements that correspond to the plaquettes in each grouping, we find that for the $U(1)$ theory, the corresponding breakup weights w_A and w_D must obey the following:

$$\begin{aligned} w_A &= 1, \\ w_D &= \exp(\epsilon t) \sinh \epsilon t, \\ w_A + w_D &= \exp(\epsilon t) \cosh \epsilon t, \end{aligned} \tag{7}$$

to satisfy detailed balance. Moreover, the choice of the breakups is such that the total sign of a configuration factorizes into a product of the signs of each cluster: $\text{Sign}\,[C] = \prod_i^{N_c} \text{Sign}[C_i]$, where the configuration C has been decomposed into N_c clusters. We can thus simulate this system by exploring a configuration space where each configuration is defined according to the combination of worldlines and breakups. By assigning breakups to all active plaquettes, clusters are formed, and then updates involve flipping all fluxes and fermions within a cluster, which generates a new worldline configuration. The algorithm begins with putting the system in a *reference configuration*, defined by the fermionic worldlines only, where the weight is known to be positive, and it is always possible to reach this configuration by appropriately flipping a subset of clusters in a given configuration. For both $U(1)$ and $\mathbb{Z}_2$ theories, the reference configuration has a staggered fermionic occupation (charge density wave, or CDW), where fermions and fluxes are stationary throughout imaginary time. Fluxes can be in any spatial configuration (because they do not contribute a sign), and the breakups are all A. Fluxes and breakups may be initially attached to the plaquettes in any way allowed by Table I. A QMC sweep is then as follows:

(1) Go through the list of the active plaquettes and update each breakup, one at a time.
   (a) If the breakup can be changed for a plaquette, change it with probability dependent on the breakup weights.
   (b) If the breakup is changed, consider the new configuration that would result from this change. If it contains a cluster where flipping the fermion occupation causes the fermions to permute in a way that produces a negative sign, then it is a *meron*. In that case, restore the breakup back to its initial state. Rules for identifying merons generalize [45,73] and are in the Supplemental Material [64].
(2) Identify the new clusters formed by the breakups in the new configuration. For each cluster, flip all fermions and fluxes with probability $1/2$.

This describes sampling of the zero-meron sector only, but sectors with other numbers of merons may become relevant depending on the observable [45]. We note that the cluster rules implement the Hamiltonian dynamics, but the constraints due to Gauss' law are not included. Like any cluster algorithm, once the detailed balance conditions have been satisfied, the meron algorithm is expected to be efficient in any space-time dimension [46,73]. We provide a demonstration of the efficiency in $(2+1)$D in the Supplemental Material [64], with an extensive investigation left for future work.

Numerical results. To illustrate the efficacy of the algorithm, we discuss results obtained by simulating the $(1+1)$D $H^{U(1)}_{N_f=1}$ model in Eq. (2), which is related to the massless quantum-link Schwinger model [57,74] and the PXP model [75,76], where quantum scars were first demonstrated experimentally [50]. We simulate the model for different temperatures $\beta = 1/T$, *without imposing Gauss' law.* A filter may then be applied to study the physics in the desired Gauss law sector. The one-dimensional nature of the problem forbids the presence of merons, providing a technical simplification. The first nontrivial result is the emergence of *two* Gauss' law sectors at low temperatures, as shown in Fig. 3. For the $\mathbb{Z}_2$ theory in $(1+1)$D, this result was also observed in [69].

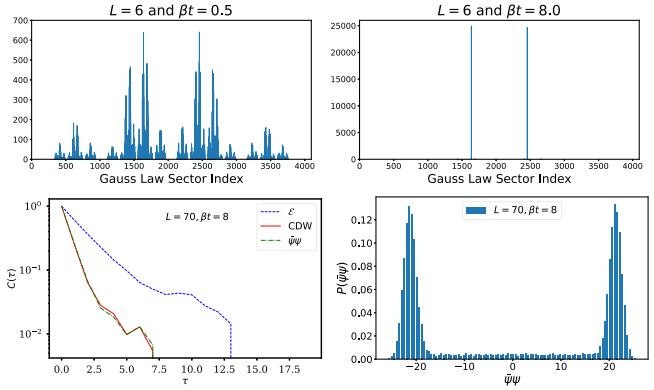


FIG. 3. Clockwise from top left: (i) and (ii) number of configurations versus Gauss law sector index $\sum_x [G_x + 2] \cdot 4^x$ (not all indices correspond to actual sectors) for 50000 equilibrated configurations. Two sectors emerge at large β: $G_x = 0$ and $G_x = (-1)^x$. (iii) The probability distribution of $\bar{\psi}\psi$, with peaks from the two emergent Gauss' law sectors, indicating that the algorithm efficiently samples all sectors. (iv) The autocorrelation functions for different operators.

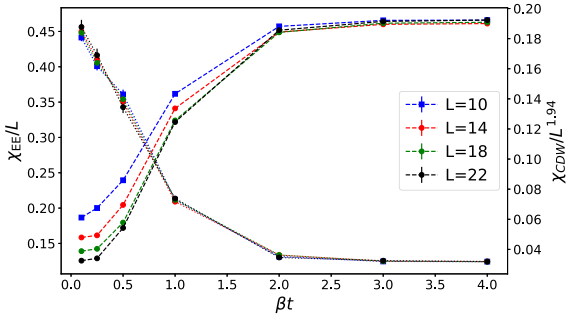


FIG. 4. Finite temperature data for $U(1)$ theory in $1+1$D. The dotted lines show the χ_{EE}, which is the susceptibility corresponding to $\mathcal{E}$. This value rapidly converges to 0.125. On the other hand, the dashed lines trace the χ_{CDW} which display more finite size effects. Thermal behavior of both observables indicate that the transition from low to high temperature is a smooth crossover.

Generating different Gauss' law sectors has the benefit that the physics in each sector can be easily studied by applying a filter. At low temperatures, this is an $\mathcal{O}(1)$ effort, but becomes exponentially difficult at higher temperatures, since exponentially many sectors will be populated. Hence, we note that the efficiency of this meron algorithm for true gauge theories (where Gauss' law is imposed) is more suited to the study of quantum phase transitions rather than finite-temperature ones. For theories where multiple nontrivial Gauss' law sectors emerge at low temperature, it is possible to study the physics in all sectors without any extra effort.

Similar to the well-studied Schwinger model [77–83], our model has the following discrete global symmetries: $\mathbb{Z}_2$ chiral symmetry, charge conjugation, C, and parity, P, [57], whose breaking depends on the strength of the four Fermi coupling. The order parameter sensitive to the P or the C symmetry is the total electric flux, $\mathcal{E} = \frac{1}{L_t}\sum_{x,t} s^3_{x,x+1}$, while the one for $\mathbb{Z}_2$ chiral symmetry is the chiral condensate, $\bar{\psi}\psi = \sum_x (-1)^x n_x$. In Fig. 3 we show the probability distribution for $\bar{\psi}\psi$, which samples the two vacua very well, indicating that at $T = 0$ the symmetry is spontaneously broken. We use these operators to check the algorithm against exact diagonalization results, as well as explore other features of the phase at low temperatures. We leave these discussions to the Supplemental Material [64]. Here we concentrate on the meron algorithm's performance measured via the autocorrelation function:

$$C_{\mathcal{O}}(\tau) = \frac{\langle (\mathcal{O}(i) - \bar{\mathcal{O}})(\mathcal{O}(i+\tau) - \bar{\mathcal{O}})\rangle}{\langle (\mathcal{O}(i) - \bar{\mathcal{O}})^2\rangle}, \tag{8}$$

where $\mathcal{O}(i)$ is the measured value at the ith step of the appropriate operator (whose average is $\bar{\mathcal{O}}$), and is the running index summed over the MC data, while the autocorrelations are measured τ steps apart. Figure 3 shows the $C_{\mathcal{O}}(\tau)$ for three different operators: $\mathcal{E}$, $\bar{\psi}\psi$, and CDW. We note that the bosonic $\mathcal{E}$ relaxes the slowest, while the fermionic operators relax faster. Even for the slowest relaxing mode, the autocorrelation decreases by more than an order of magnitude within 10 MC steps for the largest lattice at the lowest temperature, demonstrating the efficiency of the algorithm. Finally, in Fig. 4 we also show the behavior of the normalized susceptibilities corresponding to $\mathcal{E}$ and the CDW operator as a function of temperature for smaller lattices up to $L = 22$ in the $G_x = 0$ sector. We are able to capture the finite temperature crossover.

Conclusions. We have generalized the construction of the meron algorithm to cases where staggered fermions are coupled to quantum link gauge fields. This construction of the Monte Carlo algorithm is agnostic to the space-time dimension, and paves the way for *ab initio* studies of large scale gauge-fermionic system with odd or even numbers of fermionic flavors, and includes models not simulable using Determinantal quantum Monte Carlo methods. While we are able to simulate low temperatures at fixed values of gauge coupling by using two breakups, A and D, it is possible to add different microscopic terms by increasing the allowed ways of bonding the fermions and gauge links. We have also indicated how to include multiple flavors, and multiflavor interactions. Our investigations open up avenues to study quantum link gauge theories coupled to fermions in higher dimensions, which are almost certain to exhibit quantum phase transitions [84]. Since the physics of Abelian gauge fields represented by half-integer spins are sometimes related to quantum field theories at $\theta = \pi$ [60], where θ is the topological angle, our numerical method also promises to increase our knowledge of quantum field theories with nontrivial topologies. Possible future extensions include gauge fields with larger spin representation and non-Abelian gauge fields as well. Our methods can be

extended to gauge fields with larger spin representation, and hopefully to non-Abelian gauge fields as well, to tackle realistic interacting systems of increasing complexity in particle and condensed matter physics.

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