The “sign problem” (SP) is a fundamental limitation to simulations of strongly correlated matter. It is often argued that the SP is not intrinsic to the physics of particular Hamiltonians because its behavior can be influenced by the choice of algorithm. By contrast, we show that the SP in determinant quantum Monte Carlo (DQMC) is quantitatively linked to quantum critical behavior. We demonstrate this through simulations of several models with critical properties that are relatively well understood. We propose a reinterpretation of the low average sign for the Hubbard model on the square lattice away from half filling in terms of the onset of pseudogap behavior and exotic superconductivity. Our study charts a path for exploiting the average sign in QMC simulations to understand quantum critical behavior.

The first example, simulations at half-filling, where the quantum critical point (QCP) occurs, are SP-free. We introduce a small doping \( \mu \) and show, in the limit \( \mu \to 0^+ \) at temperature \( T \to 0 \), that \( \langle S \rangle \) evolves rapidly as we tune through the QCP.

Our second illustration, the ionic Hubbard model, has an SP even at half-filling. Here, the average sign undergoes an abrupt drop at the band insulator (BI) to correlated metal (CM) transition. The third example, spinless fermions on a honeycomb lattice, also features a semimetal to (charge) insulator transition but allows for an SP-free approach. Studying it with a method that contains an “unnecessary” SP lends insight into the key question of the influence of different algorithms on the connection between the SP and the physics of model Hamiltonians.

These three discussions establish a link between known physics of the models and the fermion sign. Having made that connection, we turn to the iconic square lattice Hubbard model, the physics of which has not been conclusively established. We find that the onset of the SP occurs in a dome-shaped region of the filling-temperature phase space under that of the pseudogap physics. The SP is sufficiently well controlled in the pseudogap phase to obtain reliable results for various observables, including the pairing correlations in various channels, exhibiting dominant enhancement for \( d \)-wave symmetry. Because it behaves exponentially in inverse temperature, the SP provides a rather sharp demarcation of the regime, mimicking the superconducting dome of the cuprates (23). Although the SP prevents DQMC from resolving a signal of a \( d \)-wave transition, the groundwork established for the honeycomb lattice and BI-CM models suggests that this SP dome might be linked to the onset of a superconducting phase.

The SP: Model and methodology

The origin of the SP can be understood in two related classes of algorithms, world-line QMC (WLQMC) (24) and Green’s function QMC (GFQMC) (25, 26), by considering Feynman’s path integral approach, which provides a mapping of quantum statistical mechanics in \( D \) dimensions to classical statistical mechanics in \( D + 1 \) dimensions. Paralleling Feynman’s original exposition for the real-time evolution operator \( e^{-i\hat{H}t} \), the imaginary time evolution operator \( e^{-\beta\hat{H}} \) is subdivided into \( L \), incremental pieces \( \hat{U}_m = e^{-\beta\hat{H}_m} \), where \( \hat{H} \) is the reduced Planck’s constant, \( \hat{H} \) is the Hamiltonian, and \( L\Delta \tau = \beta \) is the inverse temperature. Complete sets of states \( \hat{S}_b |S_b \rangle |S_a \rangle \) are introduced between each \( \hat{U}_m \), so that the partition function \( Z = Tr e^{-\beta\hat{H}} \) becomes a sum over the classical degrees of freedom associated with the spatial labels of each \( I_s \) and also an additional imaginary time index denoting the location \( \tau = 1, 2, ..., L \), of \( I_s \), in the string of operators \( \hat{U}_m \). The quantity being summed in the calculation of \( Z \) is the product of matrix elements \(|S_b |U_m|S_a \rangle \).

In such WLQMC/GFQMC methods, the SP arises when \( \Pi_l |S_b |U_m|S_a \rangle < 0 \). Negative matrix elements are unavailable for itinerant fermion models in \( D > 1 \) because their sign depends on the number of fermions intervening between two particles undergoing exchange, and thus changes as the particle positions are updated. The basis dependence of the SP is apparent by considering intermediate states |\( S_a \rangle \) chosen to be eigenstates \( |\phi_k \rangle \) of \( \hat{H} \), with eigenvalues \( E_k \). In that case, the matrix elements are just \( e^{-\beta E_k} \) and thus are trivially positive definite. Of course, because the eigenstates of \( \hat{H} \) are unknown, this is not a practical choice in any nontrivial situation. Moreover, the SP can generally be avoided for bosonic or spin models as long as the lattice is bipartite. Nonetheless, even bosonic and spin Hamiltonians can have negative matrix elements on frustrated geometries (27), especially for antiferromagnetic models, emphasizing that the SP is not solely a consequence of Fermi statistics.

Auxiliary field QMC (AFQMC) algorithms (28–30) typically have a much less severe SP than WLQMC (7, 31). They are based on the observation that the trace of an exponential of a quadratic form of fermionic operators can be done analytically, resulting in the determinant of a matrix of dimension set by the cardinality of fermionic operators. The determinant is the product \( \Pi_l (1 + e^{-\beta E_k}) \), where \( \epsilon_j \) is the noninteracting energy level and is always positive.

If interactions are present, quartic terms in \( \hat{H} \) are reduced to quadratic ones with a Hubbard-Stratonovich transformation. The trace of the resulting product of exponentials of quadratic forms can be performed, but now they each depend on a different, i.e., imaginary-time dependent, auxiliary field. The resulting determinant is no longer guaranteed to be positive; the consequence is the SP given that the Hubbard-Stratonovich field...
that systematic errors in sampling errors [for additional details, see servables are of the same order as statistical (spin) species of itinerant electrons hop on a same order as the bandwidth at intermediate interaction strengths (of the reasonable rule of thumb is that the average sign can be used as an alternative which is an indicator of the QCP. In all panels with data, the prediction for the ground-state phase transition occurring at $U_c/t = 3.869$ (17) is depicted by a star marker. In all data, Trotter discretization is chosen as $t \Delta t = 0.1$. See fig. S1 for additional observables and fig. S2 for the fermionic flavor-dependent average sign.

Semimetal to antiferromagnetic MI on a honeycomb lattice

On a honeycomb lattice (Fig. 1A), the $U = 0$ Hubbard Hamiltonian has a semimetallic density of states that vanishes linearly at $E = 0$. Its dispersion relation $E(k)$ has Dirac points in the vicinity of which the kinetic energy varies linearly with momentum. Unlike the square lattice that displays AF order for all $U > 0$, the honeycomb Hubbard model at $T \rightarrow 0$ remains a semimetal for small nonzero $U$, turning to an AF insulator only for $U$ exceeding a critical $U_c$. Early DQMC and series expansion calculations estimated $U_c \sim 4t$ (42), with subsequent studies (16, 17) yielding the more precise value $U_c/t = 3.869$.

The upper panel of Fig. 1B gives $\langle S \rangle$ in the $U$–$T$ plane. By introducing a small, nonzero $\mu = 0.1$, we can induce a SP that begins to develop at $T/t \sim 0.1$. As $T$ is lowered further, the average sign deviates from $\langle S \rangle = 1$ in a relatively narrow window of $U/t$ close to the known $U_c$. In turn, we show the $\langle S \rangle$ on the $U$–$\mu$ plane at fixed $T/t = 0.05$ in the lower panel of Fig. 1B. For large $\mu$, the sign is small for a broad swath of interaction values. As $\mu$
decreases, this region pinches down until it terminates close to $U_c$; the dashed white line displays the minimum $\langle S \rangle$ in the relevant range. In both panels, the behavior of the average sign outlines the quantum critical fan that extends above the QCP.

Figure 1C shows a finite size extrapolation of $\langle S \rangle$ in the $1/L-U$ plane, where $L$ is the linear lattice size. Just as $\langle S \rangle$ worsens with increasing $\beta$, it is also known to deviate increasingly from $\langle S \rangle = 1$ with growing $L$ (29). The extrapolation $L \rightarrow \infty$ clearly reveals $U_c$ in the presence of a small chemical potential. So far, we have exclusively used $\langle S \rangle$ in locating $U_c$. Original investigations used more “traditional” (and more physical) correlation functions such as the AF structure factor and conductivity. For comparison with the evolution of $\langle S \rangle$, Fig. 1D shows one example, the rate of change of the double occupancy $\langle n_{\uparrow \downarrow} \rangle$, again in the $1/L-U$ plane. A peak in $-d\langle n_{\uparrow \downarrow} \rangle/dU$ indicates where local moments ($m^2$) are growing most rapidly. The similarity between Fig. 1, C and D, emphasizes how $\langle S \rangle$ is tracking the physics of the model in a way markedly similar to $(m^2)$. The combination of the three limits, $\mu$, $\beta$, and $L$, unequivocally points out the QCP location; the supplementary materials (7) contain further discussion and other observables. Two of these limits can be simultaneously approached by fixing the ratio $L/L^*$ with $z$, the dynamical critical exponent (43).

**Ionic Hubbard BI to AF transition**

Among the different types of nonconduction states are BIs, in which the chemical potential lies in a gap in the noninteracting density of states, and MIs, in which strong repulsive interactions prevent hopping at commensurate filling. The evolution from BI to MI is a fascinating issue in condensed-matter physics (18–20, 44–46). In the ionic Hubbard model that we investigated here, a staggered site energy $\mu_i = \pm \Delta$ on the two sublattices of a square lattice (Fig. 2A) leads to a dispersion relation $E(k) = \pm \sqrt{\epsilon(k)^2 + \Delta^2}$ with $\epsilon(k) = -2t (\cos k_x + \cos k_y)$. The resulting density of states vanishes in the range $-\Delta < E < +\Delta$ in which the lattice is half-filled, resulting in a BI. The occupation of the “low-energy” sites $\mu_i = -\Delta$ is greater than that of the “high-energy” sites $\mu_i = +\Delta$, so that there is a trivial CDW order associated with an explicit breaking of the sublattice symmetry in the Hamiltonian.

An onsite repulsion $U$ disfavors this density modulation: The potential energy $U\langle n_{\uparrow \downarrow} \rangle$ is higher than that for a uniform occupation. Thus, the driving physics of the BI, the staggered site energy $\Delta$, and that of the MI, the repulsion $U$, are in competition. Although the simplest scenario is a direct BI to MI transition with increasing $U$, one of the more exotic possible outcomes is the emergence of a metallic phase when these two energy scales are in balance and neither type of insulator can dominate the behavior. Past DQMC simulations suggest that this less trivial case occurs when the DC conductivity to bound the metallic phase (46, 47).

Here, we investigated how this physics might be reflected in the average sign. Figure 2B shows $\langle S \rangle$ in the $U/t-T/t$ plane at $\Delta = 0.5t$. As $T$ is lowered, $\langle S \rangle$ deviates from unity for a range of intermediate $U$ values. Figure 2C gives the behavior in the $U/t-\Delta/t$ plane at fixed low $T = t/24$. The central result is that $\langle S \rangle$ is small in a region that maps well with the previously determined boundaries of the metallic phase (46, 47). This is emphasized.

![Image](https://www.science.org)
by comparison with Fig. 2D, which uses one of the “traditional” methods for phase boundary location, namely the behavior of the double occupancy. The BI has a low occupancy and thus very low double occupancy on the +Δ sites. Increasing U smooths out the density so that the double occupancy on the +Δ sites increases: d⟨n↑↑,n↓↓⟩/dU > 0. By contrast, in the MI region, U ≥ Δ, the physics is that of the usual Hubbard Hamiltonian and double occupancy decreases as U grows: d⟨n↑↑,n↓↓⟩/dU < 0.

In the CM region between BI and MI, however, obtaining a relevant signal-to-noise ratio for the traditional observables is exponentially challenging precisely because the average sign vanishes in this region. The “phase diagram” obtained by using ⟨S⟩ (Fig. 2C) is very similar to that given by the physical observable, the rate of change of double occupancy with U (Fig. 2D).

As in the determination of the QCP for the spinful Hubbard model on a honeycomb lattice, ⟨S⟩ emerges as more than a mere nuisance, but also as a harbinger of the physics. An in-depth similarity between these two situations is discussed in the supplementary materials (7), where we show that the BI-metal QCP is again uniquely identified by the ⟨1/L⟩ scaling of ⟨S⟩, in precise analogy with the honeycomb case. These results suggest the existence of a quantum critical region associated with the CM phase and the vanishing ⟨S⟩.

An “unnecessary” SP

We now consider spinless fermions, in which the on-site Hubbard interaction U, made irrelevant by the Pauli principle, is replaced by an intrisite repulsion Vc.

\[ \hat{H} = -t \sum_{\langle ij \rangle} \left( \hat{c}_i^\dagger \hat{c}_j + \text{H.c.} \right) + V \sum_i \hat{n}_i \hat{n}_j \] (2)

Equation 2 provides an example of a model in which the SP can be completely solved by using special techniques such as the fermion bag in the continuous time QMC approach (35) or by going to a different basis using a Majorana representation of the fermions in the AFQMC method (41), as long as the system is on a bipartite lattice and V > 0. The standard Blankenbecler, Scalapino, and Sugar approach (28), on the other hand, manifestly displays a SP in the low-temperature regime. Nevertheless, to study the sign and its connection with the underlying physics, we used a Blankenbecler, Scalapino, and Sugar–based algorithm to investigate the system on a honeycomb lattice (Fig. 3A). Consideration of this “unnecessary” SP allows us to address fundamental issues related to the influence of different algorithms on the connection between the SP and the physics of model Hamiltonians.

At T = 0, the model displays a QPT between a Dirac semimetal and an insulating staggered CDW state as the interaction is tuned through a critical value Vc (29). At large V, the repulsive interaction favors a CDW state, distinguished from that of the ionic Hubbard model by the fact that there is no staggered external field here; the CDW phase is a result of spontaneous symmetry breaking. As V is reduced, increasing quantum fluctuations caused by hopping finally destroy the CDW state, resulting in a Dirac semimetal for V < Vc. Accurate estimates based on SP-free methods yield Vc ~ 1.35t (41).

In Fig. 3B, we show a map of the temperature extrapolation of ⟨S⟩ as a function of V. The sign shows a clear reduction around the known Vc (denoted by the star). Figure 3D shows the spatial lattice size dependence of the sign, and Fig. 3C, once again, a more “traditional” local variable, the derivative of the nearest-neighbor (NN) density-density correlation ⟨δn_i δn_j⟩_{NN} with respect to V. In the CDW phase, increasing V strengthens the staggered order, reducing the NN density correlations, and thus -d⟨δn_i δn_j⟩_{NN}/dV is positive. Conversely, the effect is much smaller in the semimetal state, where the derivative is close to zero. The transition Vc is characterized by a clear downturn in this quantity, which becomes progressively sharper as L increases, as Fig. 3C shows. This variable thus serves as a physical indicator of the QPT, allowing a comparison of Fig. 3, C and D, to demonstrate the connection between the QCP and the behavior of ⟨S⟩. In this model, ⟨S⟩ is sufficiently well behaved that a study of the finite-temperature CDW transition with DQMC is feasible (7) without having to resort to SP-free approaches (48).

Square lattice Hubbard model

The essential elements of the physics of the cuprate superconductors include antiferromagnetic order at and near one hole per CuO2 cell, a superconducting dome upon doping, which typically extends to densities 0.6 ≤ ρ ≤ 0.9, and a “pseudogap”/“strange metal” phase above the dome (23, 49). There are many quantitative, experimentally based phase diagrams of different materials that determine the regions occupied by these phases (50). Likewise, there are computational studies of individual (ρ, T, U) points establishing magnetic/charge order (51), linear resistivity (52), a reduction in the spectral weight for spin excitations (53, 54), and d-wave pairing (55, 56).

Here, we reveal an “SP phase diagram” that bears notable resemblance to the experimental phase diagram. As is well known, the severity of
that occurs in a range of densities $0.4 < \rho < 1$ as $T$ is lowered (Fig. 4D), (ii) the enhancement of $d$-wave pairing (Fig. 4E) surrounding the sign dome, and (iii) the magnetic properties being also linked to the expectation value $\langle S \rangle$ dome: The trajectory tracing the peak value of $\chi(q = 0)$ as $T$ is decreased terminates precisely at the top of the dome (Fig. 4F). In isolation, the comparisons of the behavior of the sign and the pairing and magnetic responses in the square lattice Hubbard model appear likely to be coincidental. Indeed, the fact that the sign is worse precisely for optimal dopings has been previously discussed, but thought to be just “bad luck” (32, 57–59). However, that the known QCPs of the three models discussed in the preceding three sections can be quantitatively linked to the behavior of $\langle S \rangle$ suggests that the sign dome might actually be indicative of the presence of $d$-wave superconductivity.

Discussion and outlook

Early in the history of the study of the SP, a simple connection was noted between the fermionic physics and negative weights in AFQMC. If one artificially constructs two Hubbard-Stratonovich field configurations, one associated with two particle exchanging as they propagate in imaginary time and another with no exchange, one finds that the associated fermion determinants are negative in the former case and positive in the latter. This interesting observation, however, pertains to low density, that is, to the propagation of just two electrons. Another key observation is that the SP can be viewed as being proportional to the exponential of the difference of free energy densities of the original fermionic problem and the one used with the weights in the Monte Carlo sampling taken to be positive, akin to a bosonic formulation of the problem (13, 32). It highlights how intrinsic the SP is in QMC methods. A last important result is that ordered phases are often associated with a reduction in the importance of configurations that scramble the sign. This is graphically illustrated in the snapshots of (24). Although less crisp, similar effects are seen in AFQMC, for example, in considering the evolution from the attractive Hubbard model to the Holstein model with decreasing phonon frequency $\omega_0$. Reducing $\omega_0$ acts to increase the effect of the phonon potential energy term $P$ in $H$, thereby straightening the auxiliary field in imaginary time.

Here, we have shown that the behavior of the average sign $\langle S \rangle$ in DQMC simulations holds information concerning finite density thermodynamic phases and transitions between them: the QCPs in the semimetal to antiferromagnetic MI transition of Dirac fermions, the BI to CM to correlated insulator evolution of the ionic Hubbard Hamiltonian, and the QCP of spinless fermions (even though a sign-problem free formulation exists). Specifically, a rapid evolution of the sign is observed (fig. S7), different pairing channels (fig. S8), and the behavior of the spectral weight (figs. S9 and S10) is given in the supplementary materials (7). Equivalent results for $t' = 0$ are reported in fig. S11.
π flux, it can be shown that in the sign-problem free formulation, the QMC weights, when expressed in terms of the square of Pfaffians (PF), holds similar information, namely that \( \langle \text{sign}(PF) \rangle \) departs from 1 close to the QCP for this model (67). These results provide further evidence that the average sign of the QMC weights is inherently connected to the physics of the model in many mutually unrelated models and methods, but an even broader study is necessary to establish this conclusively.

Having established this connection in Hamiltonians with known physics, we have also presented a careful study of the SP for the Hubbard model on a 2D square lattice, which is of central interest to cuprate conductivity. The intriguing coincidence that the SP is the worst at a density \( \rho \sim 0.87 \), which corresponds to the highest values of the superconducting transition temperature, has been noted previously (32, 57–59). It is worth emphasizing that we have not here presented any solution to the SP. However, our work does establish the surprising fact that (S) can be used as an “observable” that can quite accurately locate QCPs in models such as the spinful and spinless Hubbard Hamiltonians on a honeycomb lattice and the ionic Hubbard model and also provides a clearer connection on a honeycomb lattice and the ionic Hubbard spinful and spinless Hubbard Hamiltonians accurately locate QCPs in models such as the ionic and spinless Hubbard model and also provides a clearer connection on a honeycomb lattice and the ionic Hubbard spinful and spinless Hubbard Hamiltonians accurately locate QCPs in models such as the ionic and spinless Hubbard model and also provides a clearer connection.

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SUPPLEMENTARY MATERIALS

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Supplementary Text Figs. S1 to S11 (References 64–67)
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Quantum critical points and the sign problem
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Unexpected benefits of the sign problem
Solving challenging problems in quantum many-body physics often involves using numerical Monte Carlo methods. However, in the most interesting regime of strong interactions and low temperatures, the so-called sign problem can make calculations intractable. Mondaini et al. studied the severity of the sign problem quantitatively in several representative models. The researchers found that quantum critical behavior in these models correlated with the regions in the phase diagram where the sign problem was most pronounced. Viewed as a diagnostic for quantum criticality, the sign problem then becomes a tool (in addition to being a nuisance). —JS

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