SUMMARY OF CHANGES

The manuscript has been revised according to the reviewers' comments. The detailed modifications are listed as follows:

1 The **title** has been changed to *"Preempting Fermion Sign Problem: Unveiling Quantum Criticality through Nonequilibrium Dynamics in Imaginary Time"*, with "in Imaginary Time" explicitly added for clarity.

2 The **abstract** has been revised to remove hyperbolic statements and to clearly emphasize that the approach is based on "imaginary-time nonequilibrium critical dynamics" to avoid possible misunderstandings.

3 **Changes in the main text:**

(1) In the **Introduction** section, on page 1, 1st paragraph, left column, the wording has been refined to better describe the sign problem and its significance.

(2) In the **Introduction** section, on page 2, 2nd paragraph, left column, the term "short-time critical dynamics" has been changed to "short-imaginary-time critical dynamics" for clarity.

(3) In the **Theoretical framework** section, on page 2, 3rd paragraph, left column, it has been clarified that the discussion focuses on zero-temperature projector QMC and imaginary-time dynamics.

(4) In the **Single-Dirac-fermion Hubbard model** section, on page 3, 2nd paragraph, left column, it has been emphasized that the discussion focuses on imaginary-time dynamics and that it is the conventional projector QMC that requires sufficiently long imaginary-time evolution. An additional note has been added to point out that similar short imaginary-time techniques have been applied in finite-temperature QMC simulations. It is also clarified that the dynamical exponent z can be independently determined.

(5) In the **Single-Dirac-fermion Hubbard model** section, on page 3, 2nd paragraph, right column, in the **Spinless t-V model** section, on page 3, 3rd paragraph, right column and page 4, 1st paragraph, left column, and in the **SU(3) Hubbard**

model section, on page 5, 4th paragraph, left column, it has been explicitly reiterated that the discussions focus on imaginary-time dynamics.

(6) In the **Spinless t-V model** section, on page 4, 1st paragraph, left column, the benefit of the flexible choice of initial states has been clarified.

(7) In the **SU(3) Hubbard model** section, on page 4, 1st paragraph, right column, previous QMC studies on the SU(3) Hubbard model have been mentioned.

(8) In the **Concluding remarks** section, on page 5, 5th paragraph, left column, the wording has been refined to better highlight the advantages of our proposed framework.

(9) In the **Concluding remarks** section, on page 5, 3rd paragraph, right column, the applicable scope and limitations of our method have been explicitly clarified.

4 **Changes in figures:**

(1) In the insets of Figure 1a, Figure 2a, and Figure 3b, the red dashed lines have been schematically extended and red legends or annotations have been added to enhance visibility.

(2) An explanation for the white dashed line has been added to the caption of Figure 1.

(3) The term "short-time critical dynamics" in the captions of Figure 2 and Figure 3 has been changed to "short-imaginary-time critical dynamics" for clarity.

(4) The blue circles in Figure 3a have been changed to light green, and the numbers "1", "2", and "3" have been added inside the circles to make it easier to visually distinguish the different fermion flavors in the schematic diagram.

5 **Changes in references:**

(1) References [52, 54, 55, 64, 65] have been newly added.

(2) The capitalization issues in References [28, 50, 51] have been corrected.

6 **Changes in Supplementary Materials:**

(1) Section I-A has been expanded to further discuss the roles and significance of imaginary time in conventional projector QMC and finite-temperature QMC,

with additional background added. The similarities and differences between our proposed framework and previous QMC methods have been clarified.

(2) Section I-B has been supplemented to discuss how the choice of Hubbard-Stratonovich transformation channel affects the structure of the fermion determinant and thus impacts the sign problem.

(3) Section I-C has been corrected to fix the typo in Equation S6.

(4) Section I-D has been newly added to provide a detailed analysis and discussion of the applicability and limitations of our method, highlighting that it makes a broad range of previously inaccessible models tractable.

(5) Section I-E has been newly added to explain in detail the guiding principles for selecting the value of τ/L^z when determining the critical point.

(6) Section II-B has been revised to adjust the notation for the structure factor on general momentum, with additional explanation clarifying the motivation for defining the fermion correlation function in momentum space.

(7) Section II-C and Figure S5 have been newly added to illustrate how to independently determine the dynamical exponent z.

(8) Section III-A has been supplemented to mention earlier cases where a larger system size can lead to a weaker sign problem.

(9) Section IV-A has been clarified to emphasize that only the λ_8 matrix is full rank.

(10) In Section IV-B and in Figure S9 and Figure S10, the mean-field calculation results have been updated with larger system size ($L = 42$), and the notation for the order parameter has been unified as $m_{\lambda_n\text{-AFM}}$.

(11) Section IV-E has been corrected to fix Equation S32, and the corresponding estimate for the efficiency acceleration factor in Figure S15c has also been updated.

Some other minor changes to enhance clarity and correct typos are not listed.

RESPONSE TO REVIEWER 1

Comment:

This paper explores an improved quantum Monte Carlo (QMC) simulation algorithm to explore phase transitions in interacting many-body systems. After describing the approach, it exhibits applications to three challenging model Hamiltonians. Two (the 'SLAC' fermion Hubbard model and the spinless t-V model) have been previously studied so that comparisons can be made and the method's correctness validated. The third, the SU(3) Hubbard model with an applied magnetic flux, has not been examined, and exhibits a transition in a very interesting and novel universality class. The manuscript is important both because the method proposed is a powerful extension to our ability to do quantum simulations and because the third application uncovers new and important properties of quantum many-body phases of matter.

I support publication of this article after the issues below are addressed.

Reply:

We are very grateful to the reviewer for recognizing our new method and new physical discoveries. We appreciate the reviewer's support for our article's publication in *Science*.

Comment:

Major comments:

[01] The key point of the paper is that phase transitions can be observed at smaller imaginary time tau, before the sign problem becomes too serious. For example, on page 3, column 1, the authors state, "In the conventional projector QMC approach, a sufficiently long evolution time should be implemented to ensure that ground state properties are accessed, resulting in the severe sign problem..." The first part of this sentence implies that one typically must use large tau to study quantum phase transitions. This is a bit misleading. It has long been understood that one can conduct simulations at fixed τ/L^z, eliminating one of the free variables in finite size scaling (FSS), and also allowing relatively small tau. One very early example is Phys. Rev. Lett. 69, 828 (1992), which examines the superconductor-insulator

transition of dirty bosons. There $\tau = (1/4)L^2$ (the dynamic critical exponent $z = 2$) so that even on a L=10 lattice a relatively small $\tau = 25$ was used, in disagreement with the authors claim of "long evolution time". In that work, because bosons are considered, there is no sign problem, but quite a few subsequent fermionic simulations have also used the idea of keeping τ/L^z fixed (and tau small) as a way to do FSS. The authors should revise their language to emphasize that their key idea is to use this to avoid the sign problem, rather than just the fact that small τ can tell the story.

Reply:

We sincerely thank the reviewer for the constructive comments.

As the reviewer rightly pointed out, our previous phrasing may lead to misunderstanding. To clarify our main idea more effectively, we would like to supplement and organize some essential concepts and background:

When using imaginary-time evolution-based QMC methods to study quantum phase transitions, two distinct types of QMC approaches are commonly employed. One is the finite-temperature QMC method (FTQMC), which considers the grand canonical ensemble. The expectation value of a physical observable is given by:

$$\langle O \rangle = \frac{\mathrm{tr}\left[\mathrm{e}^{-\beta(H-\mu N)}O\right]}{\mathrm{tr}\left[\mathrm{e}^{-\beta(H-\mu N)}\right]}. \tag{R1}$$

Here, $\beta = 1/k_{\mathrm{B}}T$ is the inverse temperature and corresponds to the imaginary-time length in the Monte Carlo simulation. FTQMC includes both quantum and thermal fluctuations. The other is the projector QMC method (PQMC), also known as the zero-temperature QMC method. The expectation value of an observable is given by:

$$\langle O \rangle = \frac{\langle \psi_0 | \, \mathrm{e}^{-\frac{\tau}{2}H} \, O \, \mathrm{e}^{-\frac{\tau}{2}H} \, | \psi_0 \rangle}{\langle \psi_0 | \, \mathrm{e}^{-\tau H} \, | \psi_0 \rangle}. \tag{R2}$$

PQMC considers only quantum fluctuations. When the imaginary-time evolution is sufficiently long, i.e., $\beta \to \infty$ or $\tau \to \infty$, both methods yield ground-state expectation values of physical observables, and hence can, in principle, be used to study quantum phase transitions. The paper mentioned by the reviewer, Phys. Rev. Lett. 69, 828 (1992), discusses FTQMC, while our manuscript focuses on nonequilibrium imaginary-time dynamics entirely within the context of PQMC.

For FTQMC, a finite β corresponds to a finite-temperature equilibrium state, which is not the nonequilibrium process we are discussing. Because β in FTQMC has such a well-defined physical meaning, it was relatively early accepted that the factor β/L^z can be used in finite-size scaling (FSS). In fact, the reviewer's statement that "it has long been understood that one can conduct simulations at fixed τ/L^z" only holds in the context of FTQMC, where what is fixed is β/L^z. Moreover, the value of β/L^z is typically not very small; $\beta = L^z$ is a common choice. In some cases, taking β/L^z to be too small may not be a sufficiently universal approach to extracting information about quantum phase transitions, because additional thermal fluctuations can obscure the quantum critical behavior. Especially for phase transitions that exist strictly at zero temperature, one only observes a continuous crossover at finite temperature. In this sense, PQMC might be a more generally applicable method.

However, within the PQMC framework, due to the lack of understanding of nonequilibrium imaginary-time dynamics, conventional PQMC simulations usually require taking τ to be sufficiently large (typically greater than two to three times L) to ensure that the wavefunction is projected onto the ground state. It is even often believed that small τ values in PQMC do not carry much physical meaning. Therefore, in PQMC, fixing τ/L^z and taking small values is not a common practice, and is only encountered in studies involving nonequilibrium imaginary-time dynamics (such as PhysRevB.89.144115, PhysRevB.96.094304), including our previous work (arXiv:2310.10601). We have carefully and systematically investigated nonequilibrium imaginary-time dynamics in Dirac fermion systems and found that, although such a setup lies beyond the conventional PQMC framework, choosing small τ values only introduces some dependence on the initial state, while the ground-state information, especially the universal quantum criticality, still manifests in the nonequilibrium dynamics. As long as one selects an appropriate initial state, quantum phase transitions can still be clearly identified even at small τ/L^z. Without additional thermal fluctuations, this method might be more general than fixing β/L^z in FTQMC. In summary, both in terms of physical interpretation and practical application, FTQMC with fixed β/L^z and PQMC with fixed τ/L^z are substantially different. The latter requires a deep understanding of nonequilibrium imaginary-time dynamics.

It is precisely based on our solid foundation in studying nonequilibrium imaginary-time

dynamics in fermionic systems that we are confident in employing this method to address the sign problem in the current work. This is fundamentally different from the idea of keeping β/L^z fixed (and β small) as a way to do FSS in FTQMC. Moreover, in addition to using smaller τ, compared to conventional PQMC and FTQMC approaches, our framework further alleviates the sign problem by flexibly choosing appropriate initial states, while the consistency of results obtained from different initial states provides a useful means of self-consistency check.

We fully agree with the reviewer that our previous wording may have been insufficient and imprecise. In the revised manuscript, we have clarified that it is the zero-temperature PQMC approach that typically requires long imaginary-time evolution [See Changes 3(3), 3(4)]. At the same time, we also acknowledge that a similar strategy has been widely applied in FTQMC simulations to probe quantum critical points [See Change 3(4)]. Following the reviewer's suggestion, we have carefully revised our relevant descriptions to emphasize that our key idea is to use nonequilibrium dynamics to avoid the sign problem [See Changes 3(3), 3(4), 3(6), 3(8), 3(9), 6(1), 6(4)]. In the Supplemental Material, we have also added more background on imaginary-time nonequilibrium dynamics to help readers unfamiliar with QMC terminology better understand our points [See Change 6(1)].

Comment:

[02] I am not sure the comments on computational efficiency (Section SM IVE) and Equation S31 are correct. It is implied there that the efficiency is linearly proportional to the sign, but in fact, the extra computational power might grow much faster than $1/\langle S\rangle$ as $\langle S\rangle$ gets small. Consider making a situation when the average sign $\langle S\rangle$ has an error bar of 0.02. If $\langle S\rangle = 0.1$ you would need to run 100 times longer to get the same accuracy on a measurement using Eq. S6 as you would if $\langle S\rangle = 1$. That is, the computational power probably grows as $1/\langle S\rangle^2$ not as $1/\langle S\rangle$. Of course, this makes the approach described in the paper even more important: the "efficiency acceleration factor" is even larger. Still, because error bars only go down as the inverse square root of the simulation time, Equation S31 seems wrong to me.

Reply:

We sincerely thank the reviewer for the careful examination and generous reminder. We confirm that Equation (S31) in the original Supplementary Materials was indeed incorrect. Following the reviewer's comment, we have corrected it [See Change 6(11)]. The correct estimate for the efficiency acceleration factor of the nonequilibrium approach compared to the equilibrium method is:

$$\text{Efficiency acceleration factor} \approx \left(\frac{1/\left\langle \text{sign} \right\rangle_{\text{eq.}}}{1/\left\langle \text{sign} \right\rangle_{\text{neq.}}} \right)^2 \frac{\tau_{\text{eq.}}}{\tau_{\text{neq.}}}. \tag{R3}$$

Below we explain how this formula is derived. For QMC simulations with the sign problem, the expectation value of an observable is computed as:

$$\langle O \rangle = \frac{\langle O \,\text{sign} \rangle_{|w|}}{\langle \text{sign} \rangle_{|w|}}. \tag{R4}$$

Thus, the statistical error of the expectation value is estimated as:

$$\Delta \langle O \rangle = \sqrt{\left(\frac{\Delta \langle O \,\text{sign} \rangle_{|w|}}{\langle \text{sign} \rangle_{|w|}} \right)^2 + \left(\frac{\langle O \,\text{sign} \rangle_{|w|}}{\langle \text{sign} \rangle_{|w|}} \frac{\Delta \langle \text{sign} \rangle_{|w|}}{\langle \text{sign} \rangle_{|w|}} \right)^2}. \tag{R5}$$

According to the central limit theorem, the Monte Carlo sampling errors $\Delta \langle O \,\text{sign} \rangle_{|w|}$ and $\Delta \langle \text{sign} \rangle_{|w|}$ scale inversely with the square root of the sample number:

$$\Delta \langle O \,\text{sign} \rangle_{|w|} \sim \frac{\alpha_1}{\sqrt{N}}, \quad \Delta \langle \text{sign} \rangle_{|w|} \sim \frac{\alpha_2}{\sqrt{N}}. \tag{R6}$$

Therefore, the statistical error in $\langle O \rangle$ can be expressed as:

$$\Delta \langle O \rangle = \frac{1}{\langle \text{sign} \rangle_{|w|}} \frac{\alpha}{\sqrt{N}}, \tag{R7}$$

where

$$\alpha \equiv \sqrt{\alpha_1^2 + \alpha_2^2 \left(\frac{\langle O \,\text{sign} \rangle_{|w|}}{\langle \text{sign} \rangle_{|w|}} \right)^2}.$$

Assuming $\alpha_{\text{eq.}} \approx \alpha_{\text{neq.}}$ (a very rough approximation, likely valid only at the order-of-magnitude level), in order to achieve the same computational accuracy, the required sample numbers in the nonequilibrium and equilibrium methods satisfy:

$$\frac{1}{\langle \text{sign} \rangle_{\text{neq.}}} \frac{1}{\sqrt{N_{\text{neq.}}}} \approx \frac{1}{\langle \text{sign} \rangle_{\text{eq.}}} \frac{1}{\sqrt{N_{\text{eq.}}}}. \tag{R8}$$

Moreover, the computational time to generate a single sample through Monte Carlo updates, T/N, is proportional to the imaginary-time length τ. Therefore, the efficiency acceleration factor of the nonequilibrium method can be estimated as:

$$\text{Efficiency acceleration factor} = \frac{T_{\text{eq.}}}{T_{\text{neq.}}} \approx \frac{N_{\text{eq.}}}{N_{\text{neq.}}} \frac{\tau_{\text{eq.}}}{\tau_{\text{neq.}}} \approx \left(\frac{1/\left\langle \text{sign} \right\rangle_{\text{eq.}}}{1/\left\langle \text{sign} \right\rangle_{\text{neq.}}} \right)^2 \frac{\tau_{\text{eq.}}}{\tau_{\text{neq.}}}. \tag{R9}$$

In the revised manuscript, we have re-calculated the efficiency gains presented in the Supplementary Materials using this corrected formula [See Change 6(11)].

Comment:

Minor comments:

[01] The authors refer to "non-equilibrium" in the introduction. To most readers this will imply real time dynamics, whereas the paper focuses on the evolution in imaginary time. This term should be eliminated or clarified.

Reply:

We sincerely thank the reviewer for the suggestion. To avoid potential misunderstandings, we have explicitly stated "in imaginary time" in the revised title [See Change 1], and clarified in the abstract that our approach is based on "imaginary-time nonequilibrium critical dynamics" [See Change 2]. In the introduction, we intentionally begin with a discussion of real-time nonequilibrium scaling and then lead into its imaginary-time counterpart (which shares the same scaling form), in order to help readers without prior experience understand our imaginary-time context. Furthermore, throughout the manuscript, we have revised instances of "short-time dynamics" to "short-imaginary-time dynamics" for clarity [See Changes 3(2), 3(5), 4(3)].

Comment:

[02] In both figures 1 and 2 the captions refer to a dashed red line. I do not see a dashed red line. Also, in figure 1a there is a dashed white line whose significance is not made clear.

Reply:

We thank the reviewer for pointing out these two issues.

The dashed red line in the figures indicates the specific imaginary-time slice and its corresponding average sign, which we use to determine the critical point. It is indeed difficult to distinguish in the small insets. In the revised manuscript, we have schematically extended the red dashed line for better visibility and added clear annotations or legends to highlight it [See Change 4(1)].

As for the dashed white line in Figure 1a, it indicates the boundary of the nonequilibrium critical region. We have added an explanation of this in the revised figure caption [See Change 4(2)].

Comment:

[03] When printed in a hard-copy, the violet and blue circles of Figure 3 are hard to distiguish, though they can be told apart on a monitor.

Reply:

We thank the reviewer for pointing out this issue. In the revised manuscript, we have changed the blue circles in Figure 3a to light green ones and added the numbers "1", "2", and "3" inside the circles to make it easier to visually distinguish between different flavors of fermions in the schematic diagram [See Change 4(4)].

Comment:

[04] In discussing the SU(3) Hubbard model, the authors should also consider citing Phys. Rev. Research 5, 043267 (2023) and Phys. Rev. A 108, 053312 (2023). The former uses CPQMC and so is not exact, but the latter used the exact DQMC method. The ordering found is similar to that of Figure 3a- one species is on one of the sublattices and a superposition of the other two species on the second sublattice.

Reply:

We thank the reviewer for recommending these two important references. Both papers study the SU(3) Hubbard model at 1/3 filling on the square lattice and reveal interesting metal-insulator transitions. The former uses CPQMC to map out the ground-state phase diagram, while the latter employs the exact DQMC method to explore various short-range ordering

patterns at finite temperature.

The λ_8-antiferromagnetic order we identified at half-filling in the ground state is qualitatively similar to the short-range two-sublattice antiferromagnetic structure observed at finite temperature in the latter work. In the revised manuscript, we have cited and briefly reviewed both of these important references in our discussion of the SU(3) Hubbard model [See Changes 3(7), 5(1)].

Comment:

[05] In the references "monte Carlo" (citations 28 and 51) and "dirac" (citation 50) should be capitalized.

Reply:

We thank the reviewer for pointing this out. We have corrected these capitalization issues in the revised manuscript [See Change 5(2)].

Comment:

[06] In the Supplemental Materials (SM), section 1A, the authors cite a review article, which is good, but it might also be appropriate to cite specific early work by Sorella etal which pioneered the PQMC method for Hubbard models, eg SORELLA S., BARONI S., CAR R. and PARRINELLO M., Europhys. Lett., 8 (1989) 663; or SORELLA S., Int. J. Mod. Phys. B, 5 (1991) 937.

Reply:

We thank the reviewer for this important suggestion. In the revised manuscript, we have cited both of these references [See Changes 5(1), 6(1)].

Comment:

[07] In the SM Section 1B , it would be good to clarify the implications of the use of different decouplings on the number of fermion determinants. Eg. with the σ_x channel (Eq. S4) spin up and down are mixed and hence there is a single fermion determinant, whereas in the $sigma_z$ channel the different flavors would each have their own determinants. This is worth

describing since in general the number of determinants can have implications for the sign problem.

Reply:

We thank the reviewer for the interesting observations and suggestions. As recommended, we have added a discussion in SM Section I-B describing the number of fermion determinants and attempted to consider its potential impact on the sign problem [See Change 6(2)]. Additionally, we noticed that the reviewer may have inadvertently referred to "(Eq. S4)" when it should have been "(Eq. S3)".

Specifically, for the single-Dirac-fermion Hubbard model, note that the free fermion hopping term involves only spin-flipping hopping (see Eq. 2 in the main text). If the interaction term in (Eq. S3) is decoupled using the off-diagonal σ_x channel, the resulting decoupled Hamiltonian contains only off-diagonal nonzero blocks. As a result, the fermion determinant in the configuration weight can be factorized into the product of two smaller determinants: $\det(M) \propto \det(M_{\uparrow\downarrow})\det(M_{\downarrow\uparrow})$. This reduction is not possible if one uses the σ_z channel decoupling for the single-Dirac-fermion Hubbard model. Correspondingly, the sign problem is more severe in the σ_z channel, as discussed in PRL 128, 225701 (2022). Since the severity of the sign problem may correlate positively with the size of the determinant, i.e., inversely with the number of reduced sub-determinants, this kind of reduction might help alleviate the sign problem.

Comment:

[08] In Eq. S6 is "sign" missing in the numerator in the last equality? That is $\langle O \rangle_{|W|}$ should be $\langle O\text{sign} \rangle_{|W|}$ in the numerator.

Reply:

We thank the reviewer for pointing out this issue. We have corrected this typo in the revised manuscript [See Change 6(3)].

Comment:

[09] In Eq. S9 I suggest not referring to $S(k)$ as the ferromagnetic structure factor since

usually that term is used for $k = 0$ only. Likewise "$S_{FM}(k)$" would be just "$S(k)$".

Reply:

We thank the reviewer for the suggestion. In the revised manuscript, we have changed the terminology to "spin structure factor" and now denote it as "$S(k)$" [See Change 6(6)].

Comment:

[10] It would be good to say a few words about why (Eq. S11) the Greens function is defined using fermionic operators which flip the spin. One often encounters also $G(i,j) = \langle c^\dagger_{i,s} c^\dagger_{j,s} \rangle$ where the fermions are the same spin. Indeed S11 is nonzero only because the σ_x decoupling was used.

Reply:

We thank the reviewer for this suggestion. In the revised manuscript, we have added an explanation for the definition of the fermionic correlation in Eq. S11 [See Change 6(6)].

First, we would like to clarify a possible misunderstanding in the reviewer's comment: Eq. S11 is nonzero not because of the σ_x decoupling, but rather due to a nonzero quasiparticle weight. This is unrelated to the choice of decoupling channel for the interaction term. In fact, in the single-Dirac-fermion Hubbard model (see Eq. 2 in the main text), the fermion hopping term itself involves spin-flip hopping. The spin-up and spin-down degrees of freedom here correspond to the two components of the massless Dirac fermion spinor. In the other two models considered in our manuscript, the two spinor components correspond to sublattice degrees of freedom, and accordingly, in Eqs. S19 and S31, we define the fermionic correlation between different sublattices.

We now explain the physical significance of the definitions used in Eqs. S11, S19, and S31. The key point is that we define fermionic correlations in momentum space, not in real space. As the reviewer noted, real-space fermionic correlations are also commonly studied. However, they typically decay with distance in an oscillatory manner. In practice, this makes the finite-size scaling analysis somewhat subtle, e.g., as it may depend on the even-odd parity of the distance or the size. In contrast, momentum-space correlations are often more straightforward and robust for analysis. Similar definitions can be found in: Phys.

Rev. X **6**, 011029 (2016); Phys. Rev. Lett. **123**, 137602 (2019); Phys. Rev. Lett. **128**, 225701 (2022); arXiv:2310.10601 (2023); arXiv:2503.15000 (2025).

Physically, the momentum-space fermionic correlation is directly related to the quasiparticle weight Z via:

$$Z = \lim_{L\to\infty} 2\left|G_{s\bar{s}}(\Delta k)\right|, \tag{R10}$$

where s and $\bar{s}$ denote the two distinct components of the massless Dirac fermion spinor, which correspond to different spin states or sublattices in different models. This shows that the fermionic correlation defined in Eqs. S11, S19, and S31 captures the occupation number jump near the Fermi surface. At critical point, it exhibits a power-law decay: $G_{s\bar{s}}(\Delta k) \sim L^{-\eta_\psi}$. In contrast, momentum-space correlations between the same spinor components are trivial, with $G_{ss}(k) = \frac{1}{2}$ for all k, due to spontaneous breaking of chiral symmetry between spinor components. For detailed derivations of these results, one can refer to Phys. Rev. X **6**, 011029 (2016) or arXiv:2310.10601 (2023).

Comment:

[11] The authors use $\tau = 0.5L^z$ for the FM initial state whereas they use $\tau = 0.3L^z$ for the DSM initial state (Figure S1 and discussion in text). It's a bit surprising to use a larger tau (0.5 vs 0.3) when the sign problem is worse. Could the authors comment?

Reply:

We thank the reviewer for pointing out this important detail. This relates to a trade-off in our nonequilibrium approach. [See Change 6(5).]

Let us begin with a general remark. If the value of τ/L^z is chosen too small, the nonequilibrium critical region becomes broad. That is, within a small range of interaction strength U near the critical point U_c, the dimensionless correlation length ratio R appears nearly independent of system size L. As a result, the crossing point of R curves (such as in Fig. 1b) becomes less sharp, and the numerical precision in determining the critical point is reduced. On the other hand, if τ/L^z is chosen too large, the sign problem becomes more severe, reducing the accessible system sizes. This can introduce finite-size effects that bias the estimate of the critical point. Therefore, when applying the nonequilibrium method to determine quantum critical points in practice, one had better tune τ/L^z to find a balance that yields

both high precision and high accuracy.

Specifically, in the case mentioned by the reviewer, we use the nonequilibrium method with both DSM and FM initial states to determine the quantum critical point of the single-Dirac-fermion Hubbard model and benchmark our results against the critical point obtained from Gutzwiller-PQMC in Ref. 56. We find that for the DSM initial state, using $\tau/L^z = 0.3$ is already sufficient to achieve accuracy and precision comparable to equilibrium methods. For the FM initial state, we slightly increase it to $\tau/L^z = 0.5$ to reach the desired level of precision. While the sign problem is more severe in the latter case, it remains manageable in the calculation of this model. Thus, this choice reflects a careful balance.

For a detailed comparison of how different values of τ/L^z affect the critical point estimates using the same initial state, one can refer to our previous work: arXiv:2310.10601 (2023).

Comment:

[12] The authors site Ozawa et al (reference 60) for a case where the SP actually gets better for large L. This has also been noted to occur in some situations in Phys. Rev. B 92, 045110 (2015).

Reply:

We thank the reviewer for providing this important reference. We have added a citation to it in the revised manuscript [See Changes 5(1), 6(8)].

As a side note, an interesting question is whether there could be a case when the sign problem actually gets better for large τ. So far, we have not observed such a phenomenon.

Comment:

[13] I am not sure the explicit forms of the Gell-Mann matrices are needed in section SMIV-A.

Reply:

We thank the reviewer for the suggestion. While we fully appreciate the value of streamlining the Supplementary Materials to keep the focus on our main results, after careful

consideration we have decided to retain the explicit forms of the Gell-Mann matrices in the SM.

There are two main reasons for this decision: 1. We wish to make it visually clear that only the λ_8 matrix is full-rank and capable of gapping out all Dirac fermions, unlike other SU(3) generators [See Change 6(9)]. 2. Some readers may not be familiar with the explicit form of the Gell-Mann matrices. When discussing SU(3) generators, they might instead think of alternative representations such as $S_{\alpha\beta} = c^\dagger_\alpha c_\beta - \frac{\delta_{\alpha\beta}}{3}\sum_\gamma c^\dagger_\gamma c_\gamma$. To ensure broad and accurate understanding of the λ_8-AFM order we report, we believe it is helpful to keep the explicit matrices included.

Comment:

[14] The authors use the notation m_{λ_n} for the order parameters in Eqs. S25 and S26 but then use m_n (without the lambda) in the text on page 16.

Reply:

We thank the reviewer for pointing out this issue. We have corrected this typo in the revised manuscript and have consistently used the notation m_{λ_n} throughout [See Change 6(10)].

Comment:

[15] The order parameter m_{λ_8} onsets very smoothly in Figure S7a. Can the authors comment?

Reply:

We thank the reviewer for pointing out this issue. The smooth onset of m_{λ_8} is due to the relatively small system size $L = 30$ used in the original self-consistent mean-field calculation in the Supplemental Materials. In the revised version, we have replaced the mean-field results with those for a larger system size, $L = 42$ [See Change 6(10)]. In the updated Figure S9a (which has been renumbered from Figure S7a in the original version), the singularity at the phase transition point is now clearly visible [See Change 6(10)].

RESPONSE TO REVIEWER 2

Comment:

In this work, Yu and coworkers suggest that the critical properties of many-body systems can be extracted from the (imaginary) short-time evolution. They consider three examples: SLAC fermions with Hubbard-U interaction, spinless fermions with nearest-neighbor interaction, and the SU(3) Hubbard model with staggered magnetic flux. The first two cases represent benchmarks to assess the accuracy of their quantum Monte Carlo calculations and a way to compare with previous calculations on the critical exponents. Indeed, the results are nice and the agreement is good. Even though they can access much larger clusters than before, the accuracy on the critical exponent is not much higher. In the third case, the claim is to obtain new exponents, not compatible with those of the Gross-Neveu universality class.

Reply:

We sincerely thank the reviewer for carefully reviewing our manuscript and for providing valuable comments. We appreciate the reviewer's positive recognition that "the results are nice and the agreement is good" for the first two benchmark models. We also acknowledge the reviewer's observation that "even though they can access much larger clusters than before, the accuracy on the critical exponent is not much higher." Here, we would like to take this opportunity to clarify the primary objective of our benchmark studies. The purpose of these calculations was not to achieve a new level of numerical precision—as existing methods are already highly accurate for these particular systems—but rather to rigorously validate our new approach by demonstrating its consistency with well-established results. Therefore, the observation that our accuracy is comparable, rather than significantly higher, is in fact the expected outcome and confirms our method's correctness. We will illustrate this point in details below.

For the first model, the single-Dirac-fermion Hubbard model, the sign problem is relatively mild and Ref. 56 employed a Gutzwiller-projected trial state to further reduce the sign problem and obtained highly accurate results. In contrast, we introduced a different and potentially more general method to mitigate the sign problem. The purpose of benchmarking

our results against Ref. 56 is to demonstrate that our method can achieve results that are at least equally accurate and consistent within the error bar.

For the second model, the spinless t-V model, Refs. 60 and 61 used continuous-time QMC and Majorana QMC respectively, both of which solve the model without sign problem and yield highly precise results. In our case, we deliberately decouple the model into a sign-problematic channel and then solve it using the nonequilibrium method. The purpose of this benchmark is to show that even when this model suffers from a sign problem, our approach can still solve it with precision and accuracy comparable to the sign-free methods.

In summary, in these two benchmarks, previous works already used specific techniques to effectively reduce or even completely eliminate the sign problem, and achieved very high accuracy. We directly applied our relatively general framework to these two models, and in terms of the performance on the sign problem, our method is not superior to those tailored approaches. Therefore, in these two benchmarks, our purpose was to align with those advanced results to demonstrate that our newly proposed framework can also reach the same level of accuracy.

No matter what, the reviewer's comment also points out a very interesting and subtle issue: why does the nonequilibrium short-time method, despite accessing larger system sizes, not show a significant improvement in accuracy? This issue does exist. A better example can be found in our earlier study on nonequilibrium dynamics in a sign-problem-free model (arXiv:2310.10601). There, we also simulated larger system sizes and obtained what we believe are more precise results, but the improvement over previous equilibrium results was not very significant. We think there are two main reasons for this. On the one hand, compared with earlier results that already reached fairly large sizes, further increasing the system size (for example, from $L = 20$ to $L = 30$) only brings marginal benefits. On the other hand, similar to finite-size effects, finite imaginary-time evolution also introduces some bias. Therefore, in cases without a sign problem, the nonequilibrium method brings only a relatively small gain in accuracy.

However, when the nonequilibrium method is applied to sign-problematic systems—which is exactly what we discuss in this work—the effect is fundamentally different. In fact, the impact of the sign problem in QMC is often not about how accurately one can compute, but

whether one can compute at all. In such cases, the computational cost of standard QMC methods scales exponentially, rendering them intractable for obtaining reliable results. For example, in the third model, the SU(3) Hubbard model, the sign problem is severe. In reality, such a model is totally inaccessible within a practically reasonable computational time via previous QMC approaches. As we show in Supplementary Materials IV-E, our method improves the computational efficiency by many orders of magnitude compared to equilibrium methods (i.e., an enormous gain in achievable accuracy under the same resource constraints). This gain is so substantial that it brings previously intractable calculations into the realm of tractable simulation.

Therefore, the key advance of our method is not a marginal increase in precision, but a qualitative leap in capability, enabling the study of models that were previously out of reach within practical resource limits.

Comment:

In my opinion, the paper is nice, but well below the standard given by Science. There have been several attempts to "solve" the many-body problem (with very "innovative" proposals and speculations) and I really do not understand from the manuscript why this one should give some advance in the field. Indeed, it could give some insight to determine (with what accuracy, in more complicated cases?) critical exponents once we know that there a QCP separating two phases, but it does not give any new input to determine the actual phase diagram of a strongly-correlated system. The latter one is a really important open question, which deserves high visibility.

Reply:

We thank the reviewer for describing our paper as "nice." We also fully agree with the reviewer that determining the phase diagram of strongly correlated systems is a truly important and open question that deserves high visibility. Right for this reason, we have demonstrated how to preempt the sign problem and determine the ground-state phase diagram in our third model, a previously unexplored and genuinely unknown system. This is an important point about our work that may not have been communicated clearly enough.

Interestingly, although our method does not completely eliminate the sign problem—in par-

ticular, it remains challenging to probe deep into the ordered phase where the sign problem is typically worse—our approach becomes remarkably effective near the phase boundaries of continuous phase transitions. This is because it relies on universal critical scaling behavior near the critical points. As a result, our method is particularly well-suited for determining the phase diagram of strongly correlated systems. For a model possessing a continuous quantum phase transition, we can precisely locate the phase transition point, and determine the symmetry breaking phases separated by this quantum critical point, thus accessing the ground-state phase diagram of the model.

In our method, the procedure for determining the phase diagram is as follows. For a strongly correlated model whose phase diagram is completely unknown beforehand—for example, the SU(3) Hubbard model in our manuscript—we need to calculate various possible order parameters and their corresponding correlation length ratios. During the nonequilibrium relaxation process, we fix τ/L^z at a relatively small value to preempt the sign problem (where the dynamical exponent z can be determined independently according to the newly added Supplementary Materials II-C in the revised version [See Change 6(7)]), and scan the tuning parameters in the model. When the system enters an ordered phase, the correlation length ratio for the corresponding order parameter will increase with system size; in the disordered phase it will decrease. If a QCP exists between them, the correlation length ratios for different system sizes will intersect at the critical point, as shown in Fig. 3b of the main text. For other trial order parameters that do not correspond to a true symmetry breaking, their correlation length ratios will not intersect, as shown in Fig. S12 in Supplementary Materials IV-C. In this way, we can determine both the location of the QCP and the phases on either side. By connecting a series of QCPs mapped out in parameter space, the complete phase diagram can be obtained, as shown in Fig. 3a.

Regarding the reviewer's question about how accurately our approach can determine critical points and critical exponents, this ultimately depends on how severe the sign problem remains after applying our method. If the sign problem is sufficiently alleviated in the short-time scaling regime, then our method can provide numerically exact results. However, if the sign problem remains severe even at very short imaginary times, then our method will also fail. In the revised version, we have added a detailed discussion on the applicability and limitations of the nonequilibrium approach in Supplementary Materials I-D [See Change

6(4)].

We sincerely thank the reviewer again for raising these important points. In response to the reviewer's feedback, we have also added a statement in the Concluding remarks section of the main text to clarify the scope of our method [See Change 3(9)]. In particular, we explicitly state that our method is applicable for determining the phase boundaries of continuous phase transitions and for identifying the phase diagram, which we hope addresses the reviewer's concern.

Comment:

In summary, even though I am sure that the work is nice and may be published in more specialized journals (as Physical Review Letters or similar), it does not meet the general criteria for being published on Science.

Reply:

We thank the reviewer for their positive assessment and for suggesting our work's suitability for a high-impact journal like *Physical Review Letters*. We have carefully revised our manuscript according to the reviewer's valuable comments, to better emphasize the value and general potential of our method for addressing the sign problem and determining the phase diagram of strongly correlated models. Encouraged by the reviewers' consensus that our findings merit publication in a high-impact journal, we have transferred the revised manuscript to *Science Advances*. We fully believe that our manuscript meets the standard of *Science Advances*.

RESPONSE TO REVIEWER 3

Comment:

This paper describes nice work on simulation studies of quantum critical points, in particular on how to determine critical exponents more accurately.

Reply:

We thank the reviewer for recognizing the value of our work.

Comment:

I'm sympathetic to the authors' desire to make a broader and more general pitch to Science, but the paper contains too much hyperbole. "The progress in overcoming sign problem will definitely lead to a great leap in various areas of modern physics." The work is not about overcoming the sign problem. For the QMC calculations that the authors are performing, the sign problem is exactly unchanged. The authors run very short imaginary time calculations so that the sign problem is not severe. That said, the authors show that by exploiting short imaginary time runs, one can in some situations obtain more accurate information near a QCP. This is great, and interesting. But the work should be presented as such. Any limitations and caveats should be clearly discussed.

Reply:

We thank the reviewer for the constructive comments and suggestions. In the revised manuscript, we have removed the hyperbolic statements and carefully revised the language throughout to present our contributions more clearly and objectively, including a more explicit discussion of limitations and caveats. [See Changes 2, 3(1), 3(9), 6(4).]

The reviewer summarizes our approach and its effect in a very clear and intuitive way. Indeed, as the reviewer points out, we do not introduce any new technique that alters or overcomes the sign problem itself. Our approach is simple and straightforward: we merely shorten the projection time in conventional PQMC so that the sign problem has not yet become severe. Compared to equilibrium methods, this allows us to reach the target accuracy with significantly improved computational efficiency. In other words, we are able

to access larger system sizes within a reasonable computational cost. The fact that such a small modification can yield strong results makes the method potentially practical and broadly applicable.

Regarding limitations and caveats, we have identified and now explicitly state two key points:

1. This method is applicable only to the continuous quantum phase transitions. For models exhibiting a continuous quantum phase transition, our approach allows us to precisely locate the phase transition point, determine the the ground-state phase diagram, and calculate the universal critical exponents. As the approach is fundamentally based on scaling theory, which is valid only near quantum critical point, it is not suitable for studying properties deep in the ordered phase.

2. One cannot take the imaginary time arbitrarily short in order to ensure that the sign problem is mild for all models. If the evolution time is too short, the system retains too much memory of the initial state, and the scaling theory breaks down. Furthermore, we currently do not have a reliable diagnostic to determine in advance whether the sign problem is sufficiently mild at the short imaginary times required by the method, without first performing exploratory simulations.

Finally, we sincerely thank the reviewer again for acknowledging that our method "is great, and interesting." In the revised manuscript, we believe we have addressed the reviewer's concerns following the suggestions provided.

Comment:

On the topic of limitations and caveats, the authors mention near the end of the manuscript "in some specific cases, although sign problem is alleviated, it remains difficult to access the critical properties with large system size in our current simulation". Why "some specific cases"?

Reply:

We thank the reviewer for pointing out this issue. The phrase "some specific cases" should be understood in connection with the following sentence in the original manuscript, which reads:

> *We should mention that in some specific cases, although the sign problem is alleviated, it remains difficult to access the critical properties with large system size in our current simulation. For example, when staggered magnetic flux is large in the* SU(3) *Hubbard model, even at short-time stage the sign problem is too severe to allow us to reach the results with high accuracy close to the QCP.*

More specifically, in this model, increasing the staggered magnetic flux ϕ shifts the critical point $U_c(\phi)$ to larger values of U (see Fig. 3a). At the same time, the sign problem becomes more severe as U increases. From the phase diagram in Fig. 3a, one can also see that in the large-U region, the error bars associated with our determination of U_c are visibly larger, which reflects the worsening of the sign problem. In this regime, even with a short projection time such as $\tau = 0.25L^z$, the sign problem is still too severe for us to reliably determine the critical point.

This is the reason why we referred to "some specific cases." There are no hidden subtleties here. What we meant by this phrase are those cases where the sign problem is so severe—decaying too rapidly with imaginary time—that it remains problematic even within the short-time scaling regime. In the current example, this includes the large-U region of the SU(3) Hubbard model. Since the severity of the sign problem varies from model to model and depends heavily on specific details, this needs to be judged on a case-by-case basis.

In the revised manuscript, we have refined this part of the language and removed such vague expressions to improve clarity. We have removed the phrase "specific" to avoid potential confusion. [See Change 3(9).]

Comment:

Isn't it a generic feature that the approach would break down if the scaling regime for the QCP requires larger system sizes L and τ where the sign problem is serious? If this is not the case, the authors should explain why not.

Reply:

We thank the reviewer for the highly accurate and concise characterization of the condition under which our approach breaks down. We fully agree with this assessment, and would like

to add a few supplemental comments.

In general, fixing a system size L for discussion, the effectiveness of our method depends on three characteristic imaginary-time scales: (1) the minimum time $\tau_{\text{neq.}}$ at which the nonequilibrium scaling theory becomes valid; (2) the minimum time $\tau_{\text{eq.}}$ required for conventional PQMC to project onto the ground state; and (3) the maximum time τ_{sign} before the sign problem becomes too severe to obtain reliable results. Empirically, $\tau_{\text{eq.}}$ varies slightly between models but is usually around two to three times the linear system size L. The time $\tau_{\text{neq.}}$ required for short-time scaling to apply is typically one or two orders of magnitude smaller than $\tau_{\text{eq.}}$. In contrast, τ_{sign} can differ drastically from model to model and is the dominant factor that determines whether our approach will be effective. This leads to three possible scenarios:

I. $\tau_{\text{neq.}} < \tau_{\text{eq.}} < \tau_{\text{sign}}$: the sign problem is mild, and equilibrium methods already work well. Our nonequilibrium method only improves computational efficiency.

II. $\tau_{\text{neq.}} < \tau_{\text{sign}} < \tau_{\text{eq.}}$: equilibrium methods fail due to the sign problem, but the nonequilibrium method still works. This is the type of situation our work is focused on.

III. $\tau_{\text{sign}} < \tau_{\text{neq.}} < \tau_{\text{eq.}}$: the sign problem is too severe even at short times. In this case, the nonequilibrium method also fails. This is the breakdown scenario described by the reviewer.

Because the sign problem behaves differently across models, τ_{sign} varies accordingly. Based on this classification, we can view sign-problematic strongly correlated models as falling into three broad categories. In particular, models of type II were previously inaccessible to unbiased numerical methods, and our new approach makes them solvable within reasonable computational cost.

Within the same model and parameter set, τ_{sign} also depends on the system size L. Typically, τ_{sign} decreases with increasing L, although exceptions may exist. Taking this size dependence into account, we can sketch a regime diagram in the (L, τ) plane with the three regimes described above, as illustrated in Fig. R1. This figure shows that the nonequilibrium method allows access to larger system sizes than traditional equilibrium QMC.

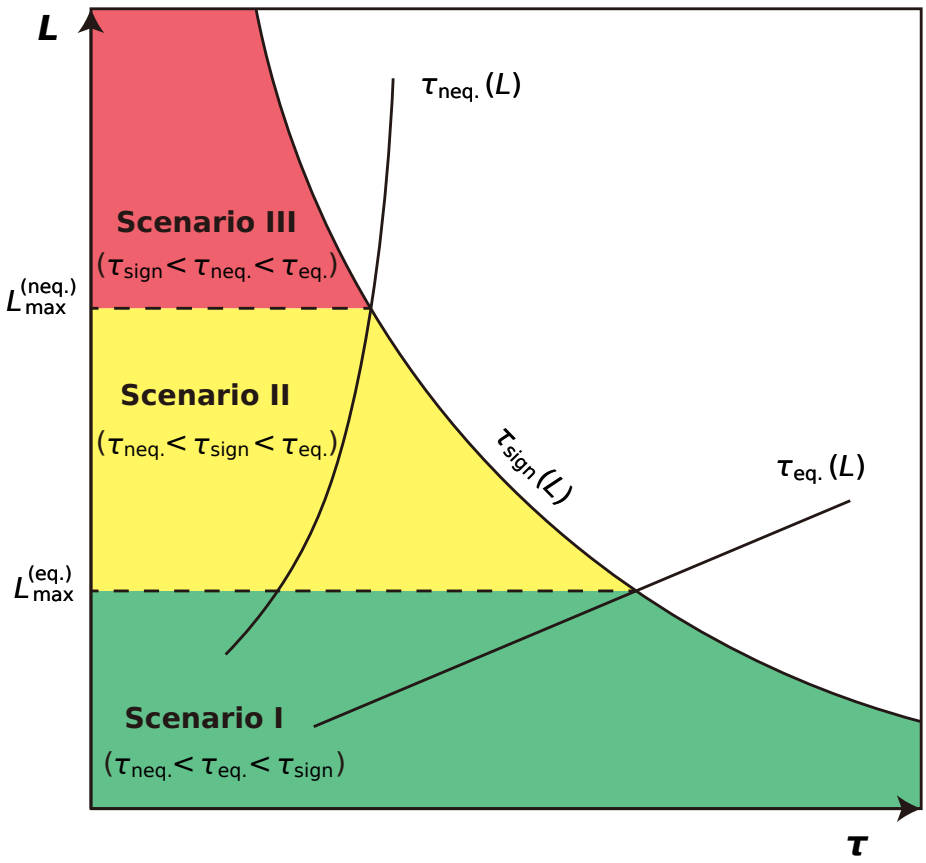

FIG. R1. Schematic illustration of the three scenarios regarding the sign problem. The shaded region indicates where the sign problem is not severe and simulations are feasible. The green region corresponds to scenario I ($\tau_{\text{neq.}} < \tau_{\text{eq.}} < \tau_{\text{sign}}$), where equilibrium methods also work. The yellow region corresponds to scenario II ($\tau_{\text{neq.}} < \tau_{\text{sign}} < \tau_{\text{eq.}}$), where only the nonequilibrium method is feasible. The red region corresponds to scenario III ($\tau_{\text{sign}} < \tau_{\text{neq.}} < \tau_{\text{eq.}}$), where even the nonequilibrium approach fails. The boundaries define the maximum accessible system sizes $L_{\text{max}}^{(\text{eq.})}$ and $L_{\text{max}}^{(\text{neq.})}$ for each method.

Nonetheless, it is important to note that in all three regimes the computational advantage of our nonequilibrium method grows exponentially with system size. This stems from the fundamental scaling of the sign problem, where the computational time required for a given accuracy is inversely proportional to the square of the average sign. For a sign-problematic model, the average sign decays exponentially as $\langle \text{sign} \rangle_{|w|} \sim e^{-c\tau L^d}$, where d is the space dimension and c is a constant independent on τ and L. As discussed previously, our nonequilibrium approach is effective with a τ value that is typically an order of magnitude smaller

than that used in equilibrium methods. Since τ is in the exponent, this seemingly small change yields an exponential reduction in computational cost. This advantage becomes dramatically more pronounced for the large system sizes of primary interest.

Again, we sincerely thank the Reviewer's valuable comments. we have added the corresponding discussions in our revised manuscript [See Change 6(4)].

Comment:

In other words, what is the argument that, in general, a QCP can be approached with sufficiently short imaginary time simulations for which the sign problem remains mild?

Reply:

Following the three-scenario classification in our previous response, the general argument that a quantum critical point (QCP) can be approached using sufficiently short imaginary-time simulations where the sign problem remains mild is valid only in models of type I and type II. It does not hold in type III models, where the sign problem is already severe even at short times. Naturally, our method is not a fully general solution to the sign problem in all cases. What it does provide is a practical and effective approach for models of type II, which were previously inaccessible due to severe sign problems in equilibrium simulations. With our method, such models become tractable [See Change 6(4)]. In our manuscript, we present three representative examples. We are currently testing the method on additional models in ongoing research.

Comment:

In the study the authors chose $\tau = 0.3L^z$ in the first two problems, and $\tau = 0.25L^z$ for the last problem. What are the guiding principles for how to choose the coefficient? What if one had chosen 0.6 instead of 0.3 in the coefficient in the first two problems? Or 0.3 instead of 0.25 in the third?

Reply:

We thank the reviewer for pointing out this important detail. When choosing the specific coefficients for $\tau = (\text{const.}) \times L^z$, we carefully balanced three considerations: the severity

of the sign problem, the validity of the scaling theory, and the numerical precision of the estimated critical point. In general, the following guiding principles apply [See Change 6(5)]:

1. **The severity of the sign problem** is the most important factor. Usually, slightly increasing the value of τ/L^z makes the sign problem significantly worse, and vice versa. Therefore, regarding the situations mentioned by the reviewer, if the coefficient 0.3 is increased to 0.6 in the first two problems, or 0.25 is increased to 0.3 in the third problem, the most noticeable effect would be that the sign problem becomes more severe, and the accessible system size becomes smaller. From this guiding principle, τ/L^z should be chosen as small as possible.

2. Another important factor is **the validity of the scaling theory**. If τ/L^z is too small, the nonequilibrium scaling theory may not hold well at currently accessible finite sizes. Specifically, for example, when it is taken below 0.1, from Figs. 1d, 2c, and 3d one can see that the data collapse gradually starts to break down, meaning finite-size effects become significant. This condition is relatively flexible. As long as τ/L^z is above a certain threshold (e.g., 0.2), the scaling holds well, and variations in the coefficient do not significantly affect the results. Values such as 0.25, 0.3, and 0.5 are typically used in the literature, such as Phys. Rev. Lett. 128, 020601 and arXiv:2310.10601. In those works, estimates of critical points at different τ/L^z values were found to agree within statistical error, providing a useful self-consistency check.

3. Another somewhat subtle factor is **the resolution of the critical point**. Even within the valid scaling regime, choosing a smaller τ/L^z broadens the nonequilibrium critical region. That is, the dimensionless correlation length ratio R appears nearly independent of L over a wider range of U near U_c, making the crossing point of R curves (such as in Fig. 1b) less sharp. This leads to reduced numerical precision in locating the critical point. Therefore, from this perspective, it is preferable to choose a somewhat larger τ/L^z to enhance resolution.

In summary, when applying the nonequilibrium approach to determine quantum critical points, one must balance these considerations within the valid scaling regime. The goal is to choose a value of τ/L^z that optimizes both precision and accuracy. In our experience, the severity of the sign problem is often the most decisive factor.

Comment:

And if one doesn't know the answer $z = 1$, shouldn't simulations with different choices of z be performed.

Reply:

We thank the reviewer for raising this important question. We have carefully considered how to apply our nonequilibrium method when the value of z is not known in advance, including how to determine z from the simulation data. In the revised Supplementary Materials, we have added a general procedure for estimating z and demonstrated its application in the single-Dirac-fermion Hubbard model under the assumption that $z = 1$ is unknown [See Change 6(7)].

Specifically, we introduce a new dimensionless ratio:

$$R_0 \equiv \frac{S(2\tau)}{S(\tau)}, \tag{R11}$$

where S is the zero-momentum structure factor (see its definition in Eq. S9 and scaling form in Eq. S14). The procedure for determining z proceeds as follows:

1. First, we choose a relatively large system size L so that the factor τL^{-z} has negligible influence on the scaling of R_0. Then, using the scaling form $R_0 = 2^{\frac{1+\eta_\phi}{z}} f_{R_0}(g\tau^{\frac{1}{\nu z}})$, we can identify the critical point by locating where $g = 0$. Note that the critical point estimated at this stage may not be highly accurate, since the effect of τL^{-z} is only approximately ignored in finite systems.

2. Second, we fix the interaction parameter at the tentative critical point found in step 1 ($g = 0$), and determine z using the scaling relation of the correlation length ratio $R = f_R(\tau L^{-z})$. At this stage, the estimate for z may still be imprecise.

3. Third, we fix the value of τL^{-z} and re-apply our nonequilibrium method as described in the main text to obtain a more accurate estimate of the critical point. With this refined critical point, we can repeat step 2 to obtain a more accurate z, and continue iterating.

By iterating steps 2 and 3, the estimates for both z and the critical point converge to

stable values. A detailed computational example is provided in the revised Supplementary Materials [See Change 6(7)].

Comment:

In that case, wouldn't there be a much smaller sign and hence much more noisy results for larger z?

Reply:

We thank the reviewer for raising this interesting question. In fact, we have not yet performed simulations for cases with larger z, so our answer here should be taken as qualitative and not definitive. Intuitively, if z is larger and we still choose $\tau = 0.3L^z$, then τ will indeed be larger compared to the $z = 1$ case. As a result, the sign problem may indeed become more severe, potentially leading to increased statistical noise in the results. Investigating the performance of our method in the case of larger z is a compelling direction for future research. Nevertheless, at least in principle, even under such conditions, the nonequilibrium approach should still offer a big advantage over equilibrium methods.

Comment:

The authors often use the word dynamics loosely, for example in the title "Unveiling Quantum Criticality through Nonequilibrium Dynamics", or in the abstract "by deviating from the conventional cognition that nonequilibrium studies should be more complicated than equilibrium cases, we propose an innovative framework based on nonequilibrium critical dynamics ..." This is confusing, and misleading. The authors are performing calculations with imaginary time dynamics, not real dynamics. The object of the study is a system in equilibrium. They are not studying "nonequilibrium dynamics" as a typical reader of Science may infer from their writing.

Reply:

We thank the reviewer for pointing out this issue. In the revised manuscript, we have followed the reviewer's suggestion and removed such ambiguous usage. To avoid any confusion, we now explicitly state "in imaginary time" in the title [See Change 1], and clarify in the abstract that our approach is based on "imaginary-time nonequilibrium critical dynamics" [See

Change 2]. In the Introduction, we begin with the general concept of (real-time) short-time critical dynamics and then introduce its imaginary-time counterpart (which shares the same scaling form) to help readers without prior experience understand that our calculations are performed in imaginary time. In addition, throughout the manuscript, we have changed all instances of "short-time dynamics" to "short-imaginary-time dynamics." [See Changes 3(2), 3(4), 3(5).]

Comment:

In summary, this work is interesting and the manuscript should be published in a good journal, but it does not have the broad appeal and has not demonstrated the milestone quality of a research paper in Science. I cannot recommend publication in Science.

Reply:

We thank the reviewer for finding our manuscript interesting and recognizing that it deserves publication in a good journal. Following the reviewer's suggestions, we have thoroughly revised the manuscript. We believe that it has now been improved in both clarity and rigor, and that it possesses sufficient broad appeal. Encouraged by the reviewers' consensus that our findings merit publication in a high-impact journal, we have transferred the revised manuscript to *Science Advances*, which we believe is an ideal venue for our manuscript.