Editors' Suggestion

Robust Fermi-Liquid Instabilities in Sign Problem-Free Models

Ori Grossman* and Erez Berg

Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel

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Determinant quantum Monte Carlo (DQMC) is a powerful numerical technique to study many-body fermionic systems. In recent years, several classes of sign-free (SF) models have been discovered, where the notorious sign problem can be circumvented. However, it is not clear what the inherent physical characteristics and limitations of SF models are. In particular, which zero-temperature quantum phases of matter are accessible within such models, and which are fundamentally inaccessible? Here, we show that a model belonging to any of the known SF classes within DQMC cannot have a stable Fermi-liquid ground state in spatial dimension $d \geq 2$, unless the antiunitary symmetry that prevents the sign problem is spontaneously broken (for which there are currently no known examples in SF models). For SF models belonging to one of the symmetry classes (where the absence of the sign problem follows from a combination of nonunitary symmetries of the fermionic action), any putative Fermi liquid fixed point generically includes an attractive Cooper-like interaction that destabilizes it. In the recently discovered lower-symmetry classes of SF models, the Fermi surface (FS) is generically unstable even at the level of the quadratic action. Our results suggest a fundamental link between Fermi liquids and the fermion sign problem. Interestingly, our results do not rule out a non-Fermi-liquid ground state with a FS in a sign-free model.

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Introduction.—The importance of reliable and practical simulations of strongly correlated fermionic systems cannot be overstated. In recent decades, substantial progress was made thanks to the development of the determinant quantum Monte Carlo (DQMC) technique [1–6]. However, this technique is often hindered by the sign problem [7,8], associated with negative or complex amplitudes in the quantum partition sum. The sign problem results in inefficient simulations, generally scaling exponentially with system size and inverse temperature [6,9] (although interesting exceptions exist [10,11]).

Interestingly, certain classes of fermionic models do not suffer from the sign problem [12–18], and hence can be solved at polynomial cost. In these models, the absence of the sign problem is guaranteed by a combination of symmetries of the fermionic action. Sign-free (SF) models were used to simulate a plethora of interesting phenomena, including fermionic quantum criticality [19–26] and unconventional superconductivity [27–30]. These developments raise the question of the physical properties and intrinsic limitations of sign problem-free models [11,31–34]. In particular, which quantum phases of matter can be accessed within SF models, and which are fundamentally inaccessible?

In this Letter, we show that all the currently known classes of sign problem-free models within DQMC cannot support a stable Fermi-liquid (FL) ground state. This is shown by demonstrating that any putative Fermi surface (FS) in a SF model is generically unstable in the presence of interactions at zero temperature. Depending on the model, the instability may be toward a fully gapped superconducting or density wave state, or toward a Dirac semimetal [35,36].

It is important to note that we cannot rule out a fine-tuned SF model with a FS (e.g., a model of noninteracting electrons). Our argument shows that in such cases, the FS is unstable, in the sense that a generic, arbitrarily small perturbation can destroy it [37]. In addition, a non-FL state with a FS (of the type that arises, e.g., at certain quantum critical points) is not ruled out.

Our main findings are summarized in Table I. In the symmetric SF classes [18] the SF property is guaranteed by the combination of two antiunitary time-reversal symmetries (TRSs) of the fermionic action matrix. A detailed description of the different SF classes is given

TABLE I. The known sign-free (SF) classes (see text for a detailed description), and the origin of the Fermi surface (FS) instability in each class. In the symmetry classes (Symm. SF), there is an interaction-induced instability of the FS that opens a gap through spontaneous symmetry breaking. In the lower-symmetry classes (lower-symm. SF), the FS is not protected (in general) by symmetry, and a gap generically opens even at the single-particle level.

	Kramers' class $\{T_1^-, T_2^-\} = 0$	Majorana class $\{T_1^-, T_2^-\} = 0$
Symm. SF	U(1) breaking	$\mathbb{Z}_2$ breaking
Lower-symm. SF	Single-particle gap	Single-particle gap

below. The product of the two TRSs defines a unitary symmetry, which is either a U(1) or a $\mathbb{Z}_2$ symmetry, depending on the class. Interactions generically lead to spontaneous breaking of the unitary symmetry, gapping out the FS. There are many known examples of these phenomena (see the Supplemental Material [38]); our Letter shows that these are general properties of SF models. There are also lower-symmetry classes where the SF is due to less strict conditions [15,16]. We show that in these cases, generically, there is no FS even at the single-particle level, since there is no symmetry to protect it. If a symmetry that protects a FS is imposed, the FS is unstable in the presence of interactions, as in the symmetric classes.

Sign-free DQMC.—DQMC is based on introducing a bosonic field ϕ via a Hubbard-Stratonovich (HS) transformation, deriving an effective action for ϕ by integrating out the fermions, and averaging stochastically over ϕ. The field ϕ mediates the fermionic interaction [6]. Alternatively, ϕ may represent a physical boson (such as a phonon). A typical action has the form of $S = S_F + S_\phi + S_{\mathrm{Int}}$ where S_F is the noninteracting fermionic action, S_ϕ is the bosonic action, and S_{Int} is a Yukawa-like interaction. We assume that $S_\phi \in \mathbb{R}$. Upon integrating out the fermions, an effective bosonic action is obtained: $S'_\phi = S_\phi + \ln\det M_\phi$, where M_ϕ is the (ϕ dependent) quadratic fermionic action matrix, $\bar{\psi} M_\phi \psi = S_{\mathrm{Int}} + S_F$. The fermionic problem has therefore been mapped to a classical statistical mechanical problem in $d+1$ dimensions for the field $\phi(\mathbf{r}, \tau)$.

However, it is not guaranteed that the statistical weights in the partition sum can be treated as probabilities, since they are not necessarily real and non-negative. This is known as the sign problem. Models that satisfy $S'_\phi \in \mathbb{R}$ (or equivalently $\det M_\phi \geq 0$) for any configuration $\phi(\mathbf{r}, \tau)$ are known as SF models.

A set of sufficient conditions is known to guarantee the absence of the sign problem [18]. These conditions are most conveniently stated using a Majorana representation, writing the complex fermion field in terms of two real (Majorana) fields: $\psi = \frac{1}{2}(\gamma_1 + i\gamma_2)$. The fermionic bilinear action takes the form $\gamma^T \tilde{M}_\phi \gamma$ where $\gamma = (\gamma_{1,1}, \ldots\gamma_{1,N}, \ldots\gamma_{2,N})$ (for N Dirac fermions) and $\tilde{M}_\phi$ is a $2N \times 2N$ skew-symmetric matrix. In addition, a Majorana TRS, T, is defined as an antiunitary operator that satisfies $[\tilde{M}_\phi, T] = 0$ for any $\phi(\mathbf{r}, \tau)$. In this framework, one can distinguish between two fundamental SF classes.

With Kramers' class, $\tilde{M}_\phi$ has two mutually anticommuting TRSs, satisfying $(T_1^-)^2 = (T_2^-)^2 = -1$. Since $(iT_1T_2)^2 = 1$, models of this class have a conserved U(1) charge, $\hat{Q} = \gamma^T iT_1T_2\gamma$. They can therefore be represented by Dirac fermions with a U(1) symmetry ($\gamma^T \tilde{M}_\phi \gamma \to \bar{\psi} M_\phi \psi$). By Kramers' theorem, the eigenvalues of M_ϕ come in complex conjugate pairs.

With the Majorana class, $\tilde{M}_\phi$ has two mutually anticommuting TRSs, satisfying $(T_1^-)^2 = -1$, $(T_2^+)^2 = 1$. Since $U = T_1^- T_2^+$ is a $\mathbb{Z}_2$ unitary symmetry, $\tilde{M}_\phi$ can be brought to the block diagonal form

$$\tilde{M}_\phi = \begin{bmatrix} B & 0 \\ 0 & B^* \end{bmatrix} \tag{1}$$

in the eigenbasis of U. Integrating out the fermions yields $\mathrm{pf}(\tilde{M}_\phi) = \mathrm{pf}(B)\mathrm{pf}(B^*) \geq 0$ (where $\mathrm{pf}(B)$ is the Pfaffian of the skew-symmetric matrix B). Models of this type may not have a U(1) symmetry, but can still have a FS of the zero energy Bogoliubov-like excitations, protected at the single-particle level by the $\mathbb{Z}_2$ symmetry.

The conditions above can be somewhat relaxed [15,16]. In the so-called lower-symmetry classes, we keep the requirement $[\tilde{M}_\phi, T_2^\pm] = 0$, but the second condition becomes $iK[T_1^-, \tilde{M}_\phi] \leq 0$ (i.e, the left-hand side is a negative semidefinite matrix), where K is complex conjugation. As before $\{T_1, T_2\} = 0$. These requirements are sufficient to guarantee $\det M_\phi \geq 0$ [16]. The limiting case where $[\tilde{M}_\phi, T_1^-] = 0$ corresponds to the symmetry classes discussed above. In the case of a strict inequality, we have two lower-symmetry SF classes: the Majorana class (T_2^+) and the Kramers' class (T_2^-).

Fermi surface instability.—We consider a general, translationally invariant model in $d \geq 2$ spatial dimension, that belongs to one of the SF classes. The model includes Majorana fermions interacting with a bosonic field via a Yukawa coupling (note that any model of fermions with a quartic interaction can be recast in this form via a HS transformation). The lattice-scale, ultra-violet (UV) action is given by

$$S_{\mathrm{UV}} = \int \mathrm{d}k \bar{\gamma}_{\alpha,k} \frac{(i\omega\delta_{\alpha,\alpha'} - h_{\alpha,\alpha',\mathbf{k}})}{2} \gamma_{\alpha',k} + S_\phi + S_{\mathrm{Int}}, \tag{2}$$

where α denotes a general fermionic flavor such as spin or Majorana flavor ($\gamma_{1,2}$), and summation over repeated indices is assumed. We have defined $\bar{\gamma}_k \equiv \gamma_{-k}$, and used the notation $k = \{i\omega, \mathbf{k}\}$, where $\mathbf{k}$ is the spatial momentum. S_ϕ is a bosonic action, and S_{Int} is given by

$$S_{\mathrm{Int}} = \int \mathrm{d}k\mathrm{d}k' \frac{1}{2} \lambda^\nu_{\alpha,\alpha',k,k'} \phi^\nu_{k,k'} \bar{\gamma}_{\alpha,k} \gamma_{\alpha,k'}. \tag{3}$$

Here ν is the index of the auxiliary field and λ is the coupling function (which depends on momenta, bosonic index, and fermionic flavor). Note that the bosonic field ϕ^ν may also be complex, but $S_\phi \in \mathbb{R}$ as the model is SF. In addition, we assume that our action corresponds to a physical Hamiltonian, i.e., Eq. (2) corresponds to a Hermitian Hamiltonian $\hat{H}(\hat{\gamma}, \hat{\phi}, \hat{\pi})$, where $\hat{\phi}, \hat{\pi}$ are canonically conjugate operators.

We use proof by contradiction, assuming that the ground state is a FL, and showing that the putative FL phase is

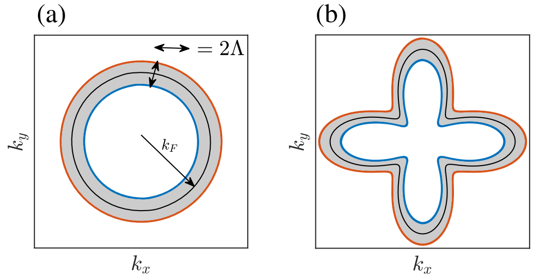

FIG. 1. A schematic plot of the fast modes integration out for a time-reversal symmetric model. The shaded region around the Fermi surface (FS) represents the slow momenta while all the rest of the Brillouin zone (fast modes) is integrated out. (a) The simple case of circular FS. (b) A generic case in which $\epsilon_{\mathbf{k}} = \epsilon_{-\mathbf{k}}$.

unstable. The proof proceeds in two steps: (1) obtaining the low-energy FL effective action and (2) showing that the SF requirement necessitates the existence of an instability of the FS.

Step 1: We divide the fermionic modes into slow modes residing within a thin shell of thickness 2Λ around the FS (shaded region in Fig. 1), and fast modes residing outside of the shell. The fast modes are integrated out, obtaining the infrared effective theory (S_{IR}) close to the FS. Note that S_{IR} is still quadratic in the fermions at this stage, as we do not integrate over ϕ at this stage [38].

The infrared action is written as

$$S_{\mathrm{IR}} = \int_{|\epsilon_{\mathbf{k},\alpha}|<\Lambda} dk \bar{\gamma}_{\alpha,k} \frac{(i\omega\delta_{\alpha,\alpha'} - h_{\alpha,\alpha',\mathbf{k}})}{2} \gamma_{\alpha',k} + S'_{\phi} + S'_{\mathrm{Int}} \tag{4}$$

with

$$S'_{\mathrm{Int}} = \int dk dk' \bar{\gamma}_{\alpha,k} \Sigma_{\alpha,\alpha',k,k'}(\phi) \gamma_{\alpha',k'}. \tag{5}$$

Here, $\Sigma(\phi)$ is the fermionic self-energy obtained from integrating out the fast modes, including all λ dependent terms (we suppress the indices of ϕ^{ν} for brevity). S'_{ϕ} is the renormalized bosonic action. More details concerning the diagrammatic representation of $\Sigma(\phi)$ and S'_{ϕ} can be found in the Supplementary Material [38]. Importantly, $\epsilon_{\mathbf{k}}$ is the "true" (renormalized) dispersion, given by the eigenvalues of the matrix $h_{\alpha,\alpha',\mathbf{k}} + \langle \Sigma_{\alpha,\alpha',k,k} \rangle_{S'_{\phi}}$ (with $\omega = 0$ within the self-energy). Hence, the exact FS is given by $\epsilon_{\mathbf{k}} = 0$.

Next, we integrate out ϕ in order to obtain a purely fermionic low-energy action. By our assumption, this action has a FL form. We assume that we are not exactly at a quantum critical point (QCP); at a QCP, singular interactions between the low-energy fermions arise, violating the FL assumption.

In the resulting fermionic action $S_{\mathrm{eff}}(\gamma, \bar{\gamma})$, we are interested only in the quartic terms, as in a FL, higher order terms are irrelevant in the renormalization group (RG) sense [41,42]. The quartic part of $-S_{\mathrm{eff}}(\gamma, \bar{\gamma})$ is written as

$$\Gamma^{\alpha,\beta,\alpha',\beta'}_{k_1,k_2,k'_1,k'_2} \bar{\gamma}_{\alpha,k_1} \bar{\gamma}_{\beta,k_2} \gamma_{\beta',k'_2} \gamma_{\alpha',k'_1} \delta(\{k\}), \tag{6}$$

where $\delta(\{k\}) = \delta_{k_1+k_2-k'_1-k'_2}$, and we can neglect the dependence of Γ on both frequency and the momentum perpendicular to the FS, since both dependencies are irrelevant [41,42]. Using the cumulant expansion, we can express Γ as

$$\Gamma^{\alpha,\beta,\alpha',\beta'}_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}'_1,\mathbf{k}'_2} = \langle \Sigma_{\alpha,\alpha',\mathbf{k}_1,\mathbf{k}'_1} \Sigma_{\beta,\beta',\mathbf{k}_2,\mathbf{k}'_2} \rangle_{S'_{\phi}} - \langle \Sigma_{\alpha,\alpha',\mathbf{k}_1,\mathbf{k}'_1} \rangle_{S'_{\phi}} \times \langle \Sigma_{\beta,\beta',\mathbf{k}_2,\mathbf{k}'_2} \rangle_{S'_{\phi}}. \tag{7}$$

Note that, due to the SF property of the model, $S'_{\phi} \in \mathbb{R}$ (see the Supplemental Material [38]).

Step 2: We now perform a stability analysis of the putative FL fixed point. The analysis closely follows the standard RG procedure for interacting fermions [41]. In the limit $\Lambda \to 0$, forward scattering processes are exactly marginal. Since the model is SF, it has at least one TRS, and hence $\epsilon_{\mathbf{k}} = \epsilon_{-\mathbf{k}}$. Then, FS instabilities may arise in the Cooper channel, corresponding to $k_1 = -k_2$, $k'_1 = -k'_2$. To obtain a compact form of the RG equations, it is convenient to define

$$\tilde{\Gamma}^{\alpha,\beta,\alpha',\beta'}_{\mathbf{k},-\mathbf{k},\mathbf{k}',-\mathbf{k}'} \equiv \frac{1}{\sqrt{v_{\mathbf{k}} v_{\mathbf{k}'}}} \Gamma^{\alpha,\beta,\alpha',\beta'}_{\mathbf{k},-\mathbf{k},\mathbf{k}',-\mathbf{k}'} \tag{8}$$

where $v_{\mathbf{k}} = |\nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}|$. We treat $\tilde{\Gamma}^{\alpha,\beta,\alpha',\beta'}_{\mathbf{k},-\mathbf{k},\mathbf{k}',-\mathbf{k}'}$ as a matrix $\tilde{\mathbf{\Gamma}}$, where the first (second) index corresponds to the set $\{\alpha, \beta, k\}$ ($\{\alpha', \beta', k'\}$). The Hermiticity of the effective FL Hamiltonian implies that the matrix $\tilde{\mathbf{\Gamma}}$ is Hermitian.

The one-loop RG equations for $\tilde{\mathbf{\Gamma}}$ take the simple form

$$\frac{d\tilde{\mathbf{\Gamma}}}{dl} = \frac{1}{4\pi} \tilde{\mathbf{\Gamma}}^2, \tag{9}$$

where $dl = -d\Lambda/\Lambda$ is the infinitesimal scaling factor. Diagonalizing $\tilde{\mathbf{\Gamma}}$, we obtain a set of differential equations for the eigenvalues (denoted by λ_i):

$$\frac{d\lambda_i}{dl} = \frac{1}{4\pi} \lambda_i^2. \tag{10}$$

A positive λ_i (corresponding to attraction in a certain channel) grows under RG, destroying the FL. Thus, a stable FL phase requires that $\lambda_i < 0$ for all i. Conversely, if there is at least one positive eigenvalue, there is no FS at $T = 0$. If $\lambda_i \leq 0$ for all i, but there is at least one zero eigenvalue, there can be a FS, but it is unstable to the addition of an infinitesimal perturbation that makes one of the eigenvalues positive (The latter case corresponds, e.g., to a noninteracting electron gas).

We now show that there exists a vector $\vec{w}$ for which $\vec{w}^T \tilde{\mathbf{\Gamma}} \vec{w} \geq 0$, and hence $\tilde{\mathbf{\Gamma}}$ has at least one non-negative eigenvalue, and the FL phase cannot be stable. As mentioned above, the model has at least one TRS. We write the

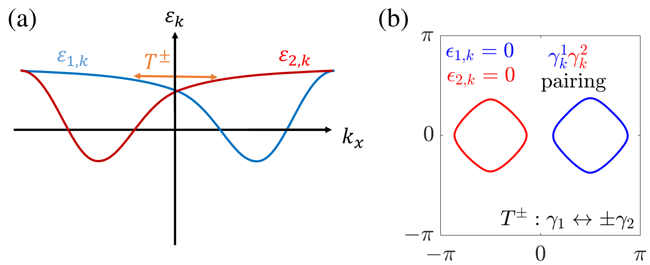

FIG. 2. Schematic description of Cooper channel instability in the sign-free classes. We demonstrate it for the simple case of two flavors. (a) The time-reversal mapping between the two bands. (b) The obtained nesting between the FSs.

corresponding TRS operator as $T = OK$, where O is an orthogonal matrix (O is real since we are dealing with Majorana fermions), and K denotes complex conjugation. Under TRS, $\gamma_{\alpha,k} \to O_{\alpha\beta}\gamma_{\beta,-k}$. Setting $w_{\mathbf{k},\alpha,\beta} = O_{\alpha\beta}\delta_{\mathbf{k},\mathbf{k}_0}$ with an arbitrarily chosen $\mathbf{k}_0$, and using the identity

$$\sum_{\alpha,\alpha'} O_{\alpha\beta}\Sigma^{\alpha,\alpha'}_{\mathbf{k}_0,\mathbf{k}_0} O_{\alpha'\beta'} = (\Sigma^{\beta,\beta'}_{-\mathbf{k}_0,-\mathbf{k}_0})^*, \tag{11}$$

which follows from the time-reversal invariance of the fermionic action under T, we obtain

$$\vec{w}^T\tilde{\mathbf{\Gamma}}\,\vec{w} = \frac{1}{v_{\mathbf{k}_0}}\sum_{\beta,\beta'}[\langle|\Sigma_{\beta,\beta',-\mathbf{k}_0,-\mathbf{k}_0}|^2\rangle_{S'_\phi} - \langle\Sigma_{\beta,\beta',-\mathbf{k}_0,-\mathbf{k}_0}\rangle_{S'_\phi} \times \langle\Sigma^*_{\beta,\beta',-\mathbf{k}_0,-\mathbf{k}_0}\rangle_{S'_\phi}] \geq 0. \tag{12}$$

Thus, the putative FL phase is either intrinsically unstable, or can be destabilized by adding an infinitesimal attractive interaction. This is our main result.

It is worth examining the key elements required for our proof. In essence, the TRS (which all presently known SF classes require) ensures that the FS has a Cooper-like instability, with states at opposite momenta being degenerate (see Fig. 2). In addition, the SF property guarantees that the effective interaction is attractive in some channel (although it may be repulsive in other channels). Therefore, the FS cannot be stable. It is natural to expect a gapped, spontaneously broken ground state as a result.

We further stress that we cannot rule out the possibility of a non-FL metal with a FS. We also do not rule out a manifold of codimension $d-2$ or lower of zero energy excitations. SF models can have a stable Dirac semimetal ground state in $d = 2$ [36,43–45], or a nodal line semimetal in $d \geq 3$.

Importantly, within our proof, we have implicitly assumed that TRS is not broken *spontaneously* [46]. If such spontaneous symmetry breaking had occurred, the FS could be stable. Reference [31] conjectured, and showed explicitly for some cases, that an antiunitary symmetry cannot be spontaneously broken in a bosonic SF model. We do not know of cases where TRS is spontaneously broken in a SF model containing fermions; whether such TRS breaking is fundamentally possible remains to be seen.

The gapped phase.—While for all SF classes, the ground state is not a stable FL, its exact nature is class dependent and model dependent. However, in both symmetry classes, it is natural to expect that as a result of the FS instability, the unitary T_1T_2 symmetry is spontaneously broken, and the FS is gapped out. In Kramers' class, this typically results in a superconducting ground state, as $\gamma^T iT_1T_2\gamma$ is the generator of a U(1) symmetry. The angular momentum of the order parameter is model specific, and both s-wave [47–53] and nodal or nodeless d-wave [27,28,30] superconductivity were found within SF DQMC. In the Majorana class, T_1T_2 is a unitary $\mathbb{Z}_2$ symmetry. Its spontaneous breaking results in a twofold degenerate ground state. In certain physical realizations, the symmetry broken phase may correspond to a charge ordered state [13,15,49,52,54,55].

It is important to note that the spontaneous breaking of T_1T_2 does not always occur; if the fermions form a band insulator or a Dirac semimetal, the symmetry unbroken phase may extend down to $T = 0$. We provide detailed examples of realizations in different symmetry SF classes and their symmetry broken phases in the Supplemental Material [38].

In the lower-symmetry SF classes, as we only have a single TRS and not a unitary symmetry, there is generically no FS already at the level of the quadratic (noninteracting) part of the action. The single-particle Hamiltonian is analogous to a Bogoliubov-de Gennes Hamiltonian with TRS, where real off diagonal pairing terms are allowed. Consequently, the codimension of the zero energy modes is at most $d-2$ (see the Supplemental Material [38]). If we add a symmetry (beyond those required by the SF property) that protects the FS at the quadratic level (e.g., a U(1) or $\mathbb{Z}_2$ symmetry), the FS is still generically unstable in the presence of interactions, just as in the symmetry classes. This is because our proof requires only a single TRS, which is present in the lower-symmetry classes. We summarize our conclusions for all currently known SF classes in Table I.

Comment regarding the Kohn-Luttinger mechanism.—We have shown that SF models cannot have a stable FL ground state, due to TRS and the presence of attraction in the Cooper channel. In this context, it is important to address the question of whether, conversely, non-SF models with TRS can support a stable FS at $T = 0$. It is well known that under a wide range of circumstances, bare repulsive interactions can lead to superconductivity at high angular momentum channel. This is the Kohn-Luttinger (KL) mechanism [56].

In general, however, the KL mechanism relies on the bare repulsion being short-ranged, i.e., exponentially decaying as a function of distance (see the Supplemental Material [38] for details). The FS can be stabilized at $T = 0$ by adding a small power-law repulsive interaction. In contrast, our proof shows that in SF models, the FS is generically unstable, even in the presence of arbitrary long-ranged interactions.

Concluding remarks.—Our arguments apply to all SF classes that are currently known within DQMC. However, these observations naturally lead to the stronger conjecture that a stable FL phase cannot be realized in any SF model. As new classes of SF models are found, this conjecture will be put to the test. For example, there are models [57] that do not have a known SF DQMC formulation, but the sign problem can be solved in a continuous time quantum Monte Carlo [14,58–60] (or the "fermion bag" approach [61,62]). None of these models have a FL ground state, as far as we know; however, our proof does not formally encompass these cases. In addition, we note that it is possible to get stable metallic phases in "mixed dimensionality" systems [63,64], where the interaction terms are subextensive. These lie beyond the scope of our results since they are not fully translationally invariant.

Looking ahead, it should be straightforward to extend our results to include quenched disorder. In this case, we expect SF models to obey a version of Anderson's theorem [65], i.e., disorder that preserves the SF property does not suppress the superconducting instability at the mean-field level.

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*ori.grossman@weizmann.ac.il

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