Emergent symmetries and coexisting orders in Dirac fermion systems

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(Received 12 November 2019; revised manuscript received 10 February 2020; accepted 13 March 2020; published 8 April 2020; corrected 8 October 2020)

We consider interacting (2+1)-dimensional Dirac fermions with competing symmetry-breaking electronic instabilities, as described by relativistic quantum field theories of the Gross-Neveu-Yukawa flavor with anti-commuting mass terms. We demonstrate, using a combination of nonperturbative field-theoretical analysis and an adapted quantum Monte Carlo approach, that such systems exhibit a strong-coupling quantum multicritical fixed point with an emerging enhanced symmetry. Moreover, an extended phase coexistence regime expands out from this high-symmetry point. Our results disagree with recent results on the presence of a deconfined quantum criticality in (2+1)-dimensional Dirac fermions for the particular case of $O(3)$ Néel and Z_2 Kekulé symmetry-breaking instabilities on the graphene lattice. The robustness of these phenomena with respect to the microscopic symmetries furthermore demonstrates their relevance for a wide range of Dirac materials of current interest, from both theory and ongoing experiments.

DOI: [10.1103/PhysRevResearch.2.022005](https://doi.org/10.1103/PhysRevResearch.2.022005)

Recent advances in the fabrication of two-dimensional electron systems, such as in twisted bilayer graphene, have exhibited the emergence of strongly correlated states [1,2], which are reminiscent of other material classes, e.g., the transition-metal oxides, where the interplay of competing electronic instabilities leads to rich phase diagrams [3,4]. In particular, these findings have renewed interest in the symmetry-broken phases of correlated Dirac fermions, due to the evidence of gap openings near charge neutrality [5–9]. Interacting Dirac fermion systems are also of fundamental interest from a general field-theoretical perspective, and are thus in focus of intensive recent research [10–15]. Based on these developments, Dirac fermion systems were argued to host markedly intriguing phenomena, such as the emergence of enhanced symmetry lines or the stabilization of quantum criticality beyond the realms of the traditional Landau-Ginzburg-Wilson (LGW) theory of critical phenomena [16]. For example, it was argued that Dirac fermions on graphene's honeycomb lattice support deconfined quantum critical points (DQCPs) [17] via the condensation of topological defects or anticommuting mass terms [18,19]. Moreover, recent theoretical calculations suggest that emergent $O(N)$ symmetries are a prevalent feature of deconfined quantum phase transitions [19–22] and beyond [23–32]. This recent progress raises two important, fundamental issues that are intimately related: (i) the stability of enhanced symmetry states in Dirac materials

and (ii) their relation to the apparent emergence of unconventional criticality in such systems.

This Rapid Communication solves both of these issues by identifying the generic features of Dirac fermions interacting with the quantum fluctuations of competing symmetry-breaking order parameters using two complementary, non-perturbative approaches. For this purpose, we formulate a relativistic quantum field theory, which we analyze using advanced renormalization group (RG) methods, and which describes both the Dirac fermions and the coupled symmetry-breaking order parameters. Remarkably, we find for such systems, rather generically, a stable quantum multicritical fixed point, which moreover exhibits an emerging enhanced symmetry. Moreover, we identify an extended phase coexistence regime to expand from the high-symmetry fixed point, in which both order parameters take on finite values simultaneously. We confirm this coexistence phase also by unbiased and controlled quantum Monte Carlo (QMC) simulations. In the following, we detail these results from our combined theoretical efforts, and we also offer a natural LGW interpretation of the proposed apparent instances of fermionic DQCPs, based on our findings.

In order to arrive at such general conclusions, we consider the generic case of (2+1)-dimensional Dirac fermions coupled to two order parameters (OPs) with $O(N_1) \oplus O(N_2)$ symmetry, following two different and complementary routes: the nonperturbative functional RG approach (FRG) [33], and a refined QMC analysis for the model in Ref. [19]. The FRG can be performed directly in $2+1$ dimensions and allows us to establish the emergence of $O(N_1 + N_2)$ symmetry at a multicritical point for all consistent values of N_1, N_2 . Also, our approach facilitates a study of the phases with broken symmetry and we find robust indications for an

intermediate coexistence phase for all such choices of N_1, N_2 . Further evidence of phase coexistence for the peculiar case of $O(3) \oplus Z_2$ symmetry breaking is derived from our refined QMC analysis, which we adapted to accurately investigate the strong-coupling regime.

Effective quantum field theory. For a general analysis of the coupled Dirac fermions, we consider the low-energy effective Gross-Neveu-Yukawa (GNY) model with two OP fields [34–41], describing interacting spin-1/2 fermions on a honeycomb lattice in the vicinity of a multicritical point. The Euclidean Lagrangian is $\mathcal{L} = \mathcal{L}_F + \mathcal{L}_B$, where

$$\begin{aligned} \mathcal{L}_F &= \bar{\psi}(-i\partial + g_1 M_\phi + g_2 M_\chi)\psi, \\ \mathcal{L}_B &= \phi_a(-\partial^2 + m_1^2)\phi_a + \chi_b(-\partial^2 + m_2^2)\chi_b \\ &\quad + \frac{u_1}{8}(\phi_a\phi_a)^2 + \frac{u_2}{8}(\chi_b\chi_b)^2 + \frac{u_3}{4}\phi_a\phi_a\chi_b\chi_b. \end{aligned} \quad (1)$$

The real OPs $\phi = (\phi_1, \dots, \phi_{N_1})$, $\chi = (\chi_1, \dots, \chi_{N_2})$ act as mass terms $M_\phi = \gamma_\phi^a \phi_a$ and $M_\chi = \gamma_\chi^b \chi_b$, interacting via Yukawa couplings $\bar{g}_{1/2}$ with eight-component Dirac fermions ψ and $\bar{\psi} \equiv \psi^\dagger \gamma_0$. Summation over repeated indices is implied. The matrices $\gamma_\phi^a, \gamma_\chi^b$ are defined as $\gamma_\phi^a = \gamma_0 \beta_\phi^a$, $\gamma_\chi^b = \gamma_0 \beta_\chi^b$, where the mass matrices $\beta_\phi^a, \beta_\chi^b$ anticommute among each other. The Lagrangian $\mathcal{L}$ exhibits an effective Lorentz invariance, which is expected to emerge in two-dimensional (2D) Dirac fermion systems at criticality [26,42], and we assume this also in the vicinity of the multicritical point. The GNY model $\mathcal{L}$ requires $d + N$ anticommuting matrices, where d is the spatial dimension, and $N = N_1 + N_2$. For the eight-dimensional representation relevant for graphene, this implies $N \leq 5$ [43,44].

The $O(N_1) \oplus O(N_2)$ symmetric system in Eq. (1) includes a symmetry-enlarged $O(N_1 + N_2)$ -invariant subspace, when $u_1 = u_2 = u_3$, $m_1^2 = m_2^2$, and $g_1^2 = g_2^2$. The leading-order ϵ expansion [39,40] studied the RG fixed point with an enlarged $O(N)$ symmetry, referred to as the isotropic fixed point (IFP). Within that approach, the IFP is found to be stable for all consistent values of N . However, it is well known from studies of purely bosonic $O(N_1) \oplus O(N_2)$ models [45,46] that the leading-order ϵ expansion severely overestimates the stability of the IFP. In contrast, FRG provides more faithful results already at truncation orders that we exploit here [47].

An important subtlety in Dirac fermion systems concerns the determination of the nature of a multicritical point. In a purely bosonic theory, a multicritical point can either be bicritical or tetracritical, and the two cases can be distinguished by the sign of the quantity $\Delta = u_1 u_2 - u_3^2$ in terms of the quartic couplings u_i at the RG fixed point, which is bicritical if $\Delta < 0$ and tetracritical if $\Delta > 0$ [45,47,48]. For the symmetry-enhanced case, $\Delta = 0$, the above classification is valid if the submanifold in coupling space determined by $\Delta = 0$ is closed under the RG flow. This is not generally the case in theories with massless fermions as can be shown using the ϵ expansion [39]: The submanifold in theory space defined by $u_1 = u_2 = u_3 =: u \neq 0$ satisfies $\Delta = 0$, but its dependence on the logarithmic RG scale t is given by $\partial_t \Delta = 2u(g_1^2 - g_2^2)^2$. Therefore, in the presence of Dirac fermions, the sign of Δ may be subject to change.

Functional renormalization group. We employ the nonperturbative FRG approach [33,49] to evaluate the generating

functional of one-particle irreducible n -point correlation functions $\Gamma^{(n)}$; see Refs. [50–60] for applications to low-dimensional GNY systems. This method allows us to calculate directly in $D = 2 + 1$ and integrate out the flow also within the ordered phases. Central to the FRG method is the exact RG flow equation $\partial_k \Gamma_k = \frac{1}{2} \text{Tr}[\partial_k R_k (\Gamma_k^{(2)} + R_k)^{-1}]$ for the average effective action Γ_k , where $\Gamma_k^{(2)}$ is the second functional derivative with respect to all field degrees of freedom, and R_k is an infrared cutoff function. This flow equation interpolates between the bare action at the ultraviolet (UV) cutoff $k = \Lambda$ and the full quantum effective action $\Gamma = \Gamma_{k=0}$.

We employ a truncation based on the original form of the microscopic action in Eq. (1), i.e.,

$$\begin{aligned} \Gamma_k &= \int d^D x \left\{ \bar{\psi}(-iZ_{\psi,k}\partial + g_{1,k}M_\phi + g_{2,k}M_\chi)\psi \right. \\ &\quad \left. - \frac{1}{2}Z_{\phi,k}\phi_a\partial^2\phi_a - \frac{1}{2}Z_{\chi,k}\chi_b\partial^2\chi_b + V_k(\rho_\phi, \rho_\chi) \right\}, \end{aligned} \quad (2)$$

which is known as the extended local potential approximation, LPA'. The scale dependence of the Yukawa couplings $g_{1,k}$ and $g_{2,k}$ as well as the wave-function renormalizations $Z_{\phi,k}$ have been made explicit. The bosonic potential V_k depends on the $O(N_1)$ and $O(N_2)$ invariant quantities $\rho_\phi = \phi_a\phi_a/2$, $\rho_\chi = \chi_b\chi_b/2$, and we expand its dimensionless form $u = k^{-D}V_k$ as a function of the dimensionless $O(N_i)$ -symmetric field variables $\tilde{\rho}_\phi = Z_{\phi,k}k^{2-D}\rho_\phi$ and $\tilde{\rho}_\chi = Z_{\chi,k}k^{2-D}\rho_\chi$ around a (running) minimum, denoted $\kappa_{\phi/\chi} = \tilde{\rho}_{\phi/\chi,\text{min}}$. A truncation up to order n_{max} in the fields will be referred to in the following as LPA' n_{max} . The nature of the minimum corresponds to three different scenarios, depending on whether the individual OP fields are in the symmetric or in the spontaneously symmetry-broken regime: (1) Both OP fields remain in their symmetric phases, i.e., the minimum of the potential is at $\kappa_{\phi/\chi} = 0$. (2) The OP ϕ acquires an expectation value, while the other OP χ remains in its symmetric phase—similarly, for the reversed situation. (3) The minimum of the potential is at nonzero expectation values for both OPs, i.e., $\kappa_{\phi/\chi} \neq 0$. Note that our ansatz for the effective action does not include topological terms, which naturally occur only when the fermions are massive and can be integrated out [61].

The FRG flow equations for the dimensionless expansion coefficients of the potential u , including the quadratic mass terms and the quartic couplings, the dimensionless Yukawa couplings $\tilde{g}_{i,k}^2 = g_{i,k}^2 k^{D-4} Z_{i,k}^{-1} Z_{\psi,k}^{-2}$, as well as the anomalous dimensions $\partial_t Z_{\psi/\phi/\chi}$ are obtained by taking the corresponding derivatives of the ansatz in Eq. (2). Flow equations for the expectation values $\kappa_{\phi/\chi}$ are obtained from the condition that they are a minimum (cf. the Supplemental Material [62] for details). This procedure yields a set of coupled flow equations of the form $\partial_t x_i = \beta_i(\{x_j\})$ in the space of coupling parameters x_j .

Stability of the symmetry-enhanced fixed point. A fixed point is defined by the condition $\forall i : \beta_i(\{x_j\}) = 0$. Here, we focus on the IFP, facilitating the symmetry enhancement $O(N_1) \oplus O(N_2) \rightarrow O(N)$. The system has two tuning parameters represented by the boson masses m_i^2 [cf. Eq. (1)]. They give rise to two relevant directions in the RG flow with scaling properties given by the critical exponents θ_1 and θ_2 obtained

TABLE I. Largest five eigenvalues θ_i of the stability matrix based on FRG calculation in LPA'8 truncation, for different values of $N_1 + N_2$. Eigenvalues that already appear in the $O(N_1 + N_2)$ symmetric models are printed in boldface.

$N_1 + N_2$	θ_1	θ_2	θ_3	θ_4	θ_5
2	0.878	0.864	-0.878	-1.087	-1.109
3	0.773	0.726	-0.924	-1.179	-1.322
4	0.734	0.580	-1.017	-1.274	-1.542
5	0.738	0.465	-1.132	-1.361	-1.732

from diagonalizing the stability matrix $\mathcal{M}_{ij} := -(\partial\beta_i/\partial x_j)|_{x^*}$ (here, x_j^* denote the fixed-point coordinates). Positive eigenvalues θ_i of $\mathcal{M}_{ij}$ correspond to relevant directions, i.e., their number indicates the number of tuning parameters. Negative θ_i correspond to irrelevant directions, attracted to the fixed point. The IFP is stable, if the third-largest eigenvalue of the $\mathcal{M}_{ij}$ is negative (called the *stability exponent*).

We report the numerical results for the five largest eigenvalues of the stability matrix in Table I, exhibiting the stability of the IFP for all consistent choices of N . In particular, the stability exponent has a sizable magnitude of $O(1)$. Therefore, any perturbation of the enhanced symmetry near the multicritical point will die out rather quickly, supporting a strong tendency towards the emergent symmetry. This strong tendency towards emergent $O(N_1 + N_2)$ is consistent with the QMC findings in Ref. [19]. Noticeable, the symmetry enhancement is naturally realized in our extended LGW approach through the fluctuations of massless Dirac fermions, i.e., without requiring the inclusion of additional topological terms. This contrasts to the case of purely bosonic $O(N_1) \oplus O(N_2)$ models [45,47], for which symmetry enhancement is supported only for $N_1 = N_2 = 1$, with an almost marginal stability exponent.

Phase diagram from field theory. The phase diagram finally can be obtained from integrating the FRG flow towards the infrared. To this end, we formulate the initial value problem at an arbitrary ultraviolet scale Λ , used to set the units. To resolve the phase diagram in the vicinity of the symmetry-enhanced quantum multicritical point, we perform a sweep of initial conditions in the vicinity of the IFP. We consider three different choices for N_1 and N_2 : (i) two coupled Ising order parameters ($N_1 = N_2 = 1$), (ii) a $O(3) \oplus \mathbb{Z}_2$ model ($N_1 = 3, N_2 = 1$), relevant to the model in Ref. [19], and (iii) a $O(3) \oplus O(2)$ model ($N_1 = 3, N_2 = 2$). The resulting phase diagrams are shown in Fig. 1, and we find that all cases exhibit extended coexistence regions, at which both OPs develop a vacuum expectation value.

In the region close to the line $\delta m_1^2 = \delta m_2^2$ in Fig. 1 emerging from the IFP, Goldstone fluctuations in both adjacent phases appear when the spontaneously broken symmetry is continuous. Their interplay with the massive modes has the tendency to drive the system out of the symmetry-broken phase. Indeed, when the adjacent symmetry-broken phases involve no massless modes (for $N_1 = N_2 = 1$), the line of exact $O(N)$ symmetry can be resolved effortlessly. In the presence of Goldstone modes and very close to $\delta m_1^2 = \delta m_2^2$, however, the expectation values $\kappa_{i,k}$ do not straightforwardly converge to definite values in the limit $k \rightarrow 0$, within our

FIG. 1. Phase diagrams from FRG for $N_1 = 1, N_2 = 1$ (left), $N_1 = 3, N_2 = 1$ (middle), and $N_1 = 3, N_2 = 2$ (right). Tuning parameters δm_i^2 measure the distance from the IFP, DSM denotes the Dirac semimetal regime, and other phases are labeled by the broken symmetry. Solid lines are continuous transitions, and coexistence regions are shown in shaded orange. Within the white areas, the FRG flow is numerically unstable.

approximation of the exact RG flow (see Ref. [62] for a more detailed discussion). Nevertheless, sufficiently away from that parameter regime, we can reliably establish the appearance of a stable coexistence region near the IFP. Moreover, exactly along the line of enhanced symmetry ($\delta m_1^2 = \delta m_2^2$), we can integrate out the renormalization group flow by exploiting the enhanced symmetry, and find that a coexistence of both orders occurs. The missing regions of the phase diagrams may be accessible to alternative FRG methods, e.g., by pseudospectral methods [56,57].

Quantum Monte Carlo. For the case of $O(3) \oplus \mathbb{Z}_2$, we obtain direct support for the coexistence region also from a refined QMC analysis for the microscopic model of Ref. [19]. For this purpose, we derive an effective quantum spin model that emerges in the strongly interacting regime of the interacting Dirac fermion model, and which can be simulated by more efficient, sign problem-free QMC methods using cluster updates and larger lattices than accessible to the QMC approach for the original fermionic model. The Hamiltonian of this effective quantum spin model, obtained by perturbation theory about the strong-interaction limit [63], reads

$$H = \sum_{\langle i,j \rangle} (J_{ij} + \chi_{ij} \sigma_{(ij)}^z) \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right) - J_l \sum_{\langle ij,kl \rangle} \sigma_{(ij)}^z \sigma_{(kl)}^z - h \sum_{\langle i,j \rangle} \sigma_{(ij)}^x,$$

in terms of Heisenberg $S = 1/2$ spins $\mathbf{S}_i$, residing on a honeycomb lattice and coupled via bond-centered strengths χ_{ij} to a transverse-field (h) Ising model of spins $\sigma_{(ij)}$, located on the nearest-neighbor bonds of the honeycomb lattice. The summation over $\langle i,j \rangle$ ($\langle ij,kl \rangle$) extends over nearest-neighbor Heisenberg (Ising model) spins. In terms of the nearest-neighbor hopping t , the Hubbard interaction U , and the fermion-spin couplings ξ_{ij} of the underlying fermionic model, we obtain $J_{ij} = 4(t^2 + \xi_{ij}^2)/U$, and $\chi_{ij} = 8t\xi_{ij}/U$ in second-order perturbation theory [62]. These relations can also be used to specify parameter values of H and compare to the results of Ref. [19].

With a staggered pattern of $\xi_{ij} = +\xi, 0, -\xi$ (cf. the inset of Fig. 2) as in Ref. [19], the model has a combined lattice inversion and Ising model spin-flip $\mathbb{Z}_2$ symmetry in addition to the $O(3)$ [SU(2)] symmetry of the Heisenberg

FIG. 2. QMC phase diagram of the $O(3) \oplus \mathbb{Z}_2$ model H in terms of the parameters $(U, 1/h)$ of the underlying fermionic model ($\xi = 0.5, J_I = 1, t = 1$). The coexistence region is shown in shaded orange. The inset shows the honeycomb lattice with the modulated pattern $\xi_{ij} = -\xi, 0, +\xi$ in different colors. Open (solid) circles denote Heisenberg (Ising) spins.

exchange. To connect to the previous results, we also fix $\xi = 0.5, J_I = 1$, and $t = 1$, and probe the strong-coupling regime for values of $U > 6$, where large single-particle gaps prevailed. We used a hybrid QMC parallel tempering scheme [62,64,65] for the Hamiltonian H on periodic lattices with N_H Heisenberg spins (and $N_I = 3N_H/2$ Ising spins), for N_H up to 2400, based on the stochastic series expansion approach [66–68]. In particular, we monitored the evolution of the ferromagnetic Ising OP $m_I = \langle |\frac{1}{N_I} \sum_{b=1}^{N_I} \sigma_b^z| \rangle$ and the antiferromagnetic Heisenberg OP $m_H = \langle |\frac{1}{N_H} \sum_{i=1}^{N_H} (-1)^i S_i^z| \rangle$ upon varying h . As an example, Fig. 3 shows the finite-size scaling of both OPs, for h in the transition region at $U = 7$. The algebraic behaviors at the order-to-disorder transitions are in accord with the anticipated asymptotic scalings for the purely bosonic Ising and Heisenberg universality classes in dimension $D = 2 + 1$, and yield two distinct critical field strengths,

FIG. 3. Finite-size scaling of m_H and m_I for h in the transition region of H for $U = 7$ ($\xi = 0.5, J_I = 1, t = 1$). Dashed lines show the asymptotic scalings $m_j \propto N_j^{-\beta_j/2\nu_j}$ for $j = I, H$, with β_j, ν_j as of Ref. [69]. For clarity, the values for m_I were multiplied by a factor of 2. The lowest and highest shown values of h are given, as well as the near-critical h values.

$h_c^I = 3.200(1)$ for m_I , and $h_c^H = 3.194(1)$ for m_H . These values are consistent also with an analysis of the corresponding Binder ratios [62].

The resulting phase diagram in the above parameter regime is shown in Fig. 2. It exhibits a narrow intermediate phase of coexisting orders between the small (large) h phase with pure $\mathbb{Z}_2$ [$O(3)$] symmetry breaking: For small h , the Ising model spins order ferromagnetically, spontaneously breaking the $\mathbb{Z}_2$ symmetry. Due to the staggered ξ_{ij} coupling, this induces a preferred dimerization pattern on the honeycomb lattice, which leads to a dominant valence-bond singlet formation of the Heisenberg spins along the stronger ($\xi_{ij}\sigma_{ij}^z > 0$) bonds. Upon increasing h , the ferromagnetic order reduces, in effect weakening also the induced dimerization, so that antiferromagnetic Heisenberg spin order can eventually set in prior to the full suppression of the ferromagnetic Ising spin order at even larger values of h . Due to the large single-particle gaps for $U > 6$, we exclude residual (charge) fluctuations in the fermionic model to qualitatively modify this basic physics. We observe in Fig. 2 that the coexistence regime widens slightly with increasing U . This thinness of the coexistence regime within the considered parameter regime explains why it was not resolved by the fermionic QMC methods [19]. It should, however, be noted that within the effective quantum spin model we cannot identify the multicritical point of the underlying fermionic theory, which was located at $(U, 1/h) \approx (4.2, 0.28)$ in Ref. [19]. Indeed, the multicritical IFP is of genuine fermionic nature (cf. the FRG results).

Discussion. We studied $(2+1)$ -dimensional Dirac fermions coupled to two compatible OPs with $O(N_1)$ and $O(N_2)$ symmetry in the vicinity of the multicritical isotropic fixed point, providing an emergent $O(N_1 + N_2)$ symmetry. Our FRG study predicts a strong irrelevance of perturbations of the $O(N_1 + N_2)$ symmetry, which is consistent with the numerical result of an emergent symmetry in the related Dirac fermion lattice model [19]. Contrary to this numerical study, however, we do not find a single line of direct, continuous order-to-order transitions. Instead, we identify a robust region of coexistence of both orders, which is separated by continuous transitions from the other phases. In the case of the $O(3) \oplus \mathbb{Z}_2$ symmetry, relevant for Ref. [19], we could furthermore support this field-theoretical analysis by large-scale QMC simulations. Therefore, our combined approach sheds light on the nature of quantum critical fermions coupled to bosonic fields as in Ref. [19], and further challenges the scenario of deconfined quantum criticality in quantum spin-Hall insulators [18]. It appears promising to also experimentally probe the physics that we uncovered here, given the very recent advances in the experimental studies of twisted bilayer graphene with Dirac points indeed located in proximity to several competing orders [70].

Acknowledgments. We are grateful to F. F. Assaad and I. F. Herbut for discussions. E.T. was supported by the Deutsche Forschungsgemeinschaft (DFG) through the Leibniz Prize of A. Rosch, RO2265/5-1. L.J. was supported by the DFG through JA2306/4-1 (Emmy Noether program, project id 411750675), SFB 1143 (project id 247310070), and the Würzburg-Dresden Cluster of Excellence *ct.qmat* (EXC 2147, project id 390858490). M.M.S. was supported by the DFG,

project id 277146847 – SFB 1238 (C02, C03). L.W. and S.W. acknowledge support by DFG under Grant No. WE/3649/4-2 of the FOR 1807 and through RTG 1995. Fur-

thermore, we acknowledge the IT Center at RWTH Aachen University and the JSC Jülich for access to computing time through JARA-HPC.

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Correction: The unnumbered equation in the “Quantum Monte Carlo” section contained an omission that had consequences for Figs. 2 and 3, the caption to Fig. 3, and the values for h_c^I and h_c^H ; all have been fixed.