p-wave superconductivity and the axiplanar phase of triple-point fermions

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(Received 6 July 2021; revised 9 October 2021; accepted 15 November 2021; published 24 November 2021)

We consider weak-coupling superconductivity in the inversion- and rotation-symmetric system of two pseudospin s = 1 low-energy fermions of opposite chirality. General contact interactions can lead to Cooper instabilities toward *d*-wave or toward a novel $2 \times 3 p$ -wave matrix order parameter. We compute the Ginzburg-Landau (GL) free energy for the latter. Remarkably, in this case the GL free energy can be minimized exactly, with the resulting ordered state being analogous to the "axiplanar" p wave, which exhibits extra degeneracy and generally breaks time-reversal symmetry. Whereas a generic GL free energy for our order parameter has only $U(1) \times SO(2) \times SO(3)$ symmetry broken down to $SO(2) \times SO(2)$ in the axiplanar ordered phase and leading therefore to six Goldstone bosons. We show how the lattice, once restored, fixes the allowed values of the magnetization in the superconducting state by locking the spatial directions implicit in the order parameter to its high-symmetry axes.

DOI: 10.1103/PhysRevB.104.L180507

Crystalline solids feature effective fermionic excitations outside the realm of possibilities of high-energy physics. Besides the ubiquitous Weyl fermions which have an effective "spin" s = 1/2 and describe crossing of two bands at a point, symmetry-protected quasiparticle excitations with s = 1 and s = 3/2 are also possible [1]. The latter Rarita-Schwinger-Weyl fermions have already been the subject of several investigations [2-4] that go beyond the noninteracting paradigm. Of great interest also are the triple-point fermions with s = 1, which may arise when a symmetry-protected crossing of three bands occurs somewhere in the Brillouin zone [1,5,6]. The two linearly dispersing bands then carry the Chern number of $C = \pm 2$, whereas the flat band has C = 0. To neutralize the topological charge, there are either (at least) two such points of triple-band crossings in the Brillouin zone with opposite helicities or other topologically nontrivial bands that cross the Fermi level elsewhere in the Brillouin zone. The possible effects of electron-electron interactions on the triple-point fermions, to our knowledge, have not been studied yet [7]. The recent detection of possible triple-point fermions in CoSi [8] brings urgency to such investigations.

In a parallel development, Cooper pairing of multiband fermions has been systematically scrutinized recently, as it may naturally lead to multicomponent unconventional superconductivity with competing ground states, possible breaking of time-reversal symmetry, or exotic quasiparticle spectra, exhibiting Bogoliubov-Fermi surfaces, for instance [9–14]. Here we consider an inversion-symmetric system of two s = 1 fermions of *opposite* chirality, which represents the minimal, albeit nonrelativistic extension of the Dirac Hamiltonian to higher spin. We show that a general contact attractive interaction may lead to a superconducting matrix order parameter with *p*-wave symmetry, which transforms under the Lie group $G = U(1) \times SO(2) \times SO(3)$. The U(1) is the usual (particle number) gauge symmetry, the SO(3) is the group of rotations, and the SO(2) is the group of transformations between the two crossing points, or valleys, of opposite chirality. The crucial observation is that the *p*-wave order parameter is only a 2×3 complex matrix because, as shown here, the opposite chirality of the two s = 1 fermions cuts off the Cooper logarithm for three of the nine components of the usual 3×3 matrix, which describes *p*-wave pairing in ³He, for example [15].

Interestingly, in spite of the large remaining twelve-realparameter space to which the order parameter belongs, we find that the derived Ginzburg-Landau (GL) free energy for the 2×3 component complex order parameter with the weak-coupling values of the coefficients of the five independent quartic terms [16] can be minimized exactly; the minima break the G symmetry completely and exhibit an additional degeneracy, not implied by the symmetry G of the GL theory, described by a single continuous parameter θ . An equivalent *p*-wave configuration has appeared in the literature before as the so-called "axiplanar" state [17], but as far as we know it has not been previously found to be a minimum of any actual free energy. The ordered phase's extra degeneracy also manifests itself in the six Gaussian zero-energy modes around the axiplanar phase instead of only five expected Goldstone bosons which would accompany the apparent symmetry-breaking pattern. This hints at a possibly larger hidden symmetry of the GL theory, and we indeed find new variables that factorize the partition function into two terms, each describing a separate three-component complex order parameter coupled to its own chiral fermion [18,19]. At each of the two triple-band crossing points, the superconducting condensate is maximally magnetized j = 1macroscopic quantum state of Cooper pairs, with average magnetization vector pointing along an arbitrary direction. The hidden symmetry-breaking pattern is in this way revealed as $U(1) \times SO(3) \times U(1) \times SO(3) \rightarrow SO(2) \times SO(2)$, which naturally accounts for the six observed massless modes by the standard Goldstone theorem.

Finally, we show that the degeneracy parameter θ is nothing but half of the angle between the two symmetry axes in the $SO(2) \times SO(2)$ residual symmetry of the axiplanar state. This means that once a discrete lattice that harbors s = 1 fermions is restored, 2θ will be given by the angle between two equivalent symmetry axes of the crystal. Reducing the rotational symmetry to the cubic symmetry, in an example we provide, leads to the preferred axes to be some of the cube's diagonals and thus ultimately the allowed values are $\theta = 0, \pi/2, ArcTan[1/\sqrt{2}], ArcCot[1/\sqrt{2}]$. These translate into average magnetization of the p-wave superconducting state as maximal (2), minimal (0), or intermediate, $2\sqrt{2/3}$ or $2/\sqrt{3}$.

Interacting triple-point fermions. Consider chiral s = 1 fermions near two points in the Brillouin zone that exhibit triple-band crossing with the low-energy Hamiltonian to the leading order in momentum,

$$H(\vec{p}) = \sigma_3 \otimes \vec{p} \cdot \vec{S},\tag{1}$$

where the momentum is measured from the crossing points $\pm \vec{K}$ related to each other by inversion. The velocity has been set to unity. The fermion field is a six-component Grassmann variable

$$\Psi(\omega, \vec{p}) = (a(\omega, \vec{K} + \vec{p}), b(\omega, -\vec{K} + \vec{p}))^T, \qquad (2)$$

with $r = (r_1, r_2, r_3)^T$, (r = a, b), and $p \ll \Lambda$, with Λ as the momentum cutoff, of the order of inverse of the lattice spacing. The matrices S_i (i = 1, 2, 3) provide an s = 1 (threedimensional) representation of the SO(3) Lie algebra, and the third Pauli matrix appearing in the left factor assures that the Chern numbers of the two degenerate eigenstates near the points $\pm \vec{K}$ cancel. The Hamiltonian is the direct sum of two s = 1 Hamiltonians near the two crossing points, in exact analogy to the Dirac Hamiltonian as a sum of two s = 1/2(Weyl) Hamiltonians. It is inversion symmetric and commutes with the inversion operator $I = \sigma_1 \otimes \mathbb{1}_3$ accompanied by $\vec{p} \rightarrow$ $-\vec{p}$. When $\vec{K} = 0$, it is also time-reversal invariant, with time-reversal operator $T = (\mathbb{1}_2 \otimes U)\mathcal{K}$ and $\vec{p} \to -\vec{p}$, where the unitary matrix U is representation dependent. Note, however, that since s is integer $T^2 = UU^* = +\mathbb{1}_6$, and therefore $H(\vec{p})$ describes spinless (or spin-polarized) fermions. Alternatively, when $\vec{k} \neq 0, H(\vec{p})$ may be taken to describe regular half-integer spin fermions, but with broken time-reversal symmetry.

We further assume a finite chemical potential μ , and $|\mu| \ll \Lambda$. The most important interactions are then those that are finite at the crossing points $\vec{p} = 0$. We may parametrize them by contact interaction terms between the triple-band fermions which, for simplicity, are assumed to respect rotational invariance. The most general interacting Lagrangian may then be written as

$$L = \Psi^{\dagger}(x)(\partial_{\tau} + H(-i\nabla) - \mu \mathbb{1}_{6})\Psi(x) - \sum_{r=s,p,d} V_{r}(\Psi^{\dagger}(x)M_{r}\Psi^{*}(x))(\Psi^{T}(x)M_{r}^{\dagger}\Psi(x)), \quad (3)$$

where $x = (\vec{x}, \tau)$. The three quartic terms are written in the "particle-particle" form to assure their linear independence [20]. Fermi-Dirac statistics requires the matrices M_r to be antisymmetric, i.e., $M_r^T = -M_r$. In the adjoint representation $S_{i,jk} = -i\epsilon_{ijk}$ they may be more conveniently written as $M_r = \Gamma_r(\sigma_2 \otimes \mathbb{1}_3)$, so that the matrices Γ_r provide either the *s*-wave ($\Gamma_s = \mathbb{1}_2 \otimes \mathbb{1}_3$) the *p*-wave ($\Gamma_{p,ij} = \sigma_i \otimes S_j$), or the *d*-wave ($\Gamma_{d,ij} = \mathbb{1}_2 \otimes T_{ij}$) pairing (with the five-component second-rank irreducible tensor $T_{ij} = \{S_i, S_j\} - (4/3)\delta_{ij}\mathbb{1}_3$ [11,19]). The repeated index summation convention is implied. We take $V_p > 0, V_s = V_d = 0$ and consider the matrix order-parameter

$$\Delta_{ij}(x) = \langle \Psi^T(x)(\sigma_2 \sigma_i \otimes S_j) \Psi(x) \rangle, \tag{4}$$

which would signal the formation of the *p*-wave superconductivity. We argue shortly that a weak-coupling V_s is irrelevant. A weak $V_d > 0$ would be relevant and would lead to a combination of the five-component *d*-wave states. This, however, was the subject of previous work on closely related systems [4,11,19].

The complex matrix order-parameter $\Delta_{ij}(x)$ is in general space and imaginary time dependent, but for the purposes of the mean-field theory it suffices to take it to be uniform. The continuous symmetry of *L* is evidently only $U(1) \times SO(2) \times$ SO(3) with U(1) being the particle number, SO(2) the intervalley, and SO(3) the rotation symmetry. Although the *p*-wave order-parameter Δ_{ij} is a 3 × 3 matrix, the Lagrangian has the symmetry smaller than the full rotational symmetry of $U(1) \times SO(3) \times SO(3)$, relevant to the *p* wave in ³He. The 2 × 3 matrix Δ_{ij} (*i* = 1, 2, *j* = 1, 2, 3) transforms as a twodimensional vector under the SO(2) acting on the left index, whereas the remaining Δ_{3j} (*j* = 1, 2, 3) is an SO(2) scalar. Both objects transform as three-dimensional vectors under the SO(3) rotations acting on the right index.

GL theory. Integrating out the fermions and expanding the result to two leading orders in powers of the uniform order parameter leads to the GL free-energy $L_{GL}(\Delta) = L_2(\Delta) + L_4(\Delta) + O(\Delta^6)$, where $L_2(\Delta)$ is quadratic in the order parameter, and

$$L_2(\Delta) = \left(\frac{\delta_{ij}}{V_p} + K_{ij}\right) \Delta_{ik}^* \Delta_{jk}.$$
 (5)

A straightforward but somewhat lengthy calculation [21] yields $K_{ij} = 0$ for $i \neq j$, as required by the symmetry, and furthermore at low temperatures *T*,

$$K_{11} = K_{22} = -\frac{2}{3}N_0 \ln\left(\frac{\Lambda}{T}\right),$$
 (6)

with $N_0 = \mu^2 / \pi^2$ as the density of states at the Fermi level. One observes the expected Cooper's logarithmic divergence as $T \to 0$. On the other hand, when $T \to 0$,

$$K_{33} = -\frac{2\Lambda^2}{3\pi^2}$$
(7)

and finite. Below the mean-field transition temperature $T_c = \Lambda e^{-3/(2N_0V)}$, $\Delta_{ij} \neq 0$ only for i = 1, 2 and j = 1, 2, 3, whereas the remaining components $\Delta_{3i} = 0$. In the limit of weak-coupling $V_p \Lambda^2 \ll 1$, the order-parameter components Δ_{3i} remain massive at T_c , and even their fluctuations are suppressed at all temperatures.

The finiteness of K_{33} may be understood by noticing that the leading-order effect of a finite Δ_{3i} would be only to shift the chemical potential and therefore not open the usual gap *anywhere*. To see this, consider the corresponding Bogoliubov-de Genness Hamiltonian with the real [22] orderparameter Δ_{3i} :

$$H_{\text{BdG}} = \sigma_3 \otimes (H(\vec{p}) - \mu \mathbb{1}_6) + \Delta_{3i} \sigma_2 \otimes \sigma_1 \otimes S_i.$$
(8)

Although not obvious, it may be easily checked that

$$\det H_{BdG} = \mu^4 (p^2 - \mu^2 - \Delta_{3i} \Delta_{3i})^4, \tag{9}$$

and thus the entire Fermi surface is inflated from $p = \mu$ in the normal phase to $p = \sqrt{\mu^2 + \Delta_{3i}\Delta_{3i}}$ in the superconducting phase. The *s*-wave channel suffers from the same problem. The superconducting instabilities of the weakly interacting Lagrangian in Eq. (3) are therefore only the truncated 2×3 *p*-wave order considered here and the *d* wave studied earlier [4,11,19].

The precise form of the superconducting condensate below T_c depends on the quartic terms in $L_4(\Delta)$,

$$L_4(\Delta) = \sum_{i=1}^5 b_i I_i(\Delta), \qquad (10)$$

where [16] $I_1 = |Tr\Delta\Delta^T|^2$, $I_2 = (Tr\Delta\Delta^{\dagger})^2$, $I_3 = Tr\Delta\Delta^T$ $(\Delta\Delta^T)^*$, $I_4 = Tr\Delta\Delta^{\dagger}\Delta\Delta^{\dagger}$, and $I_5 = Tr\Delta\Delta^{\dagger}(\Delta\Delta^{\dagger})^*$. Although the order parameter is now only a 2 × 3 matrix, these five invariants under *G* can be shown to still be linearly independent [21]. With arbitrary coefficients b_i the $L_4(\Delta)$ is the most general *G*-symmetric local quartic term. The standard one-loop diagram yields the *exact* relation between the quartic coefficients at all temperatures: $b_3 = -2b_1$, $b_2 = b_4 = -b_5$, and $b_2 > 0$ and $b_3 > 0$ [21]. In addition to the leading order in low T_c one also finds that $b_2 = b_3$, and all $b_i \sim N_0/T_c^2$, as usual [23]. These turn out to be the same relations between the quartic coefficients as in the standard weak-coupling GL free energy for ³He [16].

Mean-field solution and the axiplanar state. Writing the order parameter as $\Delta = \Delta_0 \Phi$, with Δ_0 as the complex norm and Φ is a 2 × 3 normalized matrix satisfying $Tr\Phi\Phi^{\dagger} = 1$, the $L_{\rm GL}$ is below T_c minimized by

$$|\Delta_0|^2 = -\frac{a}{2L_4(\Phi)},$$
(11)

where $a = V_p^{-1} + K_{11} \sim (T - T_c)$. At this value of Δ_0 ,

$$L_{\rm GL} = -\frac{a^2}{4L_4(\Phi)},$$
 (12)

and therefore the GL free energy is the lowest at Φ that minimizes the expression

$$L_4(\Phi) = b_2 + b_3 \left(I_3(\Phi) - \frac{1}{2} I_1(\Phi) \right) + b_2 (I_4(\Phi) - I_5(\Phi)).$$
(13)

Minimization of the last expression in terms of 3×3 matrix would lead to the Balian-Werthamer state $\Phi = (1/\sqrt{3})\mathbb{1}_3$, with the residual SO(3) symmetry and believed to be the superconducting B phase of ³He [15]. We show next that in the present case $L_{GL}(\Phi)$ has a hidden symmetry and a rather different ordered phase. First, it is easy to see that both combinations of quartic invariants appearing in $L_4(\Phi)$ are nonnegative. Since the matrix $\Phi \Phi^{\dagger}$ is 2 × 2 and Hermitian, it can be expanded in terms of Pauli matrices: $\Phi \Phi^{\dagger} = c_{\mu}\sigma_{\mu}$, $\mu = 0, 1, 2, 3$ with real c_{μ} . Then,

$$I_4(\Phi) - I_5(\Phi) = Tr\Phi\Phi^{\dagger}(\Phi\Phi^{\dagger} - (\Phi\Phi^{\dagger})^T) = 4c_2^2 \ge 0.$$
(14)

Similarly, the non-Hermitian symmetric matrix $\Phi\Phi^T$ can be written as $\Phi\Phi^T = d_\mu\sigma_\mu$ with complex d_μ , and $\mu \neq 2$. It readily follows that

$$I_{3}(\Phi) - \frac{1}{2}I_{1}(\Phi) = 2(|d_{1}|^{2} + |d_{3}|^{2}) \ge 0.$$
(15)

Since both $b_2 > 0$ and $b_3 > 0$, the configurations for which $I_4 - I_5 = I_3 - (I_1/2) = 0$, if existing, are the minima of the L_{GL} at $T < T_c$. To find such configurations, we consider the two rows of the matrix Φ_{ij} as two (complex) vectors under the *SO*(3): $\vec{\Phi}_1 = (\Phi_{11}, \Phi_{12}, \Phi_{13})$, and $\vec{\Phi}_2 = (\Phi_{21}, \Phi_{22}, \Phi_{23})$. The normalization $Tr\Phi\Phi^{\dagger} = 1$ then implies:

$$\vec{\Phi}_1 \cdot \vec{\Phi}_1^* + \vec{\Phi}_2 \cdot \vec{\Phi}_2^* = 1.$$
 (16)

The condition $I_3 - (I_1/2) = 0$ demands that $\Phi \Phi^T$ is proportional to the unit matrix, which translates into

$$\vec{\Phi}_1 \cdot \vec{\Phi}_2 = 0, \tag{17}$$

$$\vec{\Phi}_1 \cdot \vec{\Phi}_1 = \vec{\Phi}_2 \cdot \vec{\Phi}_2. \tag{18}$$

Likewise, the condition $I_4 - I_5 = 0$ requires the matrix $\Phi \Phi^{\dagger}$ to be real, for which it suffices that its off-diagonal element $\vec{\Phi}_1 \cdot \vec{\Phi}_2^*$ is real. However, a real symmetric matrix $\Phi \Phi^{\dagger}$ can always be rotated by an SO(2) rotation into a diagonal form in which a stronger but computationally more convenient condition applies:

$$\vec{\Phi}_1 \cdot \vec{\Phi}_2^* = 0. \tag{19}$$

A bit of algebra shows then that the most general solution of the Eqs. (16)–(19) [modulo a *G* transformation, time reversal (complex conjugation), or shift of θ] is given by

$$\Phi_{\theta} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & \sin \theta & 0\\ 1 & 0 & i \cos \theta \end{pmatrix}, \tag{20}$$

with an *arbitrary* θ . This is analogous to the "axiplanar" state, which may be understood as interpolating between the "axial" $(\theta = 0)$ and "planar" $(\theta = \pi/2)$ phases [17]. The axial phase for the 3 × 3 order parameter is invariant under $U(1) \times U(1)$, and it is believed to be the superconducting A phase of ³He at high pressure [15].

Since the four invariants $I_i(\Phi)$, i = 1, 3, 4, 5 separately do depend on θ , two configurations with different values of θ in general cannot be related by any symmetry transformation from *G*. The analysis of Gaussian fluctuations around Φ_{θ} confirms this: One finds *six* independent massless modes, whereas only five are implied by the symmetry-breaking pattern of Φ_{θ} , which for a general θ breaks all five generators of *G*.

Separation variables. The hidden symmetry of L_{GL} is revealed by the transformation from $\vec{\Phi}_{1,2}$ into $\vec{\Phi}_{\pm}$, defined as $\vec{\Phi}_s = \vec{\Phi}_2 + is\vec{\Phi}_1$, $s = \pm$. In terms of these variables, GL free

energy becomes $L_{GL} = L_+ + L_-$, where

$$L_{s} = \frac{a|\Delta_{0}|^{2}}{2} + \frac{b_{3}|\Delta_{0}|^{4}}{2} \left(1 + \frac{1}{2}|\vec{\Phi}_{s} \cdot \vec{\Phi}_{s}|^{2}\right), \quad (21)$$

and we imposed the normalization $\bar{\Phi}_s^* \cdot \bar{\Phi}_s = 1$ (with no summation over *s* implied hereafter) and assumed $b_2 = b_3$ in Eq. (11) as appropriate at low temperatures. It is evident that each of the two complex vector order parameters, which from Eqs. (2) and (4) are simply $\Phi_{+,i}(x) = 2\langle a^T(x)S_ia(x)\rangle$ and $\Phi_{-,i}(x) = 2\langle b^T(x)S_ib(x)\rangle$, can be gauge-transformed and rotated independently of the other, so the hidden symmetry of L_{GL} is in fact $U(1)_+ \times SO(3)_+ \times U(1)_- \times SO(3)_-$. Each condensate $\bar{\Phi}_s$ represents a spin-one macroscopic quantum state $|\Phi_s\rangle$ and couples only to the triple-point fermion of chirality *s*. Each L_s is minimized by the state for which $\bar{\Phi}_s \cdot \bar{\Phi}_s = 0$. Since in the adjoint representation,

$$\vec{\Phi}_{s} \cdot \vec{\Phi}_{s}|^{2} = 1 - (\Phi_{s,n}^{*} S_{i,nm} \Phi_{s,m}) (\Phi_{s,k}^{*} S_{i,kj} \Phi_{s,j}), \qquad (22)$$

each $\vec{\Phi}_s$ maximizes its possible average magnetization $\vec{m}_s = \langle \Phi_s | \vec{S} | \Phi_s \rangle$, i.e., it represents the m = 1 normalized state along some axis \hat{n}_s . Taking $\hat{n}_s^2 = 1$, the eigenvalue equation $(\hat{n}_s \cdot \vec{S})_{ij} \Phi_{s,j} = \Phi_{s,i}$ becomes

$$\hat{n}_s \times \vec{\Phi}_s = i \vec{\Phi}_s. \tag{23}$$

Choosing $\hat{n}_s = (0, \cos\theta, (-s)\sin\theta)$ in the x = 0 plane, for example, one finds $\vec{\Phi}_s = (1, (is)\sin\theta, i\cos\theta)/\sqrt{2}$, which yields precisely the matrix in Eq. (20). The parameter θ is thus nothing but half of the angle between the two independent axes \hat{n}_+ and \hat{n}_- . The average magnetization in the ordered state is $\hat{n}_+ + \hat{n}_-$, and therefore the parameter θ directly determines its magnitude, $2|\cos \theta|$.

Lattice symmetry. Since the two triple-point fermions of opposite chirality are still decoupled by the order parameter even in the presence of the lattice, the directions of the two axes \hat{n}_{\pm} remain mutually independent but are no longer arbitrary. The most general quartic term in each L_s that respects

cubic symmetry, for example, is

$$L_{s4} \propto |\Delta_0|^4 \left(q_1 + q_2 |\vec{\Phi}_s \cdot \vec{\Phi}_s|^2 + q_3 \sum_{i=1}^3 |\Phi_{s,i}|^4 \right).$$
(24)

For $q_2 > -q_3/2$, $\overline{\Phi}_s$ with maximal average magnetization is still the minimum of this GL free energy, but the axis of magnetization depends on the sign of q_3 : For $q_3 > 0$, it is $\hat{n}_s =$ $(\pm 1, \pm 1, \pm 1)/\sqrt{3}$, i.e., one of the cube's diagonals, whereas for $q_3 < 0$, it is $\hat{n}_s = (0, 0, 1)$ and permutations thereof, i.e., one of the C_4 axes of symmetry [21]. Reducing the symmetry to cubic by replacing $p_i \rightarrow \sin p_i$ (i = 1, 2, 3) in Eq. (1) and then rederiving the GL free energy yields $q_3 > 0$ for $s = \pm$ [21]. The two axes $s = \pm$, besides being identical or opposite, can in this particular example also be along two different diagonals of the cube. This leads to the discrete values of θ and the concomitant average magnetization quoted in the introduction.

Final remarks. The axiplanar phase breaks time-reversal symmetry, unless $\theta = \pi/2$. However, even in this case, time reversal is broken at each valley $\pm \vec{K}$ individually but in opposite ways. Since the valleys are decoupled by the axiplanar order parameter, the quasiparticle spectrum features mini-Bogoliubov-Fermi surfaces [18], as expected from general considerations [13].

Another consequence of the decoupling of the valleys is that the partition function at each valley is analogous to the one for frustrated magnets, and the finite-temperature phase transition is most likely weakly first order [24]. One also finds that the weak-coupling relations between quartic coefficients, namely $b_3 = -2b_1$ and $b_2 = b_4 = -b_5$, remain preserved under the renormalization group flow to one-loop order [25,26]. We expect these relations to persist to higher loops as well, as mandated by the enlarged symmetry that protects them.

Acknowledgments. The authors are grateful to Igor Boettcher and Julia Link for many useful discussions. This work was supported by the NSERC of Canada.

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