Bogoliubov Fermi Surfaces in Superconductors with Broken Time-Reversal Symmetry

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It is commonly believed that, in the absence of disorder or an external magnetic field, there are three possible types of superconducting excitation gaps: The gap is nodeless, it has point nodes, or it has line nodes. Here, we show that, for an even-parity nodal superconducting state which spontaneously breaks time-reversal symmetry, the low-energy excitation spectrum generally does not belong to any of these categories; instead, it has extended Bogoliubov Fermi surfaces. These Fermi surfaces can be visualized as two-dimensional surfaces generated by “inflating” point or line nodes into spheroids or tori, respectively. These inflated nodes are topologically protected from being gapped by a $Z_2$ invariant, which we give in terms of a Pfaffian. We also show that superconducting states possessing these Fermi surfaces can be energetically stable. A crucial ingredient in our theory is that more than one band is involved in the pairing; since all candidate materials for even-parity superconductivity with broken time-reversal symmetry are multiband systems, we expect these $Z_2$-protected Fermi surfaces to be ubiquitous.

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Introduction.—The theory of superconductivity is conventionally formulated in terms of the pairing of spin-1/2 fermions [1,2]. The complications introduced by additional electronic degrees of freedom, e.g., orbitals, are not usually thought to qualitatively alter the physics. This picture has recently been challenged for a number of materials. For iron-based superconductors, the role of interorbital pairing is attracting increased attention [3–6]. Another example is the nematic superconductivity of Cu$_3$Bi$_2$Se$_3$ [7], where the odd parity of the gap is encoded in the orbital degrees of freedom. Furthermore, theories of pairing in YPtBi and UPt$_3$ based on $j = 3/2$ and $j = 5/2$ fermions, respectively, have greatly enriched the allowed superconducting states [8,9].

In this Letter, we show that the presence of multiple bands qualitatively changes the nodal structure of a time-reversal-symmetry-breaking (TRSB) superconductor. Specifically, the expected line or point nodes of an even-parity superconducting gap [1,2] are replaced by two-dimensional Fermi surfaces of Bogoliubov quasiparticles, which are topologically protected by a $Z_2$ invariant. We further interpret these Fermi surfaces in terms of a pseudomagnetic field arising from interband Cooper pairs, here referred to as “interband pairing.”

Our conclusions are relevant for a wide range of candidate TRSB superconductors, such as UPt$_3$ [9–12], Th-doped UBe$_{13}$ [13,14], PrOs$_4$Sb$_{12}$ [15], Sr$_2$RuO$_4$ [16,17], URu$_2$Si$_2$ [18,19], SrPtAs [20], and Bi/Ni bilayers [21]. Remarkably, signatures of these Fermi surfaces may have already been observed in Th-doped UBe$_{13}$ [14] (and possibly in UPt$_3$ [11]), where there is evidence for a nonzero density of states at zero temperature, which appears not to be due to impurities. In addition to these known superconductors, theory has predicted TRSB superconductivity in graphene [22,23], the half-Heusler compound YPtBi [8], water-intercalated sodium cobaltate Na$_x$CoO$_2$·yH$_2$O [24,25], Cu-doped TiSe$_2$ [26], and monolayer transition metal dichalcogenides [27]. A common feature of all these materials is that the electronic structure involves multiple electronic degrees of freedom at each momentum. These four degrees of freedom can arise from either the combination of spin 1/2 and two orbitals of equal parity or from fermions with effective angular momentum $j = 3/2$. We work with a $j = 3/2$ generalized Luttinger-Kohn Hamiltonian [28] in order to make our arguments most transparent. Although these two descriptions have different symmetry properties, we show in Supplemental Material [29] that they can be unitarily transformed into each other and that our model represents a generic two-band theory including all symmetry-allowed crystal-field and spin-orbit-coupling terms. The general form of the normal-state Hamiltonian is

$$H_N = c_0 I_4 + c_{xy} J_x J_y + c_{x^2-y^2} J_x J_y + \frac{c_{xy}}{\sqrt{3}} J_x J_y + \frac{c_{x^2-y^2}}{\sqrt{3}} J_x J_y$$

where $I_4$ is the 4 × 4 unit matrix and the $J_i$ are spin-3/2 matrices given in Supplemental Material [29]. The coefficients $c_j = c_j(k)$ of the matrices in Eq. (1) are real, satisfy

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$c_i(\mathbf{k}) = c_i(-\mathbf{k})$, and transform in the same way as the corresponding matrix under spatial symmetries. $H_N$ has twofold degenerate eigenvalues $\epsilon_{N} = c_0 \pm (c_{x}^2 + c_{y}^2 + c_{z}^2)^{1/2}$. For definiteness, we discuss the case of only one of the two bands crossing the chemical potential so that there is only one normal-state Fermi surface; if there are two, identical arguments pertain to both. While our conclusions are general, numerical results are given for the spherically symmetric Hamiltonian $H_N = \alpha k^2 + \beta (k \cdot J)^2 - \mu$ [28], where $\alpha$ and $\beta$ are constants ($\beta$ is the spin-orbit coupling) and $\mu$ is the chemical potential, which leads to $c_0 = (\alpha + 5\beta/4)k^2 - \mu$, $c_{x}^2 = \beta(k_x^2 - k_y^2)/2$, $c_{y}^2 = \beta(k_z^2 - k_x^2)/2$, $c_{z}^2 = \sqrt{3}\beta k_y k_z$, $c_{x,z} = \sqrt{3}\beta k_x k_z$, and $c_{x,y} = \sqrt{3}\beta k_x k_y$.

The superconducting state is taken to have even parity. Fermionic antisymmetry permits six possible gap matrices $\eta$ in the spin-3/2 space: $\eta = U_T$, $\eta_{xy} = (J_zJ_z - J_xJ_x)/\sqrt{3}$, $\eta_{y} = (J_zJ_z + J_xJ_x)/\sqrt{3}$, $\eta_{xz} = (J_zJ_x + J_xJ_z)/U_T/\sqrt{3}$, $\eta_{xz} = (\sqrt{3}J_zJ_x + \sqrt{3}J_xJ_z)/U_T/\sqrt{3}$, and $\eta_{x, y} = (J_x^2 - J_y^2)/U_T/\sqrt{3}$, and

$$U_T = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

is the unitary part of the time-reversal operator $T = U_T K$, with $K$ denoting complex conjugation. The $\eta_1$ gap is a spin-singlet state and represents pure intraband pairing. The other gaps, however, describe spin-quintet ($J = 2$) pairs and involve both intra- and interband pairing [8]. Since we consider zero-momentum Cooper pairs, this implies that quintet pairing involves states away from the Fermi energy. A general superconducting state is a linear combination of these gap matrices with symmetry-compliant $\mathbf{k}$-dependent coefficients and is described by the Bogoliubov–de Gennes Hamiltonian

$$H(\mathbf{k}) = \begin{pmatrix} H_N(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^\dagger(\mathbf{k}) & -H_N^*(\mathbf{-k}) \end{pmatrix}. \tag{3}$$

While our results apply to all TRSB even-parity superconducting states, for concreteness we consider the gap function

$$\Delta(\mathbf{k}) = \Delta_1 \psi(\mathbf{k}) \eta_1 + \Delta_0 (\eta_{xz} + i\eta_{yz}), \tag{4}$$

where $\Delta_1$ and $\Delta_0$ are real constants. Although the latter term describes purely on-site pairing, the gap matrix $\eta_{xz} + i\eta_{yz}$ transforms under rotations as the spherical harmonic $Y_{2,1}(\hat{\mathbf{k}})$; i.e., it is chiral. It generically accompanies a spin-singlet term with a form factor $\psi(\mathbf{k})$ of the same symmetry. Being chiral, this pairing state, which we call the $k_z(k_x + ik_y)$ state, breaks time-reversal symmetry. It has the same symmetry as proposed for URu$_2$Si$_2$ [18], YPtBi [8], and UPt$_3$ [11]. For pure singlet pairing (i.e., $\Delta_0 = 0$), the gap has line nodes in the $k_z = 0$ plane and point nodes on the $k_x$ axis ($k_x = k_y = 0$). Mixing in a quintet component has a dramatic effect on the excitation spectrum: The expected point and line nodes are replaced by Fermi surfaces. In Fig. 1, we plot these Fermi surfaces for the $k_z(k_x + ik_y)$ state. We find them to be a generic feature of all the TRSB even-parity states classified in Ref. [2]. As we will see below, these Fermi surfaces bear some resemblance to those found in the presence of an exchange field [32], although they have a completely different origin.

**Existence of Fermi surfaces and $Z_2$ invariant.**—We now show that Bogoliubov Fermi surfaces are a generic feature of the Hamiltonian in Eq. (3) and construct their topological invariant. The first step is to show that $H(\mathbf{k})$ can be unitarily transformed into an antisymmetric matrix; i.e., there exists a unitary $\Omega$ such that $\tilde{H}^\dagger = -H(\mathbf{k})$ for $H(\mathbf{k}) \equiv \Omega H(\mathbf{k})\Omega^\dagger$. The main ideas of the proof are explained in the following; details and a representative $\Omega$ are given in Supplemental Material [29]. The Hamiltonian $H(\mathbf{k})$ possesses charge-conjugation symmetry $C$ and parity symmetry $P$. $C$ acts as $U_C H^T(-\mathbf{k}) U_C = -H(\mathbf{k})$ with $U_C = \tilde{\tau}_x \otimes 1_4$, where $\tilde{\tau}_x$ are the Pauli matrices in particle-hole space, while $P$ acts as $U_P H(-\mathbf{k}) U_P = H(\mathbf{k})$ with $U_P = \tilde{\tau}_0 \otimes 1_4$. Hence, $CP$ symmetry reads

![FIG. 1. Bogoliubov Fermi surfaces of the superconducting $k_z(k_x + ik_y)$ state, shown here for the case where only one band has a Fermi surface. The normal-state Fermi surface, shown as the semitransparent sphere, is gapped out by the superconductivity. The point and line nodes of the single-band theory (red dots and line, respectively), however, are “inflated” into spheroidal and toroidal $Z_2$-protected Fermi surfaces (orange surfaces).](127001-2)
with $U_{CP} = U_C U_P = \hat{1}_d \otimes 1_d$. This implies that $(CP)^2 = U_{CP} U_{CP}^* = +1$ and thus $U_{CP} = U_{CP}^T$. Any symmetric matrix can be diagonalized by a unitary congruence; i.e., there exist a unitary $Q$ and a diagonal $\Lambda$ such that $U_{CP} = Q \Lambda Q^T$ with the transposed matrix $Q^T$. Insertion into Eq. (5) gives $Q \Lambda Q^T H^T(k) Q \Lambda^2 Q^T = -H(k)$. Since $\Lambda$ is diagonal, we can define a square root $\sqrt{\Lambda}$. The sign of the root for each diagonal component of $\Lambda$ can be chosen arbitrarily and is then held fixed. This allows us to split the unitary matrices in the CP symmetry relation, which gives $[\sqrt{\Lambda} Q^T H(k) Q \sqrt{\Lambda}] = -[\sqrt{\Lambda} Q^T H(k) Q \sqrt{\Lambda}]$. This can be written as $[\Omega H(k) \Omega^T] = -[\Omega H(k) \Omega^T]$ with $\Omega \equiv \sqrt{\Lambda} Q^T$. Hence, $\tilde{H}(k) = \Omega H(k) \Omega^T$ is antisymmetric, as we wanted to show. We can then define the Pfaffian $P(k) \equiv Pf \tilde{H}(k)$. Since det $H(k) = det \tilde{H}(k) = P^2(k)$, the zeros of $P(k)$ give the zero-energy states of $H(k)$.

It has recently been shown that Fermi surfaces of Hamiltonians with $CP$ symmetry squaring to $+1$ can possess a nontrivial $Z_2$ charge, making them topologically stable against $CP$-preserving perturbations [33,34]. We now express the invariant in terms of the Pfaffian $P(k)$. The Pfaffian is real, since it is a polynomial of even degree of the components of the matrix $\tilde{H}(k)$, which is Hermitian and antisymmetric and thus purely imaginary. Regions in momentum space in which $P(k)$ has opposite signs are thus necessarily separated by a two-dimensional (Fermi) surface on which $P(k) = 0$. The existence of such Fermi surfaces is thus guaranteed if $P(k)$ changes sign, and hence we can identify $(-1)^I = \text{sgn}[P(k_\downarrow) P(k_\uparrow)]$ as the $Z_2$ invariant, where $k_\downarrow$ ($k_\uparrow$) refers to momenta inside (outside) of the Fermi surface.

Under what conditions do protected Fermi surfaces exist? In the normal state, the Pfaffian $P(k) = c^+ c^- c^+ c^-$ is always non-negative and has second-order zeros on the Fermi surface. Hence, the normal-state Fermi surface is not protected by the $Z_2$ charge. Furthermore, for time-reversal-symmetric superconductivity, $P(k)$ can also be chosen non-negative for all $k$ so that there is no nontrivial $Z_2$ invariant [33,34]. Our proof in Supplemental Material [29] simplifies the earlier proof by Kobayashi et al. [33]. For TRSB pairing, the second-order zeros of $P(k)$ are generically (i.e., in the absence of additional symmetries or fine-tuning) lifted, leading to $P(k) > 0$ in a neighborhood of the former zero, or split into first-order zeros, in which case there is a region with $P(k) < 0$. Such a region is bounded by a two-dimensional Fermi surface; as this shrinks to a point or line node in the limit of infinitesimal pairing, we call it an inflated node.

The existence of protected Bogoliubov Fermi surfaces is now illustrated for the $k_z(k_x + ik_y)$ state of Eq. (4). We restrict ourselves to pure quintet pairing, but our results hold for any gap with a nonzero quintet component; see Supplemental Material [29]. The Pfaffian is

$$P(k) = c^+ c^2 + 4\Delta_0^2 (e_+ e_- + c^z_x + c^z_y),$$

which is negative for all $k$ such that $s_- < e_+ e_- < s_+$, where $s_{\pm} = -2\Delta_0^2 \pm 2\Delta_0(\Delta_0^2 - c^2_x - c^2_y)^{1/2}$. $s_+$ and $s_-$ exist and are distinct if the radicand is positive. In the plane $k_z = 0$ and along the line $k_x = k_y = 0$, this holds for any $\Delta_0 > 0$, since symmetry dictates that $c^2_x + c^2_y$ vanishes there. We then find $s_- = -4\Delta_0^2 < 0$ and $s_+ = 0$; i.e., $s_+$ vanishes on the normal-state Fermi surface. Since $e_+ e_-$ changes sign across the normal-state Fermi surface, there is always a region with $s_- < e_+ e_- < s_+$ in this plane and along this line and, due to the continuity of the $c_i(k)$, also in their neighborhood. The resulting region with $P(k) < 0$ is bounded by a Fermi surface, as illustrated in Fig. 1.

**Stability of Fermi surfaces.**—Even-parity TRSB superconductors are usually argued to be energetically favored over time-reversal-symmetric states, because they maximize the gap in momentum space [2]. The existence of extended Bogoliubov Fermi surfaces invalidates this argument. To show that TRSB states can nevertheless be stable, we consider a model with an on-site pairing interaction of strength $V$ in both the quintet $\eta_z$ and $\eta_x$ channels. In this case, the TRSB state $\Delta_0(\eta_{z\uparrow} + i\eta_{x\downarrow})$ [i.e., the $k_z(k_x + ik_y)$ state introduced above] and the time-reversal-symmetric state $\sqrt{2}\Delta_0 \eta_{x\uparrow}$ have the same critical temperature $T_c$. To decide which is energetically stable at temperatures $T$ near $T_c$, we perform a standard expansion of the free energy $F$ in the gap $\Delta$ [35,36]:

$$F = \frac{1}{2V} \text{Tr} \Delta^\dagger \Delta + \frac{k_B T}{2} \sum_{k\omega_n} \sum_{i=1}^{\infty} \frac{1}{i} \text{Tr}[\Delta \tilde{G}(k, \omega_n) \Delta^\dagger G(k, \omega_n)]^i,$$  

where $G(k, \omega_n)$ and $\tilde{G}(k, \omega_n)$ are the normal-state electron and hole Matsubara Green’s functions, respectively. For vanishing spin-orbit coupling $\beta$, introduced below Eq. (1), the normal bands are fourfold degenerate. As was previously shown in the context of $j = 3/2$ pairing in cold atoms [35], the TRSB state is unstable towards the time-reversal-symmetric state in this limit, as it leaves two of these bands ungapped. Nonzero spin-orbit coupling partially lifts this degeneracy and allows the TRSB state to open a gap on all Fermi surfaces, reducing its energy. An analysis of the fourth-order term in Eq. (7) predicts that the TRSB $\eta_{z\uparrow} + i\eta_{x\downarrow}$ state is energetically favored for $|\beta| k_F^2 / k_B T_c \gtrsim 9.324$. Details are given in Supplemental Material [29]. Hence, the presence of the Bogoliubov Fermi surfaces does not necessarily compromise the stability of TRSB states.

**Pairing-induced pseudomagnetic field.**—To gain additional insight into the Bogoliubov Fermi surfaces, it is useful to rewrite the Hamiltonian in a basis for which the normal-state Hamiltonian is diagonal. We denote the eigenvectors of $H_N$ to the twofold degenerate eigenvalues...
conducting state is described by the Hamiltonian
\[ H = \begin{pmatrix}
    H_{N,+} & \Delta_{+} & 0 & \Delta_{+} \\
    \Delta_{+}^\dagger & -H_{N,+} & -\Delta_{+}^\dagger & 0 \\
    0 & -\Delta_{+}^\dagger & H_{N,-} & \Delta_{-} \\
    \Delta_{-}^\dagger & 0 & \Delta_{-}^\dagger & -H_{N,-}
\end{pmatrix}. \] (8)

Here, \( H_{N,+} = \epsilon_+ \hat{\sigma}_0 \) and \( \Delta_{\pm} \) are antisymmetric matrices with \( \Delta_{\pm} = \psi_{\pm}(k)i\hat{\sigma}_y \), where \( \hat{\sigma}_y \) are the Pauli matrices in pseudospin space. \( \Delta_{\pm} \) is the interband pairing potential, the explicit form of which depends on the choice of bases in the two-dimensional eigenspaces of \( \epsilon_{\pm} \) and is hence not illuminating. The intraband gap functions \( \psi_{\pm}(k) \) are obtained by transforming Eq. (4) into the pseudospin basis and are given by
\[ \psi_{\pm}(k) = \Delta_1 \psi(k) \pm 2\Delta_0 \frac{c_{\pm 2}(k) + ic_{\pm 2}(k)}{\epsilon_+(k) - \epsilon_-(k)}. \] (9)

In the absence of \( \Delta_{\pm} \), \( \tilde{H} \) would describe two decoupled pseudospin-1/2 singlet superconductors with, at most, line or point nodes. Hence, the interband pairing is responsible for the appearance of the extended Fermi surfaces. This can be shown by treating the off-diagonal interband blocks of Eq. (8) as a perturbation to the intraband Hamiltonians: Focusing on the + states (analogous results can be found for the − states if they have a normal-state Fermi surface), the second-order corrections due to the interband pairing appear only in the normal-state components, which become
\[ H'_{N,+} = [\epsilon_+ + \gamma(k)]\hat{\sigma}_0 + h(k) \cdot \hat{\sigma}, \] (10)

where
\[ \gamma(k) = \frac{2|\Delta_0|^2}{(\epsilon_+ - \epsilon_-)^2} [(\epsilon_+ - \epsilon_-)^2 - 2c_{\pm 2}^2 - 2c_{\pm 2}^2], \] (11)
\[ |h(k)| \leq \frac{4|\Delta_0|^2}{(\epsilon_+ - \epsilon_-)^2} \sqrt{c_{\pm 2}^2c_{\pm 2}^2 + c_{\pm 2}^2c_{\pm 2}^2 + c_{\pm 2}^2c_{\pm 2}^2}. \] (12)

The direction of \( h(k) \) is basis dependent and is thus not physically meaningful. The correction \( \gamma(k) \) is always present and results in a small modification of the normal-state dispersion \( \epsilon_+ \), whereas the second term \( h(k) \cdot \hat{\sigma} \) appears only for TRSB gaps. This reveals that in the TRSB state the interband pairing manifests itself as a pseudomagnetic field in the normal-state Hamiltonian.

The origin of the extended Fermi surfaces becomes clear from the excitation spectrum of the low-energy pairing Hamiltonian,
\[ E_{k,\pm} = \nu|h(k)| \pm \sqrt{[\epsilon_+(k) + \gamma(k)]^2 + |\psi_+(k)|^2}, \] (13)

where \( \nu = \pm 1 \). The pseudomagnetic field \( |h(k)| \) evidently splits the dispersion. The square root in Eq. (13) goes to zero at the intersection of the nodes of the intraband gap \( \psi_+(k) \) with the surface \( \epsilon_+ + \gamma(k) = 0 \), and the pseudomagnetic field gives rise to the Bogoliubov Fermi surfaces by shifting the nodes to finite energies \( \pm |h(k)| \). The generation of \( h(k) \) by the superconducting state itself exhibits the intrinsic nature of the Bogoliubov Fermi surfaces. This distinguishes our results from the “breached-pairing” state of population-imbalanced cold atoms or exchange-split superconductors, where the required breaking of time-reversal symmetry is extrinsic to the pairing [32,37].

The low-energy effective model also allows us to estimate the dimensions of the Fermi surfaces. Perpendicular to the normal-state Fermi surface, the Bogoliubov Fermi surfaces have a width \( \delta k_\perp/k_F \sim \Delta_0^2/\mu[\epsilon_+ - \epsilon_-] \), where \( k_F \) is the normal-state Fermi momentum. Their width in the direction parallel to the normal-state Fermi surface is \( \delta k_\parallel/k_F \sim \Delta_0^2/\mu[\epsilon_+ - \epsilon_-] \). Since we typically expect \( \Delta_0 \ll \mu \), we find that \( \delta k_\perp \ll \delta k_\parallel \), which implies oblate spheroidal Fermi surfaces near the original point nodes and flattened toroidal Fermi surfaces near the original line nodes, as seen in Fig. 1.

Pseudomagnetic fields appear in any TRSB phase of our model with interband (spin-quintet) pairs. Our analysis generalizes to other systems with multiband pairing: We expect nonvanishing contributions to the pseudomagnetic field from all the interband potentials, implying that Bogoliubov Fermi surfaces are a generic feature of such systems. Equation (12) shows that these Fermi surfaces will be largest in strong-coupling materials in which the different bands lie close to each other. These conditions are likely satisfied in heavy-fermion superconductors such as UPt_3, Th-doped UBe_13, PrOs_4Sb_12, and URu_2Si_2, which makes them ideal systems in which to search for Bogoliubov Fermi surfaces. Indeed, as mentioned in the introduction, Th-doped UBe_13 shows a large (and so far unexplained) residual density of states [14] which is consistent with our theory.

Conclusions.—We have established that broken-time-reversal even-parity superconductors generically support two-dimensional Fermi surfaces. The states at these Fermi surfaces are charge-neutral Bogoliubov quasiparticles. The Fermi surfaces are protected by a topological \( Z_2 \) invariant, which can be written in terms of a Pfaffian, and thus cannot be removed by any perturbation that is CP invariant. They are also energetically stable for plausible parameters; i.e., the corresponding state has a lower free energy than an associated time-reversal-symmetric state. The \( Z_2 \)-protected Fermi surfaces appear in multiband systems, where interband pairing produces an effective pseudomagnetic field, which inflates the expected point or line nodes. Since all
candidate materials for TRSB even-parity superconductivity have multiple relevant bands, we expect that these $\mathbb{Z}_2$-protected Fermi surfaces are ubiquitous. The existence of Bogoliubov Fermi surfaces in the superconducting state should lead to characteristic experimental consequences: A nonzero density of states at the Fermi energy, visible, for example, in tunneling and photoemission experiments, would coexist with ideal conductivity and flux expulsion. The low-temperature thermodynamic response would show a linear temperature dependence of the specific heat, and heat conduction should also be unconventional [32]. Such anomalies may have already been observed in heavy-fermion superconductors [11,14]. Our work raises many open questions; e.g., is a superconductor with Bogoliubov Fermi surfaces a Fermi liquid when residual interactions are taken into account? The search for and study of such systems thus constitutes a very promising task for future research.

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