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Multiply quantized vortices in fermionic superfluids: angular momentum, unpaired fermions, and spectral asymmetry

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We compute the orbital angular momentum L_z of an s -wave paired superfluid in the presence of an axisymmetric multiply quantized vortex. For vortices with winding number $|k| > 1$, we find that in the weak-pairing BCS regime L_z is significantly reduced from its value $\hbar N k/2$ in the BEC regime, where N is the total number of fermions. This deviation results from the presence of unpaired fermions in the BCS ground state, which arise as a consequence of spectral flow along the vortex sub-gap states. We support our results analytically and numerically by solving the Bogoliubov-deGennes equations within the weak-pairing BCS regime.

Quantized vortices are a hallmark of superfluids (SFs) and superconductors. These topological defects form in response to external rotation or magnetic field and play a key role in understanding a broad spectrum of phenomena, such as the Berezinskii-Kosterlitz-Thouless transition in two-dimensional (2D) SFs [1, 2], superconductor/insulator transitions [3–5], turbulence [6], and dissipation [7, 8]. In fermionic s -wave paired states, the structure of the ground state and low lying excitations of an axisymmetric singly quantized vortex has been established through analytical and numerical studies in both the strong-pairing regime (where the SF phase is understood as a Bose-Einstein condensate (BEC) of bosonic molecules) and in the weak-pairing Bardeen Cooper Schrieffer (BCS) regime. In the BEC regime, the microscopic Gross-Pitaevskii equation provides a reliable framework [9, 10], while in the BCS regime the (self-consistent) Bogoliubov-deGennes (BdG) theory is key in identifying the structure of the ground state [11, 12] and the spectrum of sub-gap fermionic excitations [13].

Multiply quantized vortices (MQVs) have however not received much attention. Generically in a homogeneous bulk system, the logarithmic repulsion between vortices, which scales as the square of the vortex winding number k , energetically favors an instability of a multiply quantized vortex into separated elementary unit vortices [14]. However, MQVs are of interest since under certain circumstances, the interaction between vortices is not purely repulsive and can support multi-vortex bound states, at least as metastable defects. This can happen, for instance, in type-II mesoscopic superconductors, where MQVs have been predicted [15] and experimentally observed [16–19]. In addition, it has been argued that MQVs are expected to be energetically stable in multicomponent superconductors [20, 21] and in chiral p -wave superconductors [22, 23]. In fermionic SFs, a doubly quantized vortex was predicted [24] and observed in $^3\text{He-A}$ [25]. It has further been argued that fast rotating Fermi gases trapped in an anharmonic potential will support an MQV state [26–28]. Similar vortex states

have been created in rotating BEC experiments [29–32].

Surprisingly, as we demonstrate in this Letter, there is a fundamental difference between a singly quantized vortex ($|k| = 1$) and an MQV ($|k| > 1$) in a weakly-paired fermionic s -wave SF. This difference is manifested most clearly in the orbital angular momentum (OAM) L_z , as illustrated in Fig. 1. At zero temperature in the BEC regime, a microscopic Gross-Pitaevskii calculation predicts $L_z = \hbar N k/2$, where N is the total number of fermions. Intuitively, this corresponds to a simple picture where an MQV induces a quantized OAM k per molecule. For an elementary vortex, this result also holds in the BCS regime, as confirmed within the self-consistent BdG framework [11, 12]. As we show in this Letter, for vortices with $|k| > 1$ however, the BCS ground state contains unpaired fermions which carry OAM opposite to that carried by the Cooper pairs, thereby significantly reducing the total L_z from its BEC value by an amount

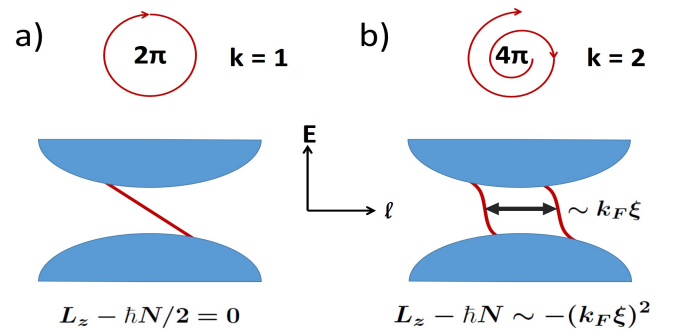


FIG. 1: Summary of main result: a) For an elementary vortex ($k = 1$), the fermionic spectrum has a vanishing spectral asymmetry and thus all fermions are paired in the ground state, resulting in $L_z = \hbar N/2$ in the BCS regime. b) In stark contrast, for an MQV ($k = 2$ pictured here as an example) mid-gap states confined to the vortex core induce a non-trivial spectral asymmetry, which leads to unpaired fermions in the ground state. These reduce L_z from its naïve value $\hbar N$ by an amount that scales quadratically with the splitting between the red branches.

$\sim (k_F \xi)^2$, where k_F is the Fermi momentum and ξ the coherence length. While the proportionality constant is non-universal and depends on the vortex core structure, the scaling with k_F and ξ is robust, being independent of any boundary effects.

To derive our main result we consider a 2D [33] s -wave paired SF in the weak-pairing BCS regime at zero temperature within the BdG framework. The mean-field Hamiltonian in the presence of an axisymmetric MQV with winding number k is $\hat{H} = \int d^2r \Psi^\dagger (-\nabla^2/2 + V(r) - \mu) \tau_3 \Psi + \int d^2r \Psi^\dagger \Delta(r) (e^{ik\varphi} \tau_+ + e^{-ik\varphi} \tau_-) \Psi$, where the Nambu spinor $\Psi = (\psi_\uparrow, \psi_\downarrow)^T$ satisfies $\{\Psi_i(\mathbf{r}), \Psi_j^\dagger(\mathbf{r}')\} = \delta_{ij} \delta(\mathbf{r} - \mathbf{r}')$. Here, τ_i are Pauli matrices, $\tau_\pm = (\tau_1 \pm i\tau_2)/2$, \hbar and the elementary fermion mass are set to unity, and μ is the chemical potential. In principle, $\Delta(r)$ should be determined self-consistently but since our results depend only weakly on its form, we use a fixed pairing term that for our numerical analysis is taken to be $\Delta(r) = \Delta_0 \tanh(r/\xi)$, where $\xi = k_F/\Delta_0$ and Δ_0 is the BCS gap.

Due to the pairing term, neither the total particle number $\hat{N} = \int d^2r \Psi^\dagger \tau_3 \Psi$ nor the OAM $\hat{L}_z = \int d^2r \Psi^\dagger (-i\partial_\varphi) \Psi$ commutes with \hat{H} , and so neither are separately conserved. Instead, as pointed out in [34, 35], the generalized OAM operator $\hat{\mathcal{L}} = \hat{L}_z - k\hat{N}/2$ generates a symmetry and thus, the BdG ground state and all quasi-particle excitations carry a sharp \mathcal{L} quantum number. More generally, in a chiral SF with pairing symmetry $\sim (p_x + ip_y)^\nu$ and with an MQV, the conserved operator is $\hat{L}_z - (k + \nu)\hat{N}/2$ (see [36]). While the OAM of vortex-free chiral paired SFs ($k = 0$) was analysed in [37–39], here we focus on s -wave SFs ($\nu = 0$) with MQVs, noting that our results readily generalize to chiral states with MQVs.

Physically, $\hat{\mathcal{L}}$ measures the deviation of OAM in the BCS ground state from its expectation value $L_z^{\text{BEC}} = kN/2$ in the BEC regime (with $N = \langle \hat{N} \rangle$). The suppression of L_z in the BCS regime will hence be reflected in the eigenvalue \mathcal{L} of $\hat{\mathcal{L}}$, evaluated in the ground state of the BdG Hamiltonian. We consider a disc geometry with Dirichlet boundary conditions, i.e., $V(r < R) = 0$ and $V(r > R) = \infty$. Expanding the fermionic operators in a single particle basis as $\psi_\sigma(\mathbf{r}) = \sum_{n,l} a_{nl\sigma} \Phi_{nl}(\mathbf{r})$ where Φ_{nl} satisfies $[-\nabla^2/2 + V(r) - \mu] \Phi_{nl}(\mathbf{r}) = \epsilon_{nl} \Phi_{nl}(\mathbf{r})$, the Hamiltonian becomes

$$\hat{H} = \sum_{\substack{l \\ n, n'}} \begin{pmatrix} a_{n,l+k\uparrow}^\dagger \\ a_{n,-l\downarrow} \end{pmatrix}^T \begin{pmatrix} \epsilon_{n,l+k} \delta_{n,n'} & \Delta_{n,n'}^{(l)} \\ \Delta_{n,n'}^{(l)*} & -\epsilon_{n,-l} \delta_{n,n'} \end{pmatrix} \begin{pmatrix} a_{n',l+k\uparrow} \\ a_{n',-l\downarrow}^\dagger \end{pmatrix} \quad (1)$$

with $\Delta_{n,n'}^{(l)} = \int d^2r \Phi_{n,l+k}^* \Delta(r) e^{ik\varphi} \Phi_{n',-l}^*$ and where n, l are the radial and angular momentum quantum numbers respectively. Denoting the single-particle Hamiltonian matrix as $H^{(l)}$, particle-hole (PH) symmetry connects the different l -sectors through $H^{(l)*} = -CH^{(-l-k)}C^{-1}$ and

the spectrum is hence PH symmetric about $l = -k/2$.

The ground state of the BdG Hamiltonian is constructed using a generalized Bogoliubov transformation [40, 41] whose main steps we present here (see [36] for details). First, we regularize the BdG Hamiltonian $H^{(l)}$ by introducing a cutoff $M \gg 1$ on n, n' . Generically, $H^{(l)}$ will have a different number of positive and negative eigenvalues, $M_+^{(l)}$ and $M_-^{(l)}$ respectively. The (unitary) Bogoliubov transformation is then written as

$$\begin{pmatrix} b_m^{(l)} \\ d_{\bar{m}}^{(l)\dagger} \end{pmatrix} = \sum_{n=1}^M \begin{pmatrix} S_{1,\bar{m}n}^{(l)} & S_{2,\bar{m}n}^{(l)} \\ S_{3,\bar{m}n}^{(l)} & S_{4,\bar{m}n}^{(l)} \end{pmatrix} \begin{pmatrix} a_{n,l+k\uparrow} \\ a_{n,-l\downarrow}^\dagger \end{pmatrix}, \quad (2)$$

where $m = 1, \dots, M_+^{(l)}$, $\bar{m} = 1, \dots, M_-^{(l)}$, and $M_+^{(l)} + M_-^{(l)} = 2M$. The Bogoliubov operator $b_m^{(l)}$ annihilates a quasi-particle with positive energy $E_m^{(l)}$, \mathcal{L} -charge [42] $l + k/2$, and spin \uparrow . Alternatively, by PH symmetry we can interpret it as the creation operator for a spin \downarrow state with negative energy $-E_m^{(l)}$ and \mathcal{L} -charge $-l - k/2$. In addition, we introduce the operator $d_{\bar{m}}^{(l)}$ that creates a spin \uparrow state with negative energy $E_{M_+^{(l)} + \bar{m}}^{(l)}$ and \mathcal{L} -charge $l + k/2$.

In terms of these operators, the ground state $|BCS\rangle \sim \otimes_l |BCS\rangle_l$ is defined as the vacuum for all positive energy quasi-particles and thus satisfies $b_m^{(l)} |BCS\rangle = 0$ and $d_{\bar{m}}^{(l)} |BCS\rangle = 0$. For systems with $M_+^{(l)} = M_-^{(l)}$, the ground state $|BCS\rangle$ closely resembles a Fermi sea with all negative energy states occupied

$$|BCS\rangle \sim \otimes_l \prod_{m=1}^M b_m^{(l)} \prod_{\bar{m}=1}^M d_{\bar{m}}^{(l)} |0\rangle, \quad (3)$$

where $|0\rangle$ is the Fock vacuum for $a_{n,l\sigma}$. This ground state can be understood in terms of Cooper pairs, where spin \uparrow quasi-particles with \mathcal{L} -charge $v = l + k/2$ (created by $d^{(l)}$) are paired with quasi-particles of the opposite spin \downarrow and with the opposite \mathcal{L} -charge $-v$ (created by $b^{(l)}$). Re-expressing the quasi-particle operators in terms of elementary fermions, we find a familiar exponential form, $|BCS\rangle_l = \exp\left(a_{n,l+k\uparrow}^\dagger K_{n,n'}^{(l)} a_{n',-l\downarrow}^\dagger\right) |0\rangle$, where $K^{(l)}$ is an $M \times M$ matrix derived in [36] and the sum over n, n' is implicit. Since $b^{(l)}$ and $d^{(l)}$ carry opposite \mathcal{L} -charge, the ground state Eq. (3) has a vanishing \mathcal{L} eigenvalue.

When $M_+^{(l)} \neq M_-^{(l)}$ however, the ground state is no longer given by Eq. (3) since there will exist an imbalance between the number of quasi-particles with \mathcal{L} -charge $l + k/2$ and with \mathcal{L} -charge $-l - k/2$. This mismatch is quantified by the spectral asymmetry of the energy spectrum $\eta_l = \sum_m \text{sgn}(E_m^{(l)}) = M_+^{(l)} - M_-^{(l)}$, where $\{E_m^{(l)}\}_{m \in \mathbb{N}}$ are the eigenvalues of $H^{(l)}$. In order to demonstrate that the presence of a non-trivial η_l leads to unpaired fermions in the ground state, we perform a judiciously chosen unitary rotation on $a_{n,l\sigma}$ to a new basis

of fermions $\tilde{a}_{j,l\sigma}$ via a conventional (non-Bogoliubov) rotation which does not mix creation and annihilation operators (see [36]). Through a separate unitary rotation, we simultaneously transform the Bogoliubov operators $b^{(l)}, d^{(l)}$ into a new basis $\tilde{b}^{(l)}, \tilde{d}^{(l)}$. The new fermions \tilde{a} and Bogoliubov quasi-particles \tilde{b}, \tilde{d} are related through a Bogoliubov transformation which, as always, takes the schematic form $\tilde{b} = U\tilde{a} + V\tilde{a}^\dagger$, where the matrix-valued coefficients U, V satisfy $|U|^2 + |V|^2 = 1$. Following [41], we find that the preceding transformations naturally distinguish between operators for which either U vanishes exactly: $U = 0, V = 1$ (*occupied* levels), or V vanishes exactly: $V = 0, U \neq 0$ (*empty* levels), with the remaining operators, for which both $U, V \neq 0$, describing *paired* levels. In the new basis, the ground state is superficially similar to Eq. (3) since it can be expressed as

$$|BCS\rangle \sim \otimes_l \prod_m' \tilde{b}_m^{(l)} \prod_{\bar{m}}' \tilde{d}_{\bar{m}}^{(l)} |0\rangle. \quad (4)$$

Importantly however, the restricted products here run only over paired and occupied levels. Bogoliubov operators \tilde{b}, \tilde{d} for empty states, which are linear super-positions of \tilde{a} 's, annihilate the bare vacuum $|0\rangle$ and are thus disallowed in Eq. (4). Conversely, occupied states contribute to Eq. (4) but since these states create unitarily rotated fermions with certainty, $\tilde{b}, \tilde{d} \sim \tilde{a}^\dagger$, they do not participate in pairing. The expression (4) is in turn equivalent to [36]

$$|BCS\rangle_l = \left(\prod_{i=1}^{M_\uparrow^{(l)}} \tilde{a}_{i,l+k\uparrow}^\dagger \right) \left(\prod_{i=1}^{M_\downarrow^{(l)}} \tilde{a}_{i,-l\downarrow}^\dagger \right) \times \exp \left(\sum_{j>M_\uparrow^{(l)}}^M \sum_{j'>M_\downarrow^{(l)}}^M \tilde{a}_{j,l+k\uparrow}^\dagger \mathcal{K}_{j,j'}^{(l)} \tilde{a}_{j',-l\downarrow}^\dagger \right) |0\rangle, \quad (5)$$

where $M_\downarrow^{(l)}$ and $M_\uparrow^{(l)}$ are the number of occupied (and also empty) $\tilde{b}_m^{(l)}$ and $\tilde{d}_m^{(l)}$ levels respectively. In terms of these parameters, the spectral asymmetry $\eta_l = 2(M_\downarrow^{(l)} - M_\uparrow^{(l)})$, with $M_{\uparrow,\downarrow}^{(l)} = \max(0, M - M_{+,-}^{(l)})$.

The exponential part of $|BCS\rangle$ explicitly illustrates the singlet pairing while $M_\sigma^{(l)} \neq 0$ signals the presence of unpaired fermions in the ground state. The eigenvalue of $\hat{\mathcal{L}}$ can now be obtained directly from Eq. (4) by summing the individual contributions of the filled quasi-particle states and noting that $\tilde{b}^{(l)}, \tilde{d}^{(l)}$ carry the same \mathcal{L} -charges as $b^{(l)}, d^{(l)}$. While contributions from the paired levels cancel out, the occupied levels lead to

$$\mathcal{L} = -\frac{1}{2} \sum_l \left(l + \frac{k}{2} \right) \eta_l. \quad (6)$$

Alternatively, this equation can be derived directly from Eq. (5), and has previously appeared in the literature in the context of chiral SFs [37, 38], where k is

replaced by the chirality ν . Physically, Eq. (6) quantifies the contribution of unpaired fermions to the OAM.

The physics originating from unpaired fermions in the ground state of a paired state was previously identified and studied in nuclear physics [41], FFLO superfluids [43], and chiral superfluids paired in higher partial waves [37–39, 44, 45]. We now demonstrate that for a weakly-paired s -wave SF with an MQV, a nontrivial η_l and the associated unpaired fermions arise as a consequence of vortex core states.

In the BCS regime, the spectrum of the vortex core (vc) states for a singly quantized vortex $|k| = 1$ was calculated analytically by Caroli-deGennes-Matricon (CdGM) [13] who found a single branch $E_{vc}^{(l)}$ (per spin projection) that crosses the Fermi level. This branch is PH symmetric with respect to itself, $E_{vc}^{(l)} = -E_{vc}^{(-l-1)}$ and at low energies ($E_{vc} \ll \Delta_0$) behaves linearly $E_{vc}^{(l)} = -\omega_0(l + 1/2)$, where the mini-gap $\omega_0 \sim \Delta_0/(k_F\xi)$. By numerically diagonalizing $H^{(l)}$ for $k = 1$, we find that $\eta_l = 0$ for all l and hence there are no unpaired fermions in the BCS ground state of an s -wave paired SF with an elementary vortex. Eq. (6) then predicts $\mathcal{L} = 0$ and thus the ground state expectation value $L_z = N/2$, which agrees with self-consistent BdG calculations [11]. The physics here is analogous to that of weakly paired $p + ip$ SFs, where there is a single PH symmetric edge mode that carries no OAM [37, 46, 47].

For an MQV with winding number k , the CdGM method can be generalized and the vortex core spectrum analytically calculated within the BdG framework (see [36]). In agreement with an argument relating the number of vortex core branches to a topological invariant [48], we find that $|k|$ branches (per spin projection) cross the Fermi level. At low energies these branches disperse linearly, $E_j(l) = -\omega_0(l - l_j)$, where $j = 1, \dots, k$ indexes the branches and the l_j 's are the angular momenta at which the branches cross the Fermi level. This is consistent with results obtained by numerically diagonalizing the BdG Hamiltonian $H^{(l)}$ (for $k = 2$, see Fig. 2a) and with previous results on MQVs in superconductors, obtained through quasi-classical approximations [48–50] and numerical simulations [51–54].

Since in the BEC regime the spectrum is completely gapped for any k , we find $\eta_l = 0$ for all l and thus the ground state OAM is exactly $L_z = kN/2$. On the other hand, in the weakly-paired regime the energy spectrum of an MQV exhibits a nontrivial spectral asymmetry. We consider the case $k = 2$ first (Fig. 2a), where there exist two vortex core branches with linear dispersions at low energies, $E_{vc,\pm}^{(l)} \sim -\omega_0(l - l_\pm)$ with $l_+ > l_-$. Under PH symmetry, these branches are exchanged as $E_{vc,+}^{(l)} = -E_{vc,-}^{(-l-2)}$ which fixes $l_- = -(l_+ + 2)$. As shown in Fig. 2b, we find that at these crossing points η_l acquires a non-zero value: $\eta_l = -2$ for $l_- < l < -1$ and $\eta_l = +2$ for $-1 < l < l_+$, with $\eta_l = 0$ at $l = -1$. Intuitively, this

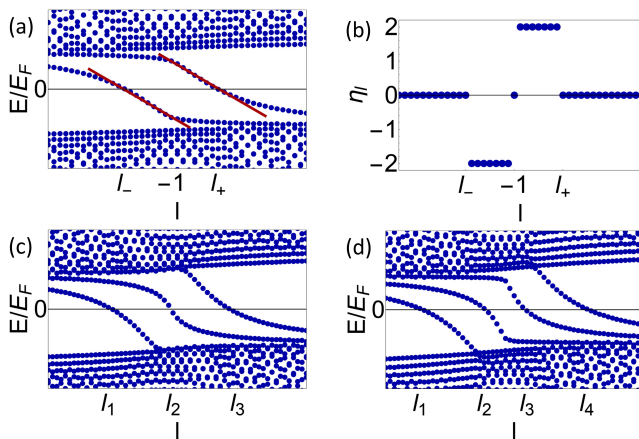


FIG. 2: BdG solution for MQVs with $\Delta_0 = 0.15E_F$, $\mu = E_F$, and $k_F R = 80$: (a) Comparison of energy spectrum for $k = 2$ with analytic approximation (in red); (b) spectral asymmetry for $k = 2$; (c) energy spectrum for $k = 3$ and (d) for $k = 4$.

can be understood as follows—at large negative l , the branches are merged into the bulk and since there are no sub-gap states, $\eta_l = 0$. On increasing l , the branches begin separating from the bulk but since both have positive energy, η_l still vanishes. At l_- however, one of the branches crosses the Fermi energy, creating a difference of precisely two between the number of negative and positive energy eigenvalues of $H^{(l)}$. At $l = -1$, η_l necessarily vanishes due to PH symmetry, which also fixes η_l for $l > -1$. In contrast with $|k| = 1$, the branches are not PH symmetric with respect to themselves, allowing the spectral asymmetry to acquire a non-zero value in the BCS regime. The fact that η_l changes from the BEC to the BCS regime can also be understood as a consequence of spectral flow along the vortex core states, since η_l (and hence \mathcal{L}) cannot change its value in any other way.

A non-zero spectral asymmetry η_l appears generally for any $|k| \geq 2$ within the BCS regime: for even k (see Fig. 2d), there are $|k|/2$ pairs of branches such that the branches within each pair are PH symmetric with each other. η_l then changes by ± 2 whenever one of these branches crosses the Fermi level; for odd k (see Fig. 2c) there are $(|k| - 1)/2$ pairs that contribute to a non-trivial η_l , since the branches within each pair go into each other under a PH transformation, while the remaining branch is PH symmetric with respect to itself and therefore does not contribute to η_l .

Having established the existence of a non-vanishing η_l , we see that there must exist unpaired fermions in the BCS ground state for $|k| \geq 2$, and as a consequence of Eq. (6), \mathcal{L} acquires a non-trivial ground state eigenvalue. For $k = 2$, this is $\mathcal{L} = -l_+^2 - l_-$, where we used PH symmetry to relate l_- to l_+ . Importantly, the analytic calculation of the vortex core states performed in [36] demonstrates that the positions of the crossing points are located at $l_{\pm} \sim k_F \xi$ with the pre-factor fixed by the form

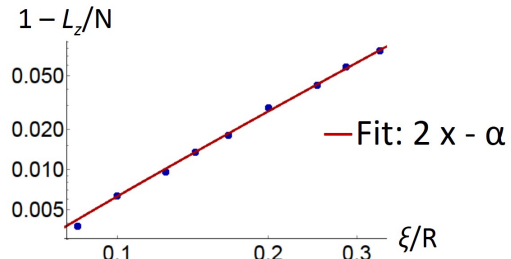


FIG. 3: The analytic prediction $L_z/N = 1 - \alpha(\xi/R)^2$ (red line) fits the numerical data (blue dots) well over a wide window within the BCS regime, $0.05 \lesssim \Delta_0/E_F \lesssim 0.25$, for an MQV with $k = 2$. The slope of the fit equals two as shown on a log-log plot.

of $\Delta(r)$. This scaling persists in self-consistent numerical calculations [52–54]. Eq. (6) along with this scaling thus establishes the reduction of the OAM of the $k = 2$ MQV in the weakly paired regime. To leading order in $k_F \xi$, $\mathcal{L} = L_z - N \sim -(k_F \xi)^2$. As a result, the OAM is significantly suppressed from $L_z^{BEC} = N$ since $k_F \xi \gg 1$ in the BCS regime ($\Delta_0 \ll E_F$). This analysis confirms that the unpaired fermions carry angular momentum opposite to that carried by the Cooper pairs. On a disc, $N \approx (k_F R)^2/2$, leading to $L_z/N \approx 1 - \alpha(\xi/R)^2$, where α is an $O(1)$ constant fixed by $\Delta(r)$. As an independent check, we have verified this behavior by numerically calculating L_z/N using the full BdG solution [36]. In Fig. 3, the quadratic scaling is shown to be in good agreement with the numerical data. We thus expect a substantial reduction of the OAM in the BCS regime, where ξ can be comparable to R [16]. We also expect that when two elementary vortices merge into a $k = 2$ MQV [49, 50], the ground state OAM decreases from $L_z = N$ by an amount $\sim (k_F \xi)^2$.

A central feature of our result is that the suppression of L_z for $|k| \geq 2$ is independent of any boundary effects and is solely determined by the splitting between the vortex core branches. Given this insensitivity to boundary details, we expect our results to hold for more general sample geometries, which may lack axial symmetry. Unlike the ground state energy, which might depend strongly on the gap profile, the OAM thus exhibits universal scaling behavior in the weak pairing BCS regime. The lack of dependence of the OAM on the system boundary is in stark contrast with weakly-paired chiral (e.g., $d+id$) SFs, where it was shown [37, 39] that the OAM is suppressed due to the topological edge modes, but that this effect is strongly dependent on the edge details [38, 44, 45, 55]. Our analysis hence suggests that s -wave SFs with MQVs may prove to be a more robust platform for investigating the intriguing suppression of the OAM in paired SFs. While the OAM has been measured in SFs [56–58], we also expect signatures of unpaired fermions—which create a current localized around the vortex core that flows counter to the superflow—in local supercurrent density

measurements in MQV states [17].

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