Stability of Half-Quantum Vortices in $p_x + ip_y$ Superconductors

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We consider the stability conditions for half-quantum vortices in a quasi-two-dimensional $p_x + ip_y$ superconductor (such as Sr_2RuO_4 is believed to be). The predicted exotic nature of these excitations has recently attracted much attention, but they have not been observed yet. We emphasize that an isolated half-quantum vortex has a divergent energy cost in the bulk due to its *unscreened* spin current, which requires two half-quantum vortices with opposite spin winding to pair. We show that the stability of such a pair is enhanced when the ratio of spin superfluid density to superfluid density ρ_{sp}/ρ_s is small. We propose using various mesoscopic geometries to stabilize and observe these exotic excitations.

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The possibility of half-quantum vortices ($\frac{1}{2}$ QV's) in $p_x + ip_y$ superconductors (SC's) has recently added a new "spin" to the interest in such exotic SCs. The prediction that such vortices in (quasi-) two-dimensional (2D) superfluids will have Majorana fermion zero modes bound at vortex cores, which render vortex statistics non-Abelian [1–4], drives the excitement. A realization of excitations with such exotic statistics is of interest in its own right. Moreover, the possibility of exploiting non-Abelian statistics for topological quantum computation [5] adds technological interest as well.

$\frac{1}{2}$ QV's are topologically allowed in triplet superfluids due to their spin degrees of freedom. They were first sought after in thin films of ^{3}He-*A* [6]: the best known example of $p_x + ip_y$ superfluid [7]. However, achieving a sufficiently thin parallel plate geometry is challenging and NMR experiments on ^{3}He-*A* thin films failed to detect $\frac{1}{2}$ QV's [8]. Sr_2RuO_4 has recently emerged as a candidate material for a quasi-2D (*ab* plane) $p_x + ip_y$ spin-triplet SC [9–12], offering an alternate system to look for $\frac{1}{2}$ QV's. References [3,4] proposed experiments for probing and exploiting the exotic nature of the Majorana fermion core states of $\frac{1}{2}$ QV's. Nevertheless, $\frac{1}{2}$ QV's have not been observed in Sr_2RuO_4 [13–15]. For $\frac{1}{2}$ QV's to be realized, it is crucial to carefully consider their energetics and schemes for stabilization.

In this Letter, we investigate the stability of the $\frac{1}{2}$ QV's and discuss routes for their realization using mesoscopic samples. Vortex energetics in the context of Sr_2RuO_4 were first considered by Kee *et al.* [16] for $\frac{1}{2}$ QV's in the *bc* plane bound to a texture in the $\mathbf{d}$ vector [Eq. (1)]. With the interest for the exotic statistics (which is only possible in 2D) in our minds, we focus on the *ab* plane vortices. Das Sarma *et al.* noted [3] that an out-of-plane field of the order of the spin-orbit decoupling field [17] can reduce the energy cost of $\frac{1}{2}$ QV's in the *ab* plane [3]. They further argued that the smaller vorticity of $\frac{1}{2}$ QV's may energetically favor them over full QV's. However, as it was remarked in Ref. [18], an isolated $\frac{1}{2}$ QV costs energy that is divergent in the system size due to its *unscreened* spin current. Indeed, fractional vortices that are allowed in multicomponent SC generally tend to be energetically unfavorable [19]. Hence free isolated $\frac{1}{2}$ QV's cannot exist in the bulk. There are two ways to cut off this divergence: (1) two $\frac{1}{2}$ QV's with opposite spin winding forming a pair in a bulk sample and (2) a $\frac{1}{2}$ QV entering a mesoscopic sample. Through explicit energetics calculations, we find that $\frac{1}{2}$ QV's can be stabilized when the ratio ρ_{sp}/ρ_s is sufficiently small.

Stability Analysis.—The order parameter of a triplet SC takes a matrix form in the spin space [12,18]:

$$\hat{\Delta}(\mathbf{k}) = \begin{bmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{bmatrix} \equiv \begin{bmatrix} -d_x + id_y & d_z \\ d_z & d_x + id_y \end{bmatrix}. \quad (1)$$

The triplet pairing requires $\Delta_{\uparrow\downarrow} = \Delta_{\downarrow\uparrow}$ and the $\mathbf{k}$ dependent vector $\mathbf{d}(\mathbf{k})$ was introduced to parametrize the gap function. For each $\mathbf{k}$, the unit vector $\hat{\mathbf{d}}(\mathbf{k})$ represents the symmetry direction with respect to the rotation of Cooper pair spin. In a $p_x + ip_y$ SC, the $\mathbf{k}$ dependence of $\mathbf{d}(\mathbf{k})$ is determined by the pairs having finite angular momentum projection $m = 1$ directed along $\hat{\boldsymbol{l}}$. Hence

$$\mathbf{d}(\mathbf{k}) = \Delta_0 \hat{\mathbf{d}} \exp(i\varphi_{\hat{\mathbf{k}}\hat{l}})|\hat{\mathbf{k}} \times \hat{\boldsymbol{l}}|, \quad (2)$$

where $\varphi_{\hat{\mathbf{k}}\hat{l}}$ is the azimuthal angle $\hat{\mathbf{k}}$ makes around $\hat{\boldsymbol{l}}$. For a (quasi-) 2D system with $\hat{\boldsymbol{l}} = \pm\hat{z}$, Eq. (2) gives the

$$\mathbf{d}(\mathbf{k}) = \Delta_0 \hat{\mathbf{d}} \exp(i\varphi_{\hat{\mathbf{k}}}), \quad (3)$$

for a single domain, where $\varphi_{\hat{\mathbf{k}}}$ is the azimuthal angle $\hat{\mathbf{k}}$ makes around the *c* axis. Notice two independent continuous symmetries associated with $\mathbf{d}(\mathbf{k})$: the spin rotation symmetry SO_2 around $\hat{\mathbf{d}}$ and the $U(1)$ symmetry combining a gauge transformation and an orbital rotation around $\hat{\boldsymbol{l}}$ [20]. For fixed $\hat{\boldsymbol{l}}$, we denote the "orbital phase" for this combined $U(1)$ symmetry by χ.

The spin degree of freedom represented by the **d** vector allows for the existence of half-quantum vortices. In a singlet (single component) superconductor, $\frac{1}{2}$ QV's are forbidden in order for the order parameter to be single valued. However, in the $p_x + ip_y$ SC, each component of the order parameter matrix can remain single valued by simultaneously rotating the **d** vector by π while the orbital phase χ winds by π. Since only χ couples to the magnetic vector potential, this type of topological defect only carries a flux of $hc/4e$, i.e., half a superconducting flux quantum $\Phi_0 = hc/2e$. From Eq. (1), one can intuitively characterize a $\frac{1}{2}$ QV as a vortex with a single unit of vorticity for one of the spin components and zero vorticity for the other [21].

In the absence of an external magnetic field, the spin-orbit (dipole) coupling favors alignment of $\hat{\mathbf{d}}$ and $\hat{\boldsymbol{l}}$, making $\frac{1}{2}$ QV's energetically costly [6,20]. However, Knight-shift measurement on Sr_2RuO_4 by Murakawa *et al.* [17] suggests that a sufficiently large magnetic field $H > 200$ G ($<H_{c2} \sim 750$ G [12]) along the c axis may neutralize the dipolar interaction by fixing the **d**-vector orientation to the ab plane (or RuO_2 plane). While this opens the possibility of $\frac{1}{2}$ QV's, the associated **d**-vector bending introduces "hydrodynamic" spin terms in the gradient free energy. In the following, we will determine their effect on the stability of half-quantum vortices.

The Ginzburg-Landau (GL) gradient free energy in its most general form in the London limit (i.e., the superfluid density is taken to be constant outside vortex cores [20]) is

$$\begin{aligned} f_{\rm grad} =& \frac{1}{2}[\rho_s v_s^2 - (\rho_s - \rho_s^{\|})(\hat{\boldsymbol{l}}\cdot\mathbf{v_s})^2] \\ &+ \frac{1}{2}\left(\frac{\hbar}{2m}\right)^2 \sum_i [\rho_{\rm sp}(\nabla \hat{d}_i)^2 - (\rho_{\rm sp} - \rho_{\rm sp}^{\|})(\hat{\boldsymbol{l}}\cdot\nabla\hat{d}_i)^2] \\ &+ K_{ij}^{mn}\partial_i \hat{l}_m \partial_j \hat{l}_n + C_{ij}(v_s)_i(\nabla\times\hat{l})_j + \frac{1}{8\pi}(\nabla\times\mathbf{A})^2, \end{aligned} \tag{4}$$

where $\mathbf{v_s}$ is the superflow velocity, m is the fermion mass, and ρ_s, $\rho_s^{\|}$ and $\rho_{\rm sp}$, $\rho_{\rm sp}^{\|}$ are components of the superfluid and spin fluid density matrix, respectively. Note that these are rank-two matrices, since there is one symmetry direction, $\hat{\boldsymbol{l}}$, for the orbital degree of freedom. For a 2D single domain, the fact that $\hat{\boldsymbol{l}}$ is fixed leads to great simplification. The superflow velocity $\mathbf{v_s}$ is then $(\hbar/2m)(\nabla\chi - 2e\mathbf{A}/\hbar c)$, as in a conventional s-wave SC. For vortex lines along the c axis, $\rho_{s\|}$ and $\rho_{sp\|}$ are projected out of the problem due to the absence of any variation along the $\hat{\boldsymbol{l}}$ direction (c axis), and the superfluid and spin current densities can be regarded as scalars. For $\hat{\mathbf{d}} = (\cos\alpha, \sin\alpha, 0)$ in the ab plane the free energy becomes

$$\begin{aligned} f_{\rm grad}^{\rm 2D} =& \frac{1}{2}\left(\frac{\hbar}{2m}\right)^2\left[\rho_s\left(\nabla_\perp\chi - \frac{2e}{\hbar c}\mathbf{A}\right)^2 + \rho_{\rm sp}(\nabla_\perp\alpha)^2\right] \\ &+ \frac{1}{8\pi}(\nabla\times\mathbf{A})^2, \end{aligned} \tag{5}$$

with the last term accounting for screening of the supercurrent, which is absent for the case of ^{3}He-A thin film [6,22].

Unlike a full QV, a single $\frac{1}{2}$ QV costs a spin current energy that diverges logarithmically [18]

$$\epsilon_{\rm sp} = \frac{\pi}{4}\left(\frac{\hbar}{2m}\right)^2 \rho_{\rm sp} \ln\left(\frac{R}{\xi}\right) \tag{6}$$

per unit length, where ξ is the core radius and R the lateral sample dimension. This divergence is due to the *absence of screening*, for the $\hat{\mathbf{d}}$ winding [the $\nabla\alpha$ term in Eq. (5)] does not couple to the electromagnetic field.

A pair of $\frac{1}{2}$ QV's with opposite sense windings in $\hat{\mathbf{d}}$ would be free of such divergent energy cost. The energy per unit length of a pair of $\frac{1}{2}$ QV's separated by r_{12} is

$$E_{\rm pair}^{\rm half}(r_{12}) = \frac{1}{2}\frac{\Phi_0^2}{16\pi^2\lambda^2}\left[\ln\left(\frac{\lambda}{\xi}\right) + K_0\left(\frac{r_{12}}{\lambda}\right) + \frac{\rho_{\rm sp}}{\rho_s}\ln\left(\frac{r_{12}}{\xi}\right)\right], \tag{7}$$

where K_0 is a modified Bessel function and $\lambda = \frac{mc}{2e\sqrt{\pi\rho_s}}$ is the London penetration depth. The first term of Eq. (7) is the *screened* self-energy of superflow. The second term accounts for the magnetic interaction between the vortices, and the third term, in which the logarithmic divergence of Eq. (6) is canceled out by the interaction term, is purely due to spin flow. However, such a pair is topologically equivalent to a single full QV [see Fig. 1(a) and 1(b)] with the self-energy

$$E^{\rm full} = \pi\left(\frac{\hbar}{2m}\right)^2 \rho_s \ln\left(\frac{\lambda}{\xi}\right) = \frac{\Phi_0^2}{16\pi^2\lambda^2}\ln\left(\frac{\lambda}{\xi}\right). \tag{8}$$

Hence the most relevant question, regarding the stability of $\frac{1}{2}$ QV's in the bulk of a SC, is whether a pair of $\frac{1}{2}$ QV's can be generated by the decay of a full QV. [Note that Eqs. (7) and (8) are approximately equal at $r_{12} = \xi$] [23].

We find that a $\frac{1}{2}$ QV pair in bulk Sr_2RuO_4 will only be stable if $\rho_{\rm sp}/\rho_s$ satisfies certain conditions. In Fig. 1, we plot $E_{\rm pair}^{\rm half}(r_{12}) - E^{\rm full}$ for $r_{12} > \xi$. We used $\kappa \equiv \lambda/\xi = 2.5$ based on $\lambda_{ab} \approx 152$ nm [12,13] and the estimated value of the Ginzburg-Landau coherence length $\xi_{ab} \sim 66$ nm [12].

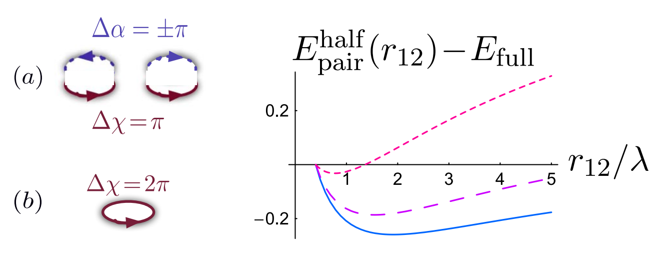

FIG. 1 (color online). Left: a schematic representation of phase winding in (a) a 1/2 QV and (b) a full QV. Right: the energy difference (see text) as a function of pair size, using $\xi = 0.4\lambda$ for Sr_2RuO_4 for different values of $\rho_{\rm sp}/\rho_s$: $\rho_{\rm sp}/\rho_s = 0.3$ (the blue solid curve), $\rho_{\rm sp}/\rho_s = 0.4$ (the purple dashed curve), and $\rho_{\rm sp}/\rho_s = 0.7$ (the red dotted curve). The energy per unit length is in units of $\Phi_0^2/16\pi^2\lambda^2$.

For all three values of ρ_{sp}/ρ_s shown, a finite equilibrium pair size $r_{equil} > \xi$ exists. However, we note that while the London approximation predicts a minimum of the energy difference $E_{pair}^{half}(r_{12}) - E^{full}$ at a finite value $r_{12} = r_{equil}$ for $\rho_{sp}/\rho_s < 1$, the London limit is only valid when ρ_{sp}/ρ_s is small enough to give $r_{equil} > \xi$.

We now discuss the ratio ρ_{sp}/ρ_s between the neutral spin superfluid density ρ_{sp} and the charged mass superfluid density ρ_s in Eq. (5). In the case of ^{3}He, this ratio has been derived theoretically in terms of Landau parameters [7,20,22,24]. Using sum rules for the longitudinal current-current correlation, Leggett showed that $\rho_{sp} < \rho_s$ [24]. This follows from the fact that the mass current is conserved even in the presence of interactions due to Galilean invariance, while the spin current is not, since a corresponding symmetry is absent. In the case of Sr_2RuO_4, the lattice breaks the Galilean invariance. However, since all interactions that scatter the mass current also must scatter spin current, but not vice versa, one still expects $\rho_{sp} < \rho_s$ [24]. While the actual value of ρ_{sp}/ρ_s is unknown for Sr_2RuO_4, it has recently been measured to be ~0.3 near $T = 0$ in ^{3}He-A [22]. Since many Fermi liquid properties of Sr_2RuO_4 are similar to that of ^{3}He [12], ρ_{sp}/ρ_s for Sr_2RuO_4 is also not anticipated to be much larger than ~0.4. If so, the $\frac{1}{2}$ QV pair would have a robust energy minimum (see Fig. 1).

Although the above analysis implies that a pair of half-quantum vortices can be stable against *combining* into a single full QV, the vortex core energy can prevent a single full QV from *decaying* into a pair of half-quantum vortices. Since the core interactions may be substantial for $r_{12} \lesssim \xi$, it is not guaranteed that the finite equilibrium separation in our analysis corresponds to a global energy minimum. When a finite separation $r_{equil} > 0$ configuration only represents a metastable state, its formation depends on the history of the sample. In this case, a full vortex would not decay into two $\frac{1}{2}$ QV's. If ρ_{sp}/ρ_s is so large that $r_{equil} \lesssim \xi$, even a local minimum might be absent. However, if $\rho_{sp}/\rho_s \sim 0.4$, as in the case of ^{3}He, this is rather unlikely.

Mesoscopic geometries.—Given that the experimentally unknown core interaction may be significant, and neutron scattering [13] and vortex imaging [14,15] found no evidence for vortex dissociation in macroscopic samples, we propose utilizing mesoscopic geometries. A sample size of order λ would promote the chance of a $\frac{1}{2}$ QV entering by cutting off the divergent spin current energy and reducing the effect of supercurrent screening. Here we discuss a thin slab and a cylinder as two examples.

We find that a slab of thickness $L = 2\lambda$ (see Fig. 2) will only permit the entry of $\frac{1}{2}$ QV if $\rho_{sp}/\rho_s < (2\xi/\lambda)K_1(2\xi/\lambda)$. Consider the Gibbs free energy for a vortex at position x in the slab (see Fig. 2), with winding numbers n_s and n_{sp} in χ and α, respectively, and a uniform applied field H: ($n_s = n_{sp} = 1/2$ and $n_s = 1$, $n_{sp} = 0$ for a $\frac{1}{2}$ QV and a full QV, respectively)

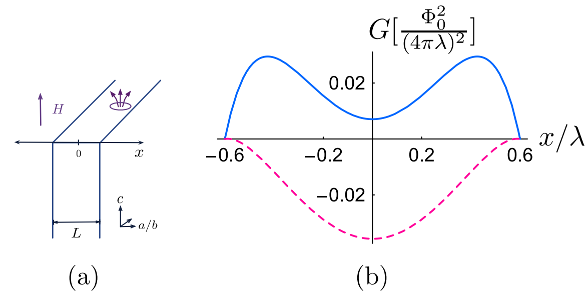

FIG. 2 (color online). (a) A slab of thickness $L = 2\lambda = 0.304$ μm in an external field H. (b) $G(x)$ [see Eq. (9)] in units of $\Phi_0^2/(4\pi\lambda)^2$ for a full-QV (blue solid curve) and for a $\frac{1}{2}$ QV (red dashed curve) at $H = 212$ G $\sim 3.0\Phi_0/4\pi\lambda^2$, for $\xi = 0.4\lambda$ and $\rho_{sp}/\rho_s = 0.4$.

$$G(x; n_s, n_{sp}) = \varepsilon_m(x; n_s) + \sum_{\delta=\mp} \sum_{j=1}^{\infty} (-1)^{j-1} \varepsilon_{bc}(|x - x_j^\delta|; n_s, n_{sp}). \quad (9)$$

Here, $\varepsilon_m(x; n_s)$ is the energy (per unit sample thickness) due to the interaction with the Meissner current:

$$\frac{\varepsilon_m(x; n_s)}{\Phi_0^2/(4\pi\lambda)^2} = n_s \frac{H}{\Phi_0/4\pi\lambda^2} \times \frac{\cosh(x/\lambda) - \cosh[(L - 2\xi)/2\lambda]}{\cosh(L/2\lambda)}. \quad (10)$$

The second line of Eq. (9) accounts for the boundary condition of vanishing current normal to each surface. We solve the boundary condition using an infinite set of image vortices at positions $x_j^\mp \equiv (-1)^j(x' \mp jL)$ for $j = 1, \ldots, \infty$ with vorticities $(-1)^j n_{s,sp}$. Between a vortex with winding number (n_s, n_{sp}) in the slab and each of its image vortices at a distance r from it, there is an interaction energy (per unit sample thickness):

$$\frac{\varepsilon_{bc}(r; n_s, n_{sp})}{\Phi_0^2/(4\pi\lambda)^2} = -n_s^2\left[K_0\left(\frac{r}{\lambda}\right) - K_0\left(\frac{2\xi}{\lambda}\right)\right] + n_{sp}^2 \frac{\rho_{sp}}{\rho_s} \ln\left(\frac{r}{2\xi}\right). \quad (11)$$

We plot $G(x; 1, 0)$ and $G(x; 1/2, 1/2)$ in Fig. 2(b) for a case when only the $\frac{1}{2}$ QV is stable inside the sample. The energy difference between the two types of vortices at the center is estimated to be much larger than $k_B T_c$ at low enough temperatures (as large as $10^4 k_B T_c/\mu$m at $T \sim 100$ mK). Hence, the entry of a $\frac{1}{2}$ QV into the slab will be favored over that of a full QV.

However, the fact that many vortices will enter the slab at different positions along its length complicates both further theoretical modeling and experiments. Thus, we also consider cylindrical samples, which can only accommodate single vortices (of either type) if the radius is small enough [25]. For example, the fabrication of a submicron disk of Sr_2RuO_4, while challenging, is within reach of available technologies such as focused ion beam (FIB) milling. The entry of a vortex or fluxoid in a cylinder or annulus geometry can be detected as an abrupt change in the magnetization as H is ramped up. As in the case of a thin slab, a $\frac{1}{2}$ QV can be energetically favored for small enough ρ_{sp}/ρ_s.

For simplicity, we only compare the free energies for fluxoids trapped in a thin, hollow cylinder. Although the fabrication of this geometry is more challenging, it has an advantage over a filled cylinder or disk of eliminating the core. For a long, thin hollow cylinder of radius R and thickness $d \ll \lambda$, R, the London approximation is nearly accurate [26], and one can obtain the Gibbs free energy per unit length for fluxoids of either type in the presence of an external field H from Eq. (5) via a Legendre transformation:

$$\frac{G(n_s, n_{sp})}{\Phi_0^2/8\pi R^2} = \beta\left[\frac{1}{1+\beta}\left(n_s - \frac{\Phi}{\Phi_0}\right)^2 + \frac{\rho_{sp}}{\rho_s}n_{sp}^2\right] - \left(\frac{\Phi}{\Phi_0}\right)^2. \tag{12}$$

We defined $\beta \equiv dR/2\lambda^2$ [27], and $\Phi \equiv \pi R^2 H$, the externally controlled flux through the cylinder. In the ground state, the values of n_s and n_{sp} minimize G for a given value of Φ. The n_{sp}^2 term in Eq. (12), which is the only difference from the s-wave case, allows for the $\frac{1}{2}$ QV possibility of $n_s = n_{sp} = 1/2$. At $\Phi/\Phi_0 = 1/2$, $G(1/2, 1/2) < G(1, 0) = G(0, 0)$ if $\rho_{sp}/\rho_s < (1+\beta)^{-1}$ and a $\frac{1}{2}$ QV will have lower energy than a full QV. The vorticity could be detected by monitoring the magnetization, as it was done for bilayer Al rings, which effectively form a two-component SC [28].

Conclusion.—We considered the vortex energetics of $p_x + ip_y$ SC in the London limit using a GL formalism. For an isolated $\frac{1}{2}$ QV, we noted the importance of controlling a logarithmically divergent energy due to the unscreened spin current. While this divergence is regulated in a pair of $\frac{1}{2}$ QV's of opposite spin winding, ρ_{sp}/ρ_s needs to be sufficiently small in order to make a finite separation in such a pair (meta-) stable. Given the fragile nature of $\frac{1}{2}$ QV's in bulk samples, we propose using mesoscopic geometries to look for $\frac{1}{2}$ QV's.

While for sufficiently small ρ_{sp}/ρ_s the pairs of $\frac{1}{2}$ QV's can be energetically stable in bulk samples and a single $\frac{1}{2}$ QV can be stable in mesoscopic samples, a number of real material features can affect the existence or complicate the observation of $\frac{1}{2}$ QV's in Sr_2RuO_4. Such features include locking of the **d** vector within the RuO_2 plane, proliferation of microscopic domain walls, significant core energy effects, and boundary scattering. Nonetheless, given the exciting promise associated with these exotic excitations, our analysis forms a point of departure in the quest of realizing $\frac{1}{2}$ QV's in Sr_2RuO_4 or other candidate materials for exotic superconductivity, such as UPt_3 [29].

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