Spin Polarization in Half Quantum Vortices

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Presentation for Bachelor Thesis Project II

Plan for Today

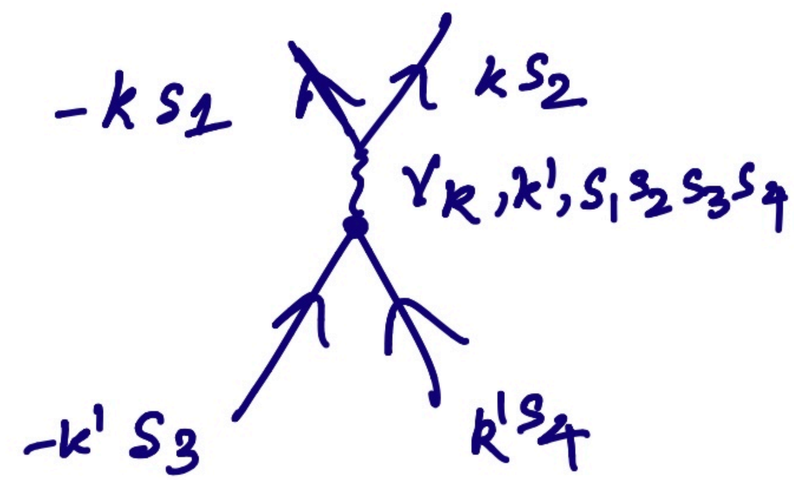
- SC states in crystals
- GL Theory for 2 component OP
- Microscopic Derivation: Example System of Bi_2Se_3
- Spin Polarization: Analysis

SC States in crystals

- BCS Theory $\Rightarrow b_{k,ss'} = \langle c_{-k\downarrow} c_{k\uparrow} \rangle$, gives rise to the gap function

$$\Delta_{\vec{k},ss'} = -\sum_{\vec{k}',s_3s_4} V_{\vec{k},\vec{k}';ss's_3s_4} b_{\vec{k},s_3s_4} \, ,$$

$$\Delta^*_{\vec{k},ss'} = -\sum_{\vec{k}'s_1s_2} V_{\vec{k}',\vec{k};s_1s_2s's} b^*_{\vec{k},s_2s_3} \, .$$



- Gap function $\rightarrow 2 \times 2$ matrix in spin space

$$\widehat{\Delta}_{\vec{k}} = \begin{pmatrix} \Delta_{\vec{k},\uparrow\uparrow} & \Delta_{\vec{k},\uparrow\downarrow} \\ \Delta_{\vec{k},\downarrow\uparrow} & \Delta_{\vec{k},\downarrow\downarrow} \end{pmatrix}$$

- One can then classify the state as singlet or triplet based on parity of the wavefunction ($b_{k,s_1 s_2} = \pm\, b_{-k,s_1 s_2}$) as

Even Parity :

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} \Delta_{\vec{k},\uparrow\uparrow} & \Delta_{\vec{k},\uparrow\downarrow} \\ \Delta_{\vec{k},\downarrow\uparrow} & \Delta_{\vec{k},\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} 0 & \psi(\vec{k}) \\ -\psi(\vec{k}) & 0 \end{pmatrix} = i\hat{\sigma}_y \psi(\vec{k})$$

$$\psi(\vec{k}) = \psi(-\vec{k})$$

Odd Parity:

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} \Delta_{\vec{k},\uparrow\uparrow} & \Delta_{\vec{k},\uparrow\downarrow} \\ \Delta_{\vec{k},\downarrow\uparrow} & \Delta_{\vec{k},\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} -d_x(\vec{k}) + i d_y(\vec{k}) & d_z(\vec{k}) \\ d_z(\vec{k}) & d_x(\vec{k}) + i d_y(\vec{k}) \end{pmatrix}$$

$$= i\left(\vec{d}(\vec{k}) \cdot \hat{\vec{\sigma}}\right)\hat{\sigma}_y$$

$$\vec{d}(\vec{k}) = -\vec{d}(-\vec{k})$$

- For an Isotropic material, one can further expand $\psi(\overrightarrow{k})$, $\overrightarrow{d}(\overrightarrow{k})$ in terms of spherical harmonics

$$\psi^l(\overrightarrow{k}) = \sum_{m=-l}^{l} a_{lm} Y_{lm}(\hat{k}) \qquad l = 0,2,4,6,8...$$

$$\overrightarrow{d}^l(\overrightarrow{k}) = \sum_{m=-l}^{l} \overrightarrow{b}_{lm} Y_{lm}(\hat{k}) \qquad l = 1,3,5,7,...$$

- In solids the orbital rotation is limited to the point group operation of the crystal lattice. Thus we will not be allowed to use the relative angular momentum *l* to label the basis functions.

- However, one can still use Irreducible representations of the crystal point group for the same expansion.

$$\psi(\vec{k}) = \sum_{l} \eta_m \psi_m(\vec{k}) \qquad \text{and} \qquad \vec{d}(\vec{k}) = \sum_{l} \eta_m \vec{d}_m(\vec{k})$$

where sum runs over all basis functions of the relevant irreducible representation.

- Landau Prescription: To construct GL functional, use η_m as order parameters in the free energy.

- As η_m transform under symmetry operations like coordinates in the basis of functions $\{\psi_m(\vec{k})\}$ or $\{\overrightarrow{d}_m(\overrightarrow{k})\}$.

- For e.g. in E_u irrep, the basis functions are given by

$$\begin{bmatrix} x \\ y \end{bmatrix}$$

- Therefore the correspond OPs η_1, η_2 transform as vectors under rotation along z-axis.

- The Landau free energy functional is then a power expansion in terms of the coefficients η_m (real, scalar functional and depending upon $\overrightarrow{A}$, T and other parameters).

- Example: Tetragonal crystal structure (D_{4h} group)

- Character Table for D_{4h}

Γ	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	I	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	Basis function
A_{1g}	1	1	1	1	1	1	1	1	1	1	$\psi = 1$
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	$\psi = k_x k_y (k_x^2 - k_y^2)$
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1	$\psi = k_x^2 - k_y^2$
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1	$\psi = k_x k_y$
E_g	2	0	-2	0	0	2	0	-2	0	0	$\psi = \{k_x k_z, k_y k_z\}$

- 4 one dimensional and one two-dimensional irreducible representations representation.

- Usual one component OP: A_{1g}, $\psi = \eta \times 1$, GL $\equiv$ conv. s-wave

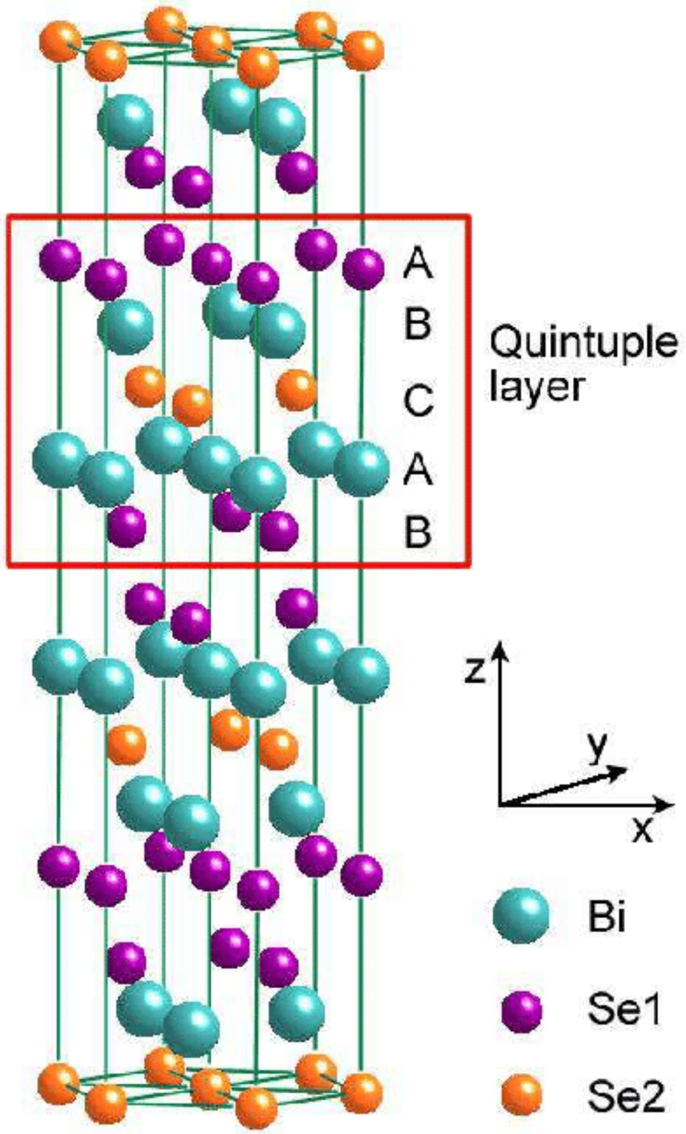
- Unusual 2 component OP: E_g, $\psi(k) = \eta_x \times k_x k_z + \eta_y \times k_y k_z$

$$
\begin{aligned}
F[\vec{\eta},\vec{A};T] = \int d^3r \Big[& a(T)|\vec{\eta}|^2 + b_1|\vec{\eta}|^4 + \frac{b_2}{2}\{\eta_x^{*2}\eta_y^2 + \eta_x^2\eta_y^{*2}\} + b_3|\eta_x|^2|\eta_y|^2 \\
& + K_1\{|\Pi_x\eta_x|^2 + |\Pi_y\eta_y|^2\} + K_2\{|\Pi_x\eta_y|^2 + |\Pi_y\eta_x|^2\} \\
& + K_3\{(\Pi_x\eta_x)^*(\Pi_y\eta_y) + c.c.\} + K_4\{(\Pi_x\eta_y)^*(\Pi_y\eta_x) + c.c.\} \\
& + K_5\{|\Pi_z\eta_x|^2 + |\Pi_z\eta_y|^2\} + \frac{1}{8\pi}(\vec{\nabla}\times\vec{A})^2 \Big]
\end{aligned}
$$

- The parameters are chosen to satisfy the symmetry condition and are in general material dependent.

Case of Odd Parity Bi_2Se_3

- Crystalline Group: D_{3d}



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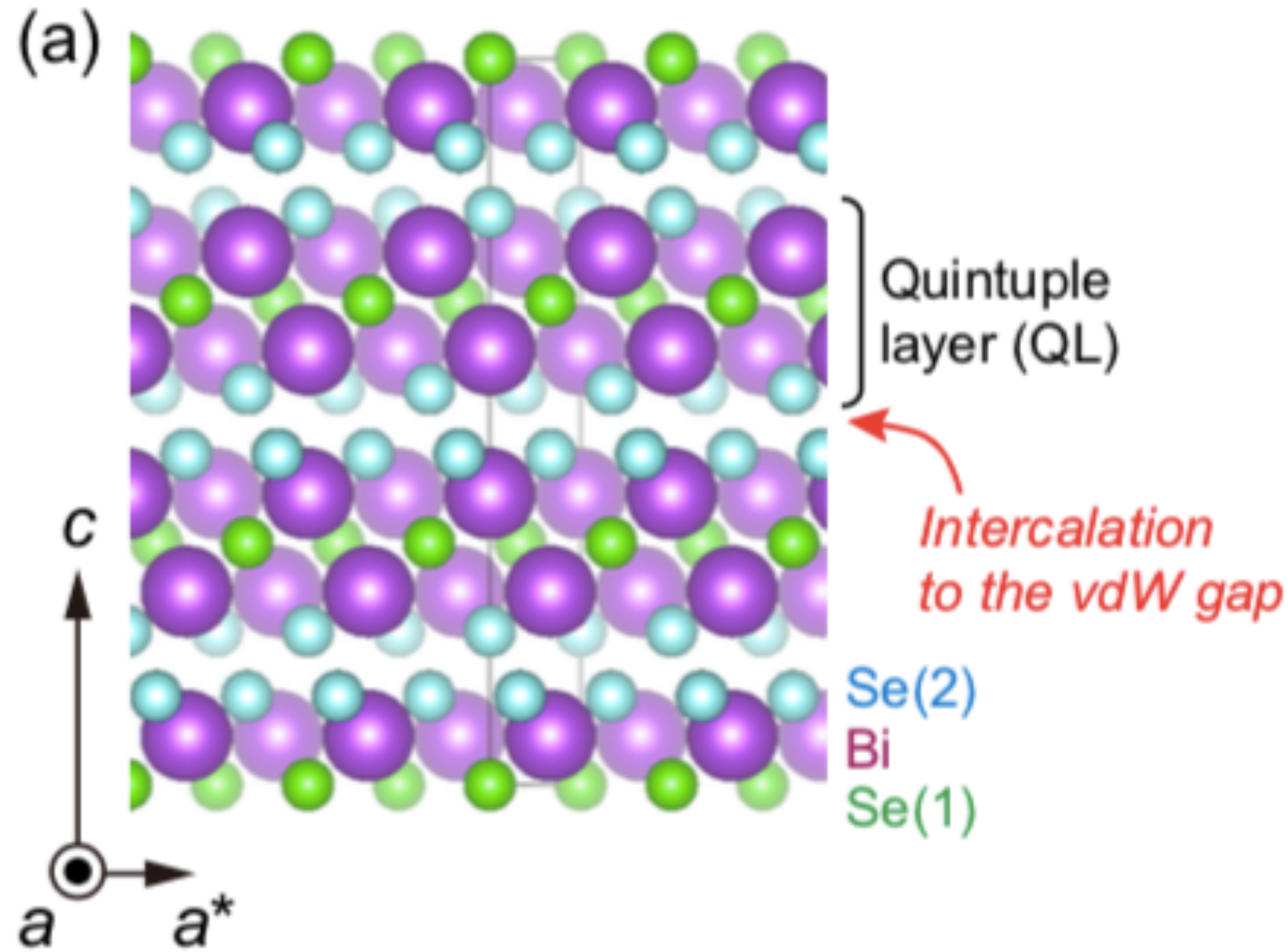


- Fu et al* pointed out (based on existing NMR and specific heat measurements) the pairing in $Cu_xBi_2Se_3$ is odd- parity pairing.

- Moreover, the proposed pairing is in the two-dimensional (2D) E_u representation.

- This requires a 2 component OP $\eta = (\eta_1, \eta_2)^T$.

- However, this proposal has turned out mixed experimental results (topological).

- Idea: Examine vortex structures in this theory - can give an additional hint about the pairing physics.

GL Functional for 2 component Order Parameter

- We start by considering a 2 component order parameter $\overrightarrow{\Delta} = (\Delta_1, \Delta_2)$ and consider the system to be uniform along $\hat{z}$ direction

$$\mathcal{F}(\Delta_1, \Delta_2) = \alpha(\Delta_1^*\Delta_1 + \Delta_2^*\Delta_2) + \frac{\beta_1}{2}[|\Delta_1|^4 + |\Delta_2|^4 + \beta|\Delta_1^2 + \Delta_2^2|^2] + \frac{(\nabla \times \overrightarrow{A})^2}{8\pi}$$
$$+ \sum_{i=1,2,j=x,y} K_1(p_i\Delta_j)^*(p_i\Delta_j) + K_2(p_i\Delta_i)^*(p_j\Delta_j) + K_2(p_i\Delta_j)^*(p_j\Delta_i)$$

- $p_{x,y} = -i\partial_{x,y} - A_i$ (choosing units s.t $\hbar = -\frac{e^*}{c} = 1$)

- Simplified form emerges when written in complex basis $\Delta_\pm = \Delta_1 \pm i\Delta_2$ and $p_\pm = p_x \pm ip_y$

$$\mathcal{F} = \frac{\alpha}{2}(|\Delta_+|^2 + |\Delta_-|^2) + \frac{\beta_1}{8}(|\Delta_+|^4 + |\Delta_-|^4) + \frac{\beta_1\delta\beta}{2}(|\Delta_+|^2|\Delta_-|^2) + \frac{K_{12}}{4}(|p_+\Delta_+|^2 + |p_-\Delta_-|^2)$$
$$+\frac{K_{12}}{4}(|p_+\Delta_-|^2 + |p_-\Delta_+|^2) + \frac{2K_2}{4}[(p_+\Delta_-)^*(p_-\Delta_+) + (p_-\Delta_+)^*(p_+\Delta_-)]$$

- $K_{12} = K_1 + K_2, \delta\beta = 1/2 + \beta$

- Stability requirement*:

  $\beta_1 > 0,\ \beta > -1,\ K_1 > 0,\ 1 > C = \dfrac{K_2}{K_1} > \dfrac{-1}{3}$

- The order parameter transforms as a 2D vector under spatial rotation.

- Also due to the 2 dimensional nature of the problem, makes it possible to have a unique perpendicular vector $\overrightarrow{\Delta_\perp}$, hence we can expect a dual theory in terms of this.

*Zhitomirskii M. E. "Magnetic transitions in a superconducting UPt3". In: *Phys. Rev. Lett.* 103 (5 July 2009), p. 057003.

Uniform and $\overrightarrow{A} \neq 0$ solutions

- Uniform Solution: Drop gradient terms

$$F = \alpha(\Delta_i^* \Delta_i) + \frac{\beta_1}{2}[(\Delta_i^* \Delta_i)^2 + \beta |\Delta_i \Delta_i|^2]$$

- Solution: $\overrightarrow{\Delta} = \Delta_\infty e^{i\chi(x)} \begin{bmatrix} cos(\theta(x)) \\ e^{i\psi(x)} sin(\theta(x)) \end{bmatrix}$

Case 1: $\beta > 0$

$$\overrightarrow{\Delta} = \Delta_\infty e^{i\chi(x)} \begin{bmatrix} 1 \\ \pm i \end{bmatrix}$$

$$\Delta_\infty^2 = \frac{-\alpha}{\beta_1}$$

Case 2: $-1 < \beta < 0$

$$\overrightarrow{\Delta} = \Delta_\infty e^{i\chi} \begin{bmatrix} cos(\theta) \\ sin(\theta) \end{bmatrix}$$

$$\Delta_\infty^2 = \frac{-\alpha}{\beta_1(1+\beta)}$$

✔ *Relevant Solution for our analysis*

Vortex States

- Consider the solution for case 2: $\vec{\Delta} = \Delta_\infty e^{i\chi} \begin{bmatrix} cos(\theta) \\ sin(\theta) \end{bmatrix}$

- 2 dofs = Orientation (θ) and phase (χ)

- A phase vortex (PV) of the usual s-wave nature involves winding of the χ by 2π around a loop. However, in this case, we can respect single-valuedness of Δ by having both χ, θ wind by π in a loop i.e

$$\chi \sim \phi/2, \;\; \theta \sim \phi/2$$

- Generically, $\chi = n_p \frac{\phi}{2}, \theta = \theta_\infty + \frac{n_0 \phi}{2}$, where (n_p, n_o) denote winding #. Shifting to chiral basis ($\Delta_\pm$) we get

$$(\Delta_+, \Delta_-) = \Delta_\infty(\; exp(i\frac{n_p + n_o}{2}\phi + i\frac{\theta_\infty}{2}), exp(i\frac{n_p - n_0}{2}\phi - i\frac{\theta_\infty}{2}) \;)$$

$\propto (e^{i\pm\phi}, 1) \; or \; (1, e^{\pm i\phi}) \rightarrow$ ***1 PV in constant background of another***

- Chiral basis reps: Allows vortex addition (n_p, n_o)

$$(\pm 1,1) + (\pm 1, -1) = (\pm 2,0)$$

- $\nabla \chi \longrightarrow$ screened at long distances due to the meissner effect $\Longrightarrow$gradient energy is localised around the PV and remains finite.

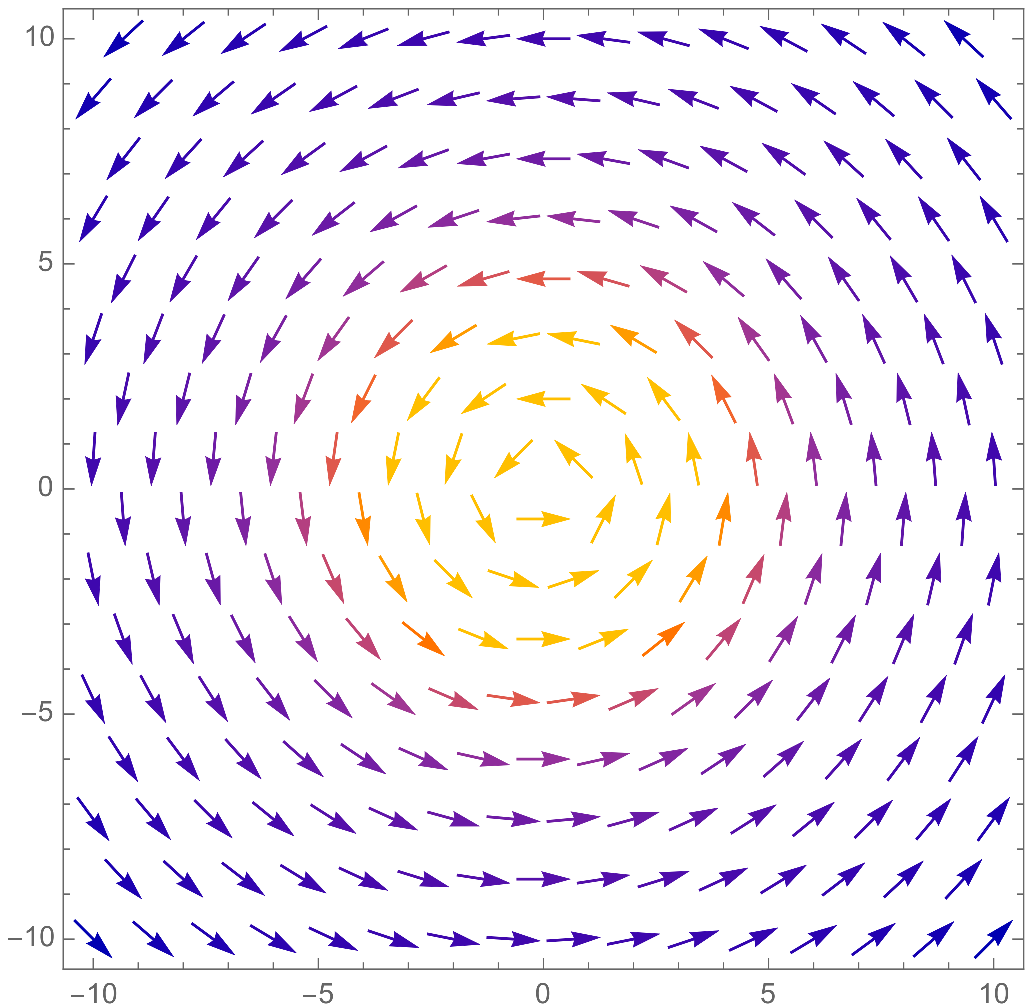
- $\nabla \theta \longrightarrow$ orientation gradient, remains unscreened (no coupling to $\overrightarrow{A}$ or anything)

  $\Longrightarrow$ energy cost associated diverges with system size.

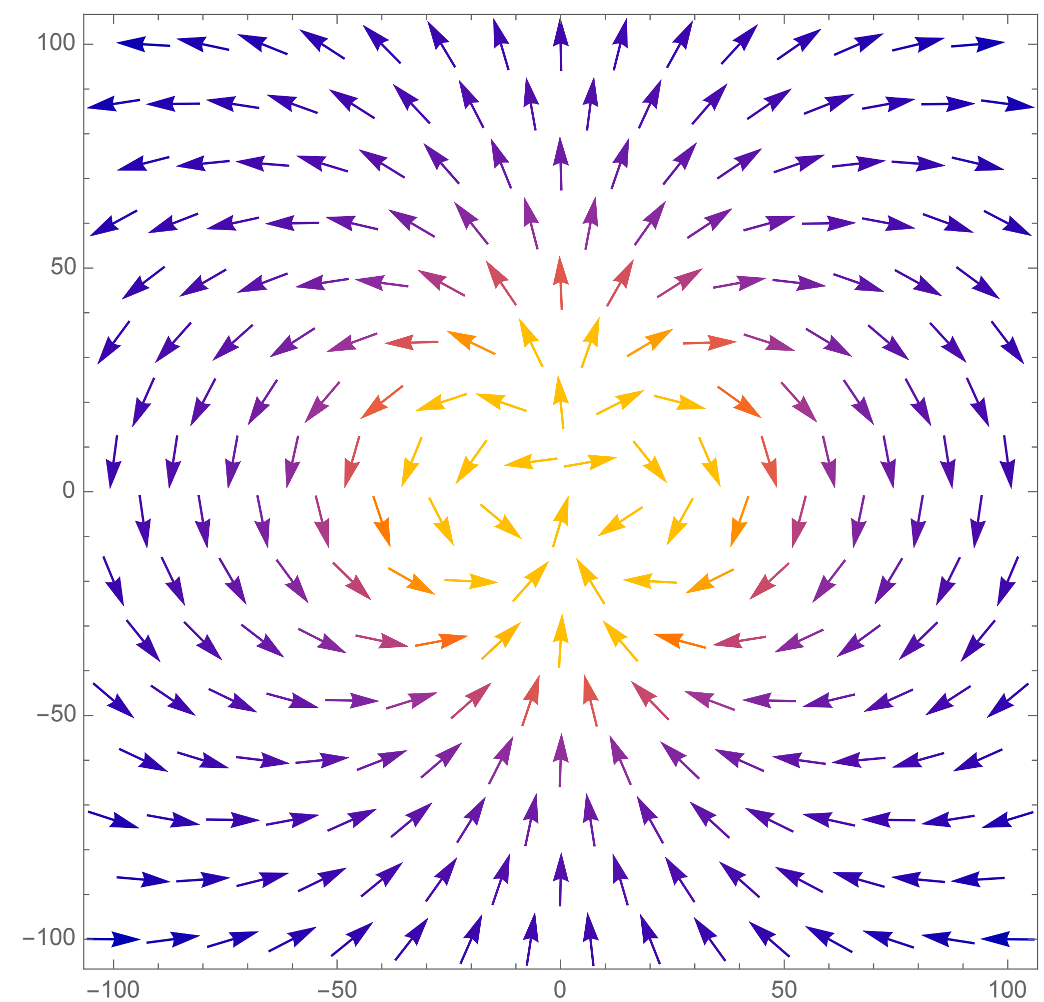
- For ∞ system, HQV then cannot exist independently. Solution?

$$\Downarrow$$

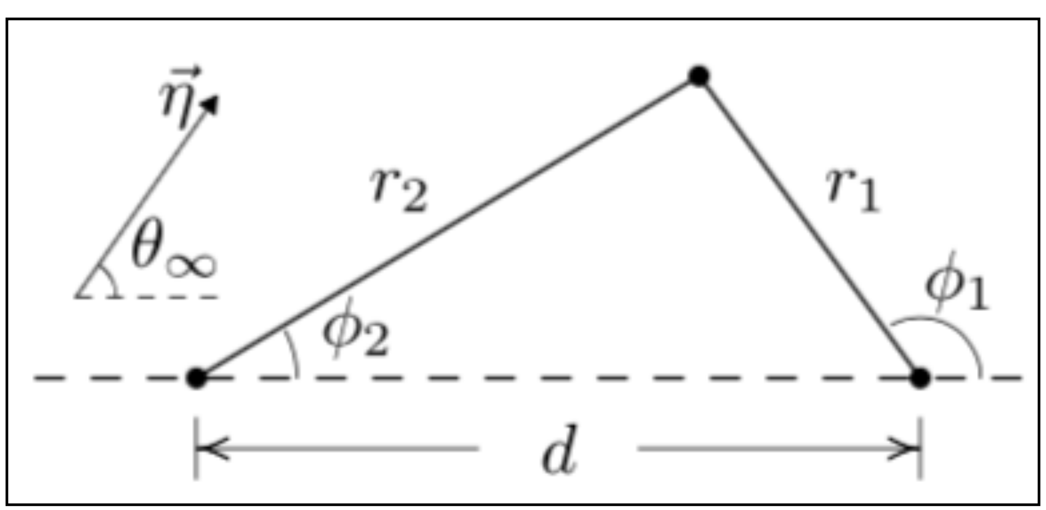
Have a pair of HQV with opposite orientation windings $(1, \pm 1)$



Isolated HQV



A pair of HQV



- Opp wounded HQV pair separation

$$\chi = \frac{\phi_1 + \phi_2}{2} + \ldots$$

$$\theta = \theta_\infty + \frac{\phi_1 - \phi_2}{2} + \ldots \to \theta_\infty$$

HQV Pair: Stability Analysis

- Depending on the phenomenological parameters, stability of vortices is decided

- Vortices -> at long distances, have attractive forces.

- At short distance -> vortices can collapse provided interaction energy of vortices don’t reduce the $F_{HQV\ pair}$ below F_{PV}.

- However, numerically, a stable bound pair of vortices have been observed in *PRL119, 167001.*

Microscopics

- Hamiltonian of the system with SOC is given by

$$H = \int d^3\vec{r}\,\Psi(\vec{r})^\dagger H(\vec{r})\Psi(\vec{r})$$

$$H(\vec{r}) = v\tau_z\big[\overrightarrow{\sigma} \times (-i\overrightarrow{\nabla} - \frac{e}{c}\overrightarrow{A})\big]] \cdot \hat{z} + v_z\tau_y\big(- i\nabla_z - \frac{eA_z}{c}\big) + m\tau_x$$

$v, v_z \Rightarrow$ Inplane and out of plane components of fermi velocity

$\overrightarrow{\sigma} \Rightarrow$ Pauli matrices corresponding to spin

$\vec{\tau} \Rightarrow$ Pauli matrices corresponding to orbitals dof (1,2)

$$\Psi(\vec{r}) = (\Psi_{\uparrow,1}(\vec{r}),\ \Psi_{\downarrow,1}(\vec{r}),\ \Psi_{\uparrow,2}(\vec{r}),\ \Psi_{\downarrow,2}(\vec{r}))$$

$$E_\pm = \sqrt{v^2p_\perp^2 + v_z^2p_z^2 + m^2}$$

BCS Pairing

- **S-wave** channel -triplet interorbital pairing

$$H_{int} = -\lambda \sum_{\sigma,\sigma'} \int d^3\vec{r}\,\Psi^\dagger_{\sigma 1}\Psi^\dagger_{\sigma' 2}\Psi_{\sigma' 2}\Psi_{\sigma 1}$$

- Define $\Delta_{\sigma\sigma'}(\vec{r}) = \lambda\left\langle \Psi_{\sigma 2}(\vec{r})\Psi_{\sigma' 1}(\vec{r})\right\rangle$

  $\Delta_{\sigma\sigma'} \rightarrow$ inter-orbital pairings.

- We pick the nambu basis as $\Phi^\dagger = \left(\Psi^\dagger, \Psi^T(\vec{r})(-i\sigma_y)\right)$

$$H_{bcs} = \int d^3\vec{r}\,\Phi^\dagger(\vec{r})\mathscr{H}_{BCS}(\vec{r})(\vec{r})\Phi(\vec{r}) + \int d^3\vec{r}\left[\sum \frac{|\Delta_{\sigma\sigma'}(\vec{r})|^2}{\lambda}\right]$$

where $\mathscr{H}_{BCS}$ is given by $\mathscr{H}_{BCS}(\vec{r}) = \begin{bmatrix} H(\vec{r}) & \Delta(\vec{r}) \\ \Delta^\dagger(\vec{r}) & -\sigma_y H^*(\vec{r})\sigma_y \end{bmatrix}$

- Pairing potential :$\Delta(\vec{r}) = \overrightarrow{\sigma} \cdot \overrightarrow{\Delta}(\vec{r})\tau_y$

  where $\overrightarrow{\Delta}(\vec{r}) = (\Delta_x(\vec{r}), \Delta_y(\vec{r}), \Delta_z(\vec{r}))$

$$\Delta_x(\vec{r}) = -i\frac{\Delta_{\uparrow\uparrow} - \Delta_{\downarrow\downarrow}}{2} \qquad \Delta_y(\vec{r}) = -\frac{1}{2}(\Delta_{\uparrow\uparrow} + \Delta_{\downarrow\downarrow}) \qquad \Delta_z(\vec{r}) = \frac{1}{2}(\Delta_{\uparrow\downarrow} + \Delta_{\downarrow\uparrow})$$

- Now derive GL functional for the case of $(\Delta_x, \Delta_y, 0)$. As before, we shift to chiral basis $\Delta_\pm = \Delta_x \pm i\Delta_y$ to get

$$F = \sum_{s=\pm}\left\{ -|\Delta_s|^2 + |D_x\Delta_s|^2 + |D_y\Delta_s|^2 + \beta_z|D_z\Delta_s|^2 + \frac{|\Delta_s|^4}{2} + \frac{\gamma}{2}|\Delta_s|^2|\Delta_{-s}|^2 \right.$$
$$\left. + \beta_\perp(D_{-s}\Delta_s)^* D_s\Delta_{-s} \right\}$$

- Same as the phenomenological expression, upto rescaling!

Spin Polarization: Calculation

- We now change gears and focus on Spin polarization.
- In order to calculate quasiparticle spin polarization, use G.Func

$$\mathbf{S}(\mathbf{r}) = \lim_{\mathbf{r}'\to\mathbf{r}} \mathrm{Tr}\ T \sum_n \frac{\boldsymbol{\sigma}}{2} G(\mathbf{r}, \mathbf{r}', \omega_n),$$

trace taken over spin and layer dof.
where now we solve for the coupled equations for G.func evolution:

$$[i\omega_n - H(\mathbf{r})]G(\mathbf{r}, \mathbf{r}', \omega_n) = \delta(\mathbf{r} - \mathbf{r}') - \Delta(\mathbf{r})\bar{F}(\mathbf{r}, \mathbf{r}', \omega_n),$$
$$[i\omega_n + \sigma_y H^*(\mathbf{r})\sigma_y]\bar{F}(\mathbf{r}, \mathbf{r}', \omega_n) = -\Delta^\dagger(\mathbf{r})G(\mathbf{r}, \mathbf{r}', \omega_n),$$

where $F_{k\uparrow}(t) = -\langle \mathcal{T} c_{-k\uparrow} c_{k\downarrow} \rangle$

- Result: $\overrightarrow{S}(\vec{r}) = C \cdot i\overrightarrow{\Delta}(\vec{r}) \times \overrightarrow{\Delta}^*(\vec{r})$, C $\equiv \vec{r}$ indpt constant

HQV Pair Spin Polarization

- Given that we've a pair of HQV as potential stable state, we now deduce the spin polarization in this situation.

- For Single HQV,

- For a two component OP, $\Delta = (\Delta_1(\vec{r}), \Delta_2(\vec{r}))^T$,

$$S(\vec{r}) = iC(\Delta_1^* \Delta_2 - \Delta_2^* \Delta_1) \sim i(\Delta_+^2 - \Delta_-^2)$$

- Specialize for HQV pair: Away from the cores, $|\Delta_+| = |\Delta_-| \Rightarrow$
$$S(\vec{r}) = 0.$$

- However, this can change in case $|\Delta_+| \neq |\Delta_-|$ is possible, which is the case for near core areas.

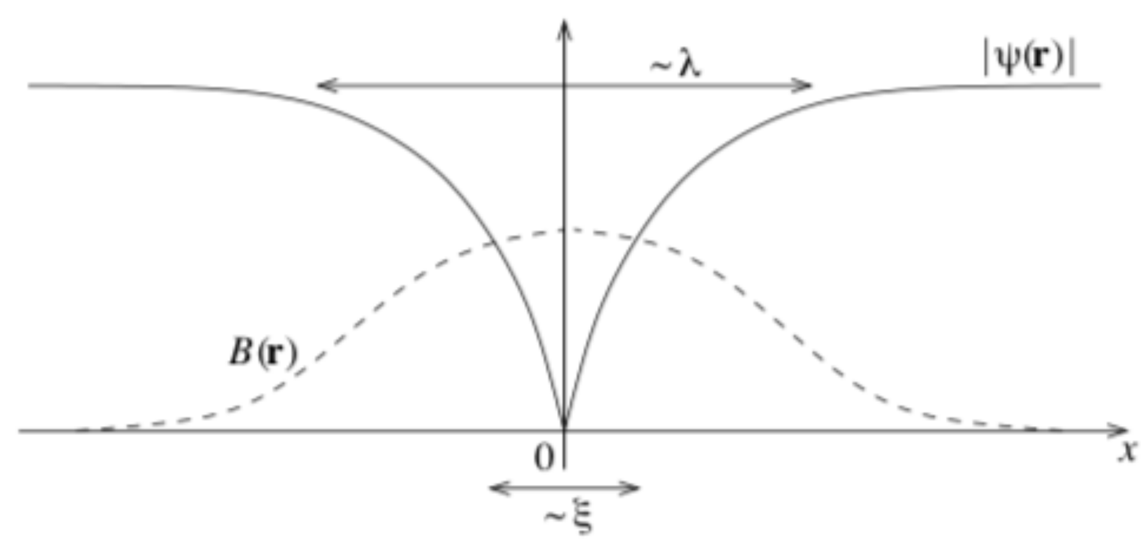
- Let's take the case that the vortices are a pair of half quantum vortices separated by $r_{12} < \lambda$. (cite the numerical observation by zyuzin etal)

- From phenom model, we set the form as
$(\Delta_+, \Delta_-) = \Delta_\infty(\ e^{i(\phi_1+\theta_\infty)} f(r_1)\ ,\ f(r_2)\ e^{i(\phi_2-\theta_\infty)}\ )$

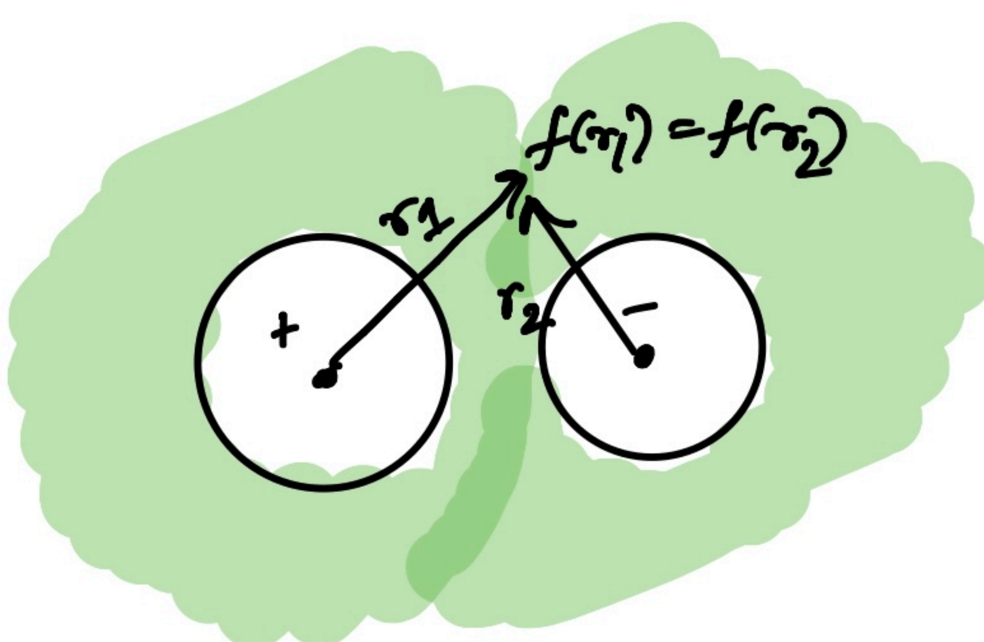
  where $f(r \to 0) \to 0$ and $f(r \to \xi^+) \to 1$.

- $\overrightarrow{S}(\vec{r}) = const \times\ (\ f(r_1)^2 - f(r_2)^2\ )$

$$f(r) \sim tanh(\frac{r}{\xi})$$



- Sketch of Spin polarization near the vortices



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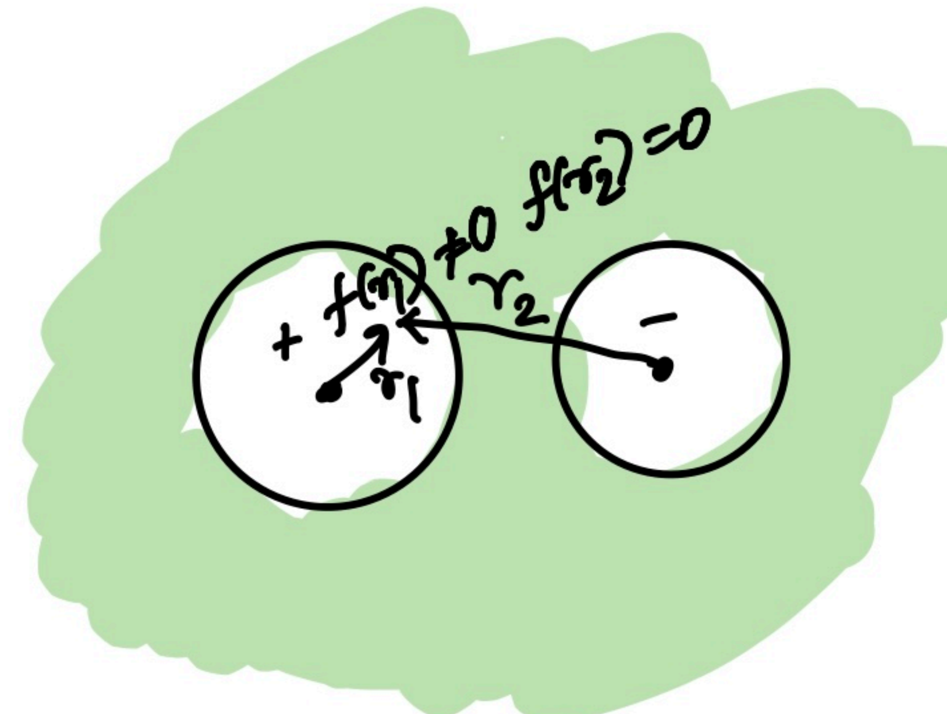

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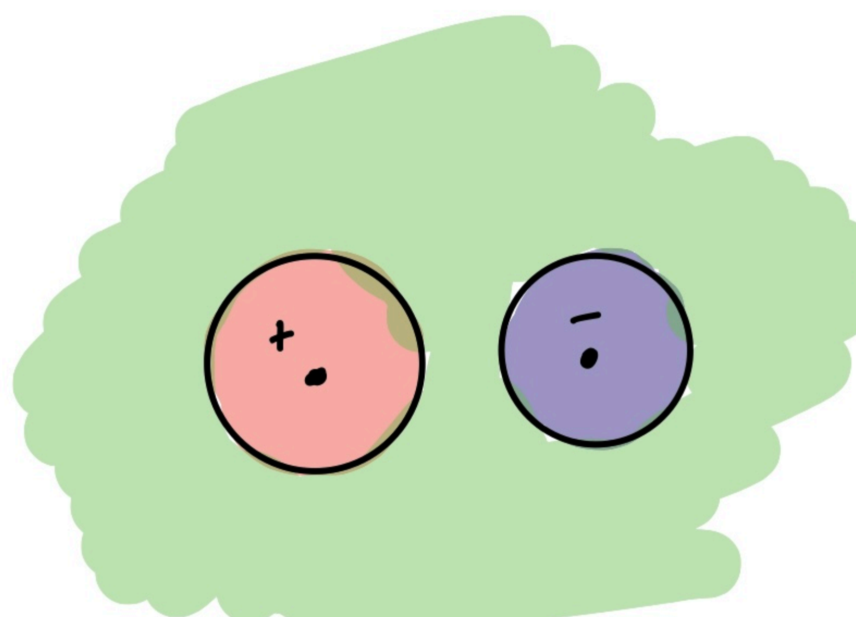

Distribution

That’s all I had to say.
Thank you!