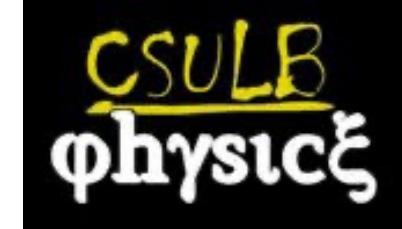




Parameter Dependence of Pair Correlations In Clean Proximity Systems



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Outline:

- ❖ Background
 - Motivation
- ❖ Method
 - Theory
- ❖ Results
 - Discrete layers
 - Continuous layers
 - Ballistic/Diffusive Comparison
- ❖ Conclusion
 - Future work

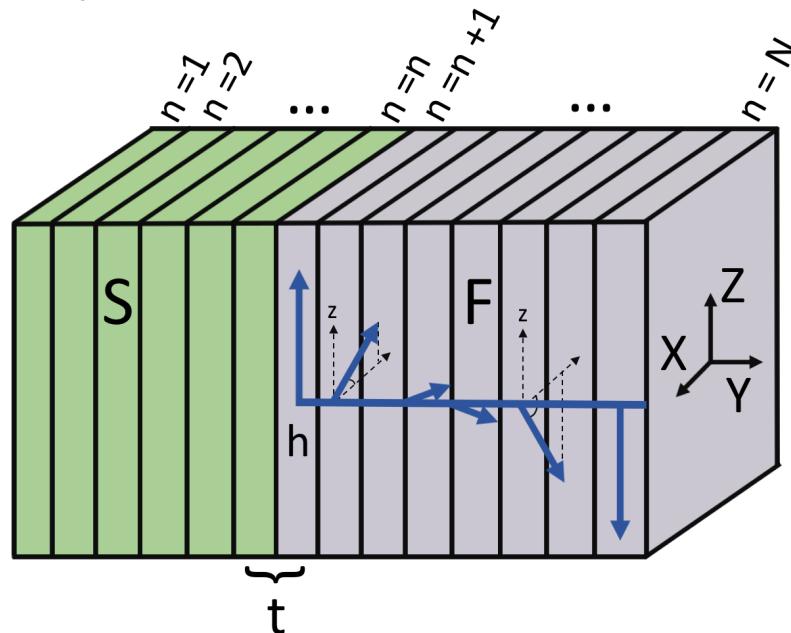
Background:

- Motivation
 - I. Focus of research
 - II. Applications

Focus of research

Question:

- How do varying magnetic configurations affect pair correlations within a Josephson junction?



Example: SF proximity system

We will be looking at different magnetic systems

Quasi one-dimensional system

Applications:

- Quantum computing
- Spintronics devices
- Memory storage
- Sensors

Method:

➤ Theory

- I. What are pair correlations?
- II. Hamiltonian
- III. Bogoliubov-de Gennes (BdG) equations
- IV. Gor'kov functions

What are pair correlations?

Singlet

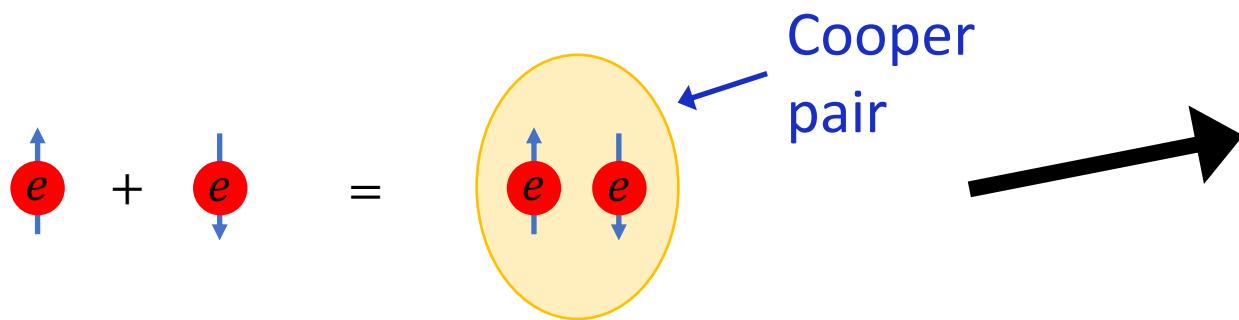
$$|0,0\rangle \propto |\uparrow\downarrow - \downarrow\uparrow\rangle, \quad |1,0\rangle \propto |\uparrow\downarrow + \downarrow\uparrow\rangle,$$

“Fast” decay

Triplet

$$|1,1\rangle = |\uparrow\uparrow\rangle, \quad |1,-1\rangle = |\downarrow\downarrow\rangle.$$

“Slow” decay



- Two fermions (spin 1/2)

$$|\Psi\rangle_{spin} = \sum_{s=0,1} \sum_{m=0,\pm 1} \alpha_{s,m} |s,m>$$

$$s = 0, 1,$$

Pair potential:

$$\Delta_{\sigma,\sigma'} = \begin{pmatrix} \Delta_{\uparrow,\uparrow} & \Delta_{\uparrow,\downarrow} \\ \Delta_{\downarrow,\uparrow} & \Delta_{\downarrow,\downarrow} \end{pmatrix}$$

$$\Delta(n) = \frac{g}{2} \langle c_{n,\downarrow} c_{n,\uparrow} \rangle$$

Pairs are bound in the superconductor and leak into the magnetic material

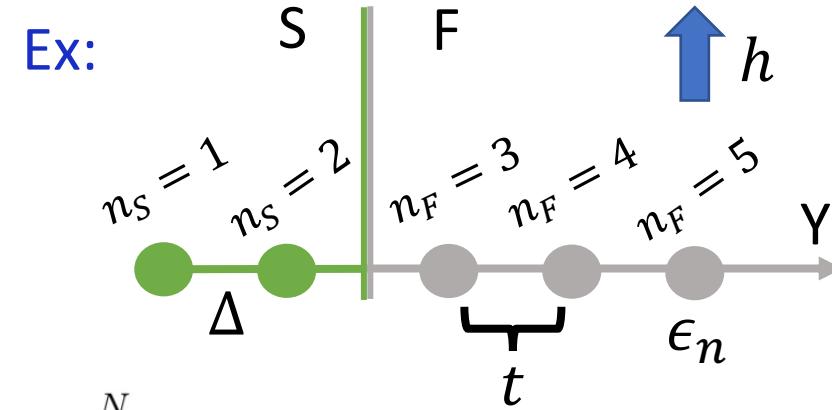
Hamiltonian

- Work is done in the Clean limit
- Formalism (Bogoliubov – de Gennes)

Non-zero in
superconducting
layers

$$\mathcal{H} = -t \sum_n^N \sum_{\sigma} (c_{n,\sigma}^\dagger c_{n+1,\sigma} + h.c.) + \sum_n^N \sum_{\sigma} (\epsilon_n - \mu) c_{n,\sigma}^\dagger c_{n,\sigma}$$

$$+ \sum_n^N \sum_{\sigma,\sigma'} \left(\Delta(n) \rho_{\sigma,\sigma'} c_{n,\sigma}^\dagger c_{n,\sigma'}^\dagger + h.c. \right) - \sum_n^N \sum_{\sigma,\sigma'} [\hat{\sigma} \cdot \mathbf{h}(n)]_{\sigma,\sigma'} c_{n,\sigma}^\dagger c_{n,\sigma'}$$



Non-zero in
magnetic layers

- t is the nearest neighbor hopping energy,
- ϵ_n is the local energy on site n , and μ the chemical potential,
- $\Delta(n)$ is the pair potential (depends on n),
- $h(n)$ is the magnetization profile in the magnetic material,
- $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices.

Solve the associated
Bogoliubov – de Gennes
equations
for the tight-binding
model.

Bogoliubov-Valatin Transformation

- The Bogoliubov-Valatin (BV) Transformation is used to diagonalize the Hamiltonian.

Creation-annihilation operators:

$$c_{n,\sigma} = \sum_J^M \left(u_{n,\sigma,J} \gamma_J - \mathcal{S}_\sigma v_{n,\sigma,J}^* \gamma_J^\dagger \right)$$
$$c_{n,\sigma}^\dagger = \sum_J^M \left(u_{n,\sigma,J}^* \gamma_J^\dagger - \mathcal{S}_\sigma v_{n,\sigma,J} \gamma_J \right)$$
$$\mathcal{S}_\sigma = \begin{cases} 1 & \text{if } \sigma = \uparrow \\ -1 & \text{if } \sigma = \downarrow \end{cases}$$



Commutation relations:

$$[c_{n,\sigma}, c_{n',\sigma'}]_+ = [c_{n,\sigma}^\dagger, c_{n',\sigma'}^\dagger]_+ = 0,$$
$$[c_{n,\sigma}, c_{n',\sigma'}^\dagger]_+ = \delta_{n,n'} \delta_{\sigma,\sigma'}.$$

Condition for diagonalizing Hamiltonian:

$$[\mathcal{H}, \gamma_J]_- = -E_j \gamma_J$$

$$[\mathcal{H}, \gamma_J^\dagger]_- = E_j \gamma_J^\dagger$$

Bogoliubov-de Gennes equations

$$u_{n,\uparrow,J} E_J = -t(u_{n+1,\uparrow,J} + u_{n-1,\uparrow,J}) + [\epsilon_n - \mu - h_z(n)]u_{n,\uparrow,J} \\ + \Delta(n)v_{n,\downarrow,J} - [h_x(n) - ih_y(n)]u_{n,\downarrow,J}$$

$$u_{n,\downarrow,J} E_J = -t(u_{n+1,\downarrow,J} + u_{n-1,\downarrow,J}) + [\epsilon_n - \mu + h_z(n)]u_{n,\downarrow,J} \\ + \Delta(n)v_{n,\uparrow,J} - [h_x(n) + ih_y(n)]u_{n,\uparrow,J}$$

$$\begin{pmatrix} H & -\hat{M} & 0 & \hat{\Delta} \\ -\hat{M}^* & H' & \hat{\Delta} & 0 \\ 0 & \hat{\Delta}^* & -H & -\hat{M}^* \\ \hat{\Delta}^* & 0 & -\hat{M} & -H' \end{pmatrix} \begin{pmatrix} U_{\uparrow,J} \\ U_{\downarrow,J} \\ V_{\uparrow,J} \\ V_{\downarrow,J} \end{pmatrix} = E_j \begin{pmatrix} U_{\uparrow,J} \\ U_{\downarrow,J} \\ V_{\uparrow,J} \\ V_{\downarrow,J} \end{pmatrix}$$

$$v_{n,\uparrow,J} E_J = t(v_{n+1,\uparrow,J} + v_{n-1,\uparrow,J}) - [\epsilon_n - \mu - h_z(n)]v_{n,\uparrow,J} \\ + \Delta^*(n)u_{n,\downarrow,J} - [h_x(n) + ih_y(n)]v_{n,\downarrow,J}$$

$$v_{n,\downarrow,J} E_J = t(v_{n+1,\downarrow,J} + v_{n-1,\downarrow,J}) - [\epsilon_n - \mu + h_z(n)]v_{n,\downarrow,J} \\ + \Delta^*(n)u_{n,\uparrow,J} - [h_x(n) - ih_y(n)]v_{n,\uparrow,J}.$$

$$U_{\sigma J} = \begin{pmatrix} u_{1,\sigma,J} \\ u_{2,\sigma,J} \\ \vdots \\ u_{n,\sigma,J} \end{pmatrix}, \quad V_{\sigma J} = \begin{pmatrix} v_{1,\sigma,J} \\ v_{2,\sigma,J} \\ \vdots \\ v_{n,\sigma,J} \end{pmatrix}$$

$u_{n,\sigma}$ and $v_{n,\sigma}$ are
particle-hole amplitudes

Block matrix for H :

$$H = \begin{pmatrix} \epsilon_1 - \mu - h_z(1) & -t & 0 & \cdots & 0 \\ -t & \epsilon_2 - \mu - h_z(2) & -t & \ddots & \vdots \\ 0 & -t & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -t \\ 0 & \cdots & 0 & -t & \epsilon_n - \mu - h_z(N) \end{pmatrix}$$

Block matrix for $\hat{\Delta}$:

$$\hat{\Delta} = \begin{pmatrix} \Delta(1) & 0 & \cdots & 0 \\ 0 & \Delta(2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \Delta(N) \end{pmatrix}$$

Block matrix for \hat{M} :

$$\hat{M} = \begin{pmatrix} h_x(1) - ih_y(1) & 0 & \cdots & 0 \\ 0 & h_x(2) - ih_y(2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & h_x(N) - ih_y(N) \end{pmatrix}$$

Physical quantities

- Using the BdG solution, other quantities can be defined in the particle-hole basis.

➤ **Pair potential:** $\Delta(n) = \frac{g}{2} \sum_J^M (u_{n,\uparrow,J} v_{n,\downarrow,J}^* + u_{n,\downarrow,J} v_{n,\uparrow,J}^*) [1 - 2f(E_j)]$

Fractional
filling

➤ **Number of particles:** $N = \sum_{n,\sigma} \sum_J^M \left\{ |u_{n,\sigma,J}|^2 f(E_j) + |v_{n,\sigma,J}|^2 [1 - f(E_j)] \right\} \rightarrow n = \frac{N}{N_{tot}}$

➤ **Local density of states:** $\rho(n, E) = \lim_{\eta \rightarrow 0} \frac{\eta}{2\pi} \sum_n^N \sum_J^M \left[\frac{|u_{n,\uparrow,J}|^2 + |u_{n,\downarrow,J}|^2}{(E - E_j)^2 + (\eta/2)^2} + \frac{|v_{n,\uparrow,J}|^2 + |v_{n,\downarrow,J}|^2}{(E + E_j)^2 + (\eta/2)^2} \right]$

➤ **Gor'kov functions:** $f_{\sigma,\sigma'}(n, \tau) = \frac{1}{2} \langle c_{n,\sigma}(\tau) c_{n,\sigma'}(0) \rangle \quad \sigma, \sigma' \in \{\uparrow, \downarrow\}$

➤ **Josephson current**

Gor'kov functions

- The pair correlations can be described by the Gor'kov functions.
- General definition:

$$\begin{aligned} s &= 0, 1, \\ m &= 0, \pm 1 \end{aligned}$$

$$f_{\sigma,\sigma'}(n, \tau) = \frac{1}{2} \langle c_{n,\sigma}(\tau) c_{n,\sigma'}(0) \rangle \quad \sigma, \sigma' \in \{\uparrow, \downarrow\}$$

Singlet:

$$f_{0,0} = f_{\uparrow,\downarrow} - f_{\downarrow,\uparrow} = \frac{1}{2} \langle c_{n,\uparrow} c_{n,\downarrow} - c_{n,\downarrow} c_{n,\uparrow} \rangle$$

$$f_{0,0}(n) = \frac{1}{2} \sum_J^M (u_{n,\uparrow,J} v_{n,\downarrow,J}^* + u_{n,\downarrow,J} v_{n,\uparrow,J}^*) [1 - 2f(E_j)]$$

Triplets:

$$f_{1,0} = \frac{1}{2} (f_{\uparrow,\downarrow} + f_{\downarrow,\uparrow})$$

$$f_{1,1} = \frac{1}{2} (f_{\uparrow,\uparrow} - f_{\downarrow,\downarrow})$$

$$f_{1,0}(n) = \frac{1}{2} \sum_J^M [u_{n,\uparrow,J} v_{n,\downarrow,J}^* - u_{n,\downarrow,J} v_{n,\uparrow,J}^*] \zeta_j(\tau),$$

$$f_{1,1}(n) = -\frac{1}{2} \sum_J^M [u_{n,\uparrow,J} v_{n,\uparrow,J}^* + u_{n,\downarrow,J} v_{n,\downarrow,J}^*] \zeta_j(\tau)$$

Time-dependence

- The triplet Gor'kov functions are time dependent.
- We apply a Fourier transform to transform the equations from the time domain to the frequency domain:

Time-dependent operators:

Triplets:

$$f_{1,0}(n) = \frac{1}{2} \sum_J^M \left[u_{n,\uparrow,J} v_{n,\downarrow,J}^* - u_{n,\downarrow,J} v_{n,\uparrow,J}^* \right] \zeta_j(\tau),$$

$$f_{1,1}(n) = -\frac{1}{2} \sum_J^M \left[u_{n,\uparrow,J} v_{n,\uparrow,J}^* + u_{n,\downarrow,J} v_{n,\downarrow,J}^* \right] \zeta_j(\tau)$$

$$c_{n,\sigma}(t) = e^{\frac{i\mathcal{H}t}{\hbar}} c_{n,\sigma} e^{-\frac{i\mathcal{H}t}{\hbar}},$$

$$c_{n,\sigma}^\dagger(t) = e^{\frac{i\mathcal{H}t}{\hbar}} c_{n,\sigma}^\dagger e^{-\frac{i\mathcal{H}t}{\hbar}}.$$

Time-dependent term:

$$\zeta_j(\tau) = \cos\left(\frac{E_j}{\hbar}\tau\right) - i \sin\left(\frac{E_j}{\hbar}\tau\right) [1 - 2f(E_j)].$$

Fourier transform:

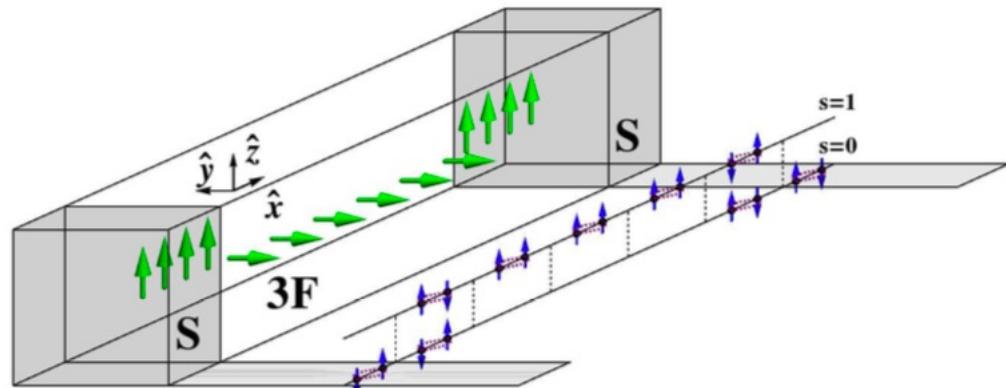
Frequency-dependent term:

$$\zeta_j(\omega) = \int_{-\infty}^{\infty} \zeta_j(\tau) e^{-i\omega\tau} d\tau, \rightarrow \zeta_j(\omega) = \pi[\delta(\omega - E_j) + \delta(\omega + E_j)] - \pi[1 - 2f(E_j)][\delta(\omega - E_j) - \delta(\omega + E_j)].$$

Discrete/Continuous configurations

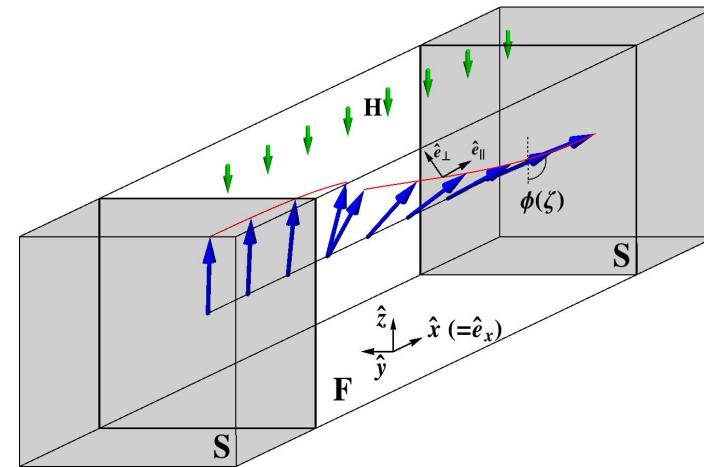
- Research done by group involves discrete and continuous layers.
- We compare the behavior of the pair correlations in both types of layers.

Discrete magnetization
(Ex: S3FS)



Ferromagnetic interface is located at specific sites

Continuous magnetization
(Ex: Helical)



Ferromagnetic interface is located at each of sites

Homogeneous vs. Inhomogeneous magnetization

$$|s,m\rangle = |0,0\rangle \quad \text{Singlet superconductor}$$

Homogeneous F $\longrightarrow \downarrow$

$$\alpha_{0,0} |0,0\rangle + \alpha_{1,0} |1,0\rangle \quad (\text{FFLO state})$$
$$+ \cancel{\alpha_{1,1} |1,1\rangle + \alpha_{1,-1} |1,-1\rangle}$$

Only the singlet and $m = 0$ triplet are seen (fast decay)

Rotation of
magnetization $\longrightarrow \downarrow$

$$\sum_{s=0,1} \sum_{m=0,\pm 1} \alpha_{s,m} |s,m\rangle$$

The $m = \pm 1$ triplets appear (slow decay) when the quantization axis is rotated (mixing)

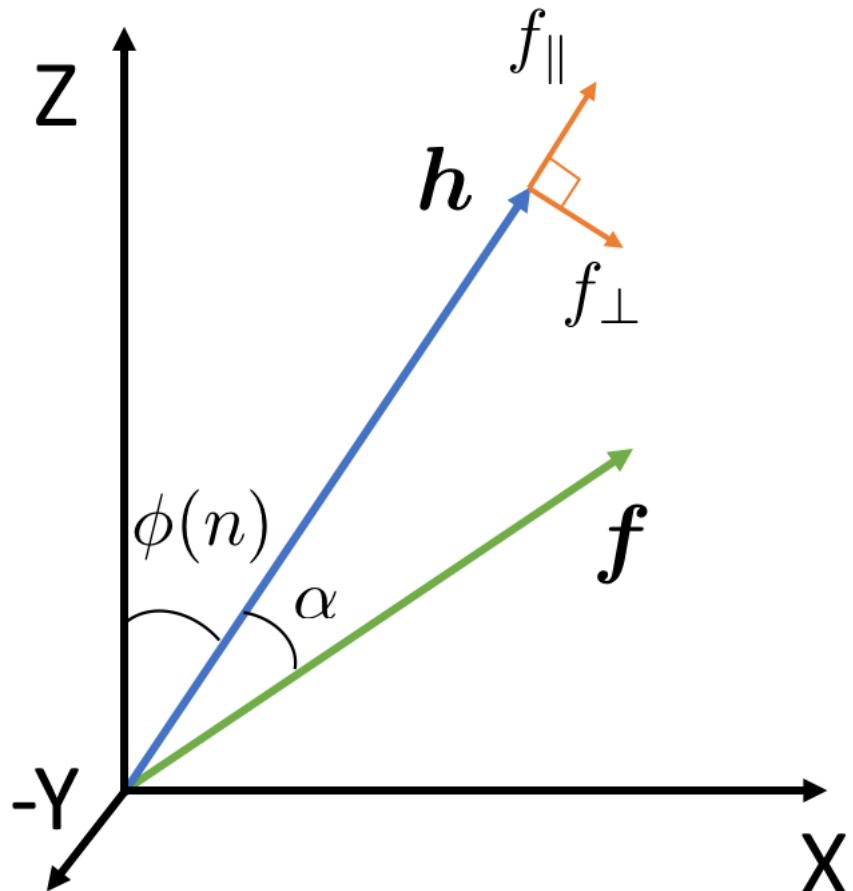
$$|0,0\rangle \Rightarrow \alpha_{0,0} |0,0\rangle + \alpha_{1,0} |1,0\rangle + \alpha_{1,1} |1,1\rangle + \alpha_{1,-1} |1,-1\rangle$$

- ✓ We study the mixing of $|s,m\rangle$ states at each rotation of the magnetization.

Rotation of quantization axis

Magnetization vector:

$$\mathbf{h}(n) = |\mathbf{h}| \sin \phi(n) \hat{\mathbf{x}} + |\mathbf{h}| \cos \phi(n) \hat{\mathbf{z}}$$



Gor'kov vector:

$$\mathbf{f}(y) = f_x(y) \hat{\mathbf{x}} + f_z(y) \hat{\mathbf{z}}$$

Gor'kov vector with angle dependence:

$$\begin{aligned}\mathbf{f}(y) &= |\mathbf{f}| [\sin(\phi + \alpha), 0, -\cos(\phi + \alpha)]_{x,y,z} \\ &= |\mathbf{f}| (\cos \alpha, 0, -\sin \alpha)_{\perp,y,\parallel}\end{aligned}$$

Transformation:

$$\begin{pmatrix} f_{\perp} \\ f_{\parallel} \end{pmatrix} = \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} f_x \\ f_z \end{pmatrix} = \begin{pmatrix} f_x \cos \phi - f_z \sin \phi \\ f_x \sin \phi + f_z \cos \phi \end{pmatrix}$$

This rotation leads to →

$$f_{1,0} = f_{\parallel}$$

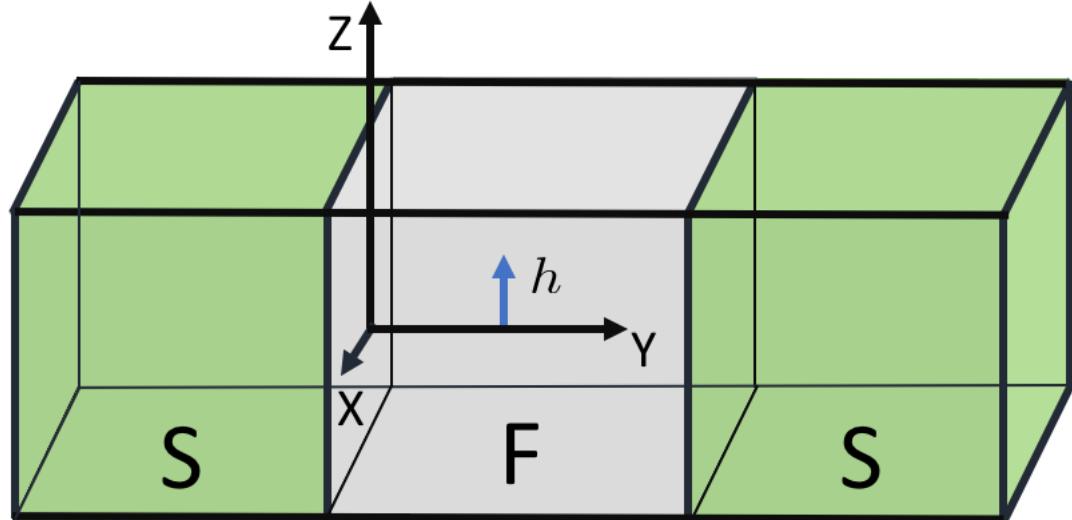
$$f_{1,1} = f_{\perp}$$

Results:

- Discrete layers
 - I. Monolayer, Trilayer, Pentalayer
- Continuous layers (Helical)
- Comparing Ballistic and Diffusive regime

Discrete layers: Monolayer (SFS)

$$|0,0\rangle \Rightarrow \alpha_{0,0}|0,0\rangle + \alpha_{1,0}|1,0\rangle$$



Functional form:

$$f_{s,0} \sim \frac{1}{y} e^{-\frac{y}{\xi_N}} \cos\left(\frac{y}{\xi_F} + s\frac{\pi}{2}\right)$$

$$\xi_N = \frac{\hbar v_F}{2\pi T}, \quad \xi_F = \frac{\hbar v_F}{2\pi h}$$

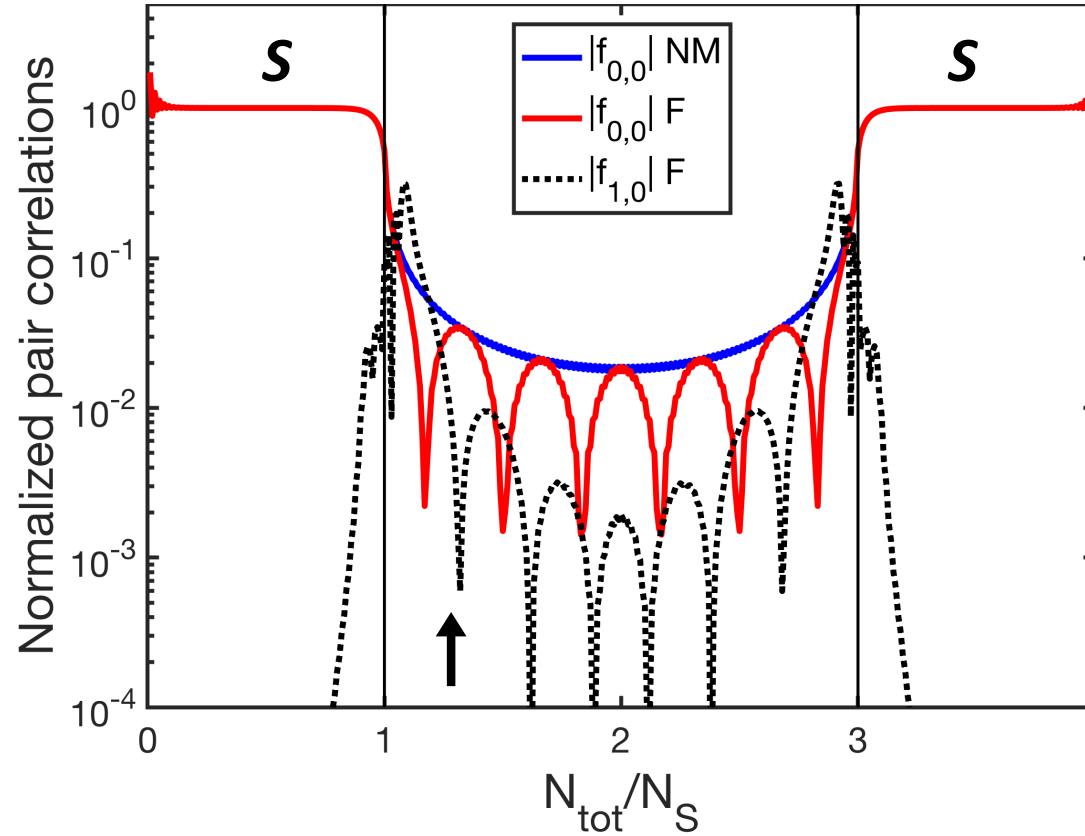
- Composed of a superconductor-ferromagnet-superconductor.
- Homogeneous magnetization along the z-axis (up).

Normalization of pair correlations:

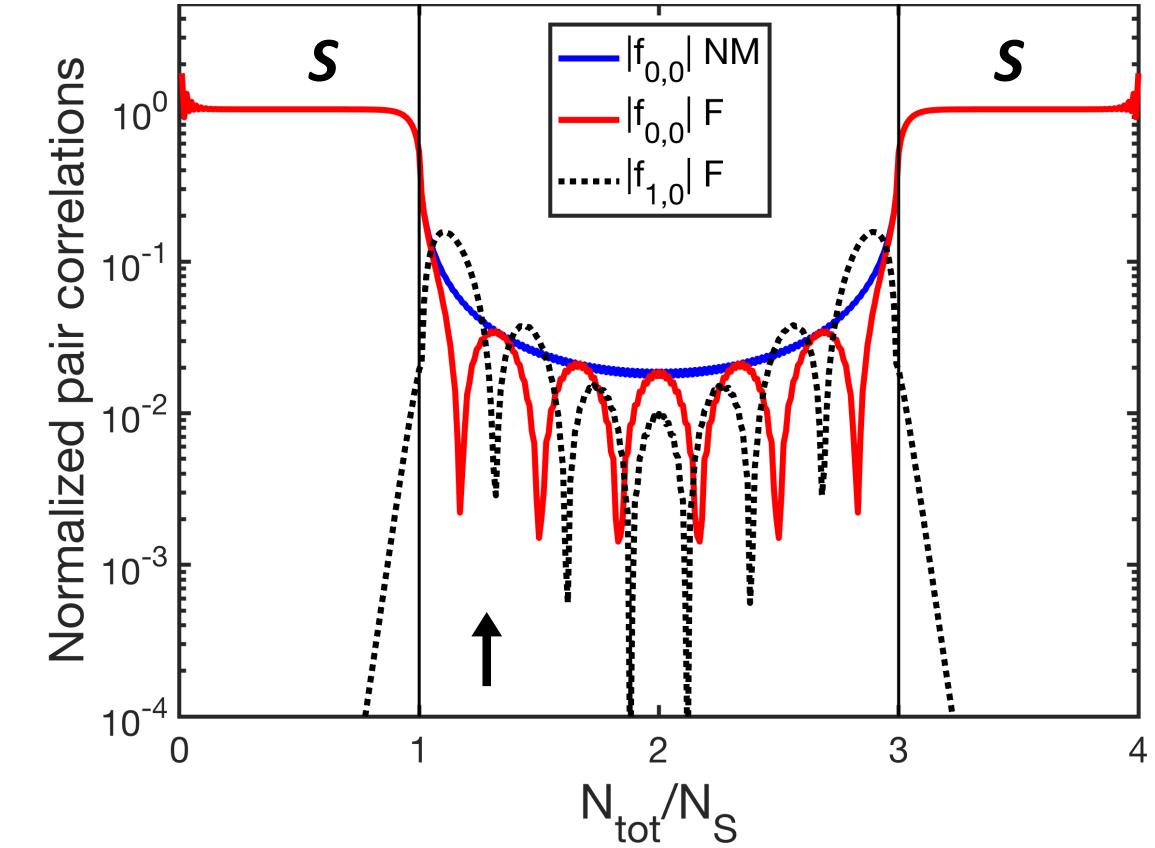
$$f_{s,m}^{norm} = \frac{f_{s,m}}{f_{0,0}^{avg}}$$

SFS Junction: Time vs. Frequency Domain

$n = 0.5$
 $h = 0.1t$



Pair correlations in the
time domain: $\tau = 10$



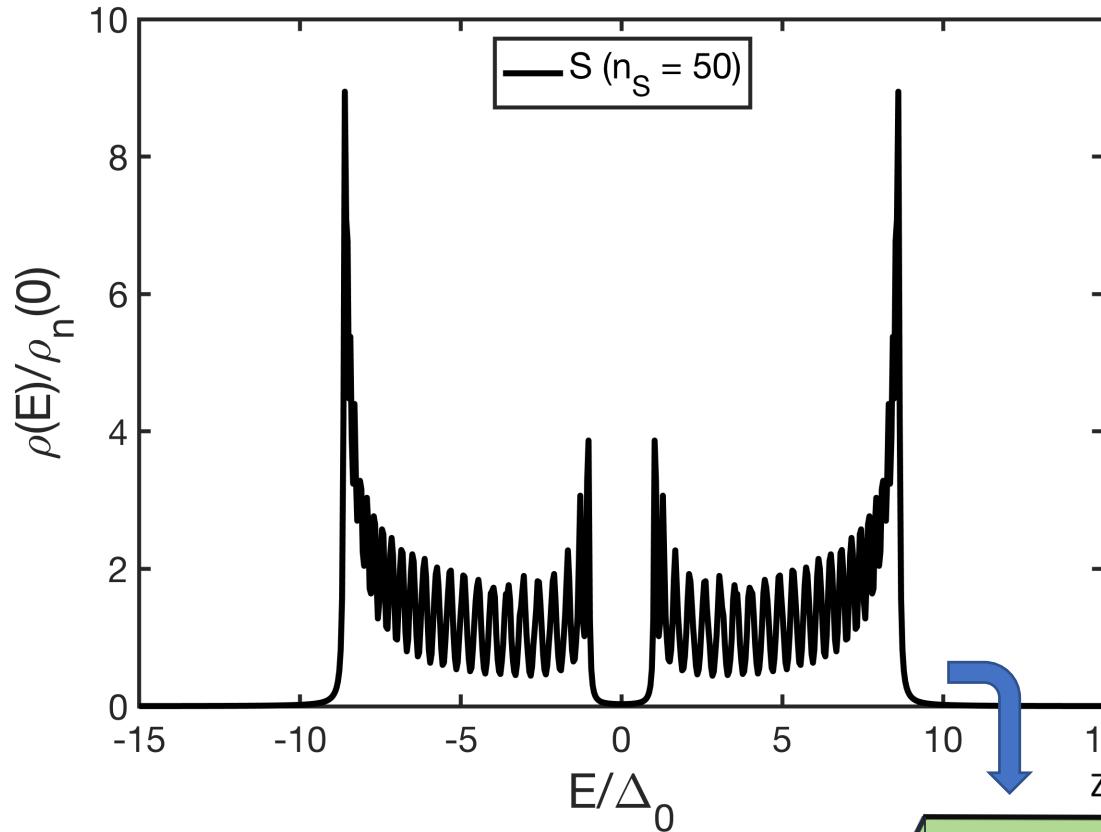
Pair correlations in the
frequency domain: $\omega = 0.1t$

We will now only present pair correlations in the frequency regime

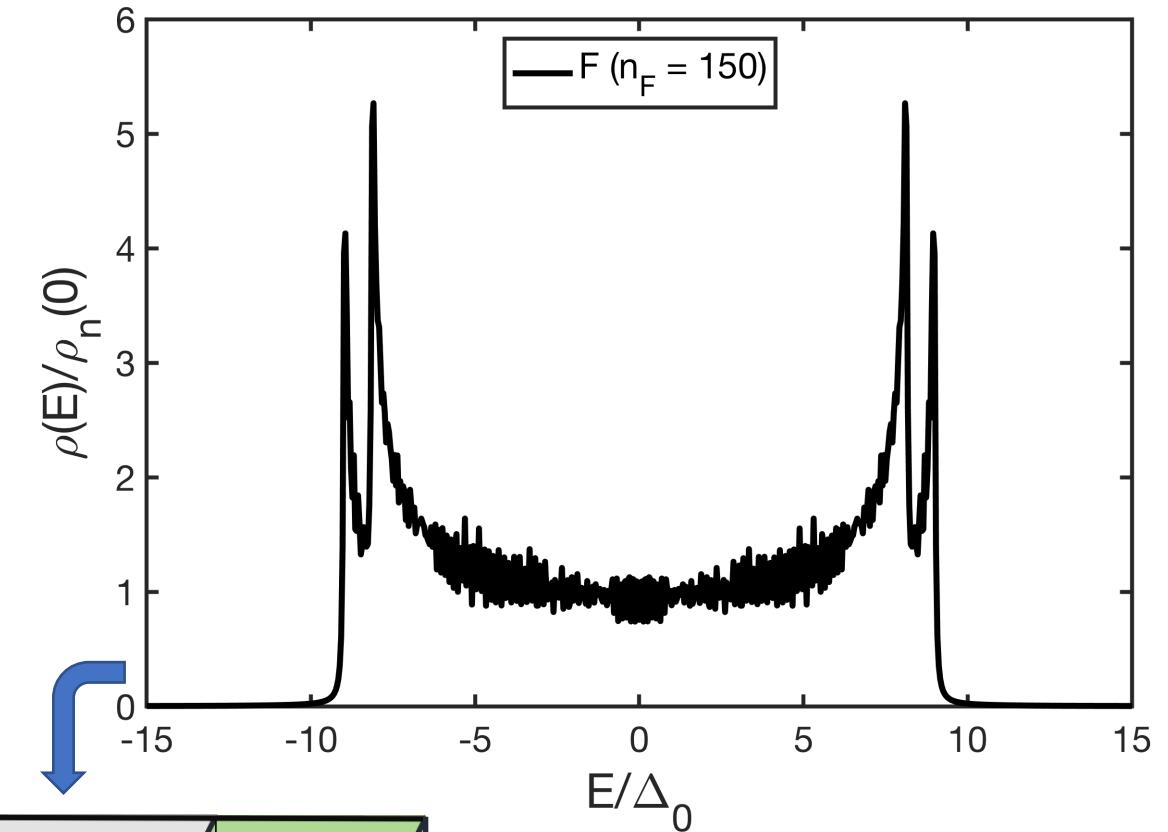
SFS Junction: Local Density of States (LDoS)

$n = 0.5$
 $h = 0.1t$

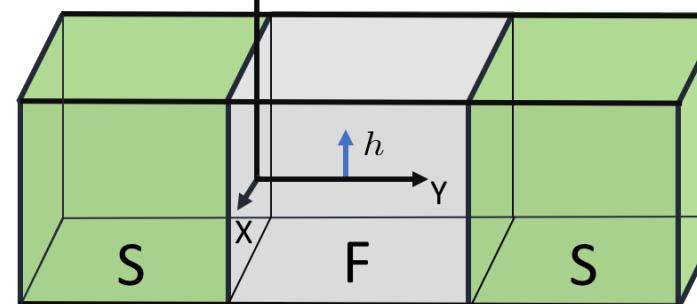
LDoS inside superconductor



LDoS inside ferromagnet



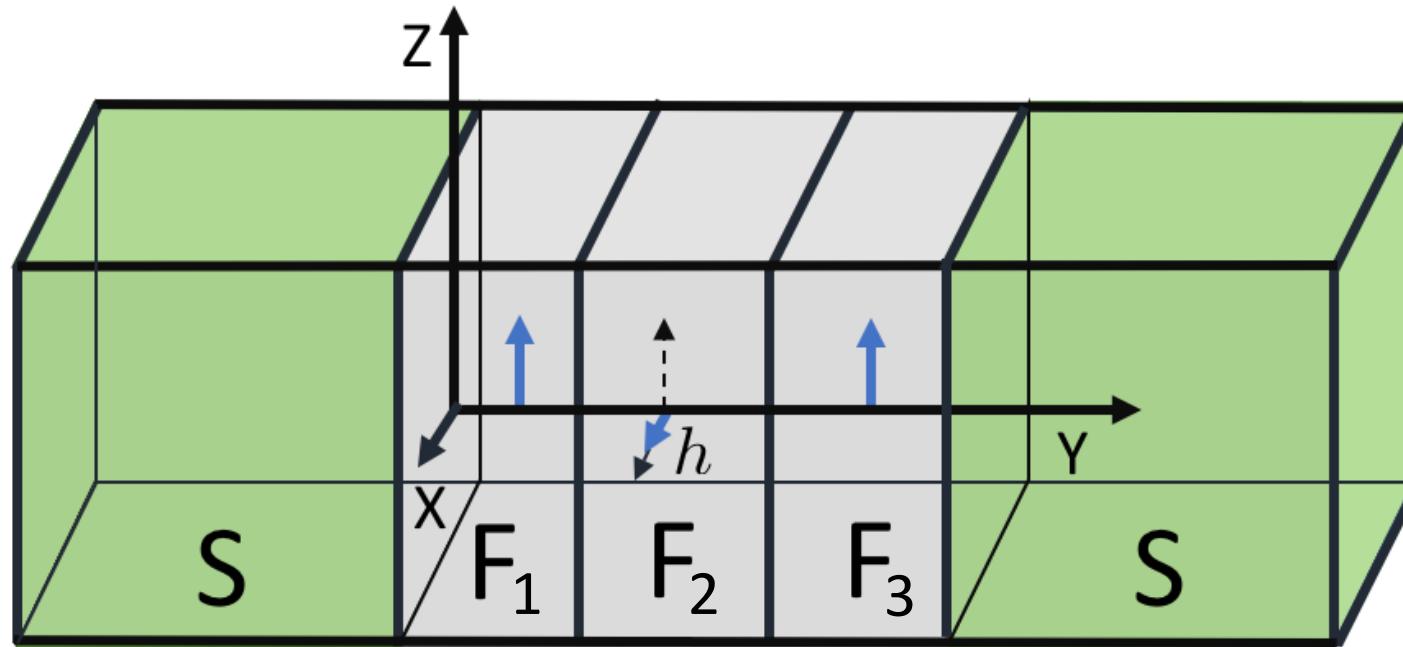
Van Hove
singularities



Spin
splitting

Discrete layers: Trilayer (S3FS)

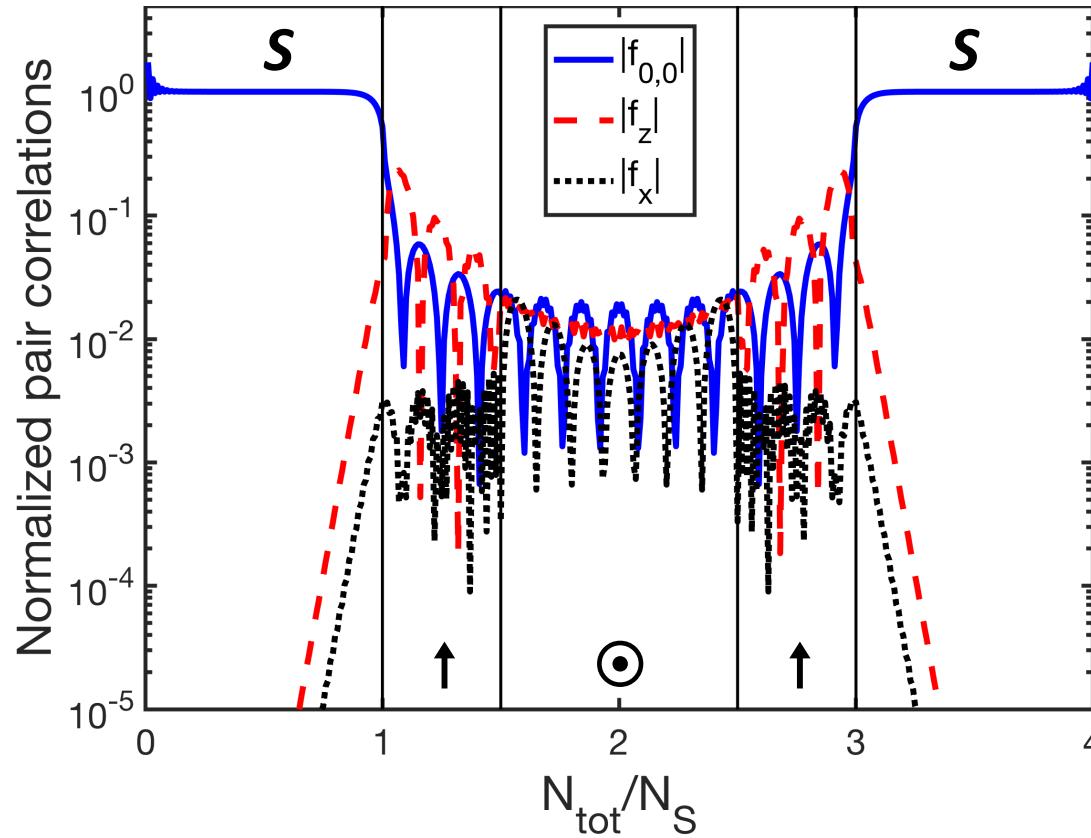
$$|0,0\rangle \Rightarrow \alpha_{0,0}|0,0\rangle + \alpha_{1,0}|1,0\rangle + \alpha_{1,1}|1,1\rangle + \alpha_{1,-1}|1,-1\rangle$$



- Josephson junction with magnetic material made up of three ferromagnets.
- Magnetization direction is up, out, up.

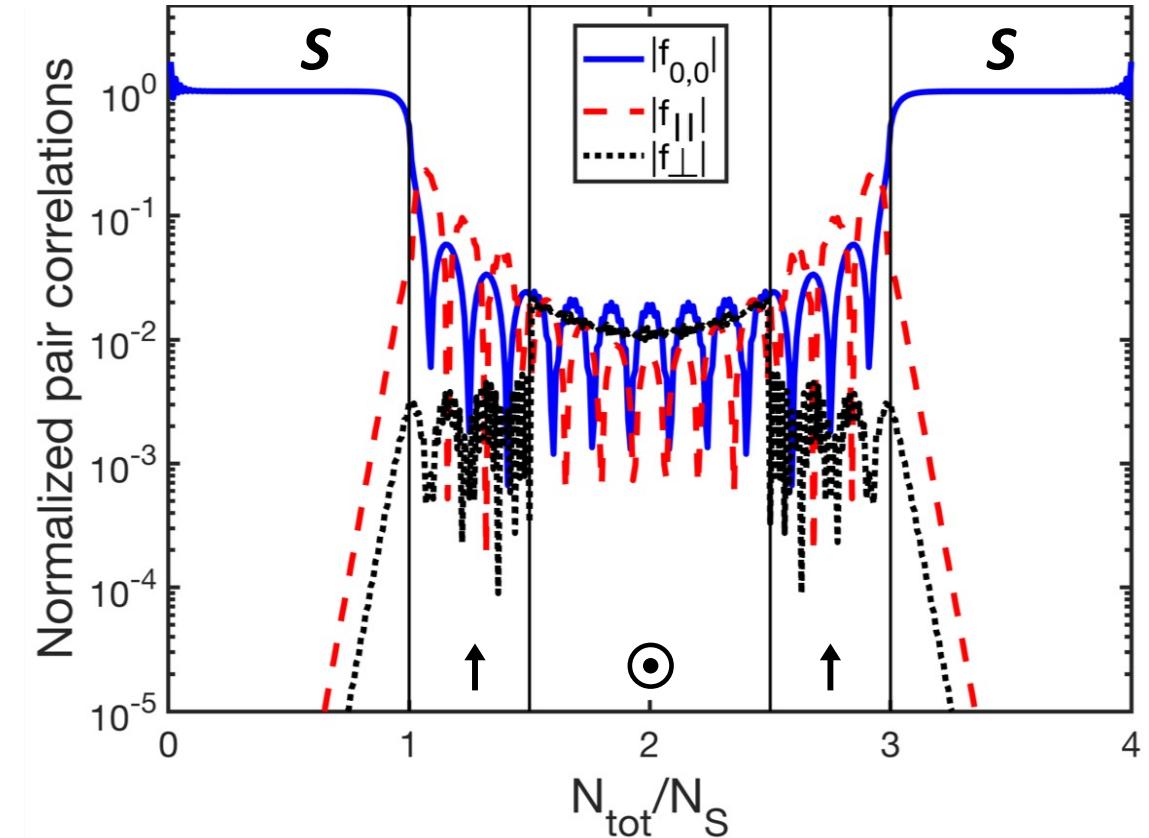
S3FS Junction: Cartesian vs. Rotating Basis

$n = 0.5$
 $h = 0.2t$
 $\omega = 0.1t$



Pair correlations in
Cartesian (static) basis

$$f_z \neq f_{1,0}, f_x \neq f_{1,1}$$

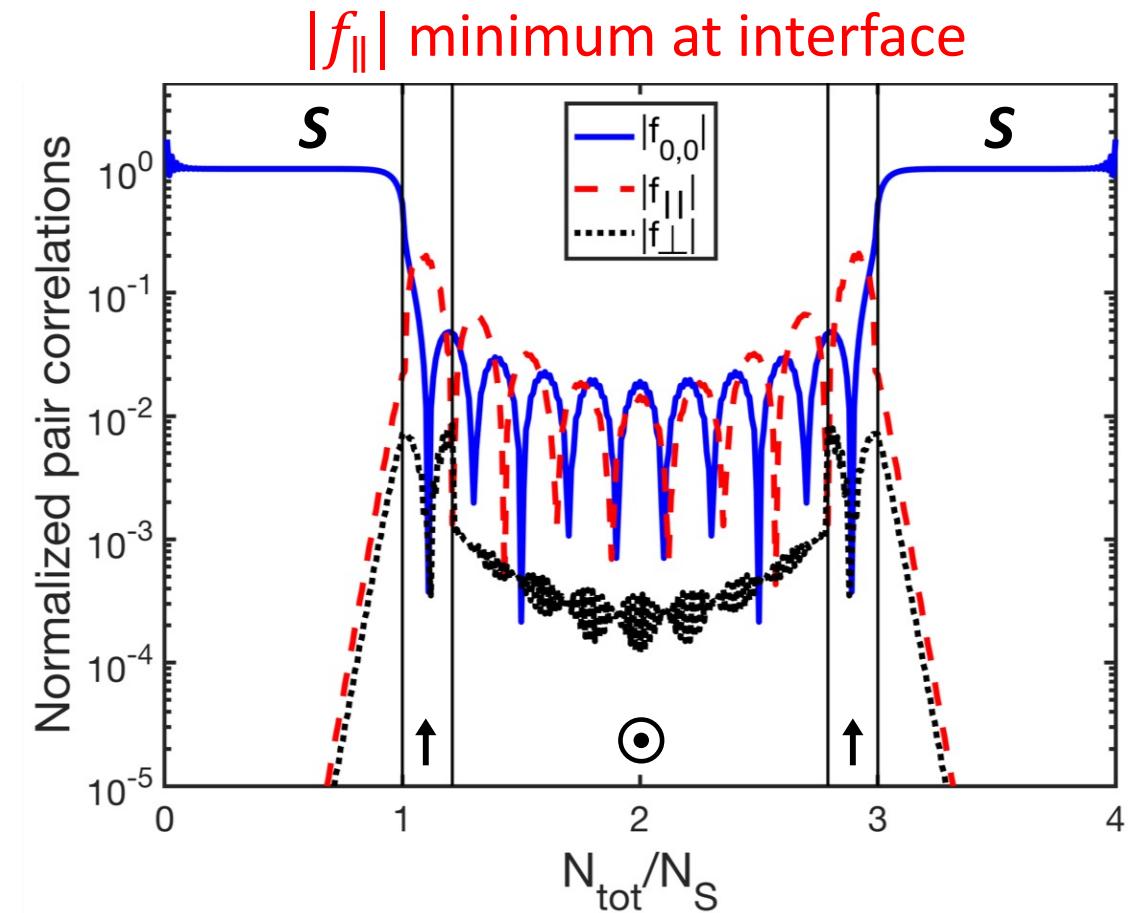
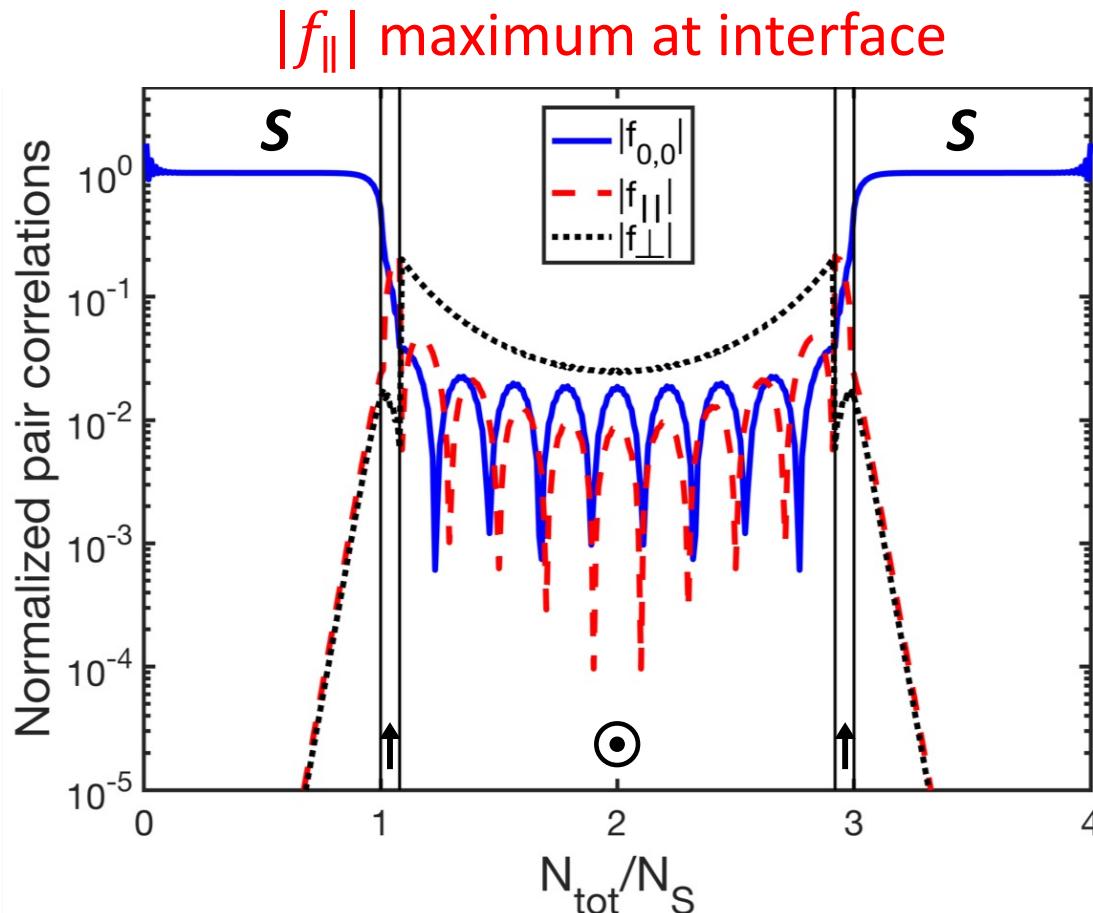


Pair correlations in
rotating basis

$$f_{||} = f_{1,0}, f_{\perp} = f_{1,1}$$

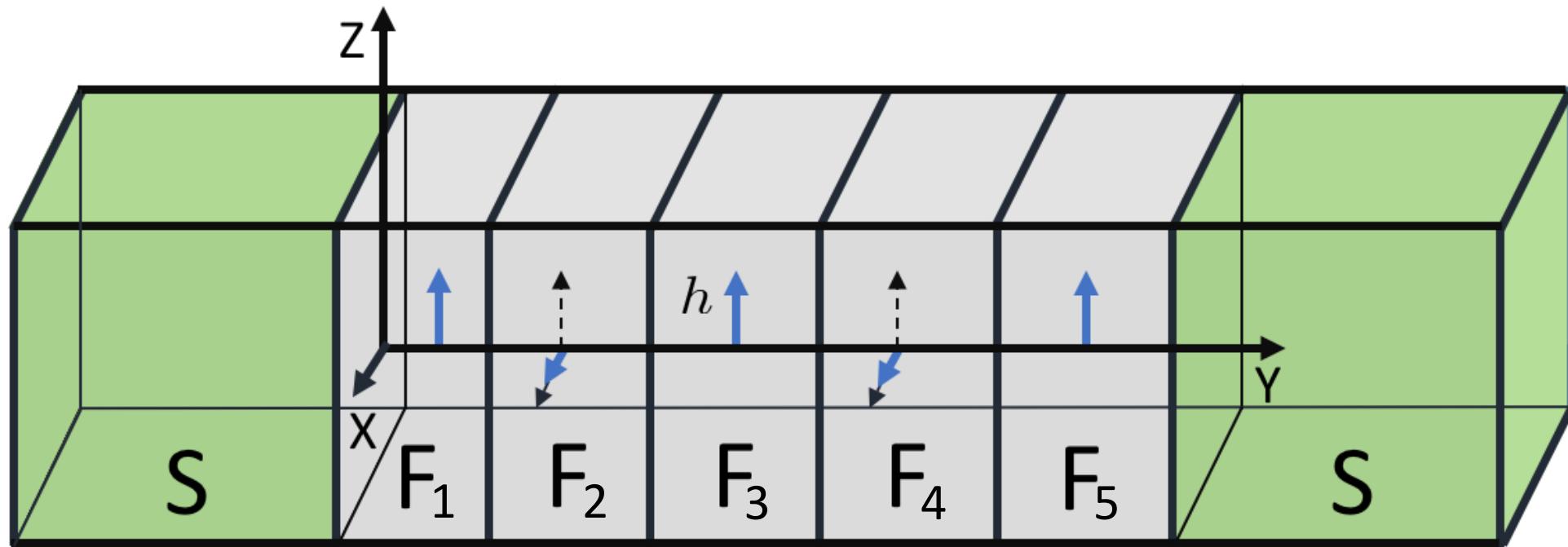
S3FS Junction: Width Dependence

$n = 0.5$
 $h = 0.15t$
 $\omega = 0.1t$



Discrete layers: Pentalayer (S5FS)

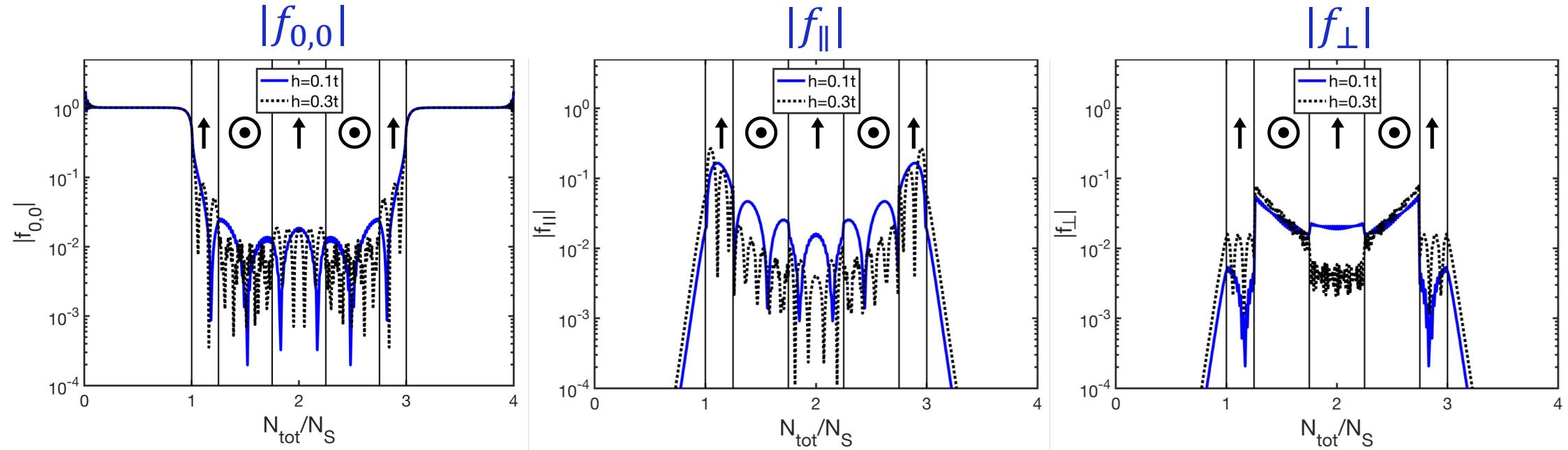
$$|0,0\rangle \Rightarrow \alpha_{0,0}|0,0\rangle + \alpha_{1,0}|1,0\rangle + \alpha_{1,1}|1,1\rangle + \alpha_{1,-1}|1,-1\rangle$$



- Josephson junction with magnetic material composed of five ferromagnets.
- Magnetization direction is up, out, up, out, up.

$n = 0.5$
 $\omega = 0.1t$

S5FS Junction: Magnetization Dependence

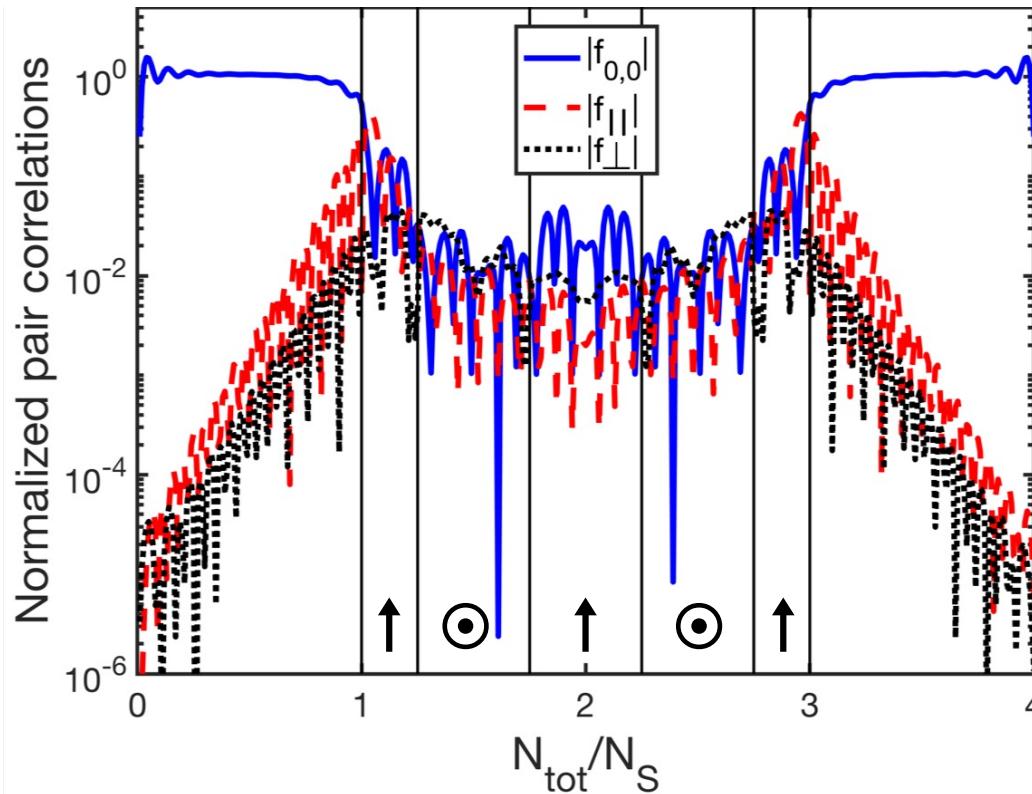


Blue smooth curve is $h = 0.1t$
Black dotted curve is $h = 0.3t$

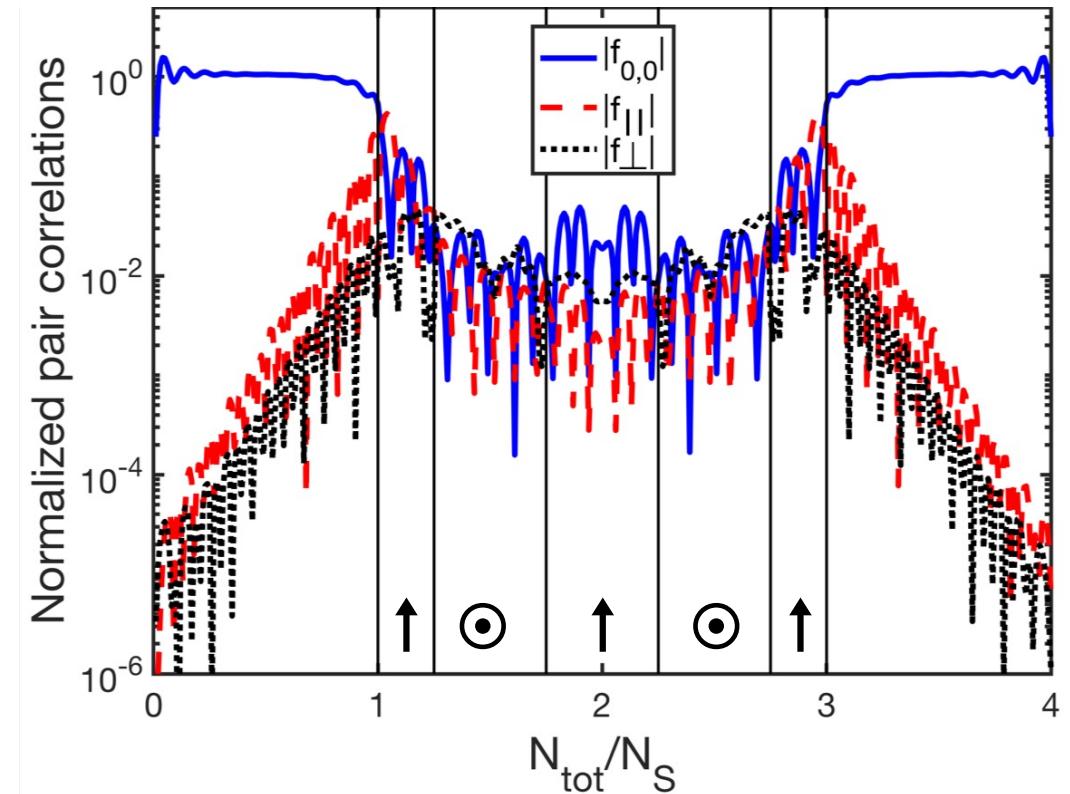
S5FS Junction: Particle-Hole Symmetry

$h = 0.1t$
 $\omega = 0.1t$

Filling: $n = 0.1$ (Nearly-empty)

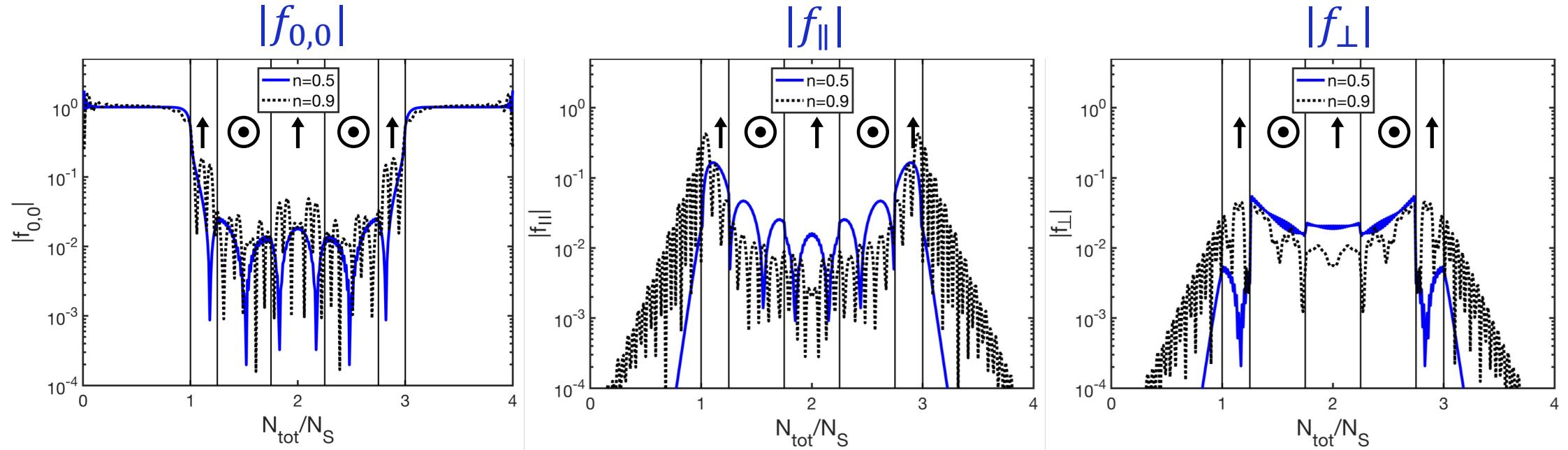


Filling: $n = 0.9$ (Nearly-full)



$n = 0.5$ $\omega = 0.1t$

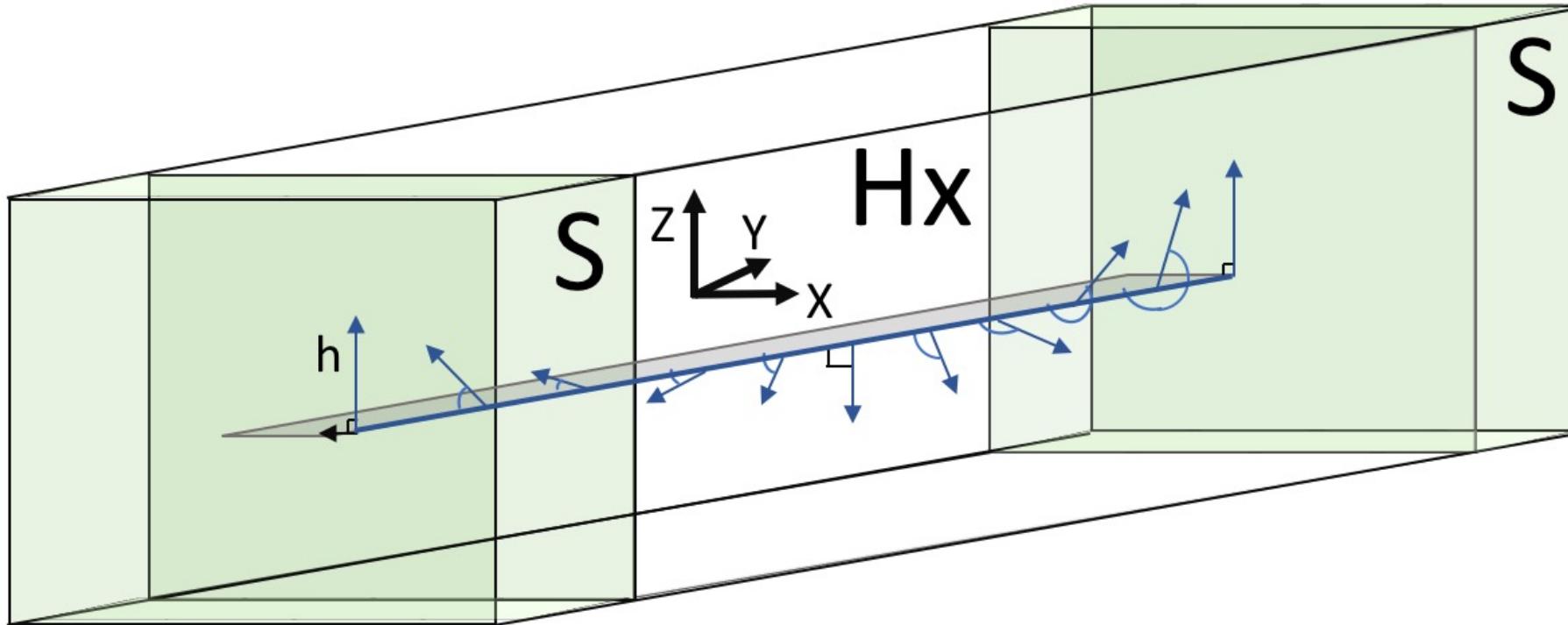
S5FS Junction: Band Filling Dependence



Blue smooth curve is $n = 0.5$
Black dotted curve is $n = 0.9$

Continuous layers: Helical configuration

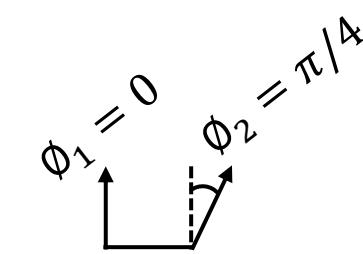
$$|0,0\rangle \Rightarrow \alpha_{0,0}|0,0\rangle + \alpha_{1,0}|1,0\rangle + \alpha_{1,1}|1,1\rangle + \alpha_{1,-1}|1,-1\rangle$$



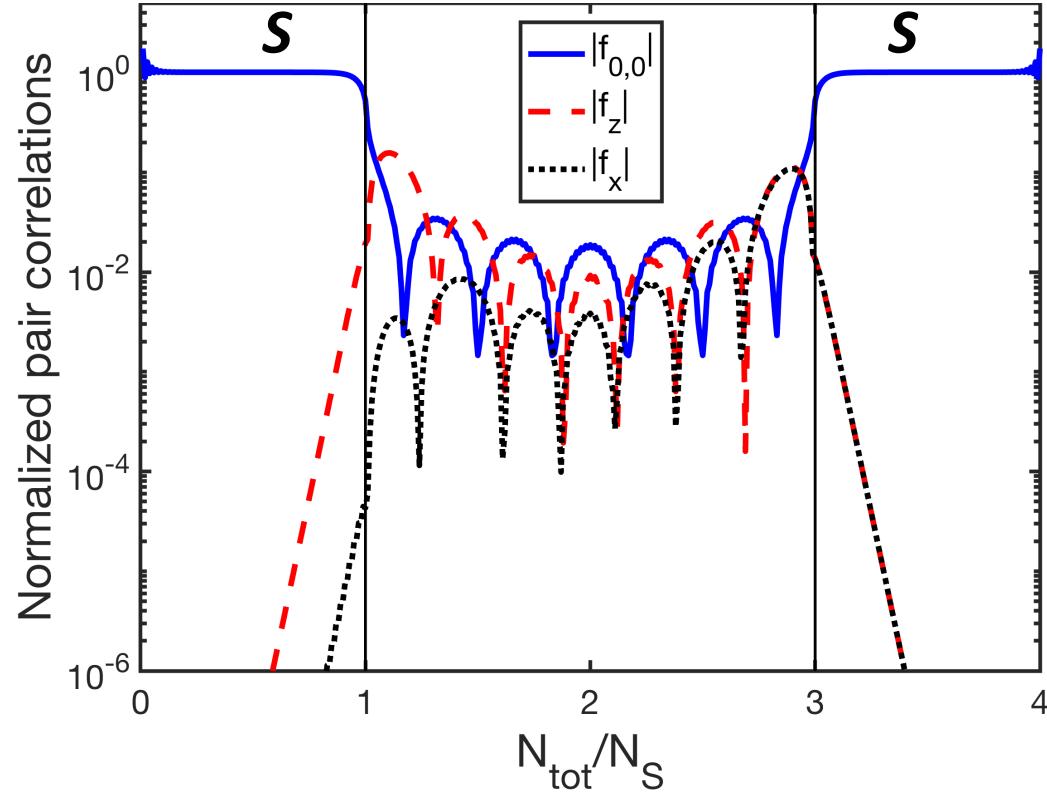
- Josephson junction with a continuous magnetic material.
- Helical configuration.

SHxS Junction: Rotating Basis

Rotation angle: $\Delta\phi = \frac{\pi}{4}$

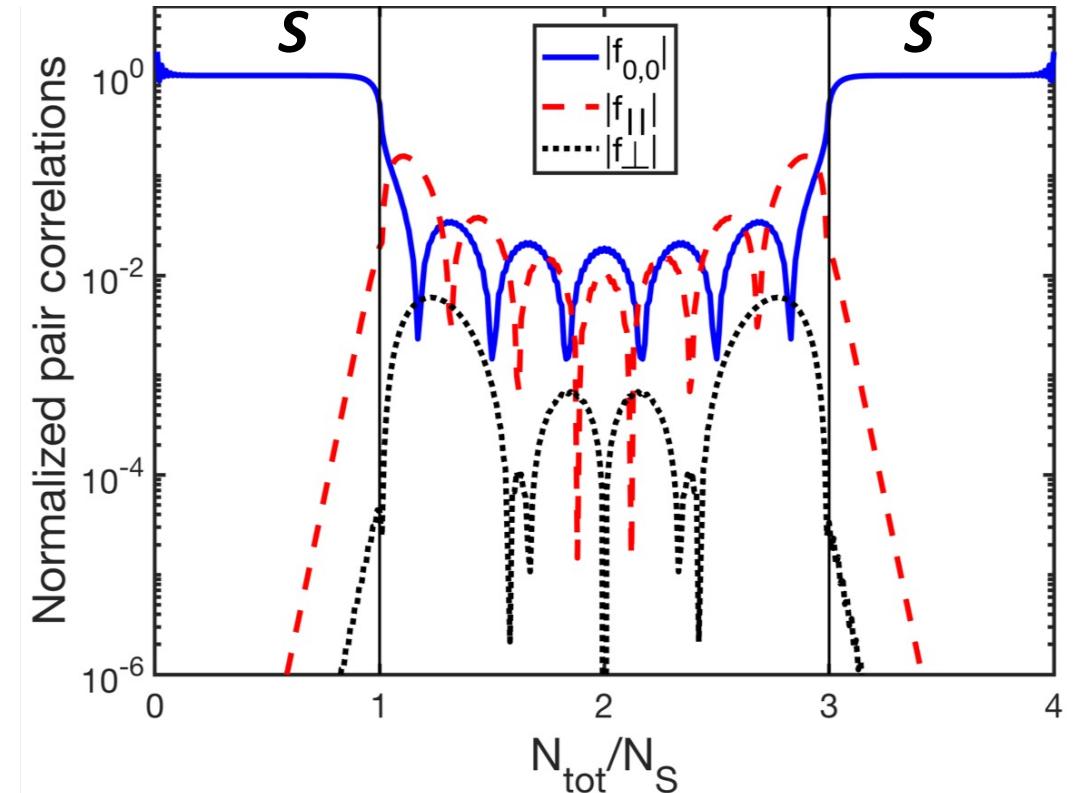


$n = 0.5$
 $h = 0.1t$
 $\omega = 0.1t$



Pair correlations in
Cartesian (static) basis

$$f_z \neq f_{1,0}, f_x \neq f_{1,1}$$

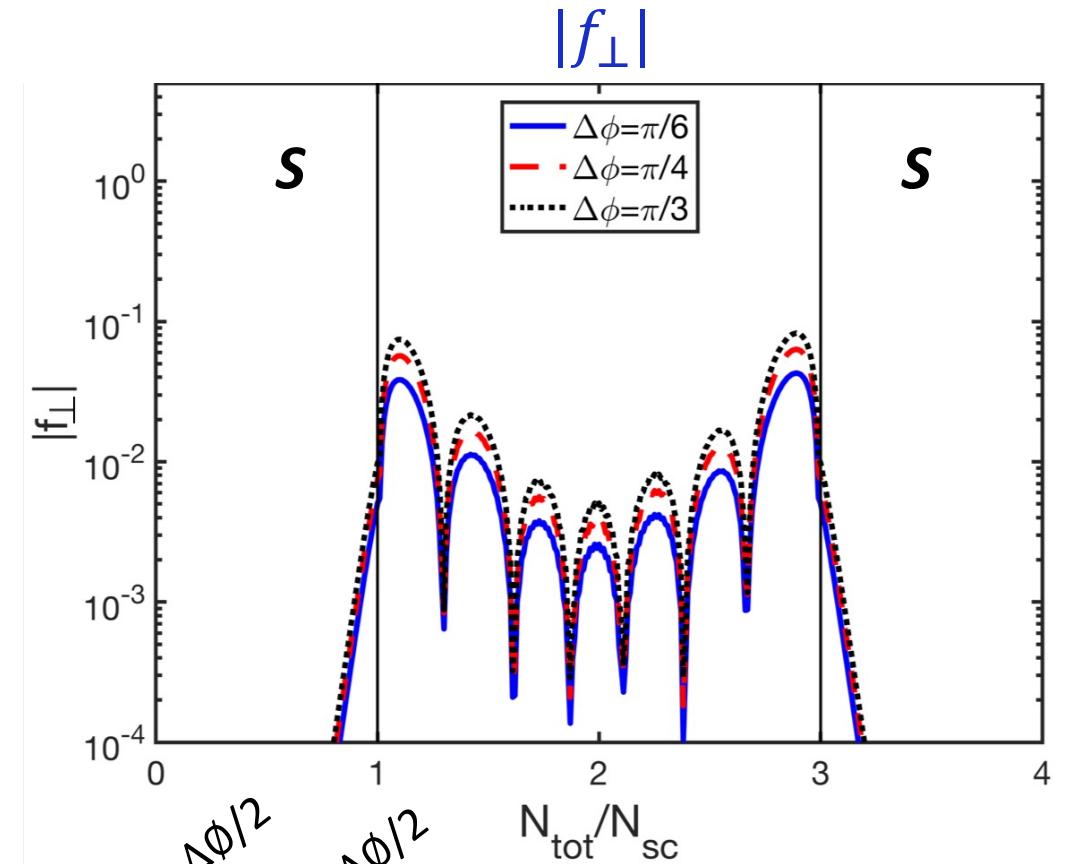
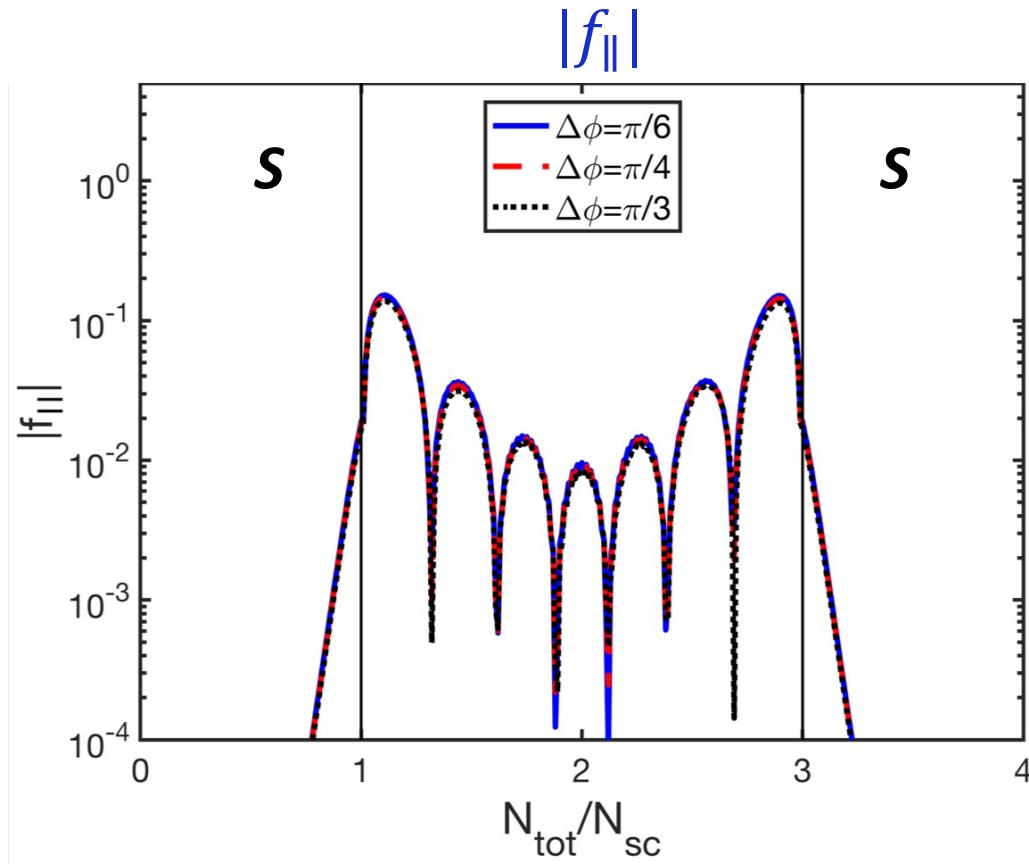


Pair correlations in
rotating basis

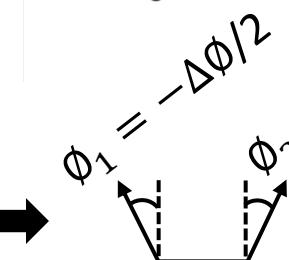
$$f_{\parallel} = f_{1,0}, f_{\perp} = f_{1,1}$$

SHxS Junction: Rotation Angle Dependence

$n = 0.5$
 $h = 0.1t$
 $\omega = 0.1t$

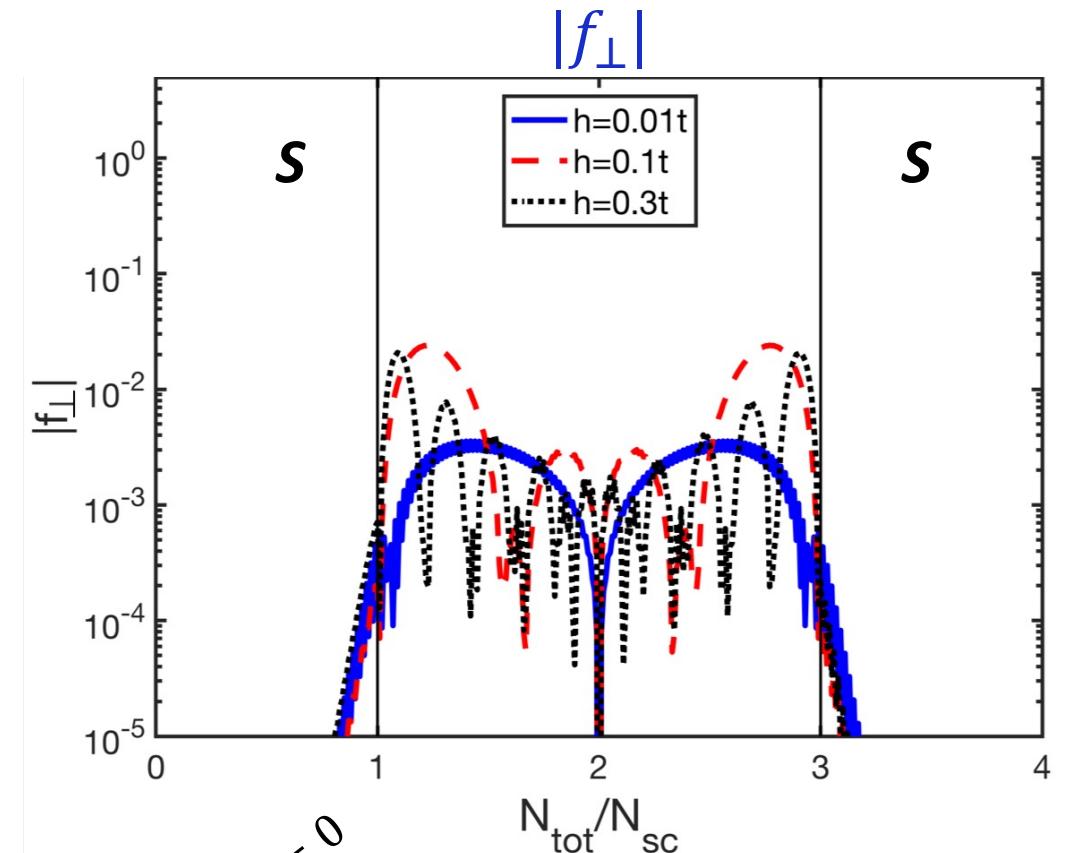
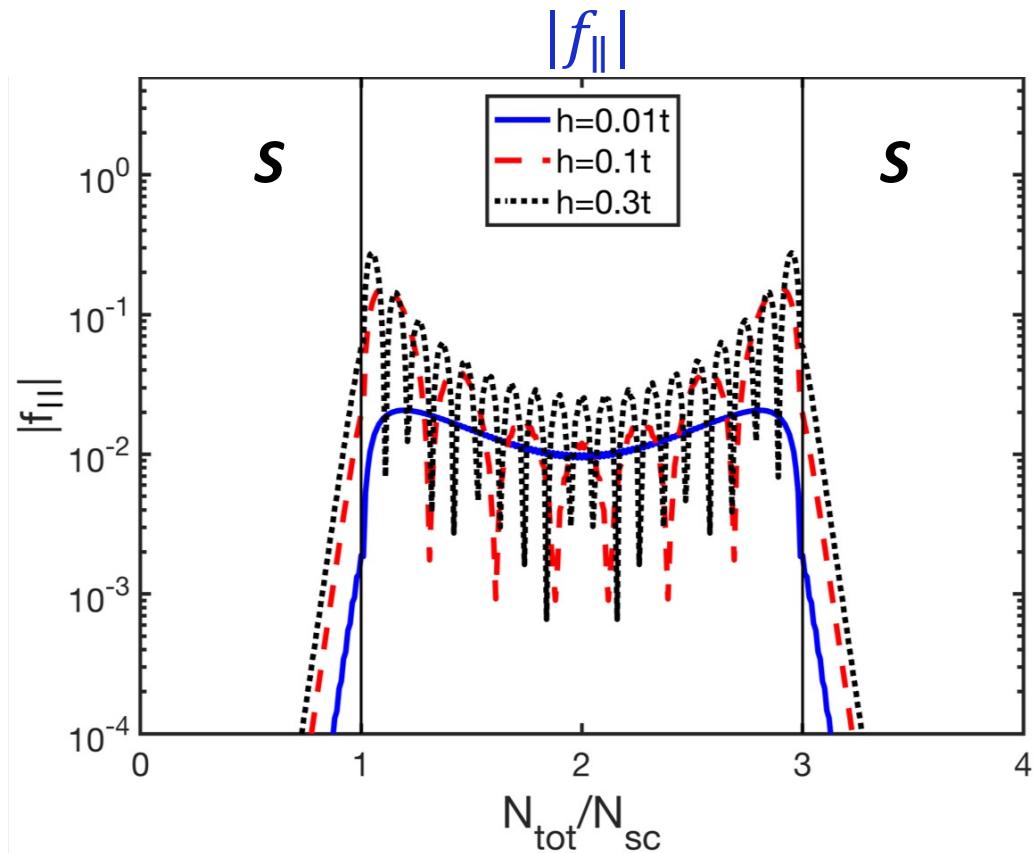


Rotation angle: $\Delta\phi$



SHxS Junction: Magnetization Dependence

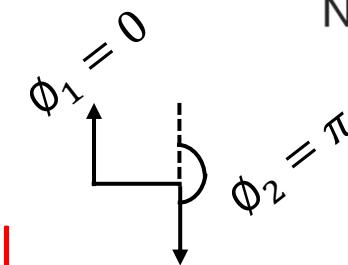
$n = 0.5$
 $\omega = 0.1t$



Rotation angle: $\Delta\phi = \pi$

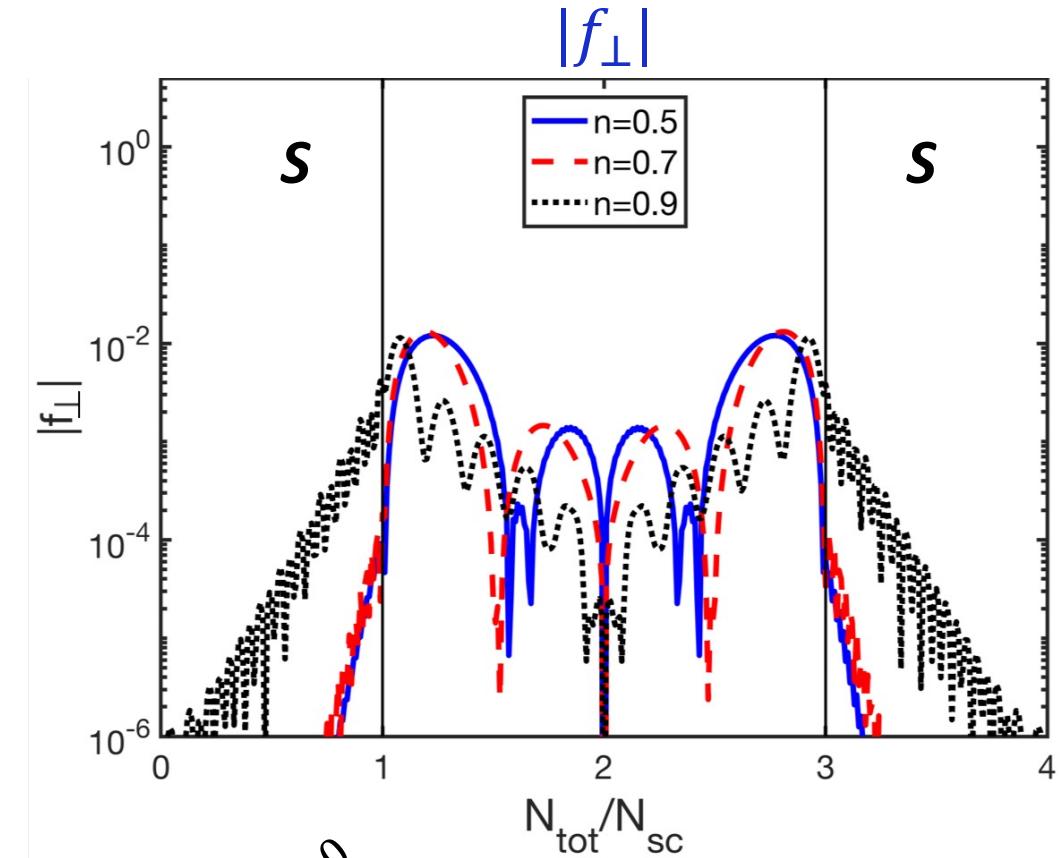
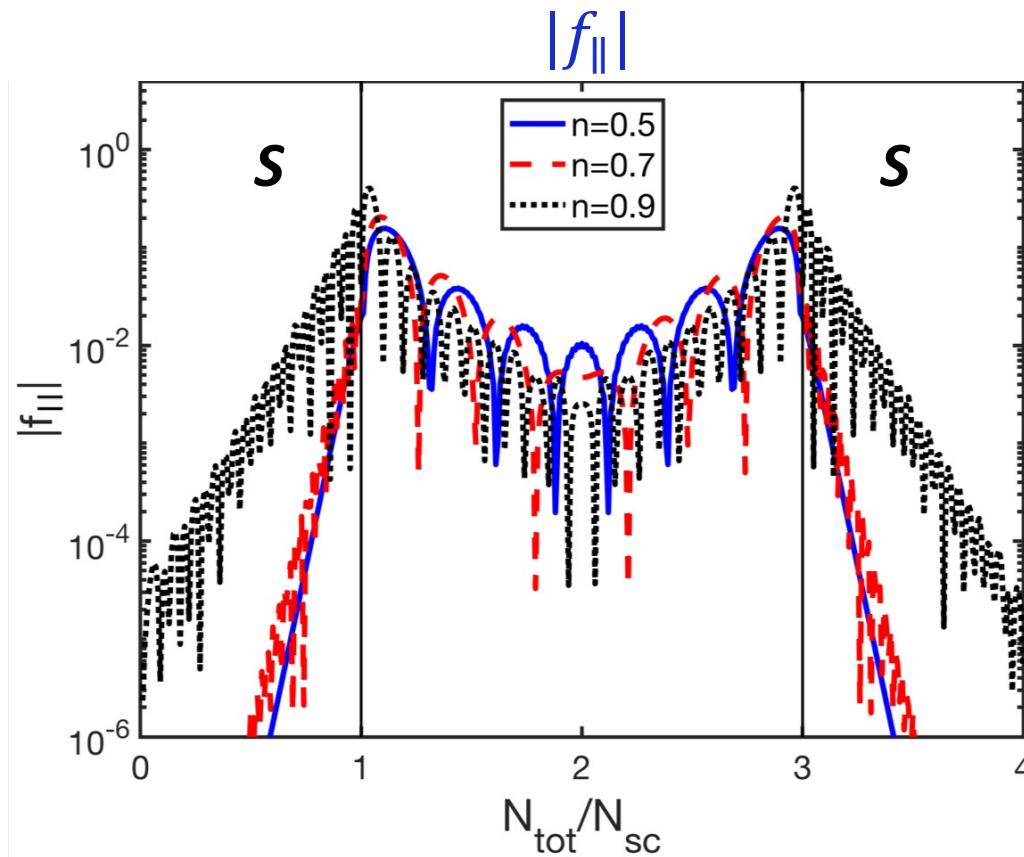


Bloch domain wall

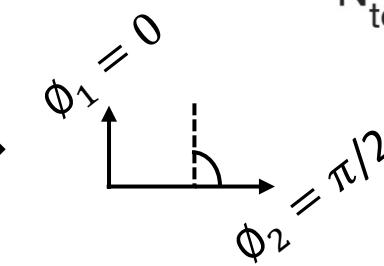


SHxS Junction: Band Filling Dependence

$h = 0.1t$
 $\omega = 0.1t$



Rotation angle: $\Delta\phi = \pi/2$



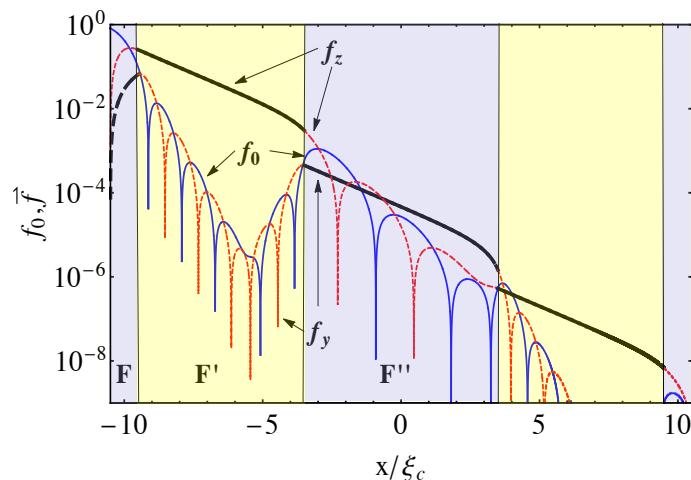
Ballistic vs. Diffusive regime: Comparison

- Diffusive regime: many nonmagnetic impurities.
- Clean regime: no impurities, strong dependence on chemical potential.

Diffusive regime

$$f_0(x) \propto e^{-x/\xi_F} \cos\left(\frac{x}{\xi_F}\right).$$

$$\xi_F = \sqrt{\frac{\hbar D_F}{2\pi h}}$$



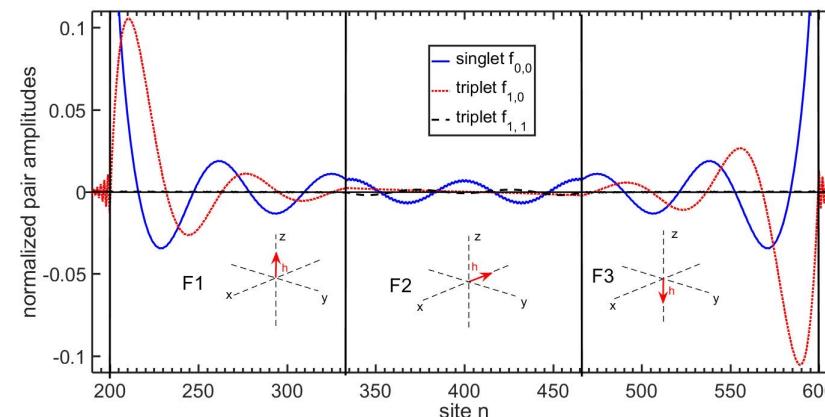
Half filling
(Log scale)

Clean regime

$$f_0(x) \propto \frac{1}{x} e^{-x/\xi_N} \cos\left(\frac{x}{\xi_F}\right)$$

$$\xi_N = \frac{v_F}{2\pi T}, \quad \xi_F = \frac{v_F}{2h}$$

v_F depends
on chemical
potential



Half filling
(Linear scale)

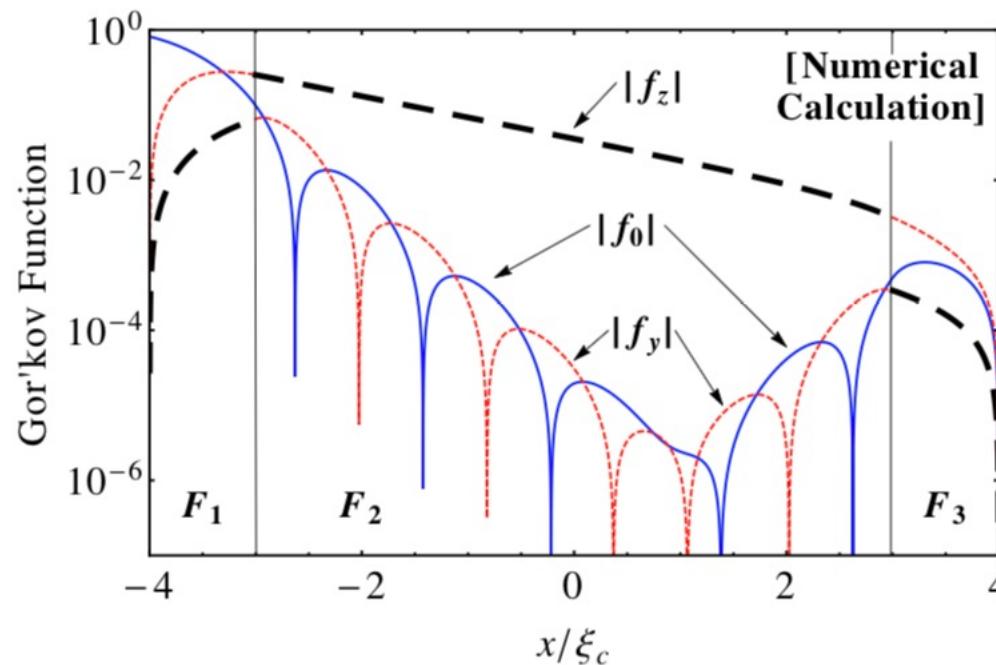
$$n = 0.5$$

$$\omega = 0.1t$$

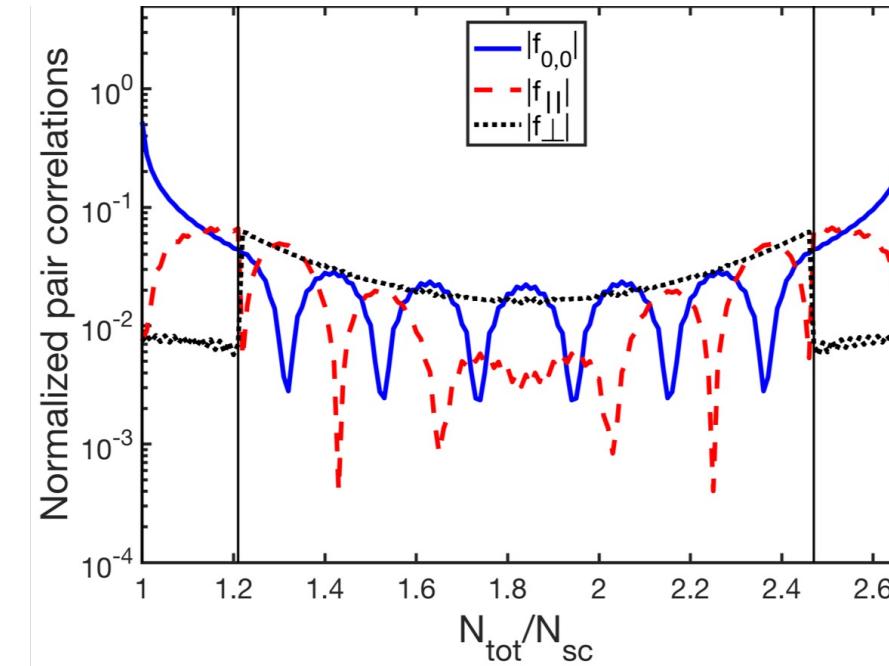
$$T = 0.4T_c$$

Ballistic vs. Diffusive Regime: S3FS Junction

- Magnetization is up, out, up



$$h_i = (3, 14, 3)\pi T_c$$



$$h_i = (13, 59, 13)\pi T_c$$

$$N_{F_i} = (1, 6, 1)\xi_c \rightarrow \xi_c = 21 \text{ sites}$$

Conclusion:

- ❖ We studied how different magnetic configurations alter the superconducting state of the hybrid structure in clean limit.
- ❖ We observe that
 - Singlet pair correlations transform into a linear combination of all four basis states of spin $\frac{1}{2}$ fermions pairs,
 - Pair correlations “bounce back” into the superconductor,
 - All pair correlations appear when the magnetization rotates.
 - A rotating basis disentangled the triplets.
 - Singlets in the clean limit behave different than in the dirty limit.

Future work:

- ❖ Determine the Josephson critical current.