Electronic Spin Susceptibility Enhancement in Pauli-Limited Superconductors

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Motivation

Superconductivity and Magnetism

-Pnictides (LaOFeAs and $BaFe_2As_2$ groups)

-Triplet superconducters ($(TMTSF)_2PF_6$, Bechgaard Salts)

-High T_c cuprates ($Ba_2Ca_4Cu_5O_{10}(F_yO_{1-y})_2$)

⇒ Heavy fermion superconductors ($CeCu_2Si_2$, $CeCoIn_5$)

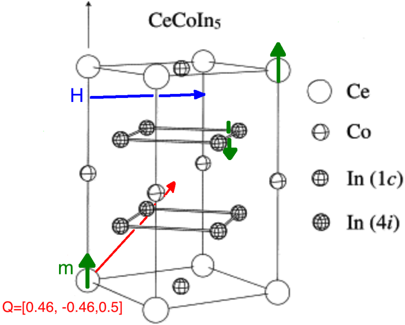
$CeCoIn_5$ Kenzelmann et al, Science (2008)

-Coexist (Q-phase)

-AntiFerromagnetic (AF)

-Pauli Limited

-D-wave symmetry



Onuki & Settai, Phys.: Condens. Matter. Kenzelmann et al, Phys. Rev. Lett. (2010)

Bianchi et al, Science (2008). Bianchi et al, Phys. Rev. Lett. (2003). Nicklas et al, Phys. Rev. B (2007).

Motivation

Q-phase Theories

-FFLO Manifestation

Yanase, Sigrist, J. Phys.: Condens. Matter (2011)(others).

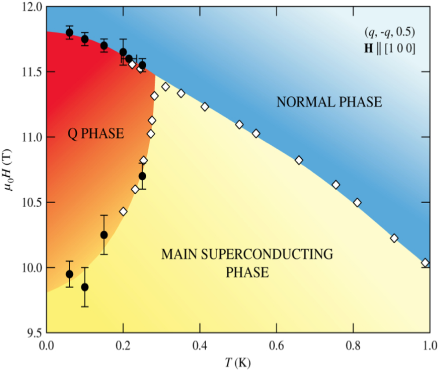
-Strong Pauli Depairing

Kato et al, Phys. Rev. Lett. (2011). Ikeda et al, Phys. Rev. B (2010).

-Strong Pauli Depairing + Vortices

Suzuki et al, Phys. Rev. B (2011).

$\Rightarrow$ **all drive Spin Density Waves**



Kenzelmann et al, Phys. Rev. Lett. (2010)

Our Goal

-Use first principles to explore itinerant electron susceptibility in superconducting and normal state systems with strong Pauli effects

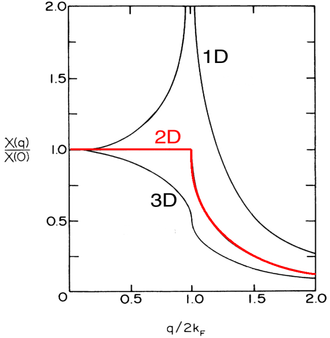
NORMAL $\Longleftrightarrow$ *Superconducting*

$$\frac{1}{\chi^N(\mathbf{q})} = \frac{1 - J_{\mathbf{q}}\chi_0^N(\mathbf{q})}{\chi_0^N(\mathbf{q})} << 1 \quad \Longleftrightarrow \quad \frac{1}{\chi^{sc}(\mathbf{q})} = \frac{1 - J_{\mathbf{q}}\chi_0^{sc}(\mathbf{q})}{\chi_0^{sc}(\mathbf{q})} = 0$$

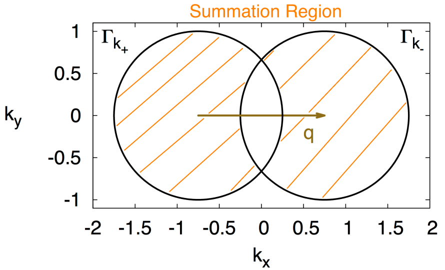
Normal State, H_0=0

LINDHARD FUNCTION (static)

$$\chi^N \propto \sum_{\mathbf{k}} \frac{f(\xi_{k_-}) - f(\xi_{k_+})}{\xi_{k_-} - \xi_{k_+}} \qquad \mathbf{k}_\pm = \mathbf{k} \pm \mathbf{q}/2$$



-Roshen and Ruvalds, Phys. Rev. B (1983)

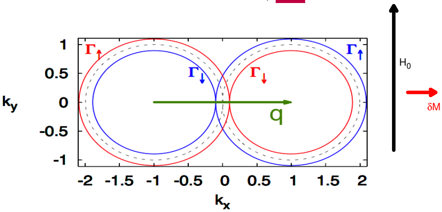


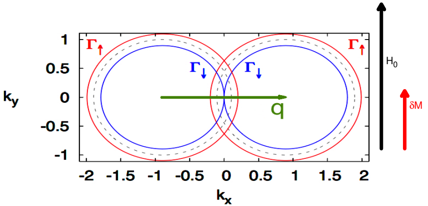
Discontinuity in $\frac{d^{d-1}}{dq^{d-1}}\chi$ (d=dimensions) occurs when the Fermi Surfaces Γ_{k_-} and Γ_{k_+} are tangent.

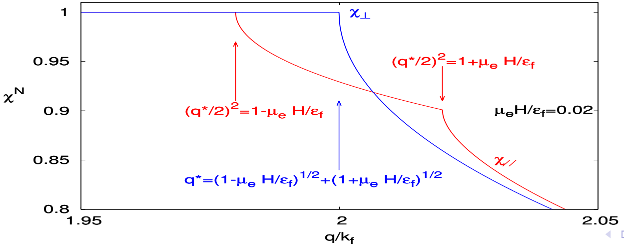
Normal State, $H = H_0 + \delta H \neq 0$

$$\boxed{\mathbf{M}_\alpha = \mathbf{M}_{0\alpha}(\mathbf{H_0}, \mathbf{q} = \mathbf{0}) + \chi_{\alpha\beta}(q)\delta \mathbf{H}_\beta}$$

$$\chi^N_\perp \propto \sum_{\mathbf{k},s} \frac{f(\xi_{k_- s}) - f(\xi_{k_+ \bar{s}})}{\xi_{k_- s} - \xi_{k_+ \bar{s}}} \qquad \chi^N_\parallel \propto \sum_{\mathbf{k},s} \frac{f(\xi_{k_- s}) - f(\xi_{k_+ s})}{\xi_{k_- s} - \xi_{k_+ s}}$$







Discontinuity

$q* \approx 2 \pm 0.02$

$q* \approx 2 - 10^{-4}$

Superconducting State

$$\chi_{\alpha\beta}(T,H,\mathbf{q}) = \mu_e^2 \sum_{ss'tt'\mathbf{k}} \sigma^{\alpha}_{ss'}\sigma^{\beta}_{tt'} \int_0^{\beta} d\tau < c^{\dagger}_{\mathbf{k+q}s}(\tau)\, c_{\mathbf{k}s}(\tau)\, c^{\dagger}_{\mathbf{k+q}t}(0)\, c_{\mathbf{k}t'}(0) >$$

Bogoliubov Transformation

$$c^{\dagger}_{\mathbf{k}\uparrow} = u_{\mathbf{k}}\gamma^{\dagger}_{\mathbf{k}\downarrow} + v^{*}_{\mathbf{k}}\gamma_{\mathbf{k}\uparrow}$$

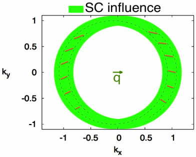
$$c_{-\mathbf{k}\downarrow} = u^{*}_{\mathbf{k}}\gamma_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\gamma^{\dagger}_{\mathbf{k}\downarrow}$$

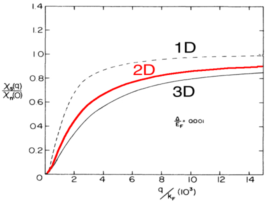
$$\epsilon_{\mathbf{k},s} = \sqrt{\Delta^2_{\mathbf{k}} + \xi^2_{\mathbf{k}}} + s\mu_e H_z$$

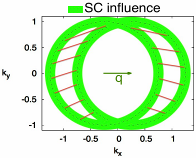
$$u^2_{\mathbf{k}} = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{\sqrt{\Delta^2_{\mathbf{k}}+\xi^2_{\mathbf{k}}}}\right)$$

$$v^2_{\mathbf{k}} = 1 - u^2_{\mathbf{k}}$$

Roshen and Ruvalds, Phys. Rev. B (1983)







Superconductivity suppresses χ for $q/k_f \lesssim \Delta/\epsilon_f$

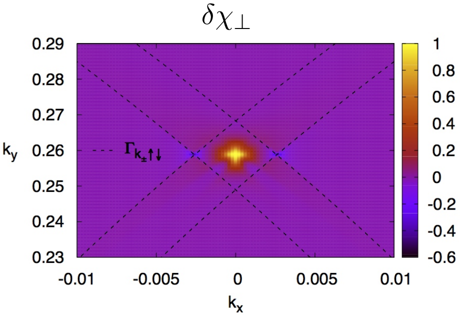
$$\chi^{SC}_{\parallel} \propto \sum_{\mathbf{k},s} \frac{(f(\epsilon_{k_-s})-f(\epsilon_{k_+s}))(u_{k_+}u_{k_-}+v_{k+}v_{k-})^2}{\epsilon_{k_-s}-\epsilon_{k_+s}} - \frac{(1-f(\epsilon_{k_-s})-f(\epsilon_{k_+\bar{s}}))(u_{k_+}v_{k_-}-v_{k+}u_{k-})^2}{\epsilon_{k_-s}+\epsilon_{k_+\bar{s}}}$$

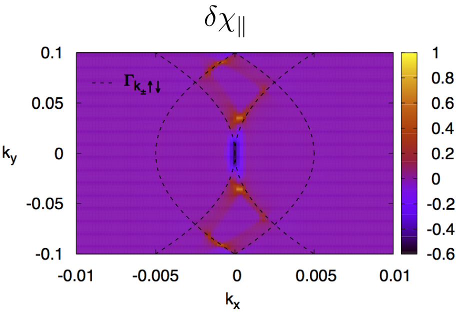
$$\chi^{SC}_{\perp} \propto \sum_{\mathbf{k},s} \frac{(f(\epsilon_{k_-s})-f(\epsilon_{k_+\bar{s}}))(u_{k_+}u_{k_-}+v_{k+}v_{k-})^2}{\epsilon_{k_-s}-\epsilon_{k_+\bar{s}}} - \frac{(1-f(\epsilon_{k_-s})-f(\epsilon_{k_+s}))(u_{k_+}v_{k_-}-v_{k+}u_{k-})^2}{\epsilon_{k_-s}+\epsilon_{k_+s}}$$

Calculation

We calculate $\boxed{\delta\chi_\alpha(q \approx 2k_f) = \chi_\alpha^{sc} - \chi_\alpha^N}$ $_{\alpha = \parallel, \perp}$ for D-wave symmetry

INTEGRAND IS STRONGLY PEAKED NEAR INTERSECTIONS OF $\Gamma_{k\pm}$





$$T = 0.005\,T_c,\ \mu_e H = 0.48\Delta_0,\ \Delta_0 = 0.01\epsilon_f,\ \text{Background} \approx 10^{-3} - 10^{-4}$$

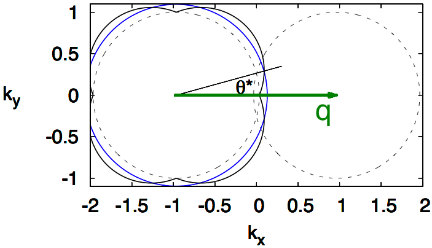
Calculation

GOAL:Maximize χ^{sc} at given T and H by varying $\mathbf{q}$

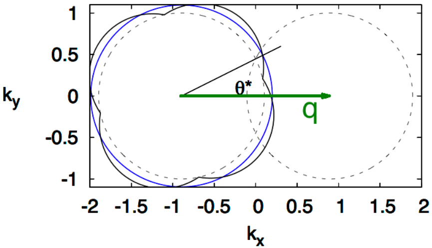
$\delta\chi \propto 1/(\text{Excitation Energies})$ $\quad \epsilon_{ks} = \sqrt{\Delta_k^2 + \xi_k^2} + s\mu_e H$

$$\epsilon_{k_-s} = \epsilon_{k_+s} = 0 \Rightarrow \boxed{\mu_e H = \Delta_{T,H} \sin 2\theta_k^*}$$

$\hat{\mathbf{q}}$=nodal direction
-Maximizes $\chi_\perp^{sc}$



$\hat{\mathbf{q}}$=off nodal direction
-Maximizes $\chi_\parallel^{sc}$

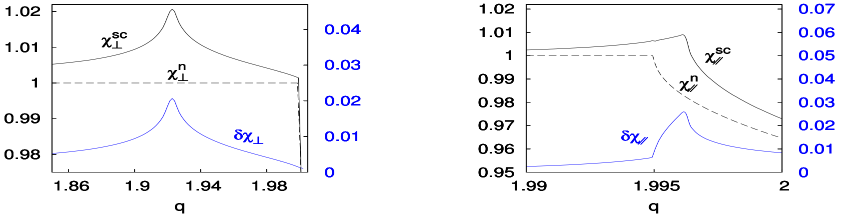


Results

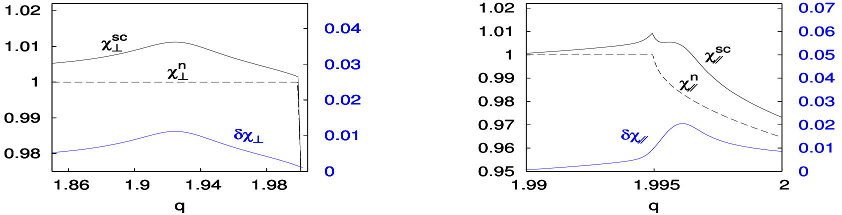
$max_{\mathbf{q}}(\delta\chi_{\perp}) = max_{\mathbf{q}}(\chi_{\perp}^{sc})$

Two possible maxima?

$T = 0.005T_c, \quad \mu_e H = 0.5\Delta_0, \quad \Delta_0 = 0.01\epsilon_f$

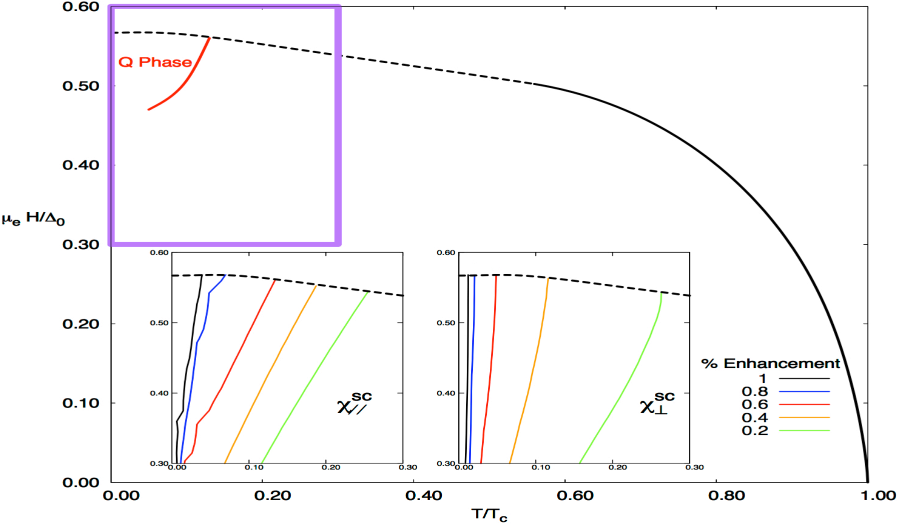


$T = 0.05T_c, \quad \mu_e H = 0.5\Delta_0, \quad \Delta_0 = 0.01\epsilon_f$



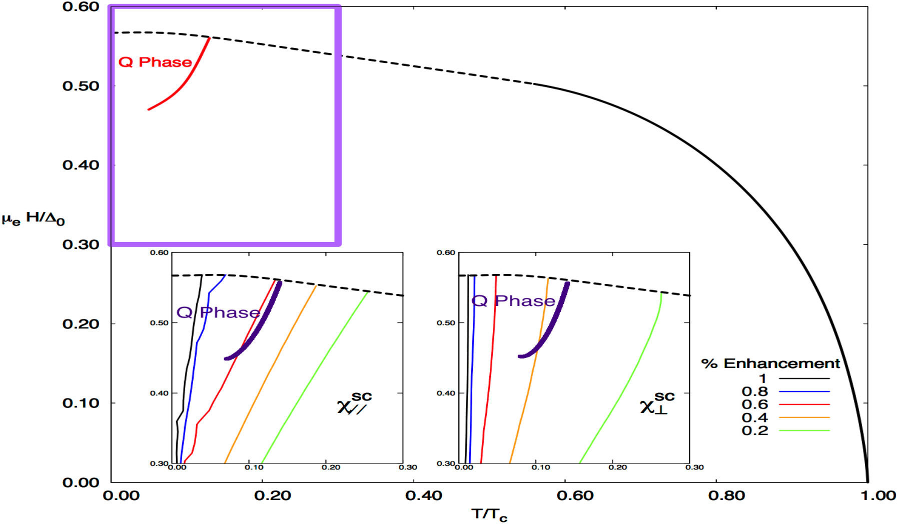
Results

% Enhancement $\mathcal{O}(\Delta/\epsilon_f)$, $\Delta_0 = 0.005\epsilon_f$,



Results

% Enhancement $\mathcal{O}(\Delta/\epsilon_f)$, $\Delta_0 = 0.005\epsilon_f$,



Conclusions

-Magnetic susceptibility in superconducting state can be enhanced compared to the normal state in high uniform magnetic fields

-This may promote AF order with $\mathbf{q} = 2k_f - \delta$ inside SC state

-Both $\chi_{\|}$ and $\chi_{\perp}$ show enhancement ($\perp$ in $CeCoIn_5$)

-χ^{sc} contours qualitatively align with Q-phase boundary

(Kenzelmann et al, Phys. Rev. Lett. (2010). Kato et al, Phys. Rev. Lett. (2011))

-Connection to order parameter:

-No enhancement seen for S-wave
-$\perp$ enhancement requires sign changing (nodal) order parameter
-$\|$ enhancement requires sufficiently small minimum in order parameter

-Possible tool to determine near nodal direction

Normal state Susceptibility

$$\frac{\chi_{\parallel}^N(q)}{\chi_0^N} = \begin{cases} 1: & q < 2\sqrt{1-\mu_e H/\epsilon_f} \\ 1 - \frac{1}{2}\sqrt{1-(\frac{2}{q})^2(1-\mu_e H/\epsilon_f)}: & q \in [2\sqrt{1-\mu_e H/\epsilon_f}, 2\sqrt{1+\mu_e H/\epsilon_f}] \\ 1 - \frac{1}{2}\sqrt{1-(\frac{2}{q})^2(1-\mu_e H/\epsilon_f)} - \frac{1}{2}\sqrt{1-(\frac{2}{q})^2(1+\mu_e H/\epsilon_f)}: & q > 2\sqrt{1+\mu_e H/\epsilon_f} \end{cases}$$

$$\frac{\chi_{\perp}^N(q)}{\chi_0^N} = \begin{cases} 1: & q < \sqrt{1-\mu_e H/\epsilon_f} + \sqrt{1+\mu_e H/\epsilon_f} \\ 1 - \sqrt{1-(\frac{2}{q})^2 + (\frac{2\mu_e H/\epsilon_f}{q^2})^2}: & q > \sqrt{1-\mu_e H/\epsilon_f} + \sqrt{1+\mu_e H/\epsilon_f} \end{cases}$$

Maximize $\delta\chi_{\perp}^{sc}$

$\hat{\mathbf{q}}$=nodal direction

$$\Delta(\mathbf{k}) = \Delta_{T,H}\sin(2\theta_k)$$

$$q^* = \sqrt{2(1+\sqrt{1-\left(\frac{\mu_e H}{\Delta_{T,B}}\right)^2}}\,\hat{x}$$

Maximize $\delta\chi_{\parallel}^{sc}$

$\hat{\mathbf{q}}$=off nodal direction

$$\Delta(\mathbf{k}) = \Delta_{T,H}\cos(2\theta_k + \eta_{q^*})$$

$$q^* \approx 2\sqrt{1-\frac{\mu_e H}{\epsilon_f}} + \delta\ \hat{x}$$

$$\eta_{q^*} \approx \sin^{-1}\frac{\mu_e H}{\Delta_{T,B}} - \sin^{-1}\left(\sqrt{1-(\frac{q^*}{2\sqrt{1+\mu_e H/\epsilon_f}})^2}\right)$$