

Reciprocal Space Magnetic Field: Physical Implications

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Outline

- 1 Introduction
- 2 Physical implications of the reciprocal space magnetic field
 - Design novel transport devices
 - Inhomogeneous phase space
 - Effective quantum mechanics
- 3 Conclusion



Effective dynamics of Bloch electron

Motivation: For a large class of crystalline materials, the equations of motion of Bloch electrons are different:

$$\begin{aligned}\dot{\mathbf{x}} &= \frac{1}{\hbar} \frac{\partial \mathcal{E}_n(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k}) \\ \hbar \dot{\mathbf{k}} &= -e\mathbf{E} - e\dot{\mathbf{x}} \times \mathbf{B}\end{aligned}$$

$\boldsymbol{\Omega}(\mathbf{k})$ – reciprocal space magnetic field. It presents in systems:

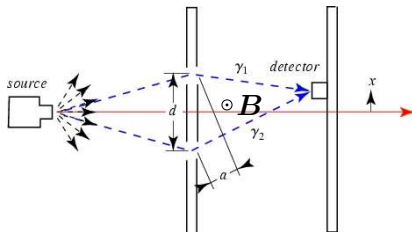
- breaking time-reversal symmetry: **magnetic materials**
- breaking spatial inversion symmetry: **surfaces, interfaces, nanotubes** ...

Sundaram and Niu, PRB **59**, 14915(1999); Marder, *Condensed Matter Physics*.

Physical consequences?



Aharonov-Bohm effect



$$\Delta\varphi_1 = \frac{e}{h} \int_{\gamma_1} \mathbf{A} \cdot d\mathbf{s}$$

$$\Delta\varphi_2 = \frac{e}{h} \int_{\gamma_2} \mathbf{A} \cdot d\mathbf{s}$$

$$\Delta\varphi = \Delta\varphi_2 - \Delta\varphi_1 = \frac{e}{h} \oint_{\gamma} \mathbf{A} \cdot d\mathbf{s}$$

$$\oint_{\gamma} \mathbf{A} \cdot d\mathbf{s} = \int_S (\nabla \times \mathbf{A}) \cdot d\mathbf{S} = \int_S \mathbf{B} \cdot d\mathbf{S} \equiv \phi_B$$



Berry phase

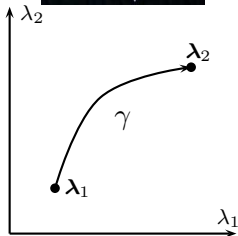
Considering a quantum system controlled by a set of parameters that are slowly varying with time:

$$H \equiv H[\boldsymbol{\lambda}(t)]$$

At t_1 : $|\psi(t_1)\rangle = |\psi[\boldsymbol{\lambda}(t_1)]\rangle$

At t_2 : $|\psi(t_2)\rangle \equiv \exp(i\varphi) |\psi[\boldsymbol{\lambda}(t_2)]\rangle$

$$\varphi = -\frac{1}{\hbar} \int_{t_1}^{t_2} E[\boldsymbol{\lambda}(t)] dt + \varphi_B$$

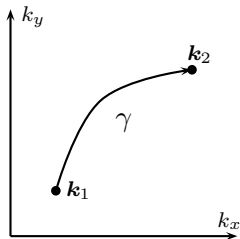


Berry Phase:

$$\varphi_B = i \int_{\gamma} d\boldsymbol{\lambda} \cdot \langle \psi(\boldsymbol{\lambda}) | \nabla_{\boldsymbol{\lambda}} \psi(\boldsymbol{\lambda}) \rangle$$



Berry phase and k -space magnetic field



$$\psi(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} u_{n\mathbf{k}}(\mathbf{x})$$

$$\hat{H}(\mathbf{k}) u_{n\mathbf{k}} = \epsilon_n(\mathbf{k}) u_{n\mathbf{k}}$$

$$\hat{H}(\mathbf{k}) = \frac{(-i\hbar\nabla + \hbar\mathbf{k})^2}{2m} + V(\mathbf{x})$$

Berry phase:

$$\varphi_B = i \int_{\gamma} \left\langle u_{n\mathbf{k}} \left| \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right. \right\rangle \cdot d\mathbf{k}$$

A-B phase in real space:

$$\varphi_{AB} = \frac{e}{\hbar} \int_{\gamma} \mathbf{A}(\mathbf{r}) \cdot d\mathbf{s}$$

k -space magnetic field: $\mathcal{A}_{\mathbf{k}}(\mathbf{k}) = i \left\langle u_{n\mathbf{k}} \left| \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right. \right\rangle$

$$\Omega(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}_{\mathbf{k}}(\mathbf{k}) = i \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \left| \times \right| \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right\rangle$$



Symmetry consideration

$$\boldsymbol{\Omega}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}_{\mathbf{k}}(\mathbf{k}) = i \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \left| \times \right| \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right\rangle$$

With time-reversal symmetry:

$$\boldsymbol{\Omega}(\mathbf{k}) = -\boldsymbol{\Omega}(-\mathbf{k})$$

With spatial inversion symmetry:

$$\boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\Omega}(-\mathbf{k})$$

With both symmetry:

$$\boldsymbol{\Omega}(\mathbf{k}) = 0$$



Implication

Theory of everything:

$$\hat{H} = \sum_i \frac{[\hat{\mathbf{p}}_i + e\mathbf{A}(\mathbf{r}_i)]^2}{2m_e} + \sum_\mu \frac{[\hat{\mathbf{P}}_\mu - Z_\mu e\mathbf{A}(\mathbf{R}_\mu)]^2}{2M_\mu} - \sum_{i\mu} \frac{Z_\mu e^2}{|\mathbf{r}_i - \mathbf{R}_\mu|} + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

More realistic approach – Effective Hamiltonian:

$$\hat{H} = \sum_i \frac{[\hat{\mathbf{p}}_i + e\mathbf{A}(\mathbf{r}_i)]^2}{2m_e^*} + \sum_{i<j} V_{ee}(\mathbf{r}_i - \mathbf{r}_j) + \hat{H}_{e-ph} + \hat{H}_{ph}$$

Examples: BCS theory; Quantum Hall effect ...

With the k -space magnetic field:

?



Directions for exploration

- **Applications** – the presence of an extra reciprocal field provides new freedom for designing novel devices.
- **Fundamentals** – concept of phase space; effective quantum mechanics
- **Physical effects** – Luttinger's theorem; orbital magnetization; magnetoresistance; superconductivity...



Outline

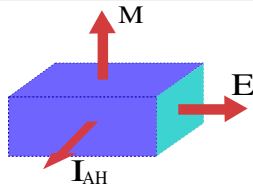
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Anomalous Hall effect

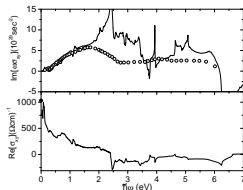
Hall effect in ferromagnetic metal:

$$\rho_{xy} = R_0 B + (4\pi M) R_s$$



Intrinsic contribution:

$$\begin{aligned} \dot{\mathbf{x}} &= \frac{1}{\hbar} \frac{\partial \mathcal{E}_n(\mathbf{k})}{\partial \mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k}) & I_{AH} &\equiv -e \langle \dot{\mathbf{x}} \rangle \\ \hbar \dot{\mathbf{k}} &= -e \mathbf{E} & &= -\frac{e^2}{\hbar} \mathbf{E} \times \int_F \frac{d\mathbf{k}}{(2\pi)^d} \boldsymbol{\Omega}(\mathbf{k}) \end{aligned}$$



Karplus, Luttinger (1954); Jungwirth, Niu, MacDonald (2002); Fang et al. (2003); Yao et al. (2004).



Anomalous Hall insulator

$$\sigma_{AH} = -\frac{e^2}{\hbar} \int_F \frac{d\mathbf{k}}{(2\pi)^d} \boldsymbol{\Omega}(\mathbf{k})$$

For a fully occupied 2D band (band insulator):

$$\sigma_{AH} = -\frac{e^2}{\hbar} \int_{BZ} \frac{d\mathbf{k}}{(2\pi)^2} \Omega_z(\mathbf{k})$$

$$\int_{BZ} d^2\mathbf{k} \Omega_z(\mathbf{k}) = 2\pi C_n$$

Quantized anomalous Hall effect:

$$\sigma_{AH} = -\frac{e^2}{h} C_n$$

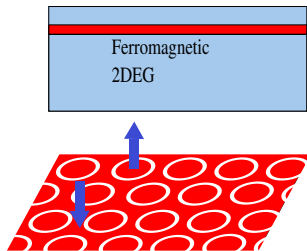
Protected by the **band gap**, extraordinarily robust!



Design an anomalous Hall insulator

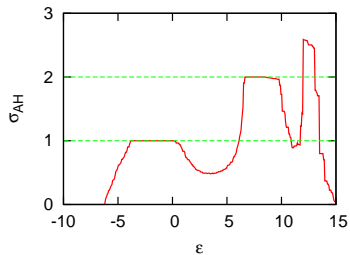
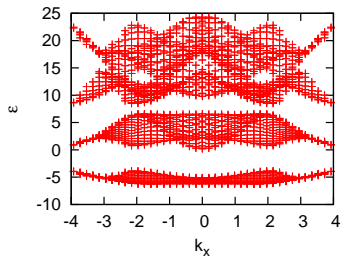
Objective: A 2D ferromagnetic band insulator

- A ferromagnetic 2DEG confined in an **asymmetric quantum well**
- Patterned with non-magnetic rings arranged as a triangular lattice
- Electron density tunable by the gate voltage

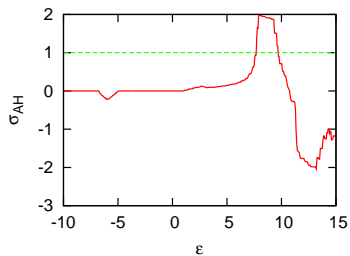
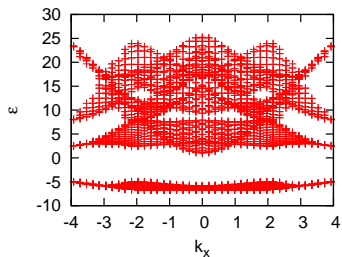


Parameters: Strength of Rashba spin-orbit coupling; Exchange interaction between electron and magnet; Lattice constant; ring radius





Reversed magnetization



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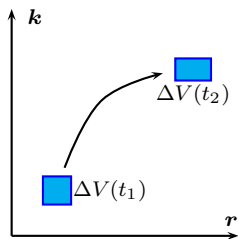


Breakdown of Liouville's theorem

Liouville's theorem: Ensemble density in phase space is conserved.

$$\Delta V = \Delta r \Delta k$$

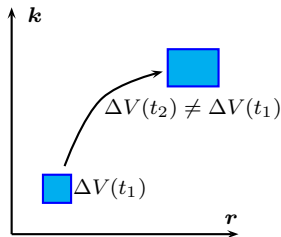
$$\frac{1}{\Delta V} \frac{d\Delta V(t)}{dt} = \nabla_{\mathbf{x}} \cdot \dot{\mathbf{x}} + \nabla_{\mathbf{k}} \cdot \dot{\mathbf{k}} = 0$$



With k -space magnetic field:

$$\frac{1}{\Delta V} \frac{d\Delta V(t)}{dt} \neq 0$$

$$\Delta V(t) = \frac{\Delta V(0)}{1 + (e/\hbar) \mathbf{B} \cdot \boldsymbol{\Omega}(\mathbf{k})}$$



Non-uniform phase space

Phase volume of a quantum state:

$$(2\pi)^d \quad \longrightarrow \quad \frac{(2\pi)^d}{1 + (e/\hbar)\mathbf{B} \cdot \boldsymbol{\Omega}(\mathbf{k})}$$

Statistical Physics – Phase space measure:

$$D(\mathbf{r}, \mathbf{k}) = \frac{1}{(2\pi)^d} \quad \longrightarrow \quad D(\mathbf{r}, \mathbf{k}) = \frac{1}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}(\mathbf{k}) \right)$$

Physical quantity:

$$\langle \hat{O} \rangle = \int d\mathbf{r} d\mathbf{k} D(\mathbf{r}, \mathbf{k}) \mathcal{O}(\mathbf{r}, \mathbf{k}) f(\mathbf{r}, \mathbf{k})$$

$f(\mathbf{r}, \mathbf{k})$ — Distribution function

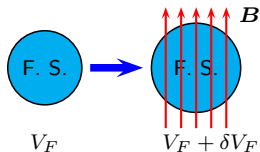


Physical effects

Fermi sea volume:

$$n_e = \int_{V_F + \delta V_F} \frac{d\mathbf{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega} \right)$$

$$\delta V_F = -\frac{e}{\hbar} \int_{V_F} \mathbf{B} \cdot \boldsymbol{\Omega}$$

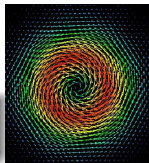


Luttinger's theorem breaks down!

Orbital magnetization:

$$E(\mathbf{B}) = \int_{V_F + \delta V_F} \frac{d\mathbf{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega} \right) [\epsilon_0(\mathbf{k}) - \mathbf{B} \cdot \mathbf{m}(\mathbf{k})]$$

$$\mathbf{M} = -\frac{\partial E}{\partial \mathbf{B}} = \frac{e}{2\hbar} \int_{V_F} \frac{d\mathbf{k}}{(2\pi)^d} i \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \left| \times \left[2\mu - \epsilon(\mathbf{k}) - \hat{H} \right] \right| \frac{\partial u_{n\mathbf{k}}}{\partial \mathbf{k}} \right\rangle$$



Confirmed by: Thonhauser, Ceresoli, Vanderbilt, Resta, cond-mat/0505518



More physical effects

Density of states at Fermi surface and specific heat:

$$\rho(\mu, \mathbf{B}) = \int \frac{d\mathbf{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega} \right) \delta(\epsilon(\mathbf{k}) - \mathbf{B} \cdot \mathbf{m}(\mathbf{k}) - \mu)$$

$$C_e = \frac{\pi^2}{3} k_B^2 T \rho(\mu, \mathbf{B})$$

Magnetoresistivity in linear B :

$$\sigma_{xx} = e^2 \rho(\mu, \mathbf{B}) v_F^2(\mu, \mathbf{B}) \tau(\mu, \mathbf{B})$$

$$v_F(\mu, \mathbf{B}) = \frac{v_F^0(\mu) - \mathbf{B} \cdot [\partial \mathbf{m}(k_F) / \partial k_F]}{1 + (e/\hbar) \mathbf{B} \cdot \boldsymbol{\Omega}}$$

$$\frac{1}{\tau(\mu, \mathbf{B})} = \int_{\mu} \frac{d\mathbf{k}'}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega} \right) W_{\mathbf{k}\mathbf{k}'} \left(1 - \frac{\mathbf{k} \cdot \mathbf{k}'}{k^2} \right)$$



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Effective quantum mechanics

Conventional:

$$i\hbar \frac{\partial \psi}{\partial t} = \left[\mathcal{E}_n \left(-i\nabla + \frac{e}{\hbar} \mathbf{A} \right) - e\phi(\mathbf{r}) \right] \psi$$

With k -space magnetic field:

$$\hat{H} = \mathcal{E}_n(\hat{\mathbf{k}}) - e\phi(\hat{\mathbf{r}})$$

$$[\hat{x}_\mu, \hat{x}_\nu] = i \frac{\epsilon_{\mu\nu\gamma} \Omega_\gamma}{1 + (e/\hbar) \mathbf{B} \cdot \boldsymbol{\Omega}}$$

$$[\hat{k}_\mu, \hat{k}_\nu] = -i \frac{(e/\hbar) \epsilon_{\mu\nu\gamma} B_\gamma}{1 + (e/\hbar) \mathbf{B} \cdot \boldsymbol{\Omega}}$$

$$[\hat{x}_\mu, \hat{k}_\nu] = i \frac{\delta_{\mu\nu} + (e/\hbar) B_\mu \Omega_\nu}{1 + (e/\hbar) \mathbf{B} \cdot \boldsymbol{\Omega}}$$

$\boldsymbol{\Omega} = 0$ – Pierles substitution:

$$\hat{\mathbf{k}} \rightarrow -i \frac{\partial}{\partial \mathbf{r}} + \frac{e}{\hbar} \mathbf{A}(\mathbf{r})$$

$\mathbf{B} = 0$:

$$\hat{\mathbf{r}} \rightarrow i \frac{\partial}{\partial \mathbf{k}} + \mathcal{A}_k(\mathbf{k})$$

General case: Quantum mechanics in **non-commutative geometry**



Many-body Hamiltonian

Theory of everything:

$$\hat{H} = \sum_i \frac{[\hat{\mathbf{p}}_i + e\mathbf{A}(\mathbf{r}_i)]^2}{2m_e} + \sum_\mu \frac{[\hat{\mathbf{P}}_\mu - Z_\mu e\mathbf{A}(\mathbf{R}_\mu)]^2}{2M_\mu} - \sum_{i\mu} \frac{Z_\mu e^2}{|\mathbf{r}_i - \mathbf{R}_\mu|} + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

More realistic approach:

$$\hat{H} = \sum_i \frac{[\hat{\mathbf{p}}_i + e\mathbf{A}(\mathbf{r}_i)]^2}{2m_e^*} + \sum_{i<j} V_{ee}(\mathbf{r}_i - \mathbf{r}_j) + \hat{H}_{e-ph} + \hat{H}_{ph}$$

With the k -space magnetic field:

$$\hat{H} = \sum_i \frac{\hbar^2 \hat{\mathbf{k}}_i^2}{2m_e^*} + \sum_{i<j} V_{ee}(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j) + \hat{H}_{e-ph}(\hat{\mathbf{r}}) + \hat{H}_{ph}$$

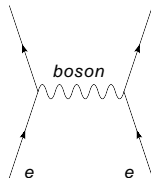
$$[\hat{\mathbf{r}}_i^\mu, \hat{\mathbf{r}}_i^\nu] \neq 0$$



Superconductivity – Boson exchange mechanism

Theory of superconductivity:

- Electrons develop attractive interaction through exchanging bosons (collective excitation).
- Cooper pairs

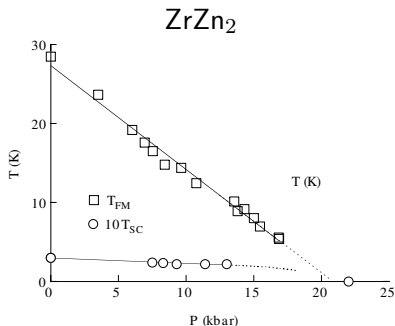
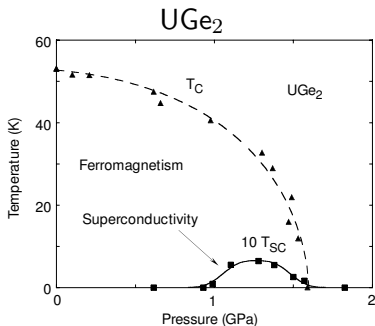


Bosonic excitations responsible for the superconductivity:

- Phonon – conventional BCS superconductivity
- Charge density wave – Kohn and Luttinger, PRL, 1965
- Spin fluctuation – ^3He ; heavy-fermion superconductors; high- T_c superconductors? ...



Ferromagnetic superconductors



Sexena et al., Nature, 2000

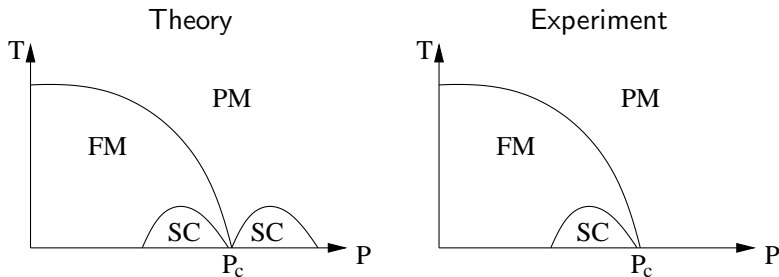
Pfleiderer et al., Nature, 2001

Prevailing picture: Attractive e-e interaction induced by the enhanced **spin fluctuation** near a quantum critical point.



Spin fluctuation?

Puzzle: The superconducting state is only observed in the ferromagnetic phase, not in the paramagnetic phase.



Alternative theory?



Effective quantum mechanics

Quantum mechanics in **non-commutative geometry**:

$$[\hat{x}_\mu, \hat{x}_\nu] = i \frac{\epsilon_{\mu\nu\gamma} \Omega_\gamma}{1 + (e/\hbar) \mathbf{B} \cdot \boldsymbol{\Omega}} \rightarrow i \epsilon_{\mu\nu\gamma} \Omega_\gamma$$

$$[\hat{k}_\mu, \hat{k}_\nu] = -i \frac{(e/\hbar) \epsilon_{\mu\nu\gamma} B_\gamma}{1 + (e/\hbar) \mathbf{B} \cdot \boldsymbol{\Omega}} \rightarrow 0$$

$$[\hat{x}_\mu, \hat{k}_\nu] = i \frac{\delta_{\mu\nu} + (e/\hbar) B_\mu \Omega_\nu}{1 + (e/\hbar) \mathbf{B} \cdot \boldsymbol{\Omega}} \rightarrow i \delta_{\mu\nu}$$

Zero B field limit:

$$\hat{x}_\mu \rightarrow i \frac{\partial}{\partial k_\mu} + \mathcal{A}_\mu(\mathbf{k})$$

Electron-electron interaction:

$$V_{ee}(\mathbf{x}_i - \mathbf{x}_j) \rightarrow V_{ee}(\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j)$$

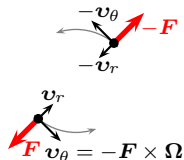


Electron-electron interaction – Classical picture

Scattering between two electrons:

$$\dot{\mathbf{x}} = \frac{1}{\hbar} \frac{\partial \mathcal{E}_n(\mathbf{k})}{\partial \mathbf{k}} - \mathbf{F}_{ee} \times \boldsymbol{\Omega}(\mathbf{k})$$

$$\hbar \dot{\mathbf{k}} = \mathbf{F}_{ee}(\mathbf{r} - \mathbf{r}')$$



“Screw” scattering – transient pairing of electrons with finite angular momentum

Superconductivity with unconventional pairing?



Quantum approach – Second quantization

$$V_{ee}(\mathbf{x}_i - \mathbf{x}_j) \rightarrow v(\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j)$$

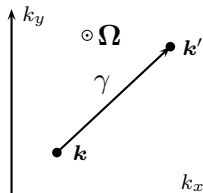
$$\hat{x}_\mu \rightarrow i \frac{\partial}{\partial k_\mu} + \mathcal{A}_\mu(\mathbf{k})$$

$$V = \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}\mathbf{k}'\mathbf{K}} u(\mathbf{k}, \mathbf{k}'; \mathbf{K}) c_{\frac{\mathbf{K}}{2} + \mathbf{k}'}^\dagger c_{\frac{\mathbf{K}}{2} - \mathbf{k}'}^\dagger c_{\frac{\mathbf{K}}{2} - \mathbf{k}} c_{\frac{\mathbf{K}}{2} + \mathbf{k}}$$

$$u(\mathbf{k}, \mathbf{k}'; \mathbf{K}) = v(\mathbf{k}' - \mathbf{k}) e^{i\gamma(\frac{\mathbf{K}}{2} + \mathbf{k}', \frac{\mathbf{K}}{2} + \mathbf{k}) + i\gamma(\frac{\mathbf{K}}{2} - \mathbf{k}', \frac{\mathbf{K}}{2} - \mathbf{k})}$$

Aharonov-Bohm phase under the
 \mathbf{k} -space magnetic field

$$\gamma(\mathbf{k}, \mathbf{k}') = \int_{\mathbf{k}}^{\mathbf{k}'} \mathcal{A}(\mathbf{k}) \cdot d\mathbf{k}$$



Application to a simple ferromagnetic metal

Model: An isotropic two-dimensional ferromagnetic metal with a constant topological field $\Omega_z(\mathbf{k}) = \Omega_0$

Bare electron-electron interaction:

$$v(\mathbf{r}) = V_0 \frac{\exp[-\kappa_{TF}(\sqrt{r^2 + a^2} - a)]}{\sqrt{(r/a)^2 + 1}}$$

Berry phase:

$$\gamma(\mathbf{k}, \mathbf{k}') = \frac{1}{2} \Omega_0 k k' \sin \theta$$

Effective e-e interaction:

$$u(\mathbf{k}, \mathbf{k}'; \mathbf{K} = 0) = v(|\mathbf{k} - \mathbf{k}'|) \exp [i\Omega_0 k k' \sin \theta] = \sum_m u_m(k, k') e^{im\theta}$$



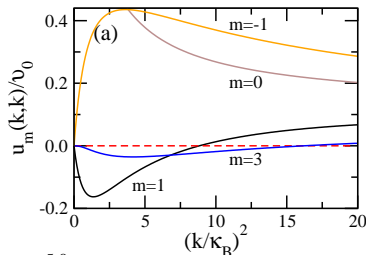
Effective electron-electron interaction

For channel m : $\kappa_u \equiv \kappa_{TF}/\sqrt{1 + \kappa_{TF}a}$, $\phi_\Omega \equiv \Omega_0\kappa_u^2$

$$u_m(k, k') \propto \begin{cases} I_m \left(\frac{kk'}{\kappa_u^2} \sqrt{1 - \phi_\Omega^2} \right), & |\phi_\Omega| \leq 1 \\ (-1)^m J_m \left(\frac{kk'}{\kappa_u^2} \operatorname{sgn}(\phi_\Omega) \sqrt{\phi_\Omega^2 - 1} \right), & |\phi_\Omega| > 1 \end{cases}$$

Attractive interaction:

- $|\Omega_0|\kappa_u^2 > 1$
- m is odd
- The angular momentum is parallel to the Ω -field.



More realistic model:

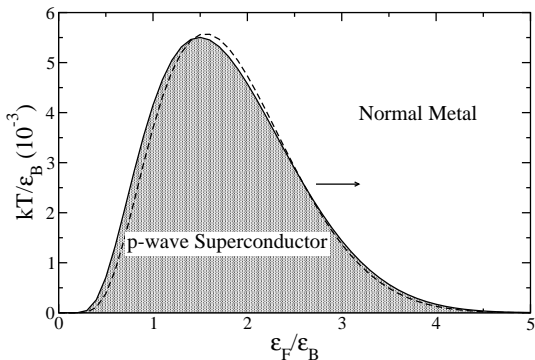
$$\Omega(k) = \frac{\Omega_0\kappa_B^2}{(k^2 + \kappa_B^2)^2}$$



Superconductivity

$$\Delta(\mathbf{k}) = -\frac{1}{2} \sum_{\mathbf{k}'} u(\mathbf{k}, \mathbf{k}') \frac{\tanh \frac{\beta \mathcal{E}(\mathbf{k}')}{2}}{\mathcal{E}(\mathbf{k}')} \Delta(\mathbf{k}')$$

Pairing is determined by the most attractive m -channel.



$$\Delta(\mathbf{k}) \sim k_x + ik_y$$

$$\frac{\Delta_F(0)}{kT_c} \approx 1.76$$

$$\Delta_F(0) \sim (\epsilon_F + \epsilon_B)$$

$$\times \exp \left[-\frac{1}{\rho_F u(\epsilon_F, \epsilon_F)} \right]$$



Conclusion

Reciprocal space magnetic field:

- **Design novel transport devices** – anomalous Hall insulator
- **Inhomogeneous phase space** – Breakdown of Luttinger theorem; Fermi-surface related phenomena; orbital magnetization...
- **Quantum mechanics in non-commutative geometry** – Unconventional superconductivity in ferromagnetic metals...

Collaborators: Q. Niu and D. Xiao (UT-Austin)

Publication: Phys. Rev. Lett. **95**, 137204 (2005); More is coming



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Thank You For Your Attention!

