Magnetostatics and optics of noncentrosymmetric metals

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Metals without inversion



E.Bauer et al, 2004 $CePt_3Si$ $CeRhSi_3$, $CeIrSi_3$ $G=C_{4v}$ $Li_2(Pd_{1-x}Pt_x)_3B$ G=OUIr $G=C_{2v}$

Curent in media without inversion

$$\mathbf{j}_{d} = \frac{\varepsilon}{4\pi} \frac{\partial \mathbf{E}}{\partial t}$$

$$\mathbf{j}_{d} \rightarrow \mathbf{j}_{d} + \mathbf{j}_{g}$$

$$\mathbf{j}_{d} \rightarrow \mathbf{j}_{d} + \mathbf{j}_{g}$$

$$\mathbf{j}_{g} = \lambda \operatorname{rot} \mathbf{E} + \nu \mathbf{B}$$

$$\lambda = \lambda(\frac{\partial}{\partial t}) - \operatorname{odd} \operatorname{function}$$

$$\nu = \operatorname{const}$$

$$t \rightarrow -t \quad \mathbf{j}_{g} \rightarrow -\mathbf{j}_{g}$$

$$\mathbf{r} \rightarrow -\mathbf{r} \quad \mathbf{j}_{g} \rightarrow \mathbf{j}_{g}$$

 $\varepsilon_{ij}(\omega,\mathbf{q}) = \varepsilon_{ij}(\omega,0) + i\gamma_{ijl}q_l \qquad \gamma_{ijl} = -\frac{4\pi i}{\omega}\lambda(\omega)e_{ijl} \quad \text{Space dispersion}$

Current and magnetic moment

Normal metal

$$S_g = -\frac{1}{2c} \int dt d^3 \mathbf{r} \{ \mathbf{B} \lambda \mathbf{E} \}$$

$$\mathbf{j}_g = -c\frac{\delta S_g}{\delta \mathbf{A}} = \lambda rot \mathbf{E}$$

$$\mathbf{M}_g = -\frac{\delta S_g}{\delta \mathbf{B}} = \frac{1}{2c} \lambda \mathbf{E}$$

Superconductor

$$S_g = -\frac{1}{2c} \int dt d^3 \mathbf{r} \left\{ \mathbf{B} \lambda \mathbf{E} + \mathbf{B} \nu \left[\mathbf{A} - \frac{\hbar c}{2e} \nabla \varphi \right] \right\}$$

$$\mathbf{j}_g = -c\frac{\delta S_g}{\delta \mathbf{A}} = \lambda rot\mathbf{E} + \nu\mathbf{B}$$

$$\mathbf{M}_g = -\frac{\delta S_g}{\delta \mathbf{B}} = \frac{1}{2c} \lambda \mathbf{E} + \frac{1}{2c} \nu \left[\mathbf{A} - \frac{\hbar c}{2e} \nabla \varphi \right]$$



London magnetostatics

$$rot\mathbf{B} = \frac{4\pi}{c}\mathbf{j} \qquad \qquad \mathbf{j} = -\frac{c}{4\pi\delta^2}\left(\mathbf{A} - \frac{\hbar c}{2e}\nabla\varphi\right) + \nu\mathbf{B}$$

$$rotrot\mathbf{B} = -\frac{1}{\delta^2}\mathbf{B} + \frac{4\pi}{c}\nu\mathbf{B}$$

London equation

$$\mathbf{B}^{int} - \mathbf{B}^{ext} = 4\pi \mathbf{M} = \frac{2\pi\nu}{c} \mathbf{A} \qquad B_x^{int} = H, \qquad B_y^{int} = \frac{2\pi\nu}{c} A_y^{int} \qquad \text{boundary conditions}$$

$$B_x + iB_y = H(1 + i\tan\beta)\exp\left(-\frac{ze^{i\beta}}{\delta}\right) \approx H(1 + i\beta)\exp\left(-\frac{i\beta z}{\delta}\right)\exp\left(-\frac{z}{\delta}\right)$$

$$\sin\beta = \frac{2\pi\nu\delta}{c}$$

Levitov, Nazarov, Eliashberg, 1985

(i)
$$at \ z = 0 \quad B_x = H \quad B_y = \beta H$$
 (ii) H rotates

$$\nu = \frac{4}{3}\mu_B e\gamma N_0 \frac{n_s(T)}{n}$$

$$\beta(T=0) = \frac{2}{3\pi} \frac{e^2}{\hbar c} \frac{\gamma}{c} k_F \delta \approx 10^{-3} \qquad \frac{\delta}{\beta} = 10^3 \delta$$

V.Edelstein, 1995 C.-K.Lu and S.Yip, 2008

The mountain gave birth to the mouse

Metals without inversion. Spectrum.



CePt₃Si - P4mm; CePt₃B-type

E.Bauer et al, 2004 $CePt_3Si$ $CeRhSi_3$, $CeIrSi_3$ $G=C_{4v}$ $Li_2(Pd_{1-x}Pt_x)_3B$ G=OUIr $G=C_{2v}$

Spin-orbit interaction

Pauli
$$-\mu\sigma\mathbf{H} = -\frac{\mu}{c}(\mathbf{v}\times\mathbf{E})\sigma = \frac{\hbar\mu}{mc}(\mathbf{E}\times\mathbf{k})\sigma$$
Rashba $\gamma(\mathbf{k})\sigma, \quad \gamma(-\mathbf{k}) = -\gamma(\mathbf{k})$ Spectrum $\xi_{\alpha\beta}(\mathbf{k}) = \xi_0(\mathbf{k})\delta_{\alpha\beta} + \gamma(\mathbf{k})\sigma_{\alpha\beta}$

Band splitting



Two band superconductivity



In the simplest model with BCS pairing interaction $v_g(\mathbf{k}, \mathbf{k}') = -V_g$, the gap functions are the same in both bands: $\tilde{\Delta}_+(\mathbf{k}) = \tilde{\Delta}_-(\mathbf{k}) = \Delta$ and we deal with pure singlet pairing

Current

$$\mathbf{v}_{\alpha\beta}(\mathbf{k}) = \frac{\partial \xi_{\alpha\beta}(\mathbf{k})}{\partial \mathbf{k}} \quad (m_{ij}^{-1})_{\alpha\beta} = \frac{\partial^2 \xi_{\alpha\beta}(\mathbf{k})}{\partial k_i \partial k_j}$$

 $K_{\pm} = (\Omega_m \pm \omega_n/2, \mathbf{k} \pm \mathbf{q}/2) \quad \omega_n = 2\pi n T$
 $\Omega_m = \pi (2m+1-n)T$

$$-e^{2}Tr\left[\mathrm{T}\sum_{m=-\infty}^{\infty}\int\frac{d^{3}k}{(2\pi)^{3}}\{\hat{v}_{i}(\mathbf{k})\hat{G}^{(0)}(K_{+})\hat{v}_{j}(\mathbf{k})\hat{G}^{(0)}(K_{-})+\hat{v}_{i}(\mathbf{k})\hat{F}^{(0)}(K_{+})\hat{v}_{j}^{t}(-\mathbf{k})\hat{F}^{+(0)}(K_{-})\}+\hat{m}_{ij}^{-1}\hat{n}_{e}\right]A_{j}(\omega_{n},\mathbf{q})$$

$$\hat{v}_j = v_j + \hat{w}_j + \hat{u}_j \qquad \qquad v_j = k_j/m \qquad \hat{w}_j = \gamma \hat{\sigma}_j \qquad \hat{u}_j = i\mu_B \frac{c}{e} q_m \hat{\sigma}_l e_{lmj}$$

Diamagnetic current and diamagnetism Landau

 $v_i \hat{G} v_j \hat{G} + v_i \hat{G} \hat{w}_j \hat{G} + \hat{w}_i^d \hat{G} \hat{w}_j^d \hat{G} \qquad \qquad \mathbf{j}_d + crot \mathbf{M}_d = \mathbf{j}_d + c \chi_L rotrot \mathbf{A}$

Paramagnetism Pauli

$$\hat{u}_i \hat{G} \hat{u}_j \hat{G}$$
 $\mathbf{j}_p = crot \mathbf{M}_p = c \chi_P rotrot \mathbf{A}$

Gyrotropic current

 $\hat{w}^o_i\hat{G}\hat{w}^o_j\hat{G}+\hat{u}_i\hat{G}\hat{w}_j\hat{G}+\hat{u}_i\hat{G}v_j\hat{G}$

Residual spin susceptibility at T=0



$$\mathbf{j}_p = crot \mathbf{M}_p = c \chi_P rotrot \mathbf{A}$$

$$\chi_{ij} = \frac{2}{3} \mu_B^2 N_0 \left(2 + Y(T)\right) \delta_{ij}$$

$$H_p = \sqrt{\frac{3}{2}} \ \frac{\Delta_0}{\mu_B}$$

K.Samokhin 2008

Susceptibility anisotropy

Spin susceptibility in tetragonal crystal with broken space parity, point group C_{4v} , possesses orthorhombic anisotropy

$$\chi_{xx}(\mathbf{q}) - \chi_{yy}(\mathbf{q}) \approx \mu_B^2 N_0 \gamma_\perp^2 (q_x^2 - q_y^2) (1 + f(\mathbf{q})) / \varepsilon_F^2$$

$$\boldsymbol{\gamma}(\mathbf{k}) = \gamma_{\perp}(k_y\hat{x} - k_x\hat{y}) + \gamma_{\parallel}k_xk_yk_z(k_x^2 - k_y^2)\hat{z}$$

Spin susceptibility in a crystal with cubic symmetry and broken space parity loses diagonal form

$$\chi_{xy} \approx \mu_B^2 N_0 (\gamma^2 q_x q_y / \varepsilon_F^2 + i \gamma q_z / \varepsilon_F + \dots)$$

 $\gamma(\mathbf{k}) = \gamma \mathbf{k}$

T.Takemoto 2008 theory B.Fåk et al 2013 experiment

$$\begin{aligned} \mathbf{Gyrotropy\ current,\ finite\ frequency} & \mathbf{j}_g = \lambda rot \mathbf{E} \\ \lambda &= -\frac{ie^2\omega}{48\pi^2 m\gamma^2} \left\{ m\gamma \left(\frac{k_+ + m\gamma}{k_+^2 - a^2} + \frac{k_- - m\gamma}{k_-^2 - a^2} \right) + \frac{3}{2} \ln \frac{k_+^2 - a^2}{k_-^2 - a^2} - a^2 \left(\frac{1}{k_+^2 - a^2} - \frac{1}{k_-^2 - a^2} \right) \right\} + \dots \\ \mathbf{Notations} & k_{\pm} - Fermi\ momenta & a = \frac{\omega}{2\gamma} \end{aligned}$$

 $\gamma k_F \approx \gamma k_+ \approx \gamma k_- - band \ splitting \ at \ \gamma k_F << \varepsilon_F$

$$\lambda \approx \frac{i}{8\pi^2} \frac{e^2}{\hbar} \frac{\hbar\omega}{\gamma k_F} \qquad \hbar\omega < \gamma k_F$$

$$\lambda \approx \frac{4i}{\pi^2} \frac{e^2}{\hbar} \left(\frac{\gamma k_F}{\hbar\omega}\right)^3 \qquad \quad \hbar\omega > \gamma k_F$$

Natural optical activity

$$\varepsilon_{ij}(\omega, \mathbf{q}) = \varepsilon_{ij}(\omega, 0) + i\gamma_{ijl}q_l$$

$$\gamma_{ijk}(\omega, \mathbf{q}) = e_{ijk}\gamma(\omega, \mathbf{q})$$

$$\Theta = \frac{\gamma\omega^2}{2c^2} l$$

Optical activity and natural optical activity





Kerr angle estimation

$$\theta_{Kerr} \approx \frac{32}{\pi} \frac{e^2}{\hbar c} \frac{\omega}{\omega_p^2 \tau} \left(\frac{\gamma k_F}{\hbar \omega}\right)^3$$

$$\omega_p = \sqrt{rac{4\pi n e^2}{m}}$$
 $\omega_p au > \omega au >> 1$ $\omega > \gamma k_F$

For example
$$\omega_p au pprox 10^3$$
 $\omega/\omega_p pprox 1/10$ $\gamma k_F/\hbar\omega pprox 1/3$

 $\theta_{Kerr} \approx 1 \mu rad$

Kerr and CDW in High Tc

Short range CDW order (detected in x-ray diffraction studies) first shows above the background at about the same temperature as the Kerr signal.

J.Chang et al, Nat. Phys. (2012) A.Achkar et al, PRL (2012) G.Chiringhelli et al, Science (2012)







The Kerr angle in all cuprates measured to date cannot "trained" by cooling through the transition in externally applied magnetic field. The Kerr angle sign is the same for reflection on opposite surfaces.

Another desription of noncentrosymmetric metal



$$H = \sum_{\mathbf{k}} E(\mathbf{k}; z) \psi_{\mathbf{k}, z}^{\dagger} \psi_{\mathbf{k}, z} - t_{\perp} \sum_{\mathbf{k}, z} (\psi_{\mathbf{k}, z}^{\dagger} \psi_{\mathbf{k}, z+1} + \text{H.c.}),$$

$$E(k;z) = \frac{1}{2m} \{k^2 + [k \cdot n(z)]^2\} - E_F$$

P.Hosur et al, PRB 87, 115116 (2013)

Spinless mechanism – cholesteric type charge density ordering of spinless electrons

$$\vec{n}(\vec{r}) = n_0[\cos(\pi Q z), \sin(\pi Q z), 0]$$

$$\lambda_{Hosur} \approx \frac{i}{4\pi} \frac{e^2}{\hbar} \frac{n_o^4 t_\perp^2 E_F}{(\hbar\omega)^3}$$

$$n_0 << 1, \qquad t_{\perp}^2 << n_0^2 E_F, \qquad |t_{\perp}| << \hbar \omega$$

Spin-orbital mechanism

$$\lambda \approx \frac{4i}{\pi^2} \frac{e^2}{\hbar} \left(\frac{\gamma k_F}{\hbar\omega}\right)^3 \qquad \hbar\omega > \gamma k_F$$

Conclusion

The Kerr onset seen in the pseudogap phase of a large number of cuprate high temperature superconductors arising at about the same temperature as short range Charge Density Wave order can serve as an evidence of gyrotropic ordering that breaks inversion symmetry preserving time-reversal invariance.

I have proposed the simplest microscopic model of isotropic metal where inversion symmetry breaking reveals itself due to spin-orbital coupling lifting the spin degeneracy and creating the electron band splitting: V.P.Mineev unpublished (2013) ; V.P.Mineev, Yu.Yoshioka, PRB, 81, 094525 (2010). The magnitude of the Kerr angle in infrared frequency region is proved to be in reasonable correspondence with recently reported observations of the Kerr effect in high Tc materials.

There are also alternative explanations of the same phenomenon related with cholesteric liquid crystal type charge ordering that is chiral ordering of spinless electrons:

P.Hosur et al, PRB 87, 115116 (2013), and J.Orenstein and J.Moore, PRB 87, 165110 (2013). As well with loop-current model:

S.Pershiguba et al, Arxiv: 1303.2982, and V.Aji, Y.He and C.M.Varma, PRB 87, 174518 (2013).