Interband Theory of Kerr Rotation in Unconventional Superconductors

Robert Joynt (姜巴比)

University of Wisconsin-Madison;
Peking University,
International Center for Quantum Materials

Wen-Chin Wu

Taiwan Normal University

KITS WORKSHOP
BEIJING
28 MARCH, 2017

Outline

- Unconventional Superconductivity
  - Gauge, Time-reversal, Rotation, Chirality, Breaking
  - UPt_3, (possible states of), Sr_2CuO_4 , etc.
- Kerr Rotation
  - Experimental Results
  - General Theory
  - Interpretations
- Superconductivity in Unoccupied Bands
  - Standard 2-band theory
  - Order parameter in unoccupied band
- Response Function
- Ginzburg-Landau
- Conclusions

Unconventional Superconductivity

Breaking of gauge symmetry is accompanied by breaking of *other* symmetries, for example

Rotation: $\Delta(\mathbf{k}) = \Delta_p\, k_x$ or $\Delta(\mathbf{k}) = \Delta_d\, (k_x^2 - k_y^2)$

Time-reversal: $\Delta(\mathbf{k}) = \Delta_0 + i\, \Delta_d\, (k_x^2 - k_y^2)$

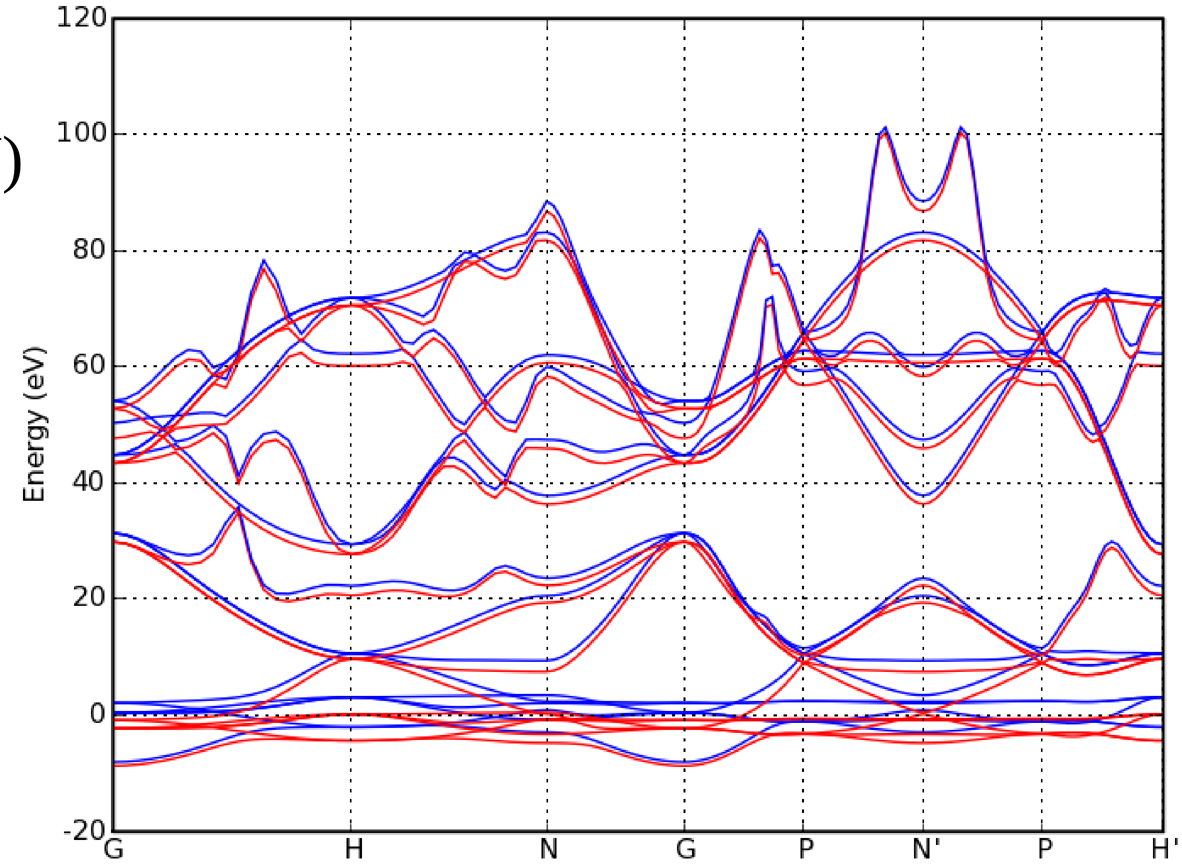
Chirality: $\Delta(\mathbf{k}) = \Delta_0\, (k_x + i\, k_y)$, *topological*

The Unconventional Superconductor UPt_3

- UPt_3 has multiple indirect indications of unconventionality, e.g. ,
  - Power Law (not exponential) Response Functions at low T and ω
  - Split Second-order Transition
- Some Candidate Pair Functions:
  - Spin Singlet (scalar gap function)
    - E_{1g} : $\Delta(\mathbf{k}) = \Delta_d \, k_z \, (k_x + ik_y)$
  - Spin Triplet (2 × 2 gap function)
    - E_{1u} : $\boldsymbol{\Delta}(\mathbf{k}) = \Delta_p \, \sigma_x \, (k_x + ik_y)$
    - E_{2u} : $\boldsymbol{\Delta}(\mathbf{k}) = \Delta_f \, \sigma_x \, k_z \, [k_x \, k_y + i \, (k_x^2 - k_y^2)]$

Order Parameter in Unoccupied Bands: Band Structure of bcc Iron

Energy (eV)



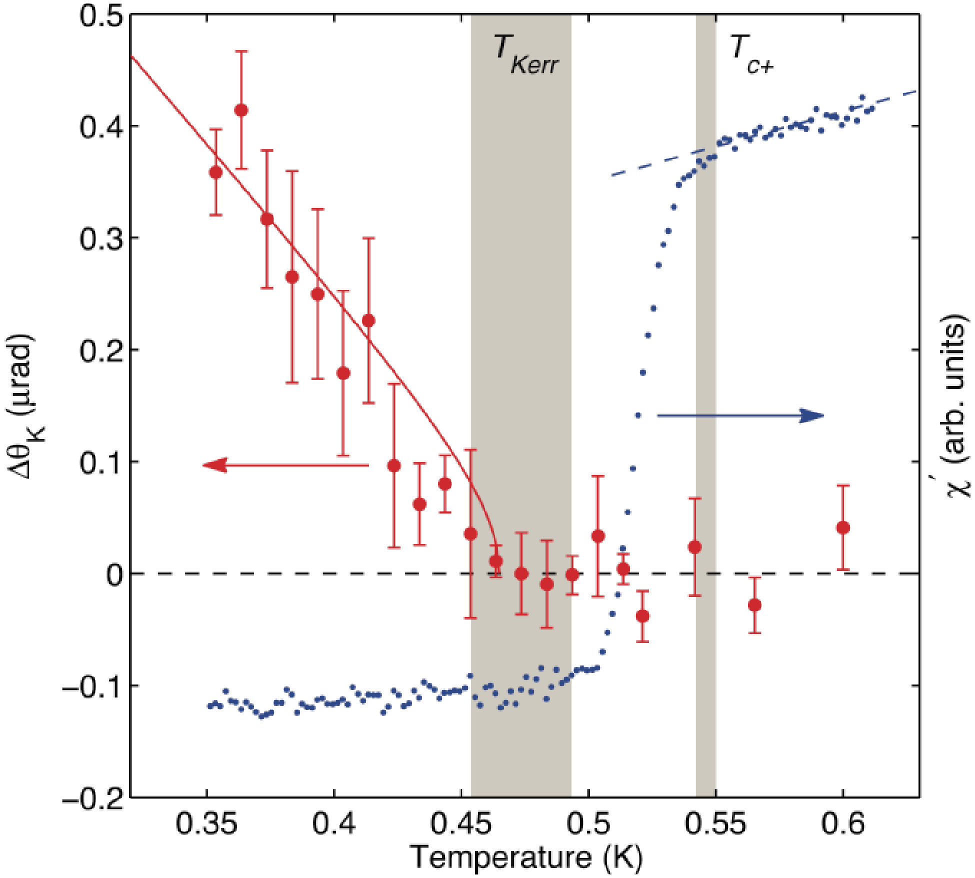
ε_F

k

red = up spins and blue = down spins

REF. https://quantumwise.com/documents/manuals/ATK-2008.10/chap.ironspin.html

Kerr Rotation Angle θ_K and Susceptibility

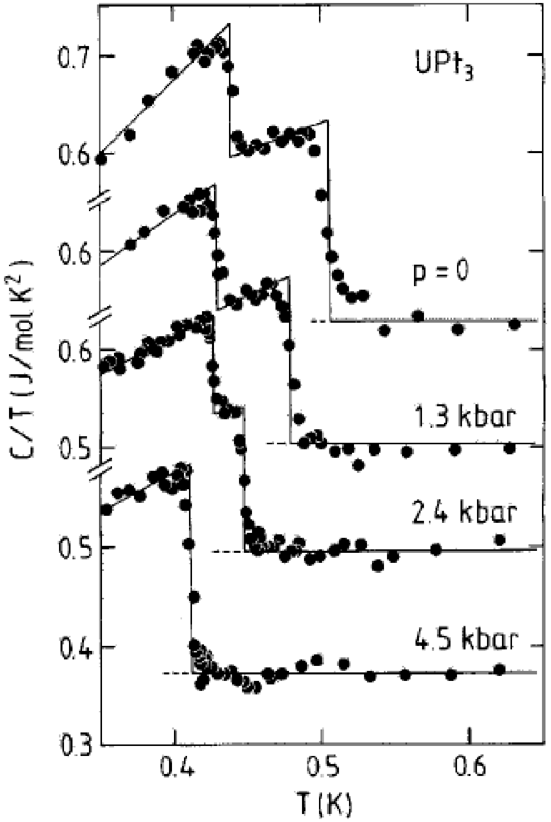


Laser Frequency is 0.8 eV

Note slight offset – actually very important !

E. R. Schemm, W. J. Gannon, C. M. Wishne, W. P. Halperin, A. Kapitulnik, Science **345**, 190 (2014)

Specific Heat of UPt_3:Split Transition



T. Trappmann, H. von Löhneysen, and L. Taillefer, Phys. Rev. B **43**, 13714 (1991)

Electrodynamics of θ_K

The Onsager relation for a small time-reversal symmetry-breaking field H_a is

$$\varepsilon_{xy}(H_a) = cH_a = \varepsilon_{yx}(-H_a) = -cH_a$$

and with the hexagonal symmetry of UPt_3 we have

$$\varepsilon_{ij} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{yx} & \varepsilon_{xx} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix} \rightarrow \begin{pmatrix} \varepsilon & \varepsilon_{xy} & 0 \\ -\varepsilon_{xy} & \varepsilon & 0 \\ 0 & 0 & \varepsilon_{z} \end{pmatrix}$$

when the symmetry gets broken. ε_{ij} becomes non-Hermitian!

For propagation of the light in the z-direction of the hexagonal system the normal modes in the metal are the two circularly - polarized modes with slightly different indices of refraction n_+ and n_- and therefore slightly different reflection coefficients .
This allows us to compute the Kerr angle θ_K.

Expression for θ_K

For |n| >>1, the Kerr angle is given by

$$\theta_K = \mathrm{Re}\left(\frac{1}{\sqrt{\varepsilon_{xx}}}\frac{\varepsilon_{xy}}{\varepsilon_{xx}}\right)$$

The ellipticity (ratio of minor to major axis) of the reflected wave (not measured so far) is

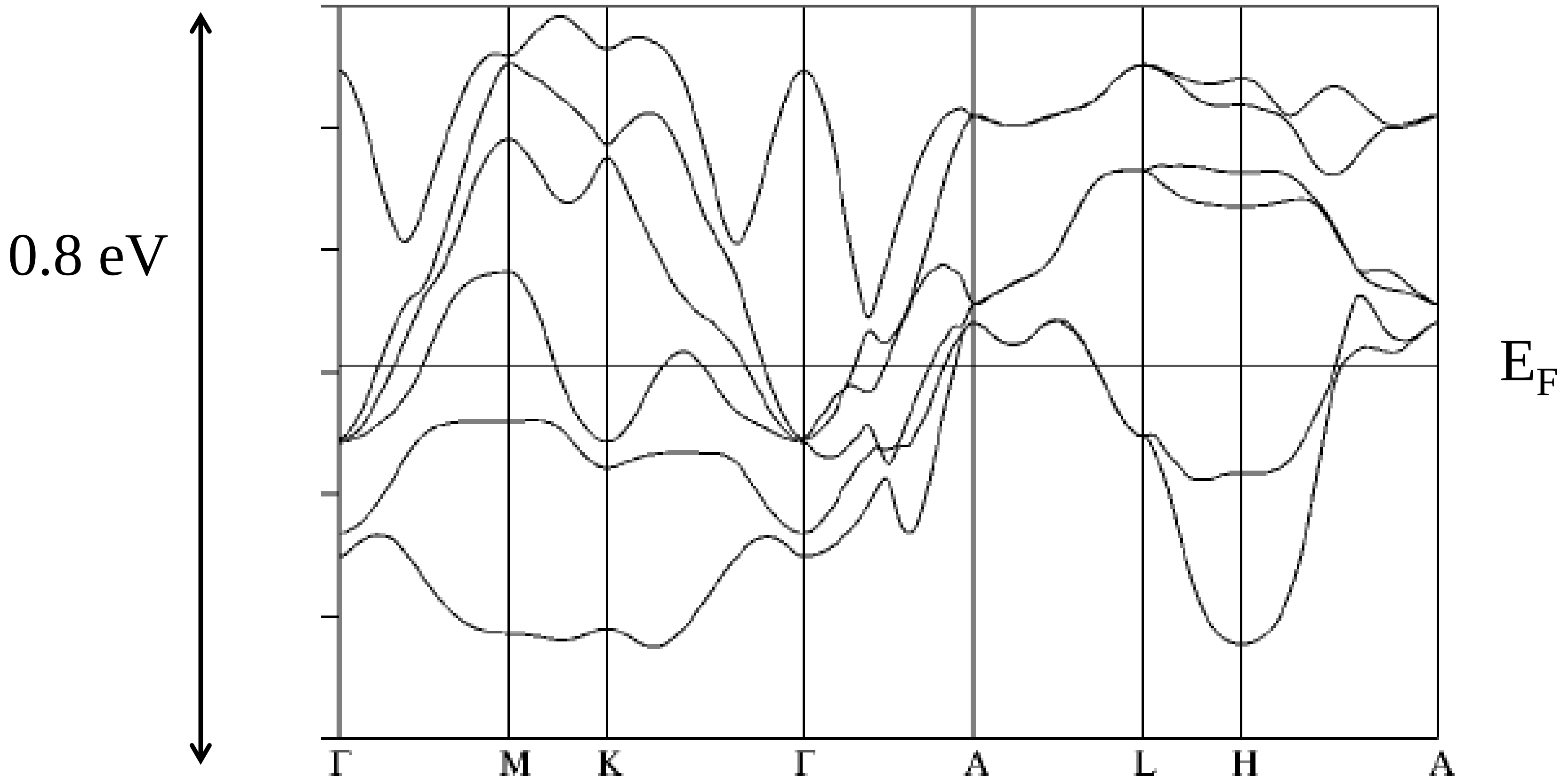
$$\mathrm{Ellipticity} = \mathrm{Im}\left(\frac{1}{\sqrt{\varepsilon_{xx}}}\frac{\varepsilon_{xy}}{\varepsilon_{xx}}\right)$$

So we first need the dielectric function ε_{xx} (ω) at ω = 0.8 eV.

(Low-Energy) Theories of Kerr Effect in Superconductors

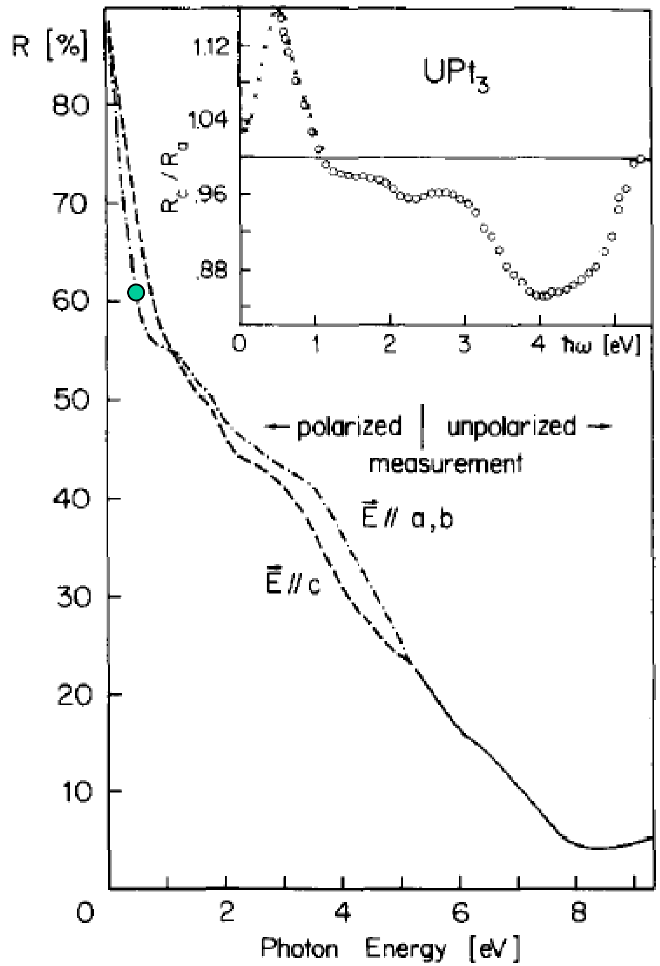
- Collective Modes (high-T_c)
  - Yip S K and Sauls J A, J. Low Temp. Phys. **86,** 257 (1992)
  - Flapping modes of the order parameter
  - Drawback: $\omega / \Delta \sim 10^4$
- Impurity Scattering (Sr_2RuO_4)
  - Lutchyn R M, Nagornykh P and Yakovenko V M Phys. Rev. B **80** 104508, Koenig and Levchenko, PRL **118**, 027001 (2017)
  - Skew scattering ~ $n_i U^3$
  - Drawback: $\omega / \Delta \sim 10^4$
- Interband pairing in partially occupied bands (Sr_2CuO_4)
  - Wysokinski et al., Phys. Rev. Lett. **108**, 077004 (2012)
  - Taylor E and Kallin C, Phys. Rev. Lett. **108**, 157001(2013)
- **Perhaps OK in Sr_2RuO_4, but not in UPt_3.**

Energy Bands of UPt_3



Wang *et al*., Phys. Rev. B **35**, 7260 (1987)

Reflectivity of UPt_3



R ≈ 0.6 for propagation in the z-direction

J. Schoenes and J.J.M. Franse, Physica B**130**, 69 (1985)

Analysis of $\varepsilon(\omega)$

As with all metals, the reflection coefficient
$R(\omega) = |(1 - n(\omega))/(1 + n(\omega))|^2$
shows an overall decrease with ω as ω increases toward the UV.
In addition Re $n(\omega)$ / Im $n(\omega)$ also increases.

UPt_3 is well modeled by the Lorentz formula
$\varepsilon = 1 + (4\pi ne^2/m)\ \Sigma\ f_i / (\omega_i^2 - \omega^2 - i\omega/\tau_i)$.

A minimum of 6 bands, indexed by i, are necessary to fit the data.

(So there definitely are bands at 0.8 eV above ε_F!)

Finally: Re $\varepsilon_{xx}(\omega = 0.8\text{ eV}) \approx 3$, Im $\varepsilon_{xx}(\omega = 0.8\text{ eV}) \approx 25$

Gap in an Unoccupied Band (s-Wave Theory)

If there is a gap Δ_g in a partially occupied "g" band from a pairing interaction of strength g, then the Coulomb interaction of strength g′ between electrons in the e and g bands can induce a 'gap' Δ_e in an unoccupied "e" band. The equations are

$$\begin{aligned}\Delta_g\left[1-gF_g\left(\Delta_g\right)\right] &= \Delta_e g' F_e\left(\Delta_e\right)\\ \Delta_e &= \Delta_g g' F_g\left(\Delta_g\right)\end{aligned}$$

with

$$\begin{aligned}F_g\left(\Delta_g\right) &= \frac{1}{2}\sum_{\vec{p}}\Theta\left(\omega_c-\left|\xi_{\vec{p}}\right|\right)\tanh\left(\frac{E_{\vec{p}}}{2k_BT}\right)\frac{1}{E_{\vec{p}}}\rightarrow N\left(\varepsilon_F\right)\ln\left(\frac{\omega_c}{\Delta_g}\right), \text{ for } T\rightarrow 0\\ F_e\left(\Delta_e\right) &= \frac{1}{2}\sum_{\vec{p}}\frac{1}{\varepsilon_{\vec{p}}} \text{ in the unoccupied band.}\end{aligned}$$

The result is that $\Delta_e = \dfrac{g'}{g}\Delta_g$

And since g′ and g can be the same order, so can Δ_g and Δ_e .

Computation of ε_{xy}

Need indirect method: calculate the ratio

Re ε_{xy} / Im ε_{xx} in which unknown factors largely cancel -

$$\begin{aligned}
\operatorname{Im}\varepsilon_{xx}(\omega) &= \frac{32\pi}{V\omega^2}\sum_{\vec{p}} j_x(\vec{p})\, j_x(\vec{p})\;\delta\left[\omega-(\varepsilon_e(\vec{p})-\varepsilon_g(\vec{p}))\right] \\
&= \frac{32\pi f_e R_n}{\omega^2}\frac{e^2 p_F^2}{m^2} D(\omega)
\end{aligned}$$

$$\begin{aligned}
\operatorname{Re}\varepsilon_{xy}(\omega) &= \frac{64\pi}{V\omega^2}\sum_{\vec{p}} j_x(\vec{p})\, j_y(-\vec{p})\,\frac{\operatorname{Im}\left[\Delta_g^*(\vec{p})\,\Delta_e(\vec{p})\right]}{E_g(\vec{p})\,E_e(\vec{p})}\delta\left[\omega-E_e(\vec{p})-E_g(\vec{p})\right] \\
&= \frac{64\pi f_e R_s}{\omega^2}\frac{e^2 p_F^2}{m^2} D(\omega)\,\frac{\Delta_g^*\Delta_e}{(\omega/2)(\omega-B)}
\end{aligned}$$

Here $f_e < 1$ is the oscillator strength, D is the joint density of states of the two bands, B is the bandwidth and $R_{n,s} \approx 1$ are angular integrals.

Estimate of θ_K

Using our estimates for ε_{xx} , noting that B ≈ 0.2 eV and ω = 0.8 eV, and setting $\Delta_g = \Delta_e$ = 2 kT_c,
we find that

$$\frac{\mathrm{Re}\,\varepsilon_{xy}}{\mathrm{Im}\,\varepsilon_{xx}} \sim \frac{\Delta_g \Delta_e}{(\omega - B)\,B} \log\left(\frac{\omega_c}{\Delta_g}\right) \times \frac{R_s}{R_n} \approx 5 \times 10^{-7} \times \frac{R_s}{R_n}$$

$$\frac{R_s}{R_n} \lesssim 1$$

As long as R_s does not vanish by symmetry !
Setting R_s/R_n = 1 we finally find at T = 0 that

$$\theta_K = 2 \times 10^{-7}$$

Pattern of Symmetry Breaking: Group Representation

Time reversal symmetry breaking is not enough!*

In order that R_s not vanish, it is necessary for $\mathrm{Im}[\Delta_g(\mathbf{p})^*\Delta_e(\mathbf{p})]$ to transform as $k_x k_y$ under the operations of the point group.

In the E_{1g} representation of D_{6h}, we need

$\Delta_g(\mathbf{p}) \sim p_x + ip_y$ and $\Delta_e(\mathbf{p}) \sim p_x - ip_y$,

More generally, $k_x k_y \rightarrow E_{2g}$, $\Delta_g(\mathbf{p})^* \rightarrow \Gamma_g$ and $\Delta_e(\mathbf{p}) \rightarrow \Gamma_e$.

For $\boldsymbol{\varepsilon}_{\mathbf{xy}}$ not to vanish, it is necessary that $a_1 \neq 0$ in the decomposition $E_{2g} \times \Gamma_g \times \Gamma_e = a_1 \Gamma_1 + a_2 \Gamma_2 + \ldots$

The Kerr rotation experiments provide useful information as to which representation is manifested in the system.

*Y. Wang, A. Chubukov, R. Nandkishore, PRB **90**, 205130 (2014)

Pattern of Symmetry Breaking: Ginzburg-Landau Theory

Since we know little about the pairing interaction, we can only make a general symmetry analysis and list the possibilities. The form of GL theory depends on the representation.

For E_{1g}:

$$\begin{aligned}\Delta_g\left(\vec{p}\right) &= h_g\left(\vec{p}\right)p_z\left(\eta_x^g p_x+\eta_y^g p_y\right)\\ \Delta_e\left(\vec{p}\right) &= h_e\left(\vec{p}\right)p_z\left(\eta_x^e p_x+\eta_y^e p_y\right)\end{aligned}$$

$$F=\alpha_g\left(T-T_c\right)\vec{\eta}^g\cdot\vec{\eta}^{g*}+\beta_1^g\left(\vec{\eta}^g\cdot\vec{\eta}^{g*}\right)^2+\beta_2^g\left|\vec{\eta}^g\cdot\vec{\eta}^g\right|^2+\alpha_e\vec{\eta}^e\cdot\vec{\eta}^{e*}+\gamma\left(\vec{\eta}^g\cdot\vec{\eta}^{e*}+\vec{\eta}^{g*}\cdot\vec{\eta}^e\right)$$

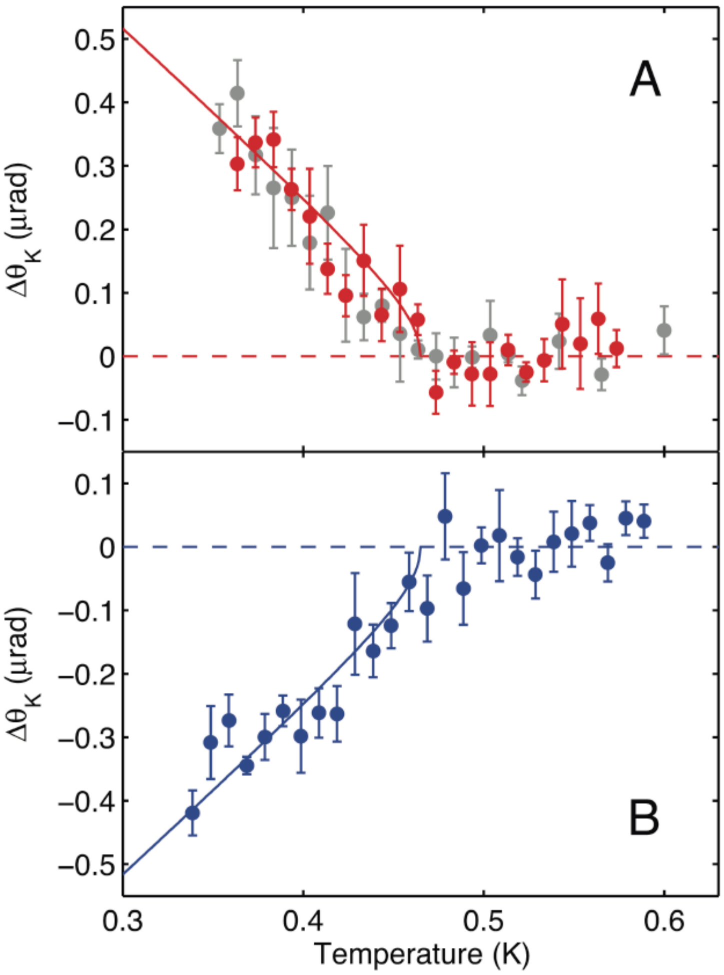
To break TR we need $\beta_2^g > 0$. Also $\alpha_e > 0$ because the superconductivity in the upper band is induced, not intrinsic.

Finally we must have $\gamma > 0$ to get $\boldsymbol{\eta}_g = \eta_g(T)\,(1,i)$ and $\boldsymbol{\eta}_e = \eta_e(T)\,(1,-\,i)$ which gives the finite Kerr rotation, while $\gamma <$ does not.

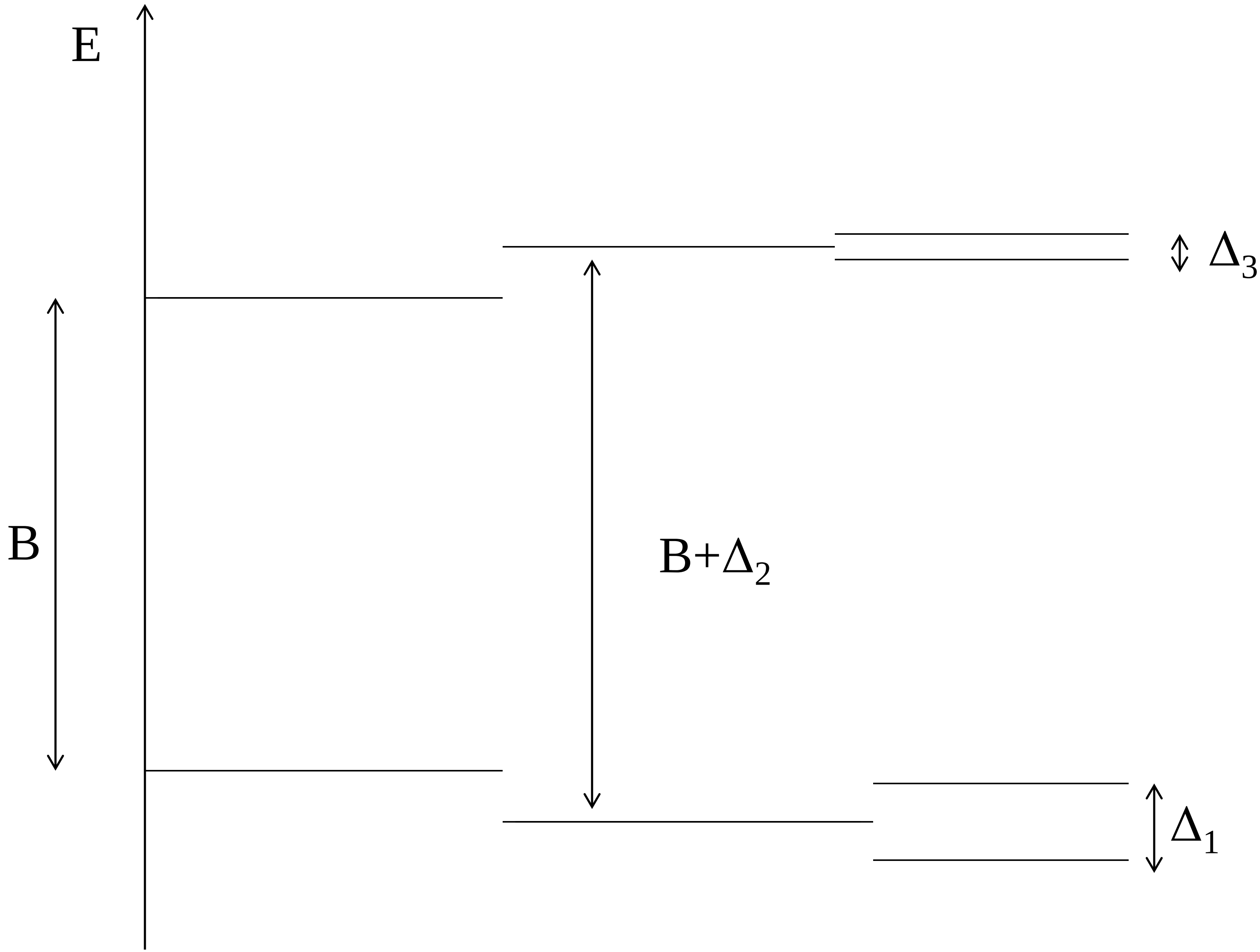
Conclusions

- Ultrasensitive Kerr rotation is a *uniquely* valuable tool for detection of symmetry breaking in unconventional superconductors
- So far this is at *optical* frequencies, so it does not probe solely the conduction (g) band (as in most theories)
- Overall optical response must be understood before the experiments can be properly analyzed
- Details of the Cooper pair wavefunction – the pairing symmetry - can be probed by these experiments
- Superconducting order parameter field has been detected for the 1st time in a superconductor

Field Training



E. R. Schemm, W. J. Gannon, C. M. Wishne, W. P. Halperin, A. Kapitulnik, Science **345**, 190 (2014)



E
B
B+Δ_2
Δ_3
Δ_1