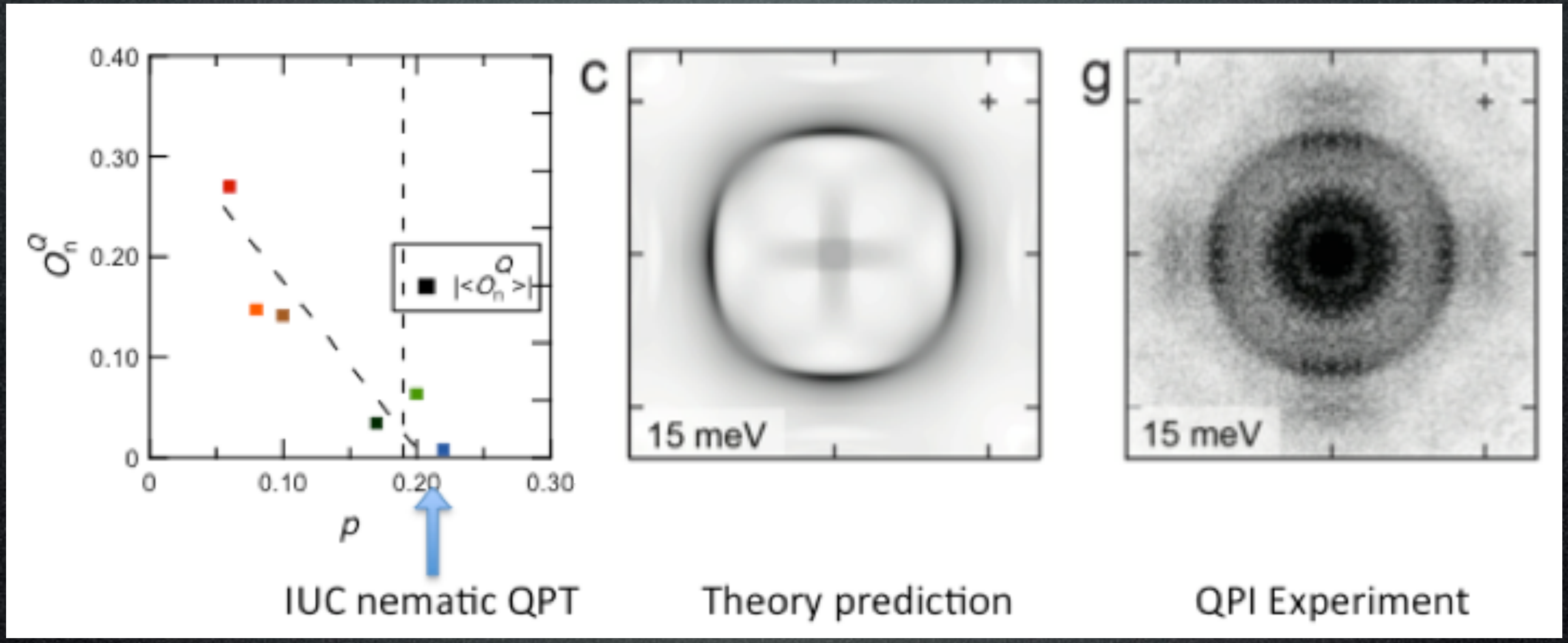
Recent Theoretical Advances in the Study of High-T_c Superconductivity using a 'Middle-top/down' Approach

Eun-Ah Kim



Penn State, Oct 2, 2014

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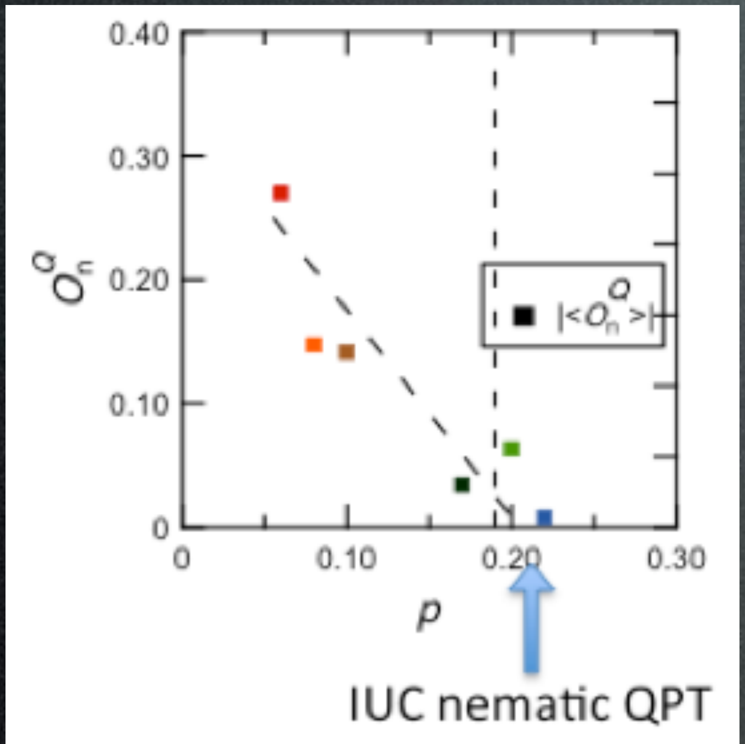

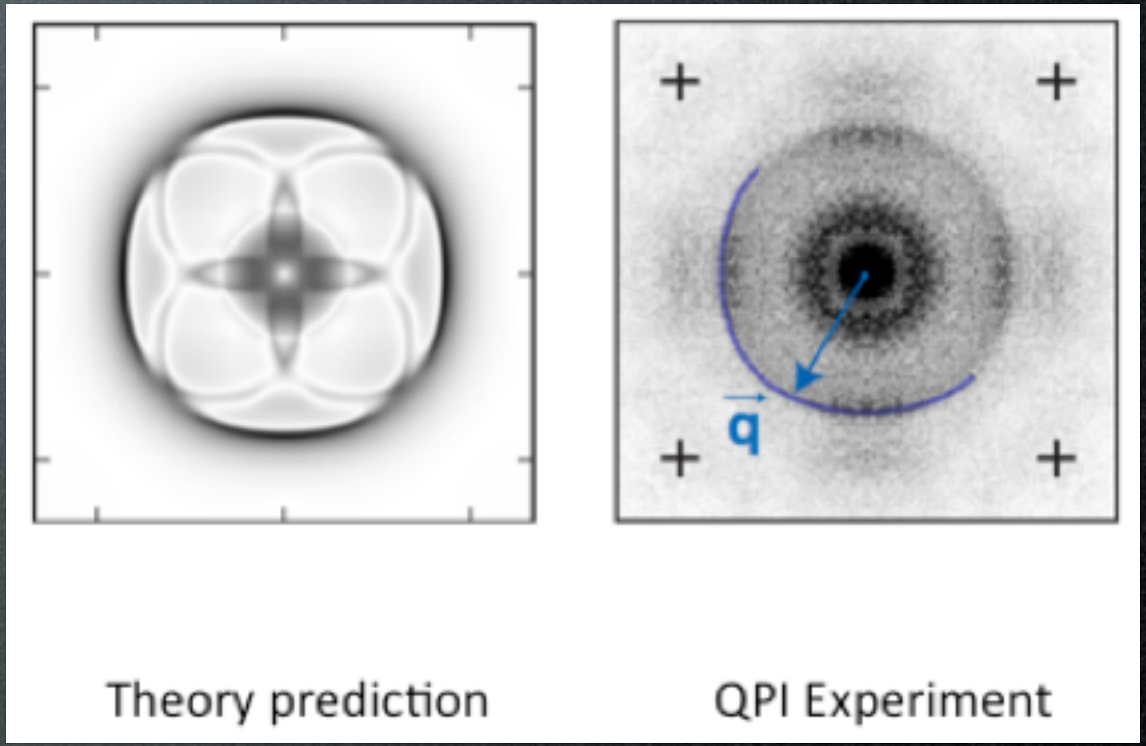

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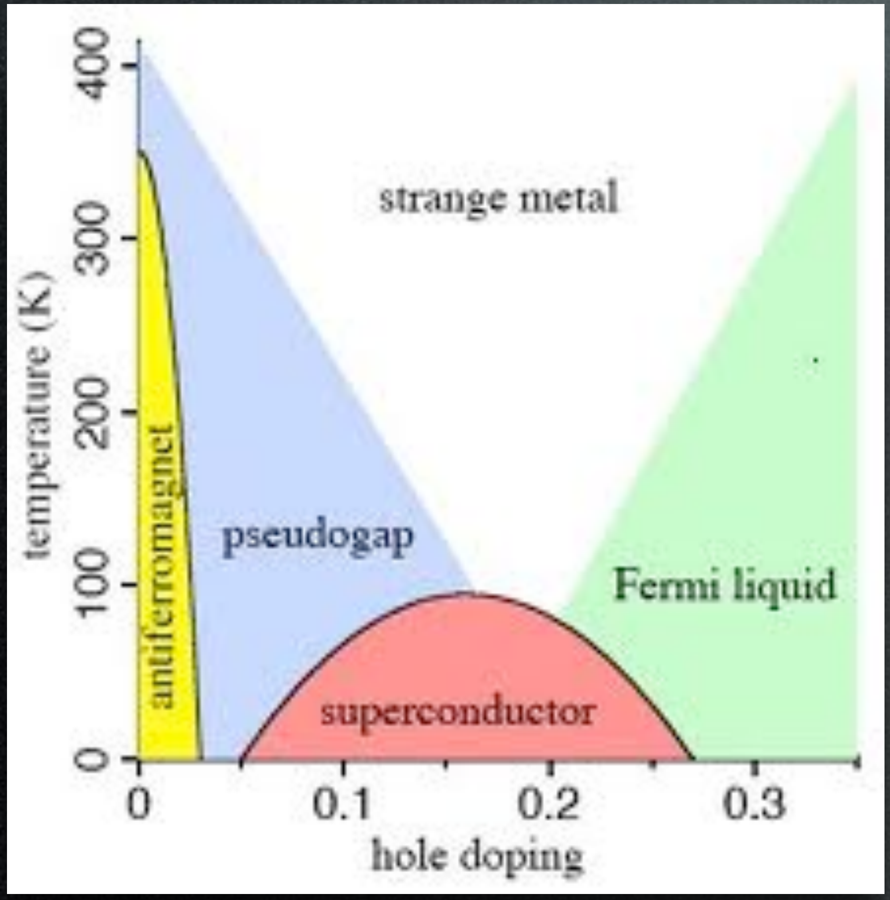
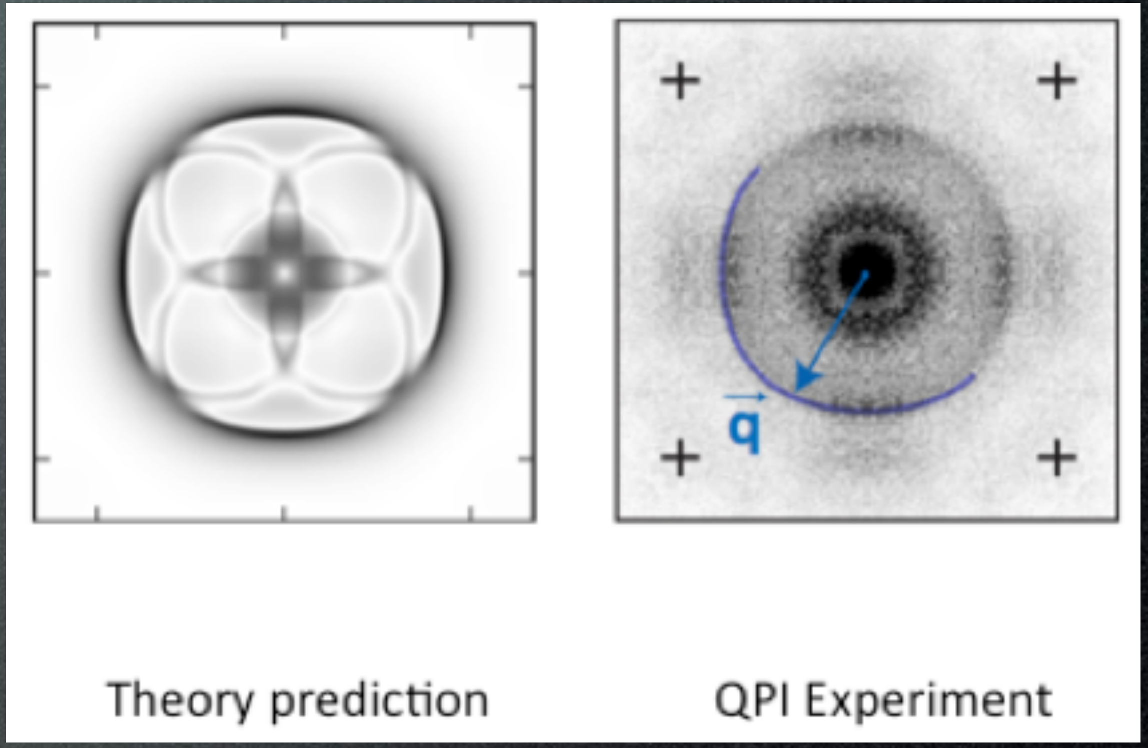
The Phase Diagram





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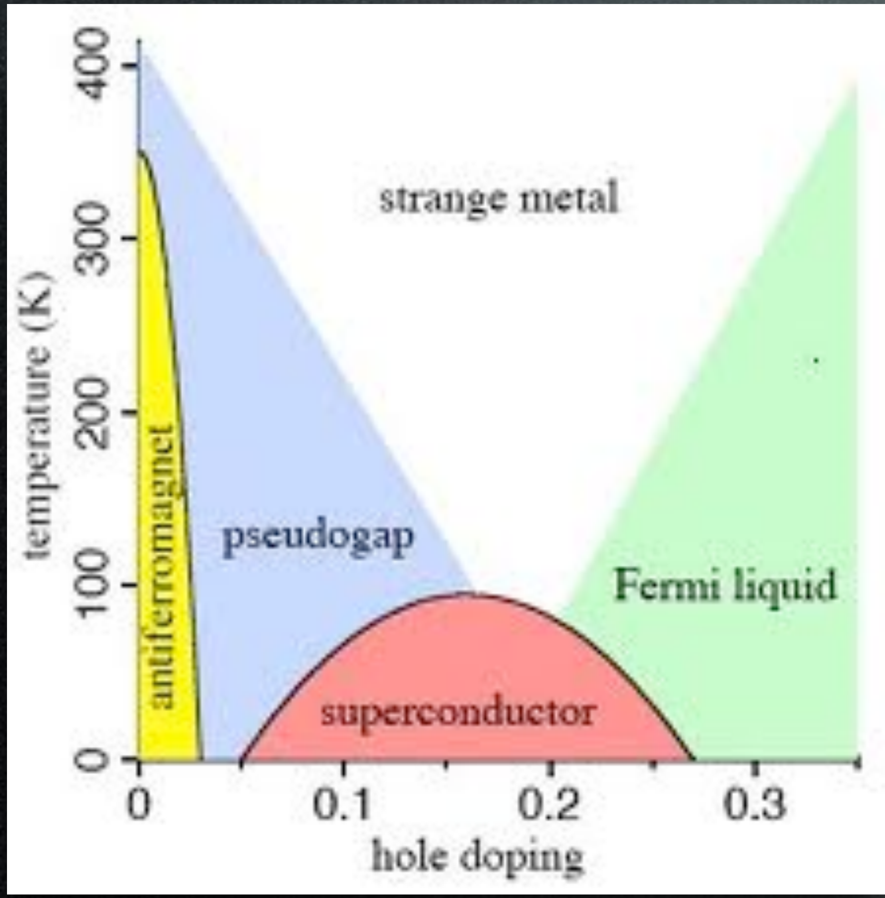
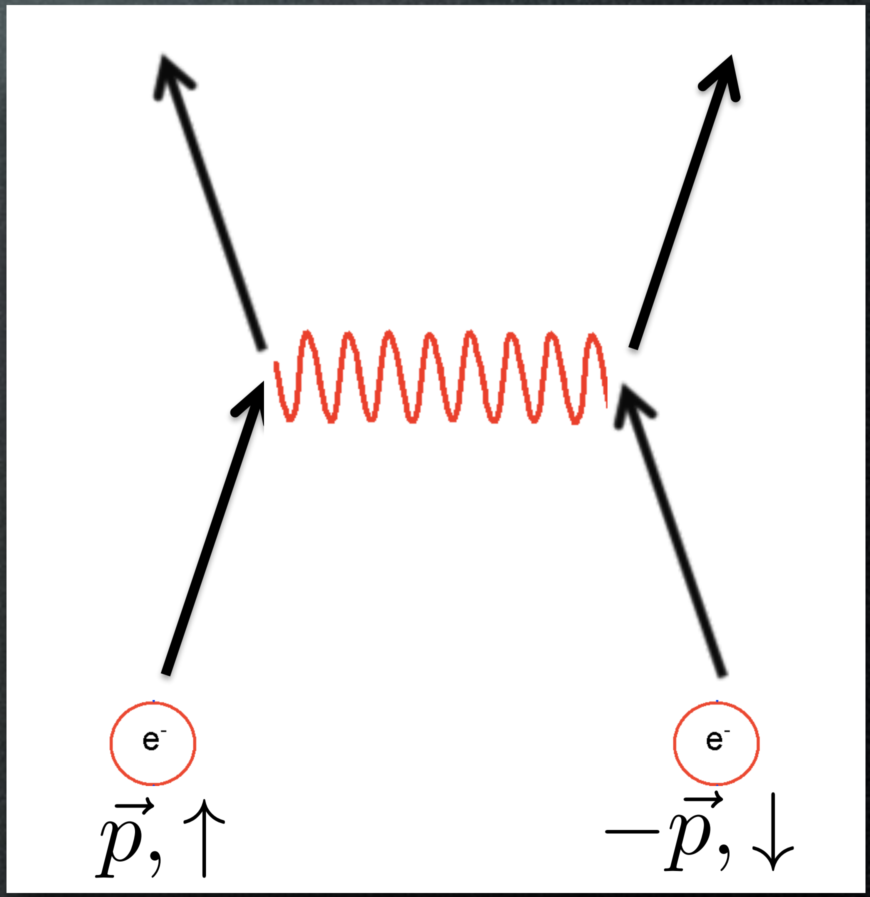


The Mechanism



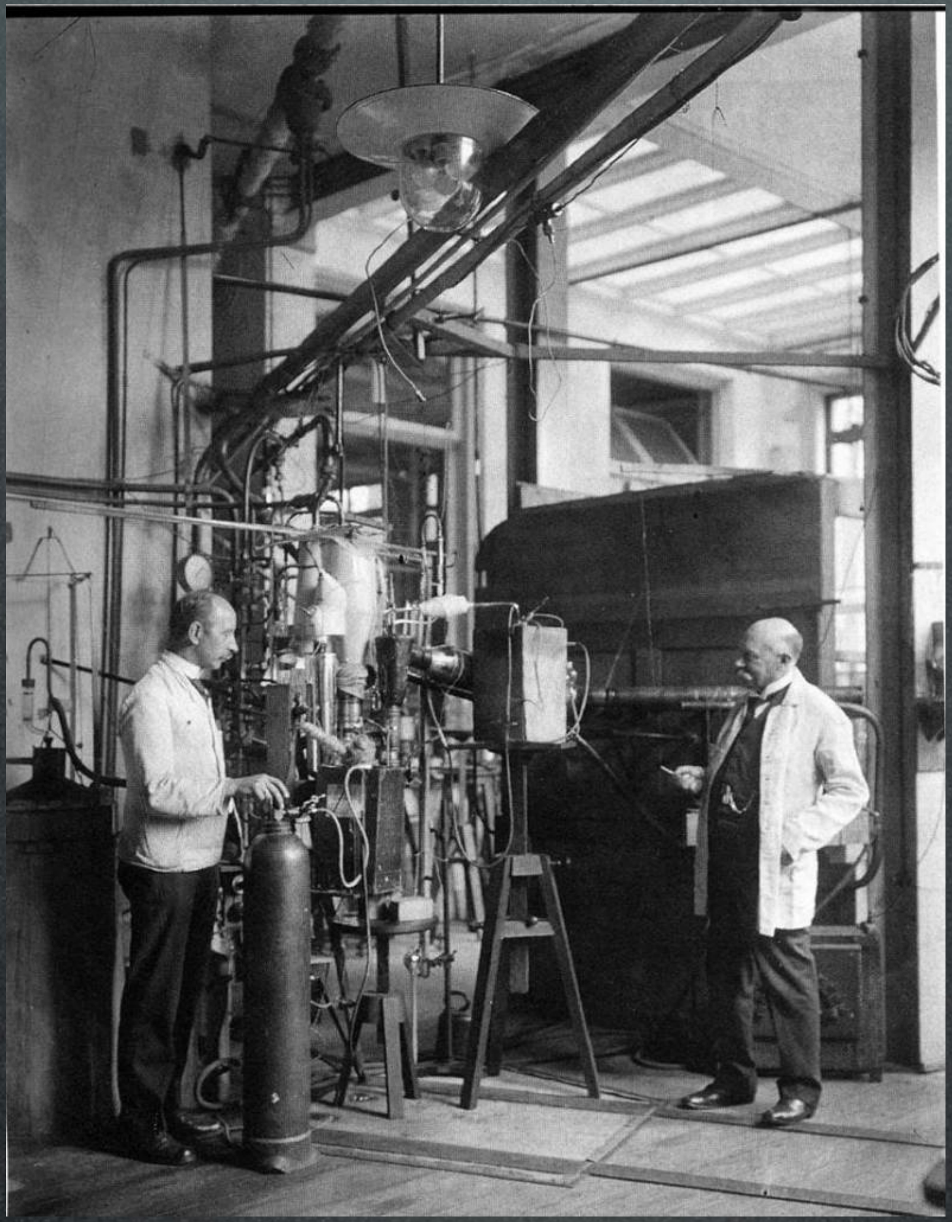
Please STOP ME and ASK QUESTIONS

CONVENTIONAL SUPERCONDUCTIVITY

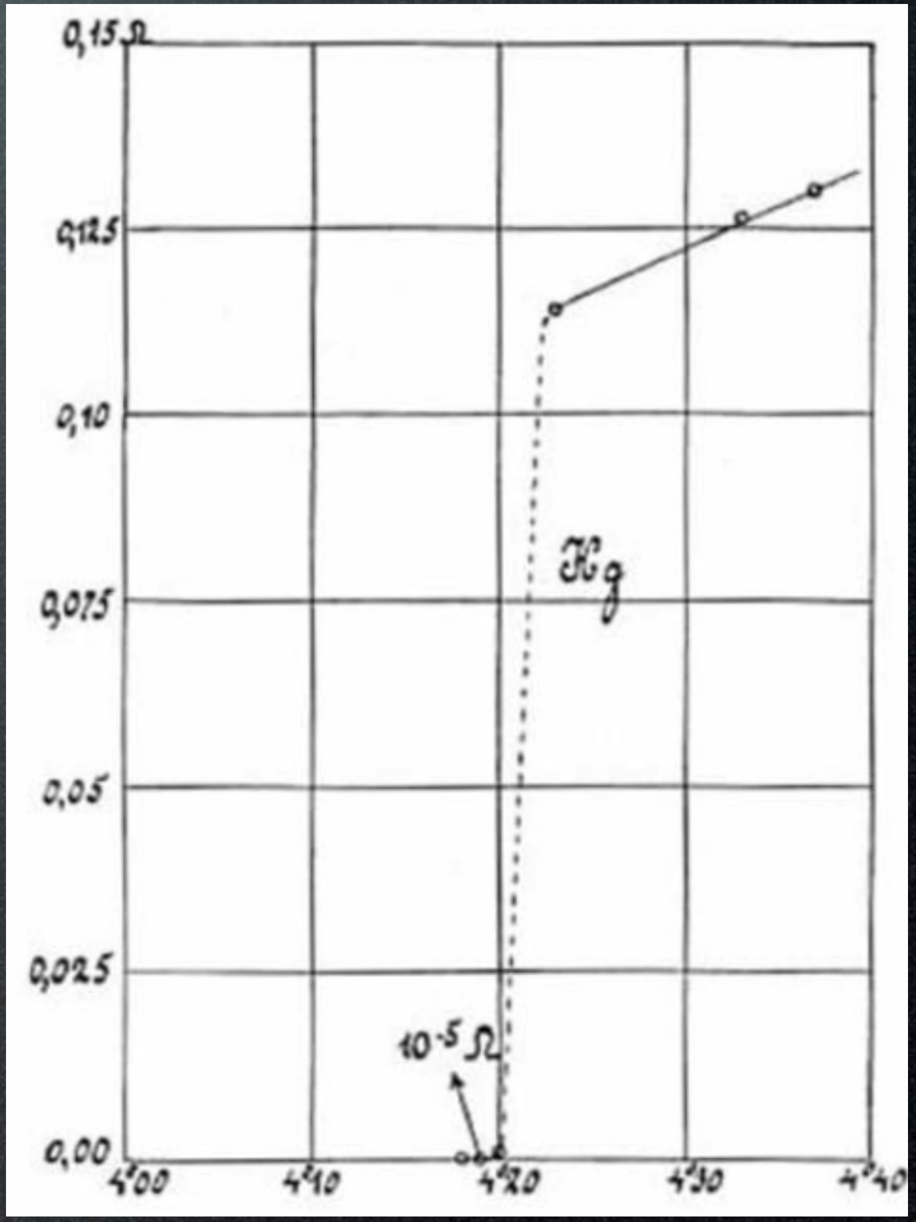
Heike Kamerlingh Onnes

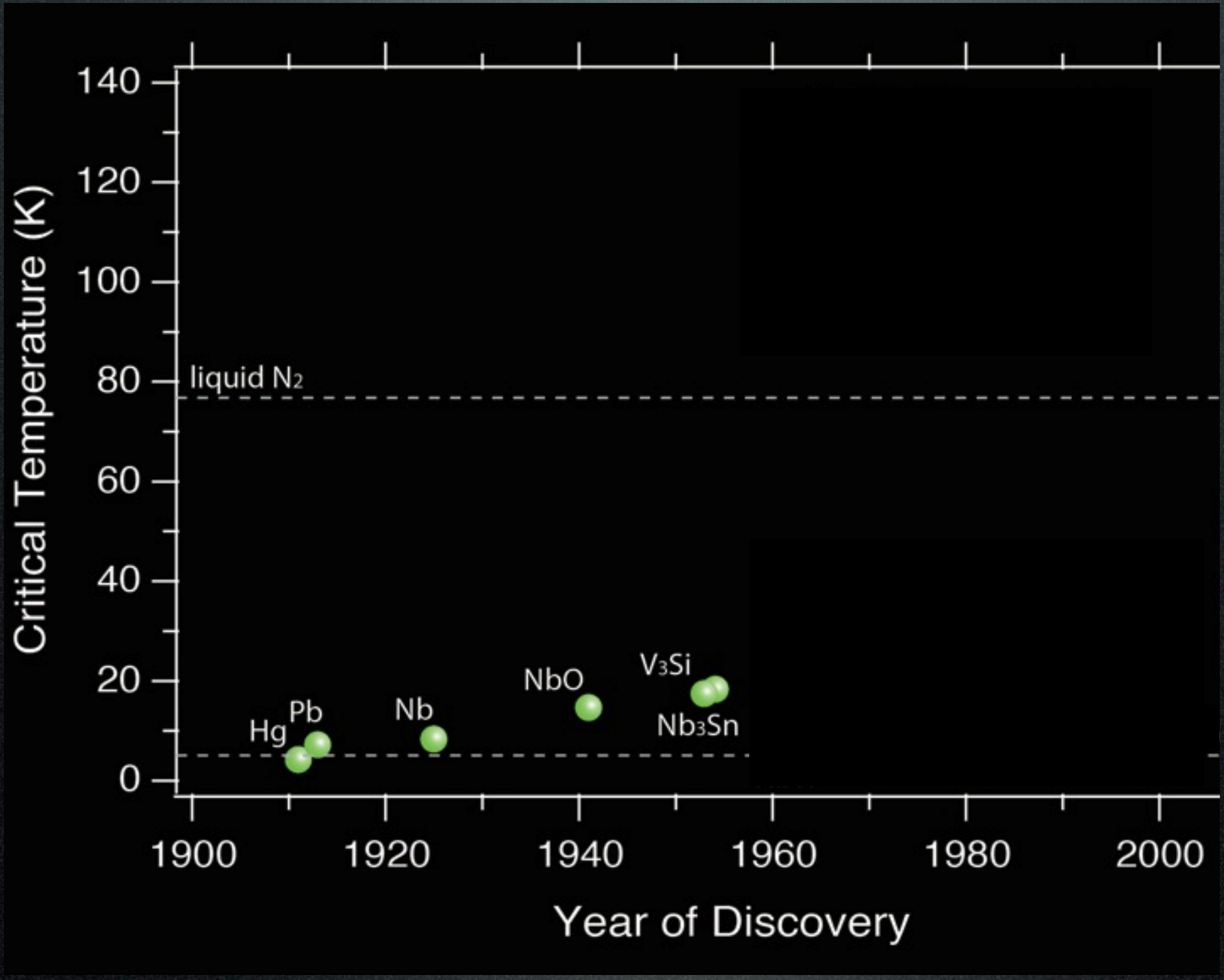
Verslagen van de Afdeeling Natuur-kunde der Kon. Acad. van Wetenschappen te Amsterdam, pp. 1479, 28 April 1911.

Liquefied Helium in 1908



Superconductivity 1911





Critical Temperature (K)
140
120
100
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liquid N2
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Nb
NbO
V3Si
Nb3Sn
1900
1920
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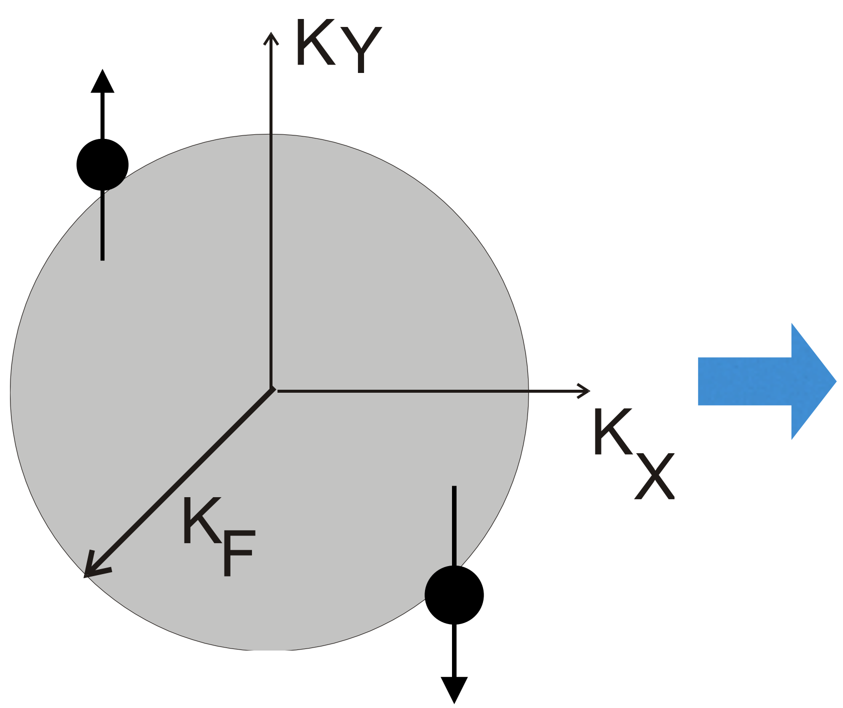
Year of Discovery

BCS theory of conventional superconductivity

BCS, Phys Rev 108, 1175 (1957)

Bogoliubov, Nuovo Cimento 7, 794 (1958)

Normal State (Metal)



Degenerate
~free electron gas

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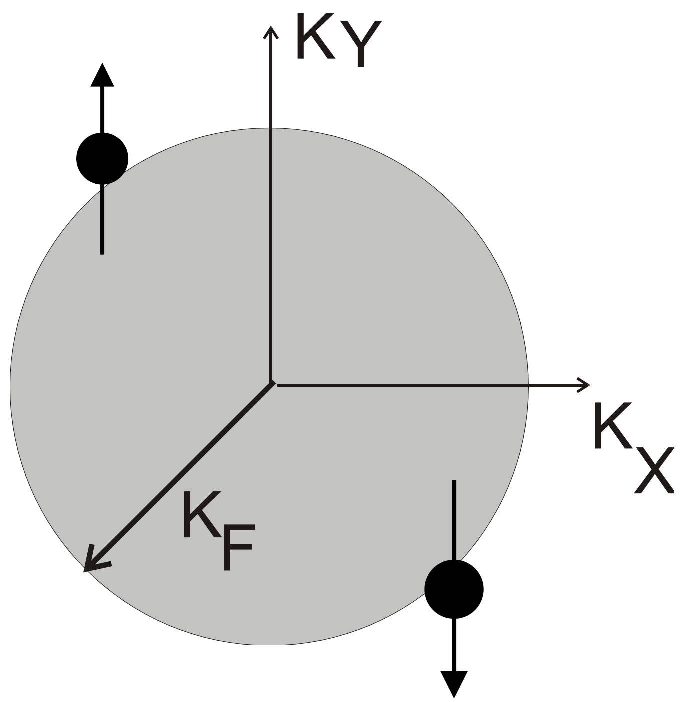

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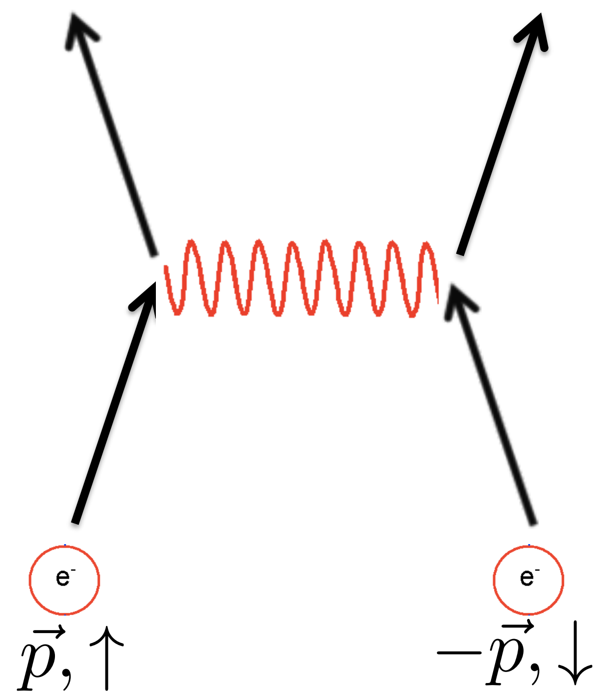

Electrons interacting with
Lattice Vibration Mode

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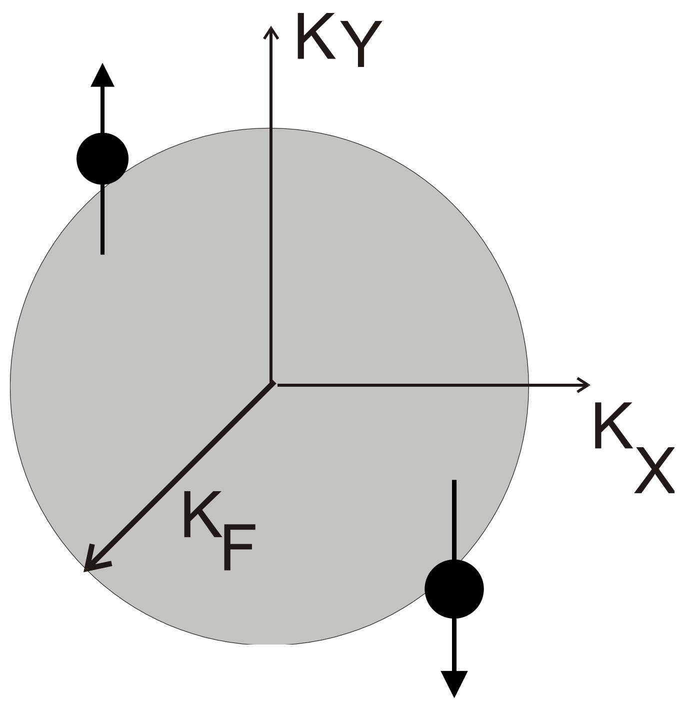

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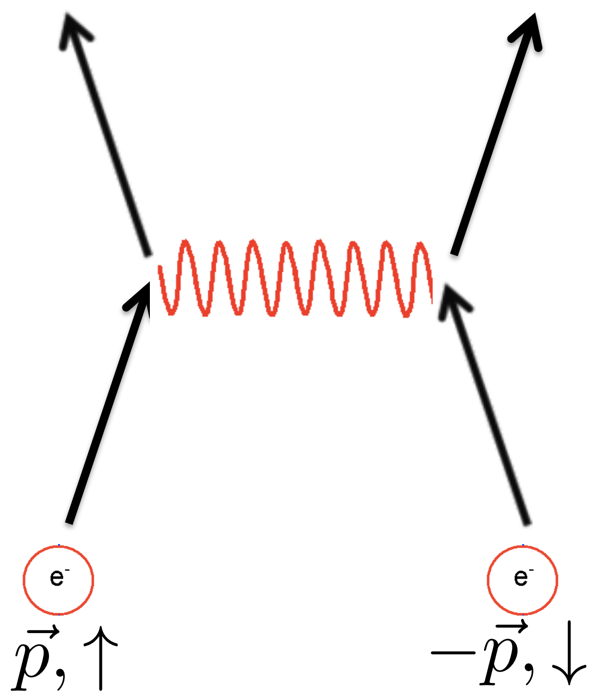
Weak coupling instability



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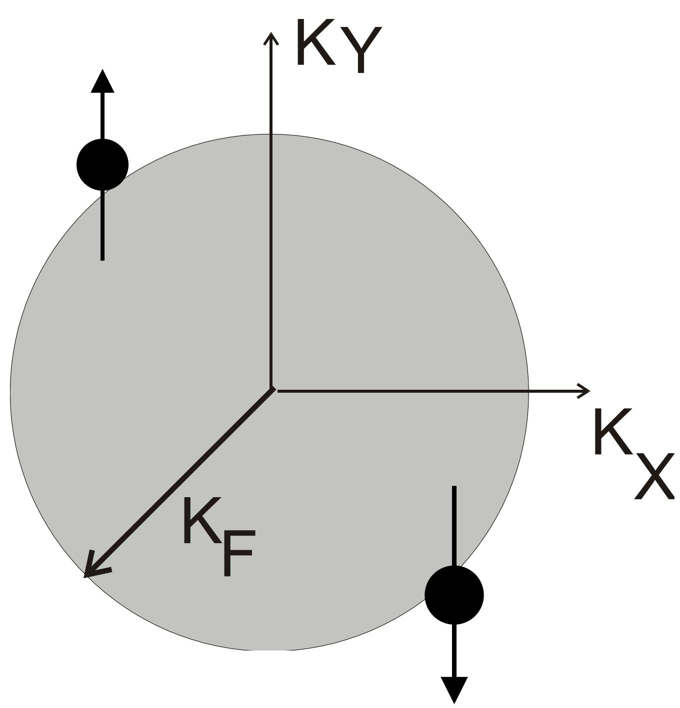

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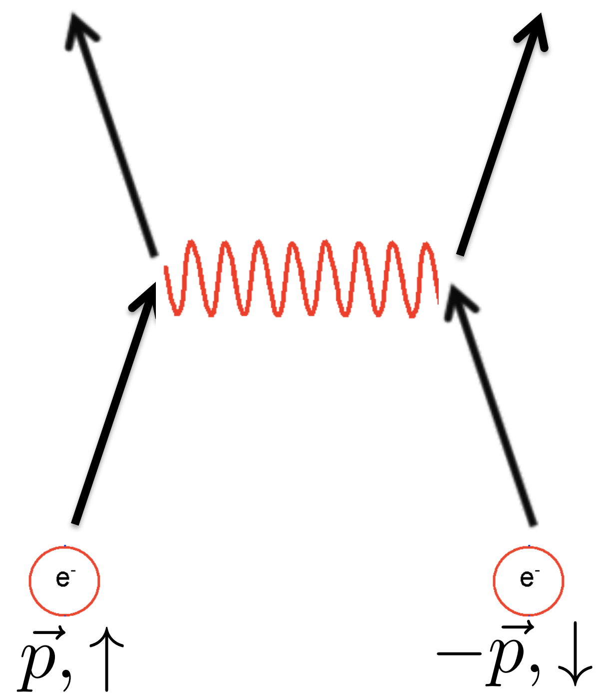

Electrons interacting with
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Low T- Superconducting
Ground/Excited States

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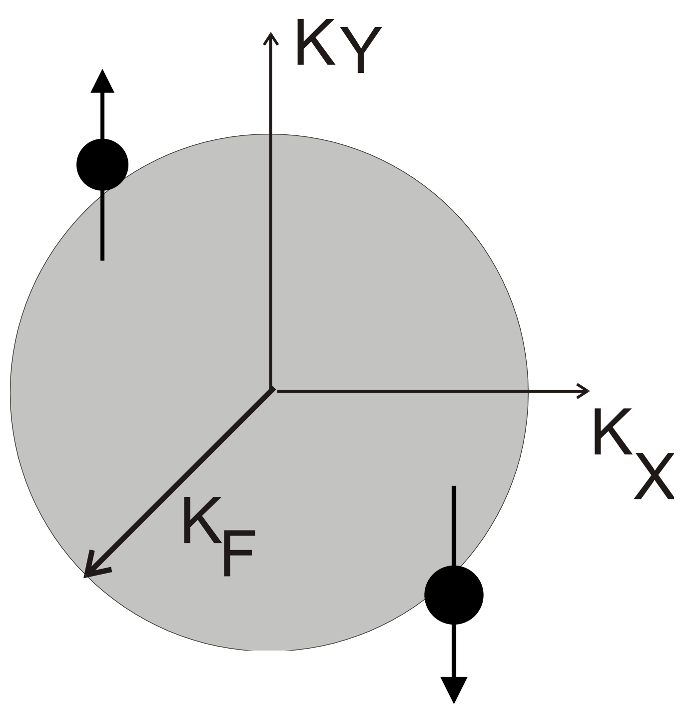

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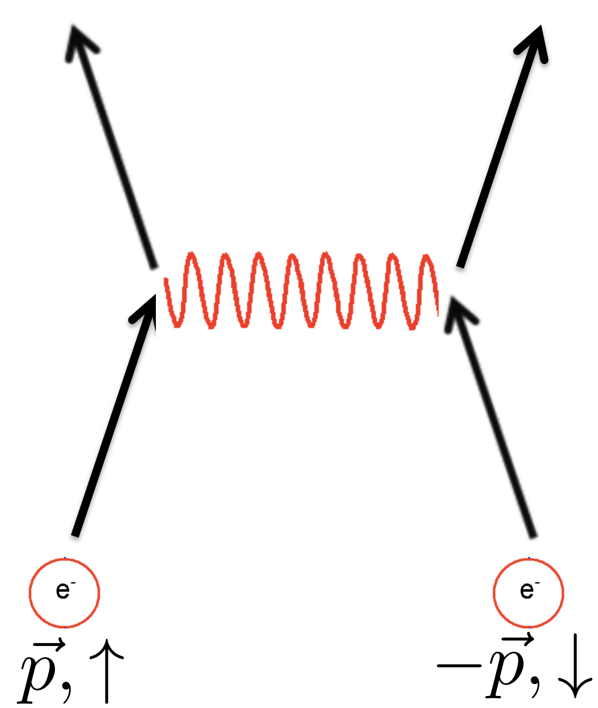

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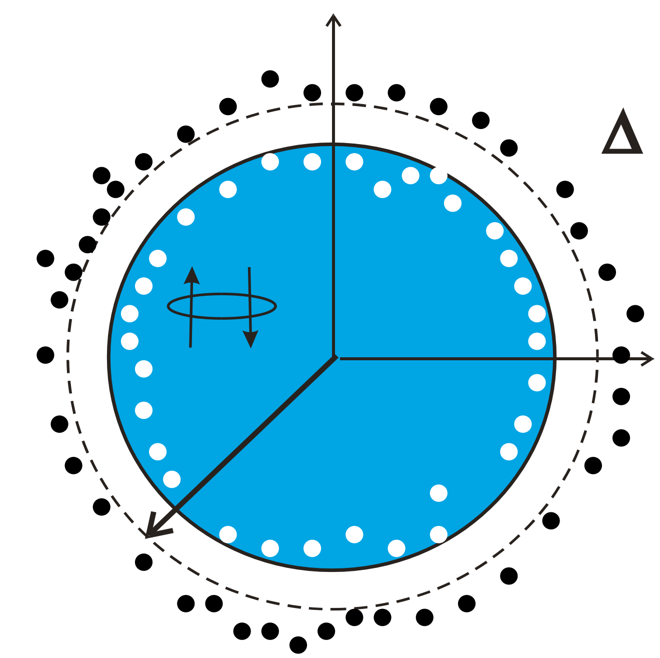
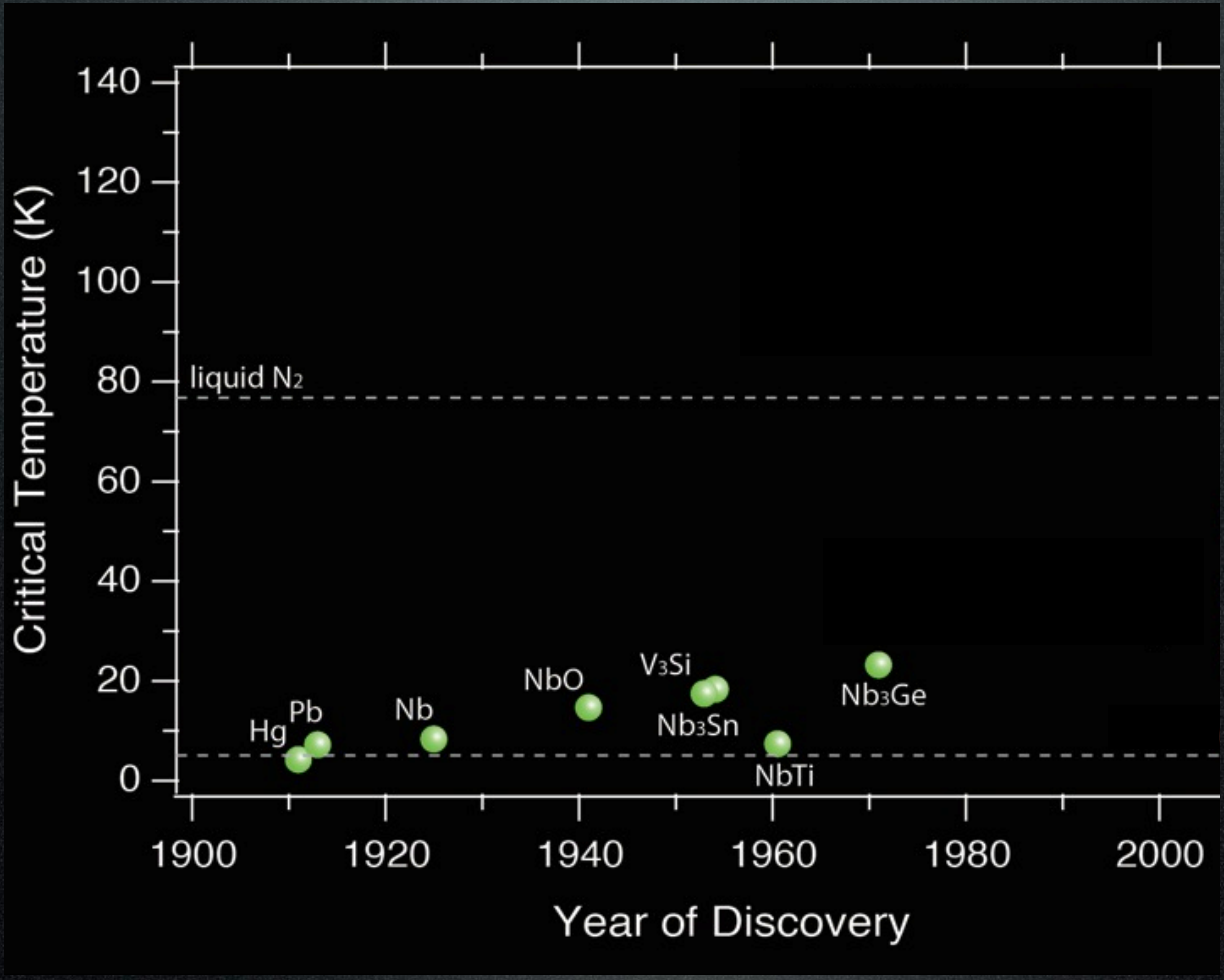


- Gas of Cooper Pairs
- Pair-Energy Gap Δ
- Bog. quasiparticles



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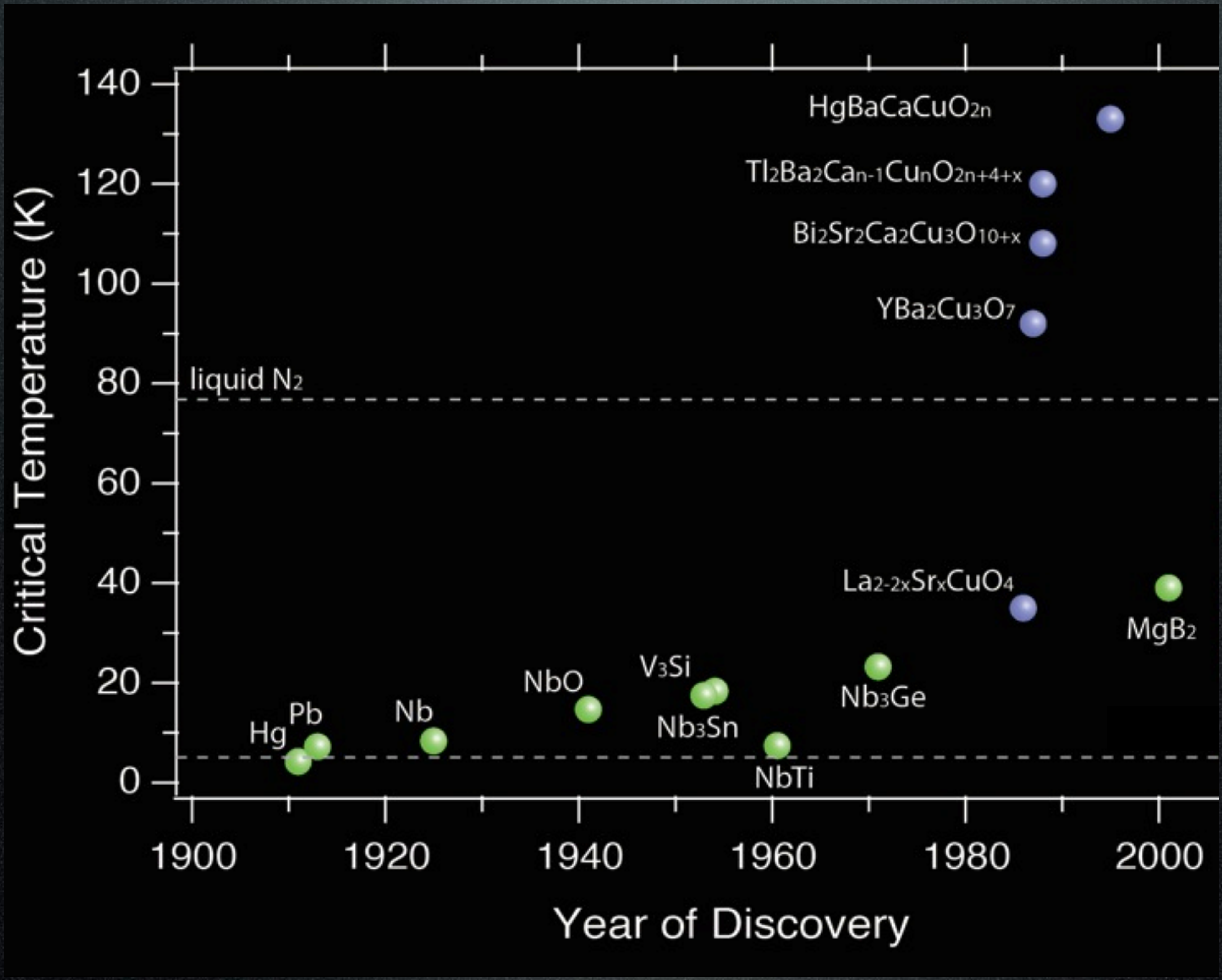
Correlated (High-T_c) Superconductivity



Key Questions in High-T_c Superconductivity:

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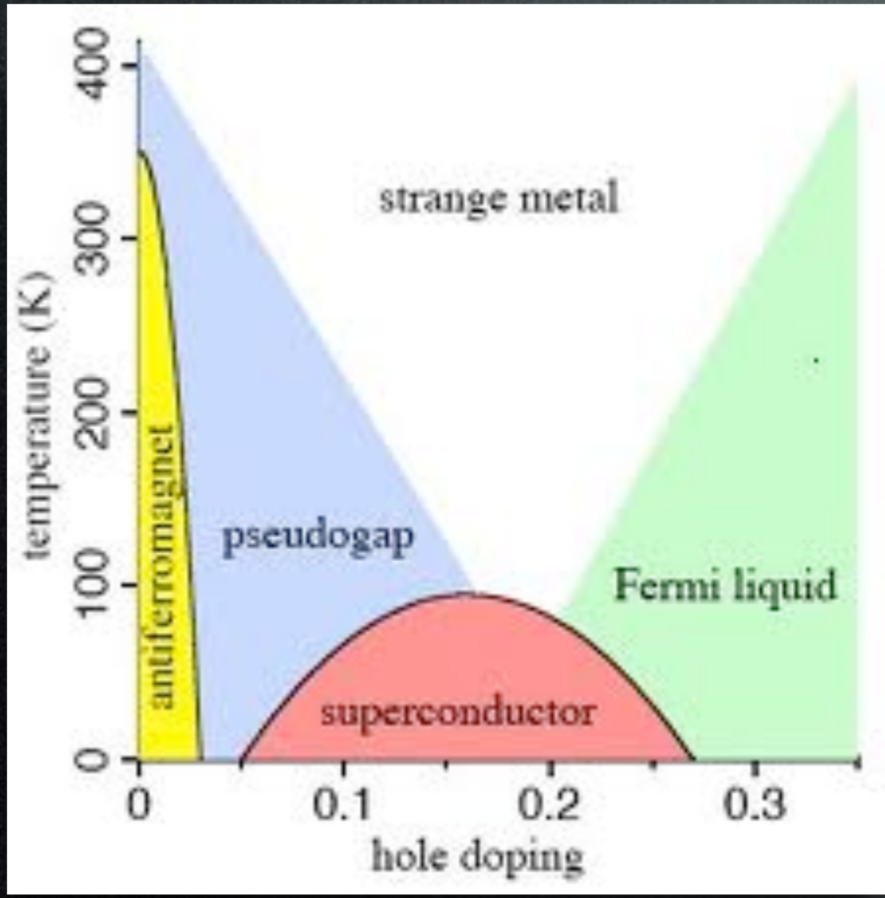

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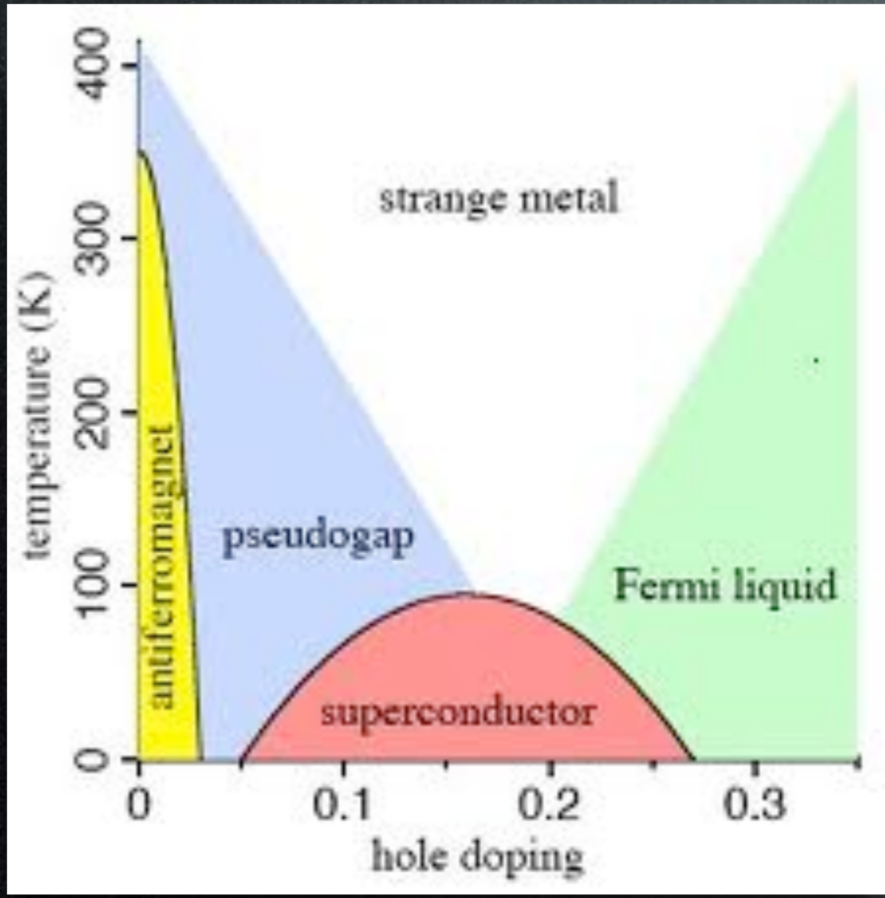

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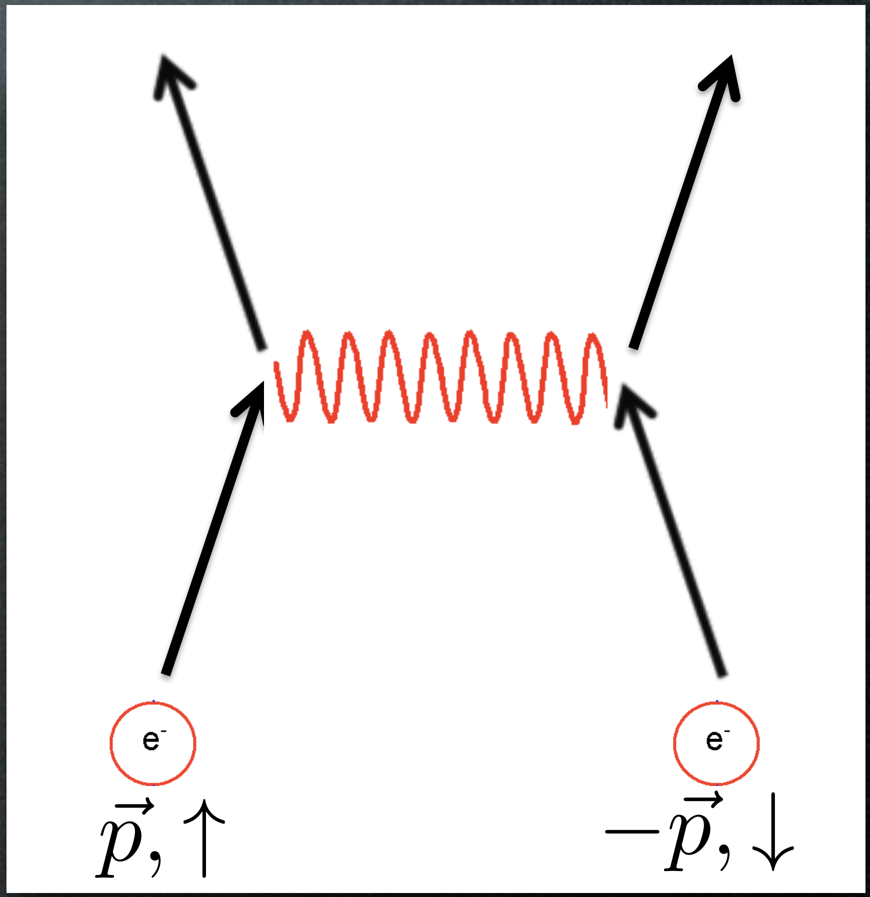

The Challenge of Strong (Intermediate) Coupling

Interaction Energy vs Kinetic Energy

Liquid

$$V_{int} \ll E_{kin}$$

- Weak interaction
- K-space

Interaction Energy vs Kinetic Energy

Crystal

$$V_{int} \gg E_{kin}$$

- Strong interaction
- Real space

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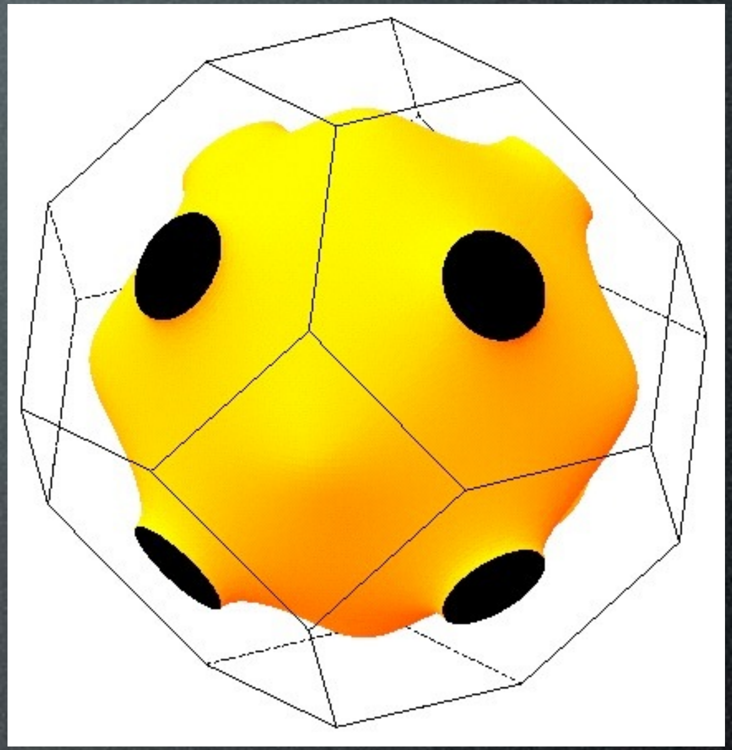
Freezing

Interaction Energy vs Kinetic Energy

Landau Fermi Liquid (1956)



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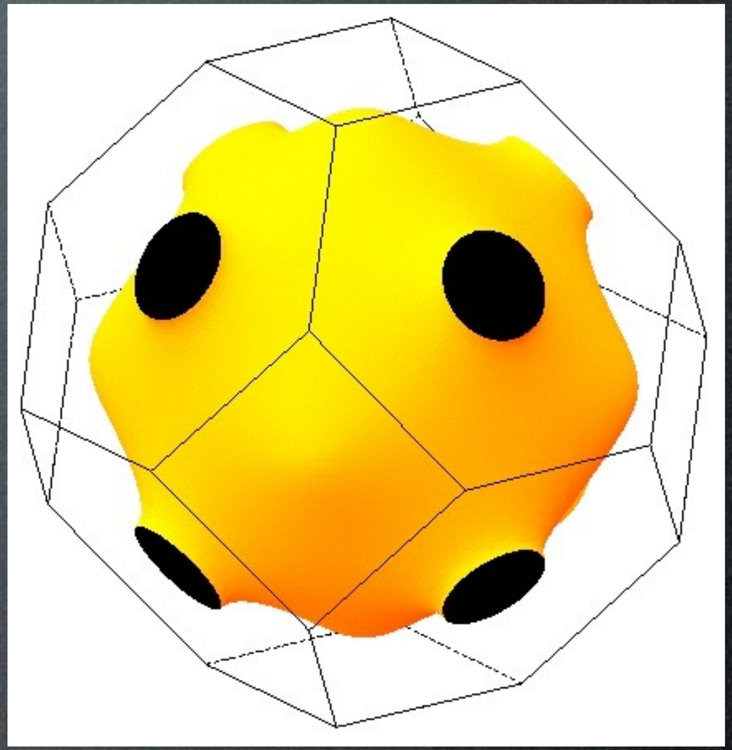

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Fermi surface instabilities

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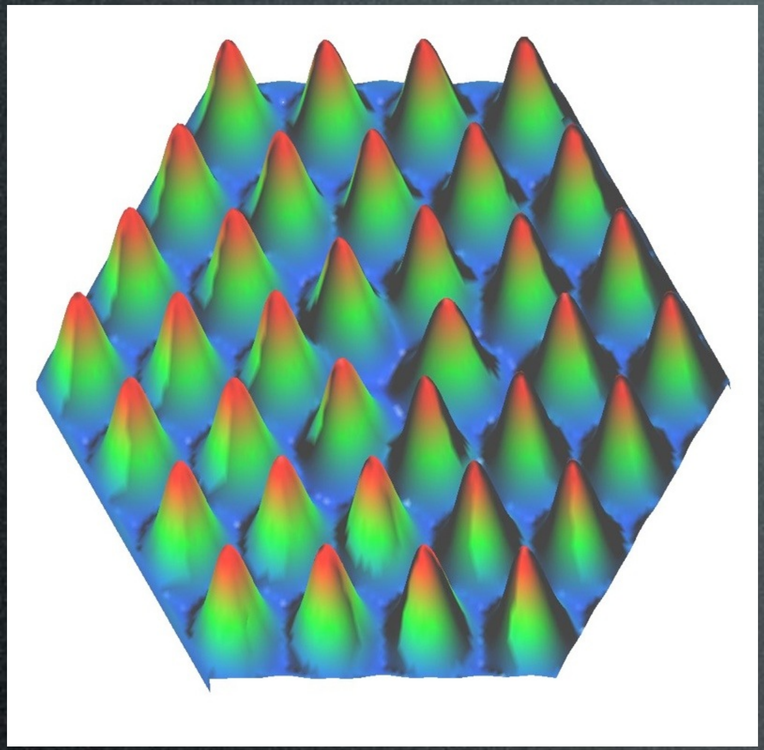

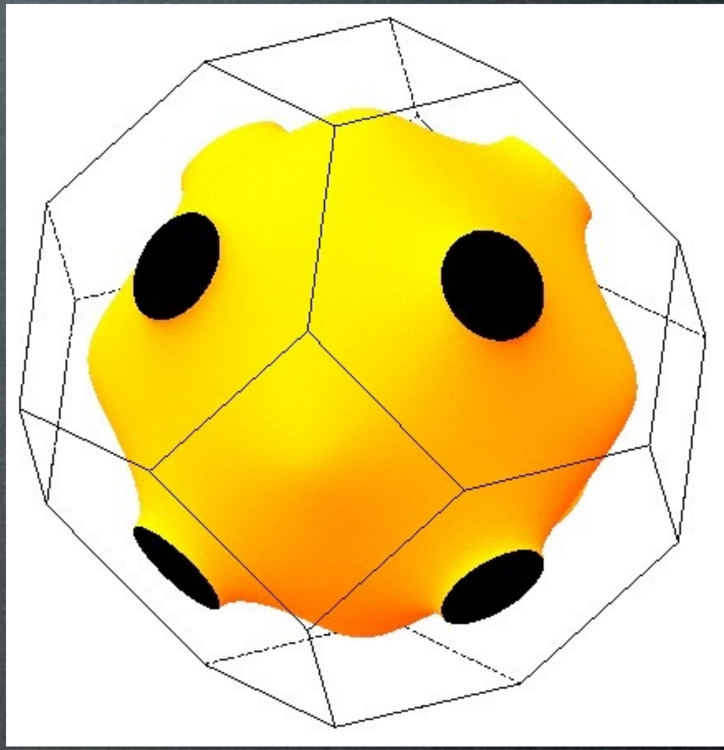

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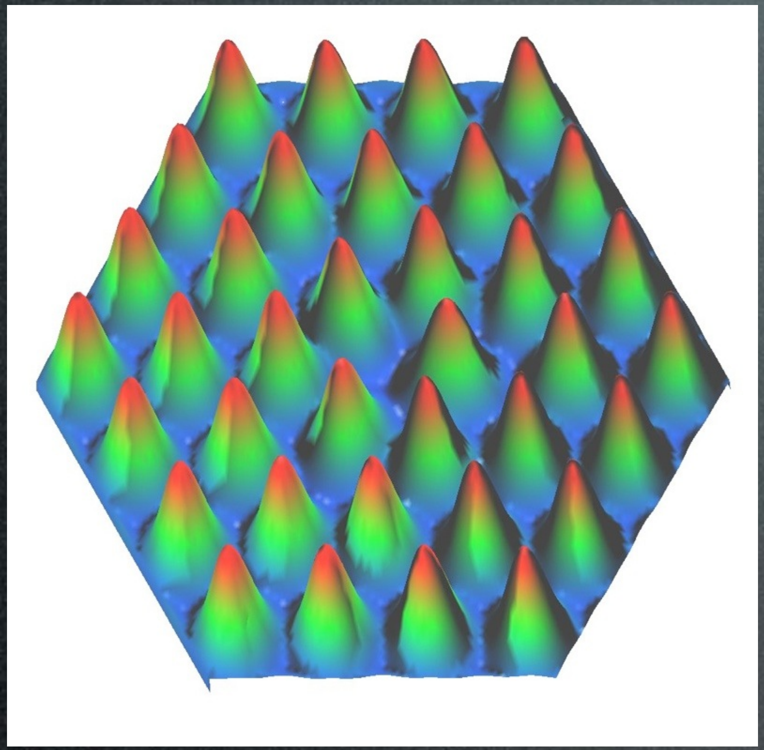

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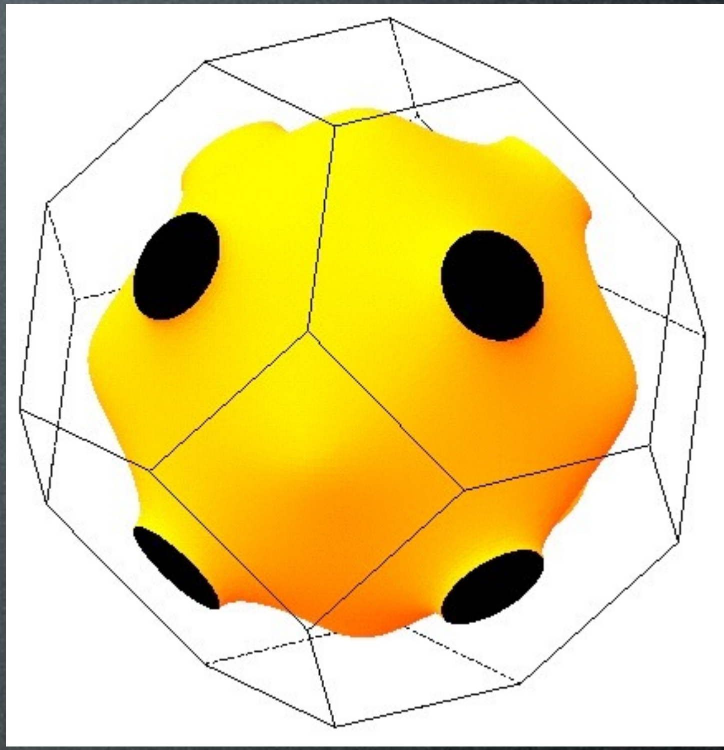

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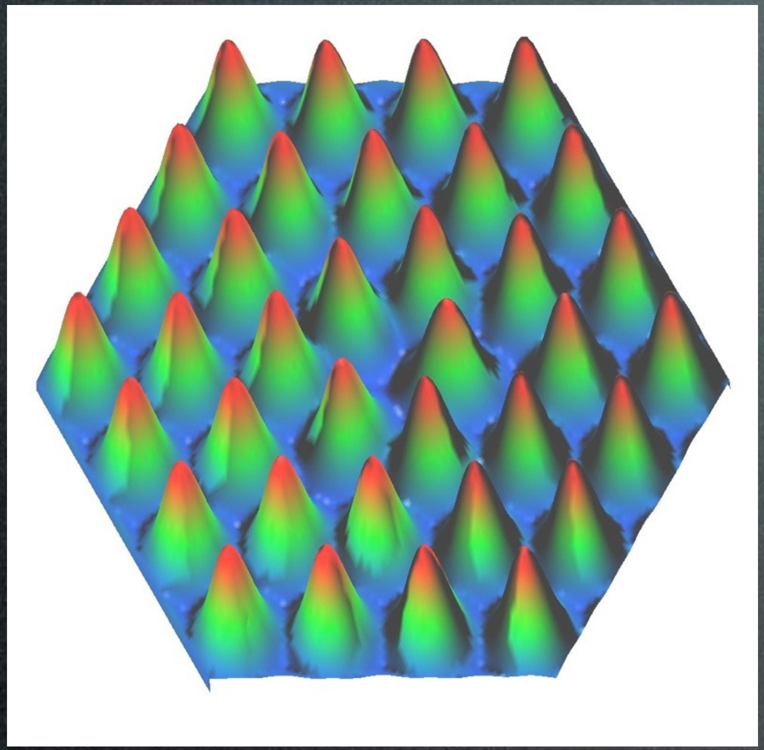
Interaction Energy vs Kinetic Energy

Wigner Crystal (1930)

Mott Insulator (1937)



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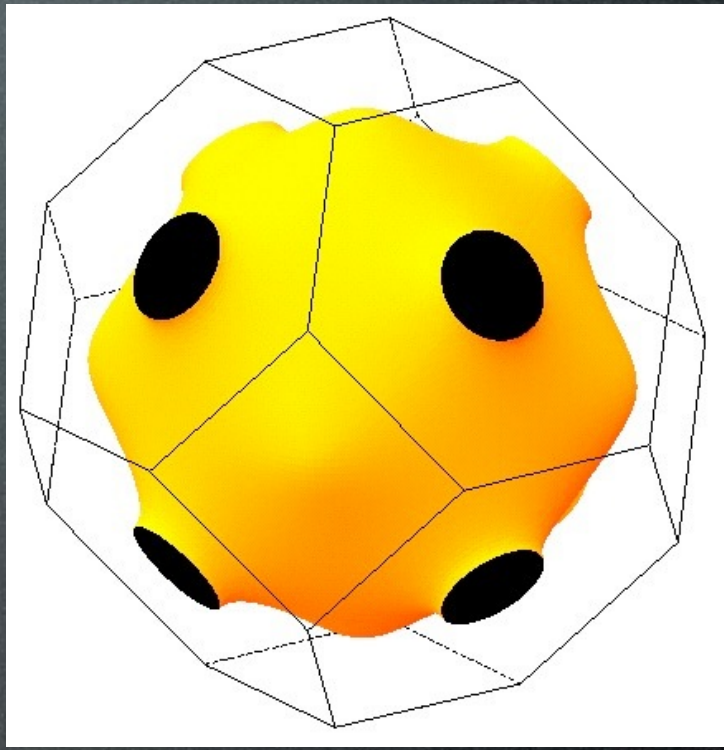

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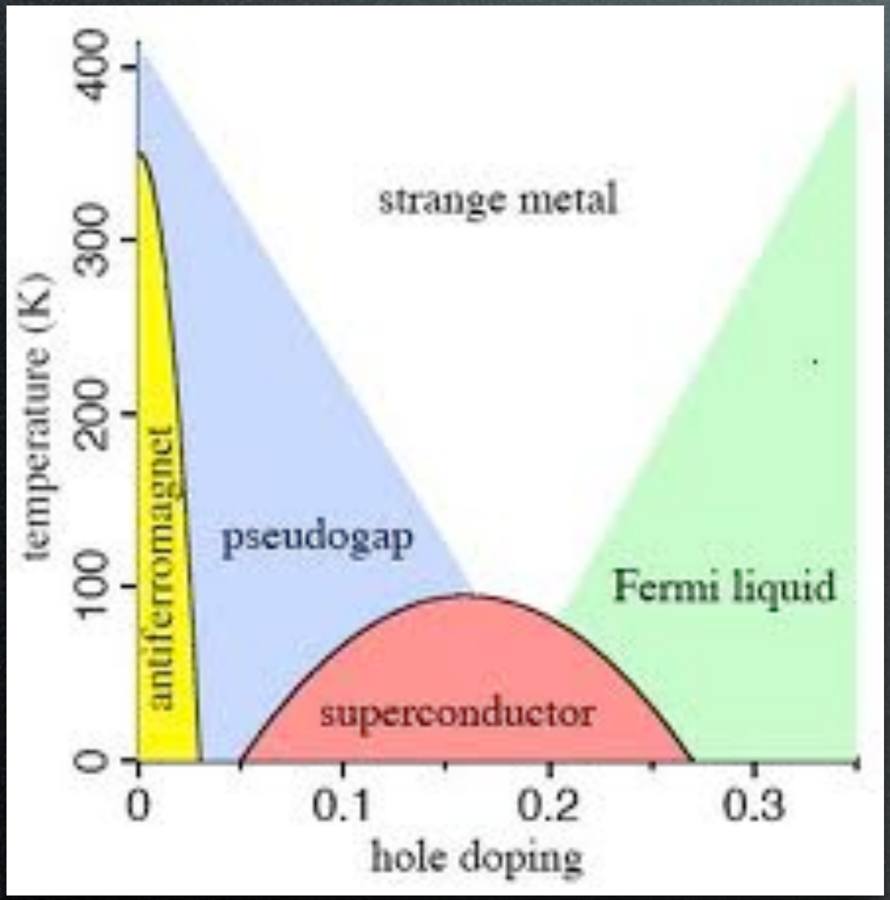

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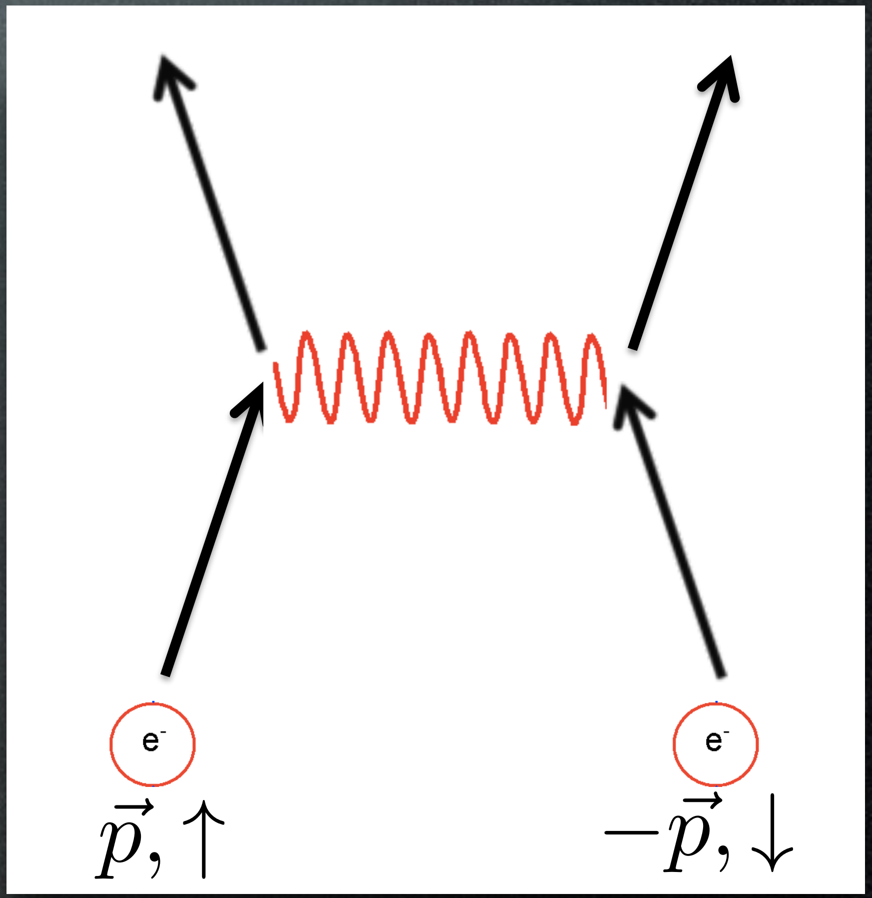

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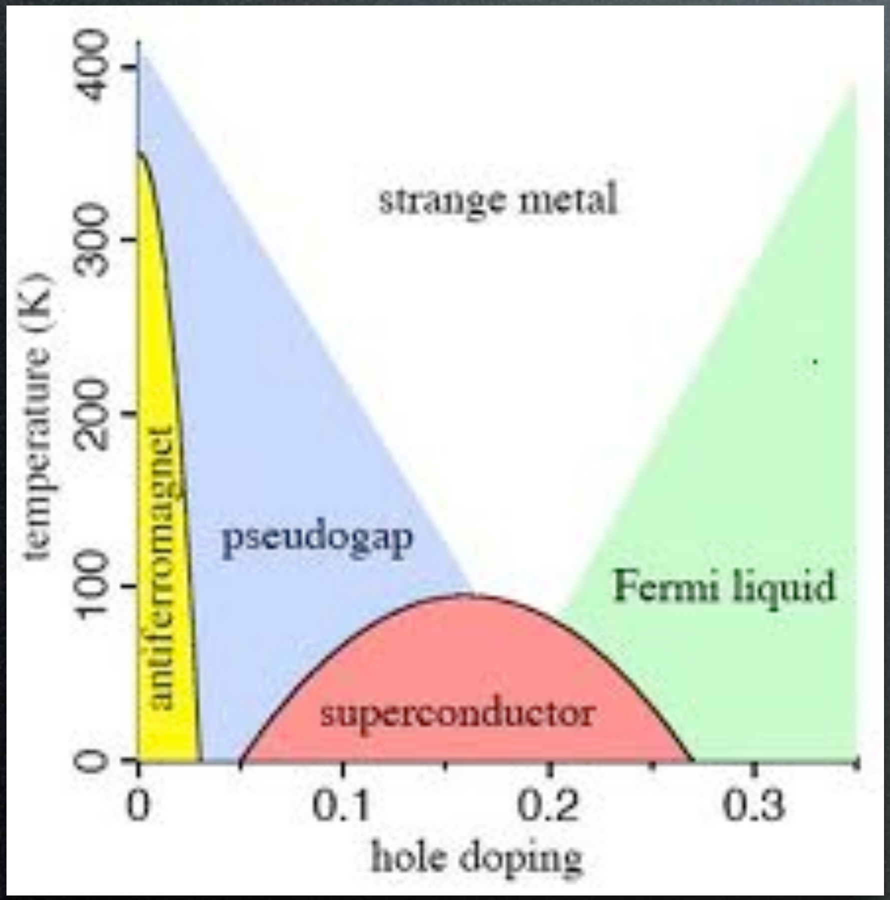

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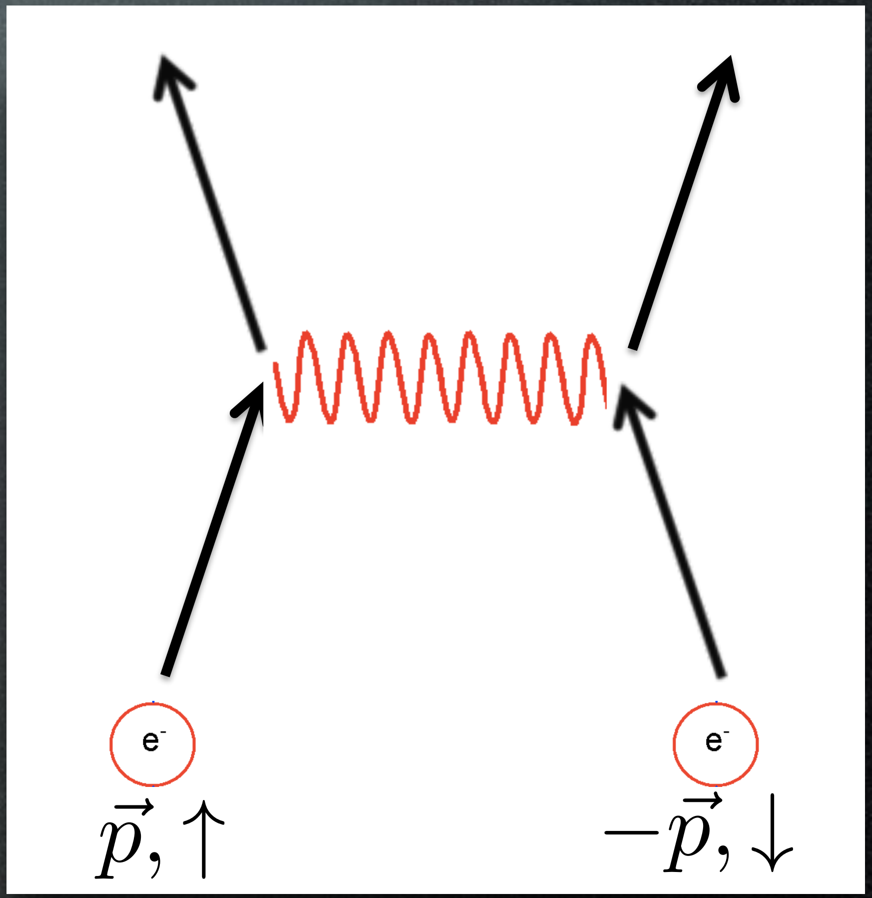
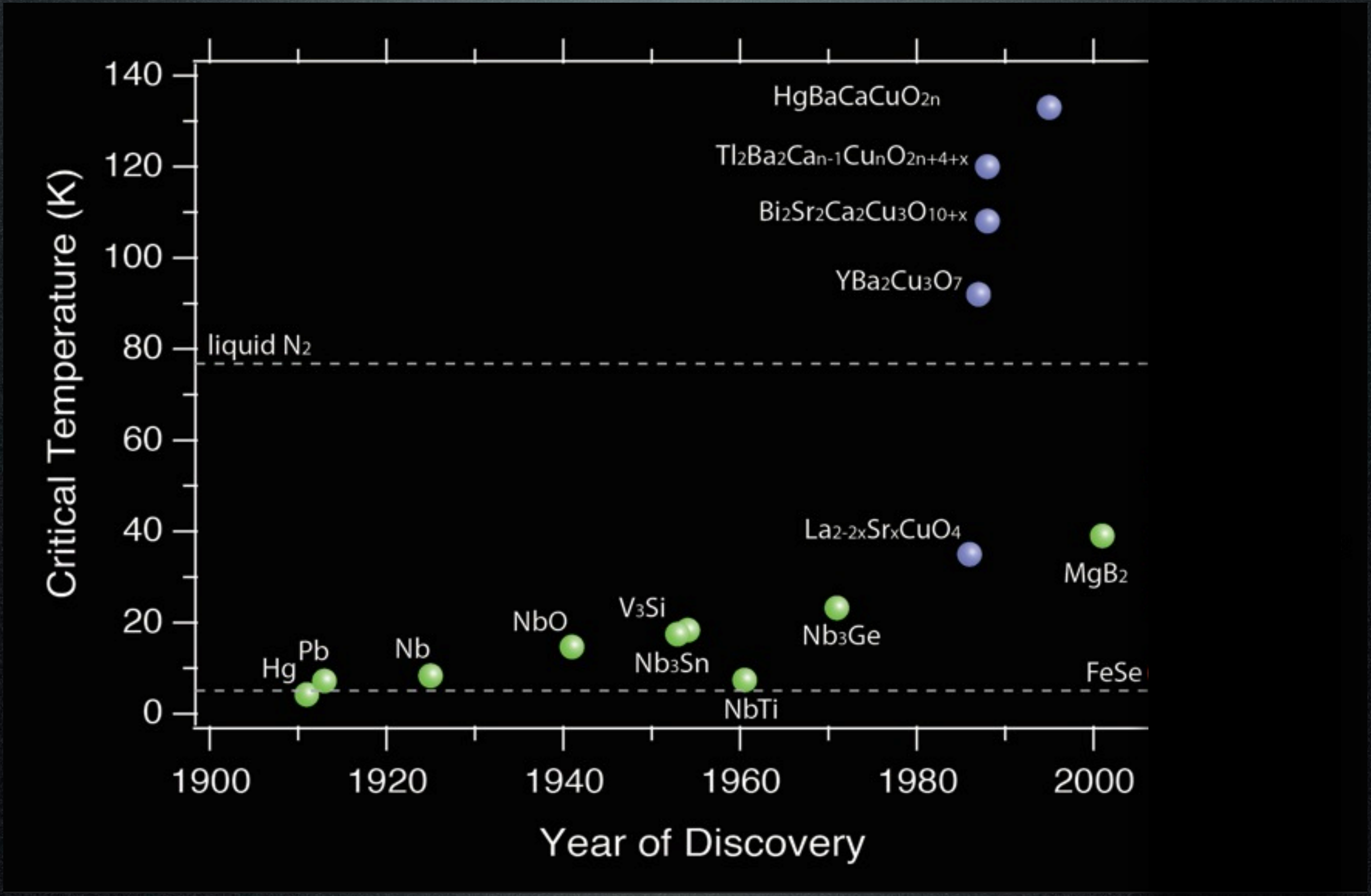


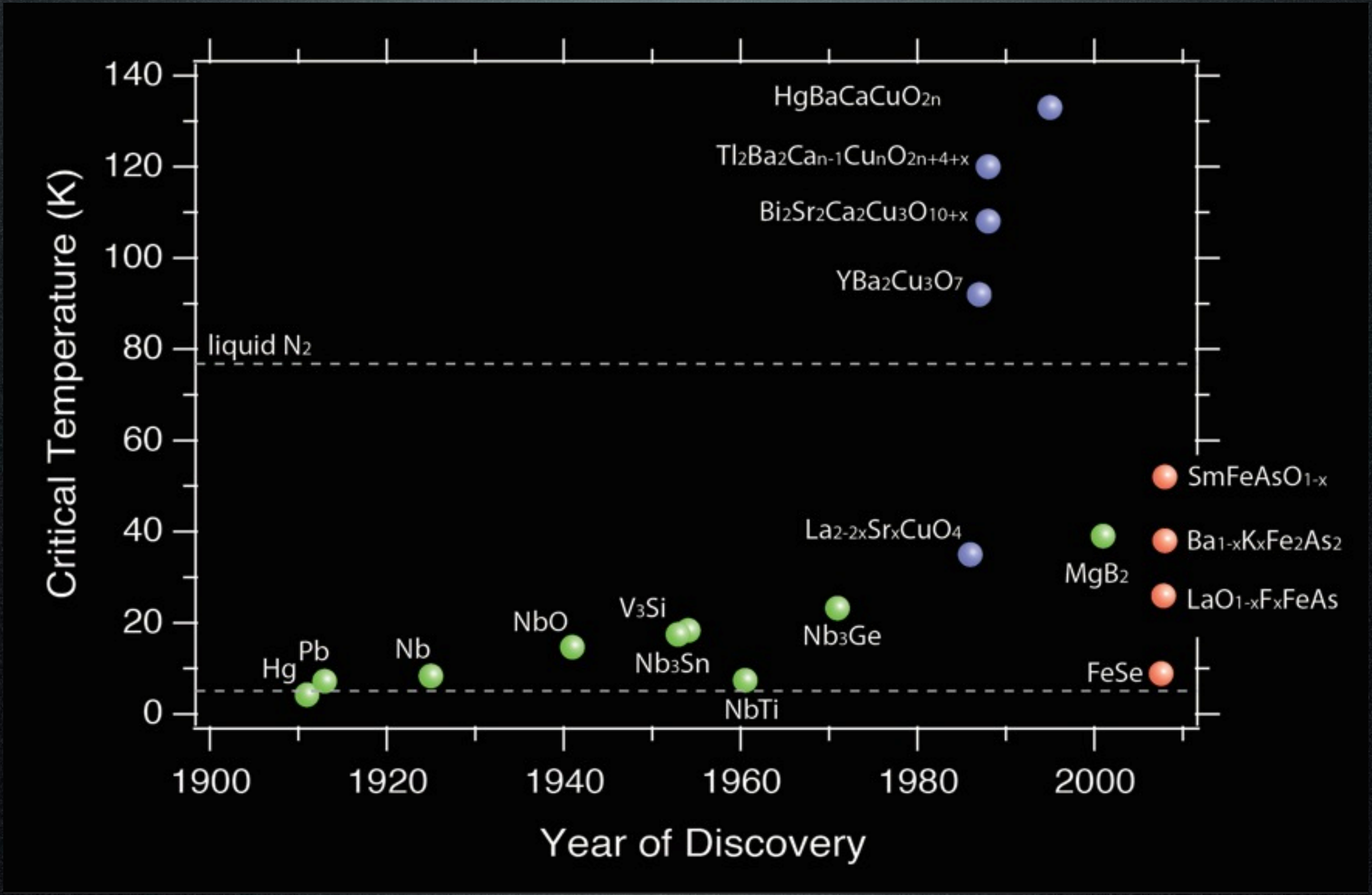
New Physics in the Intermediate Regime!

Recent Advances in Materials



Recent Advances in Materials

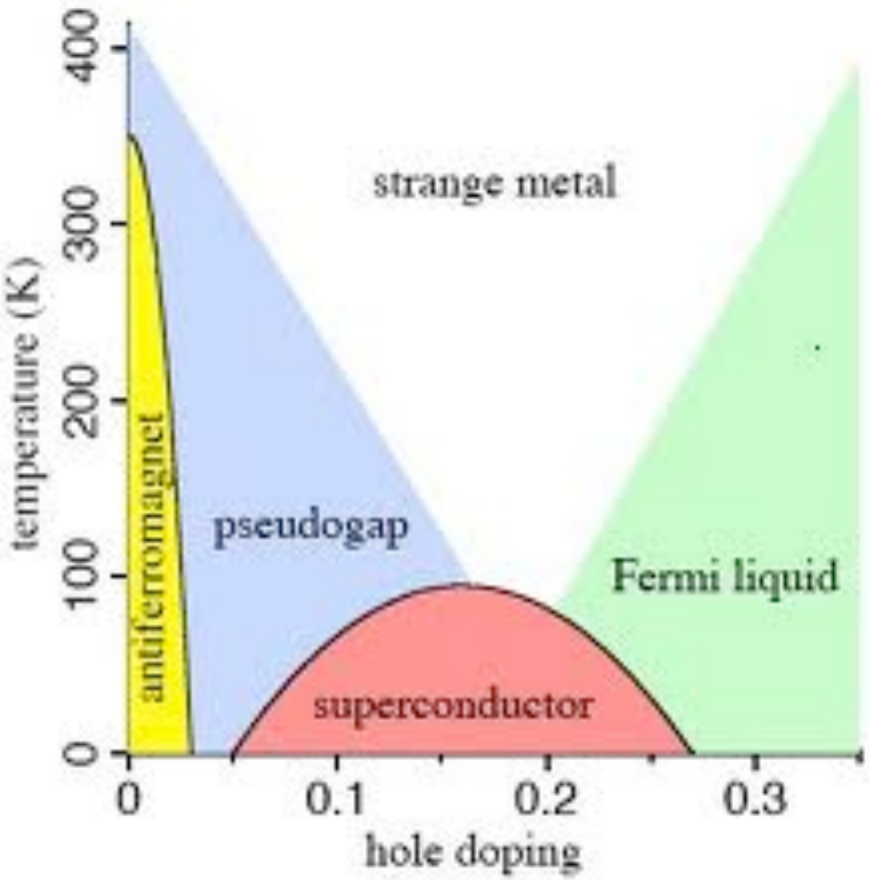
Discovery of Fe-pnictide



Copper-oxide vs Iron-pnictide

Copper-oxide
(d-wave)

Iron-pnictide
(s±-wave?)



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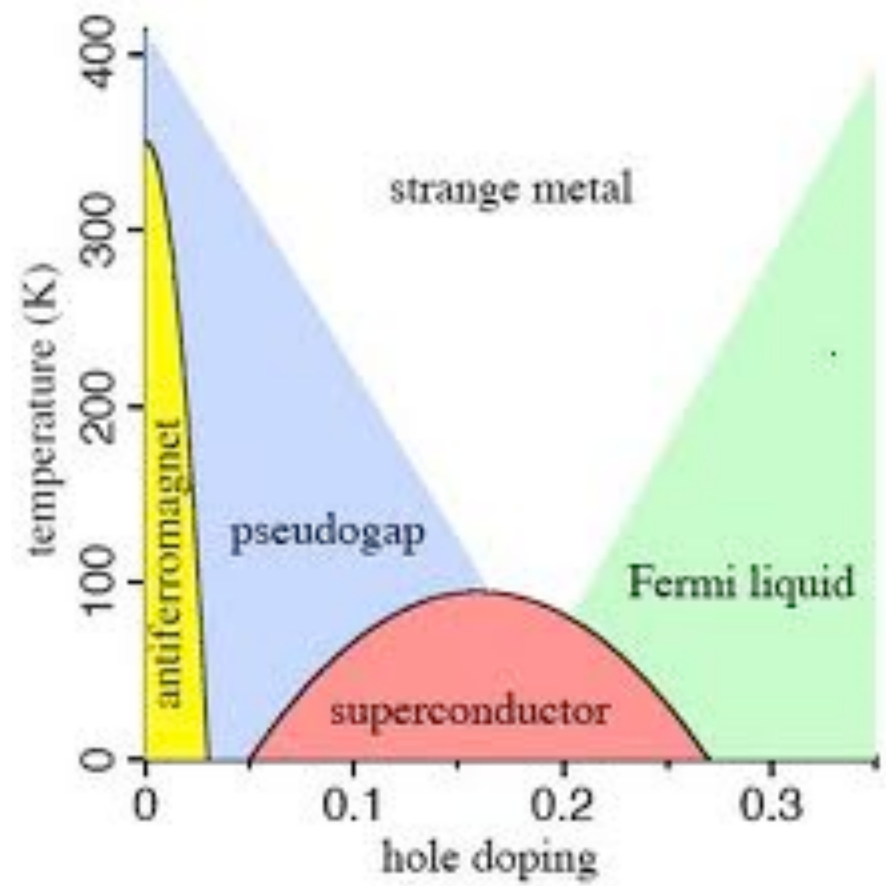

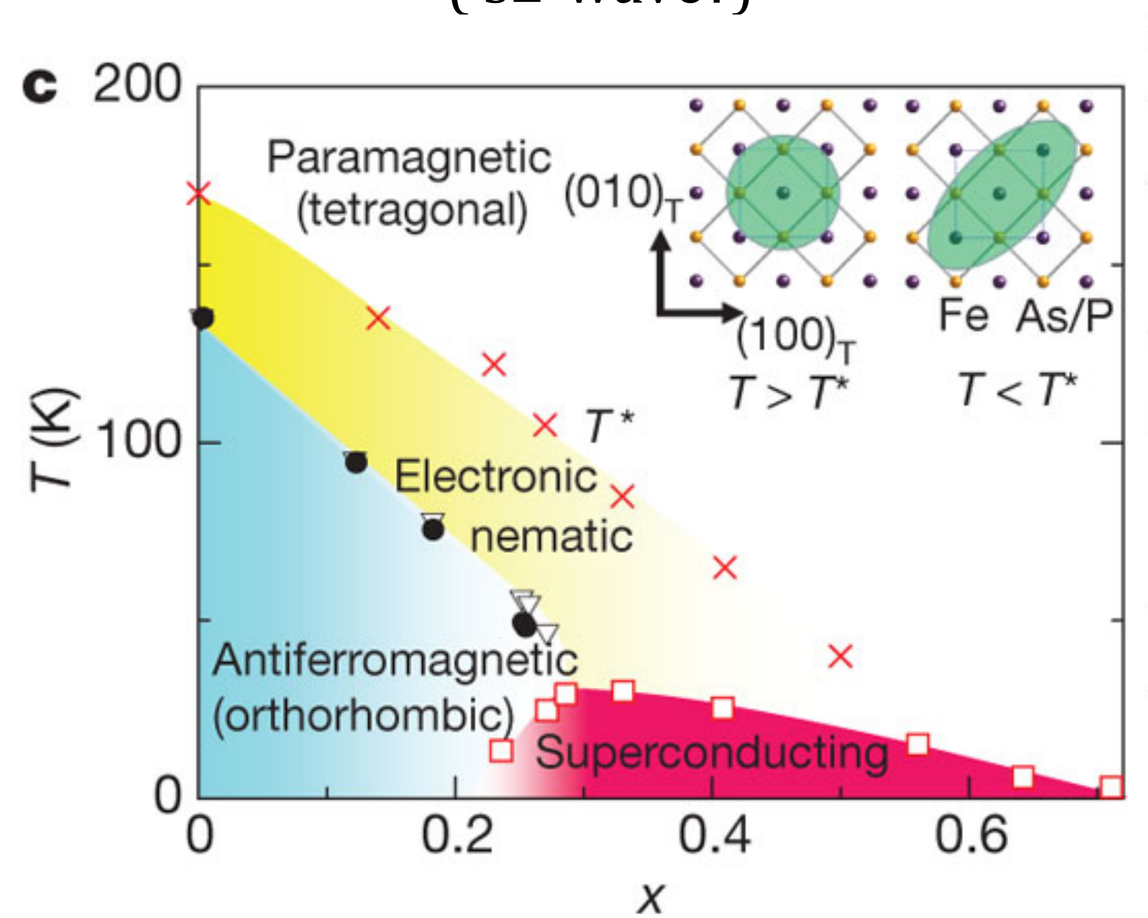

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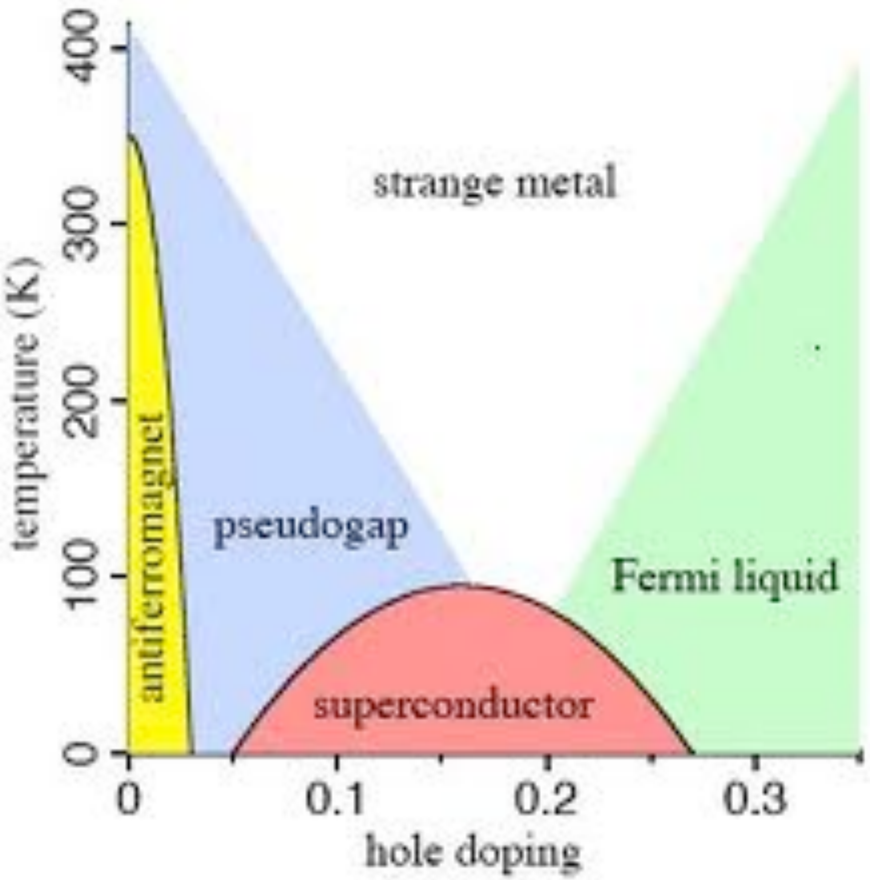

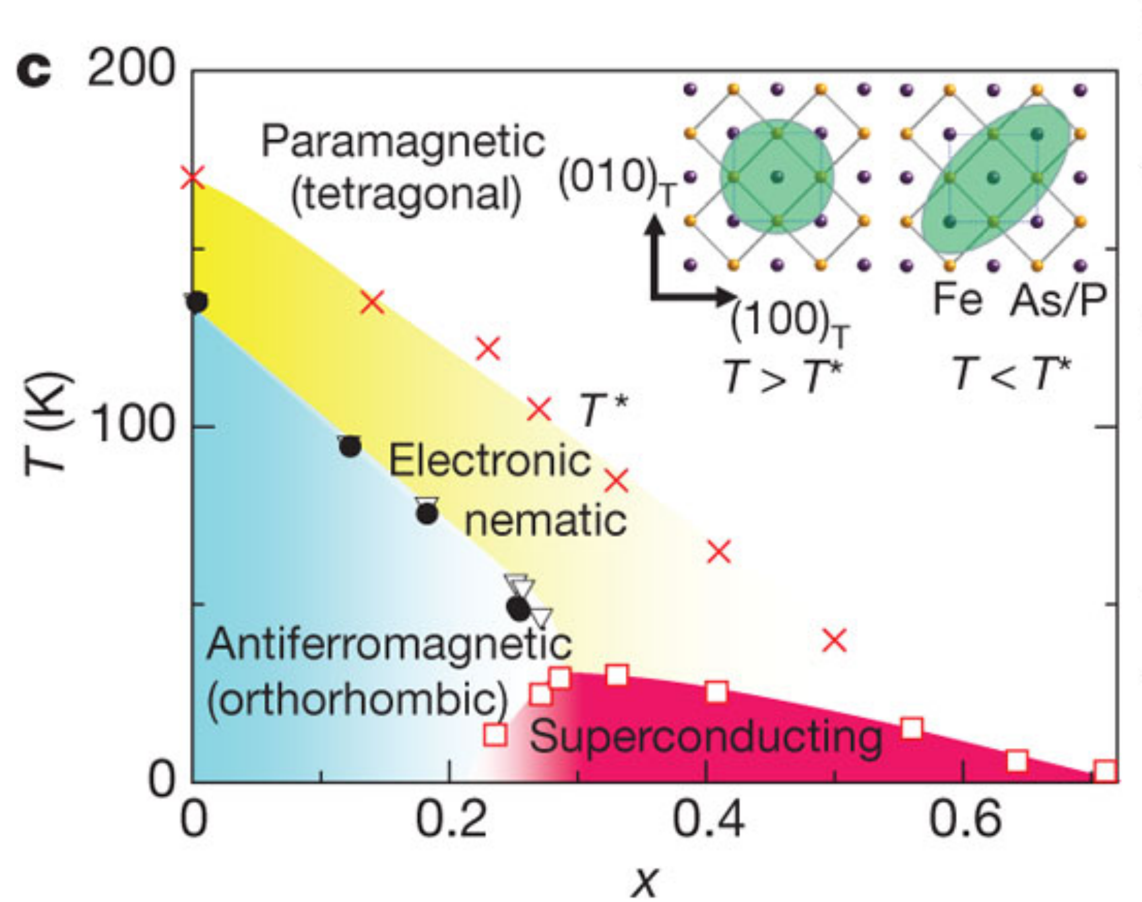

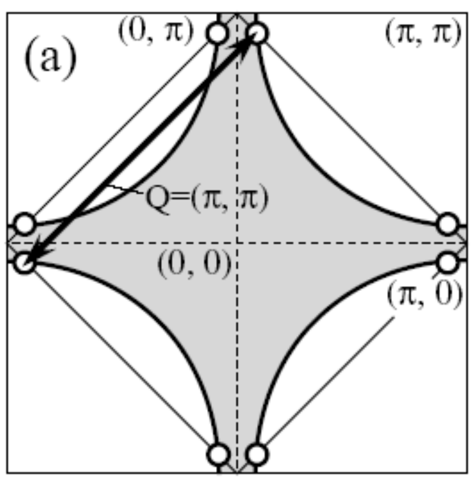

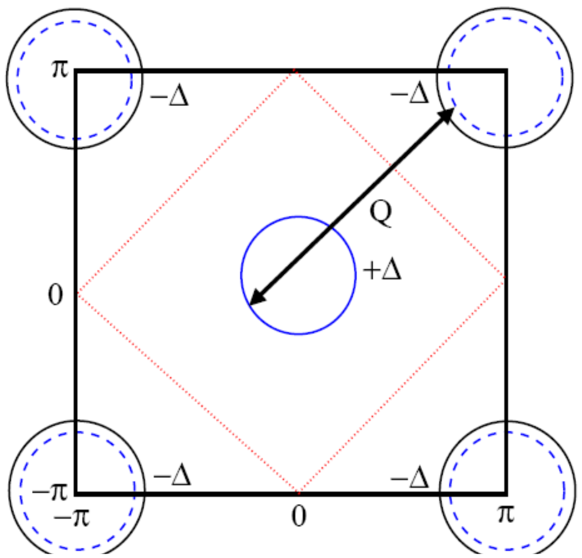

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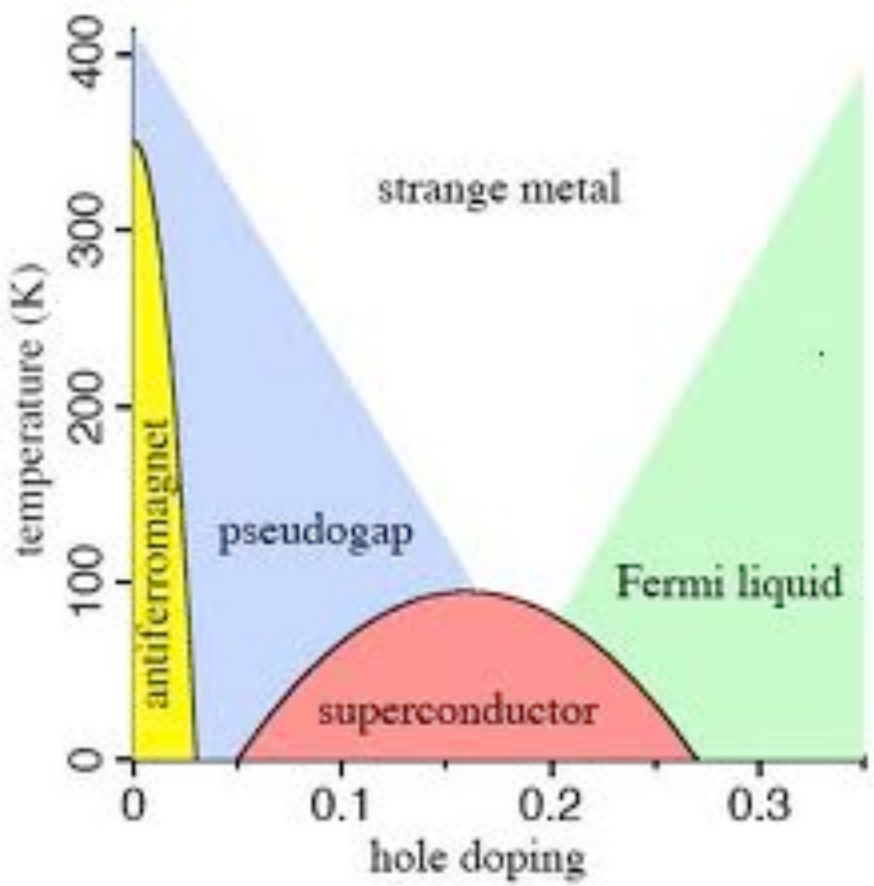

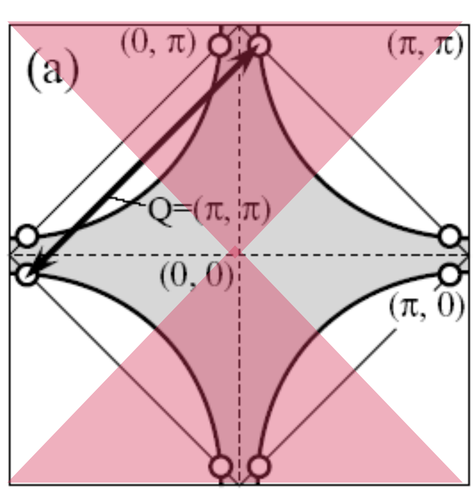

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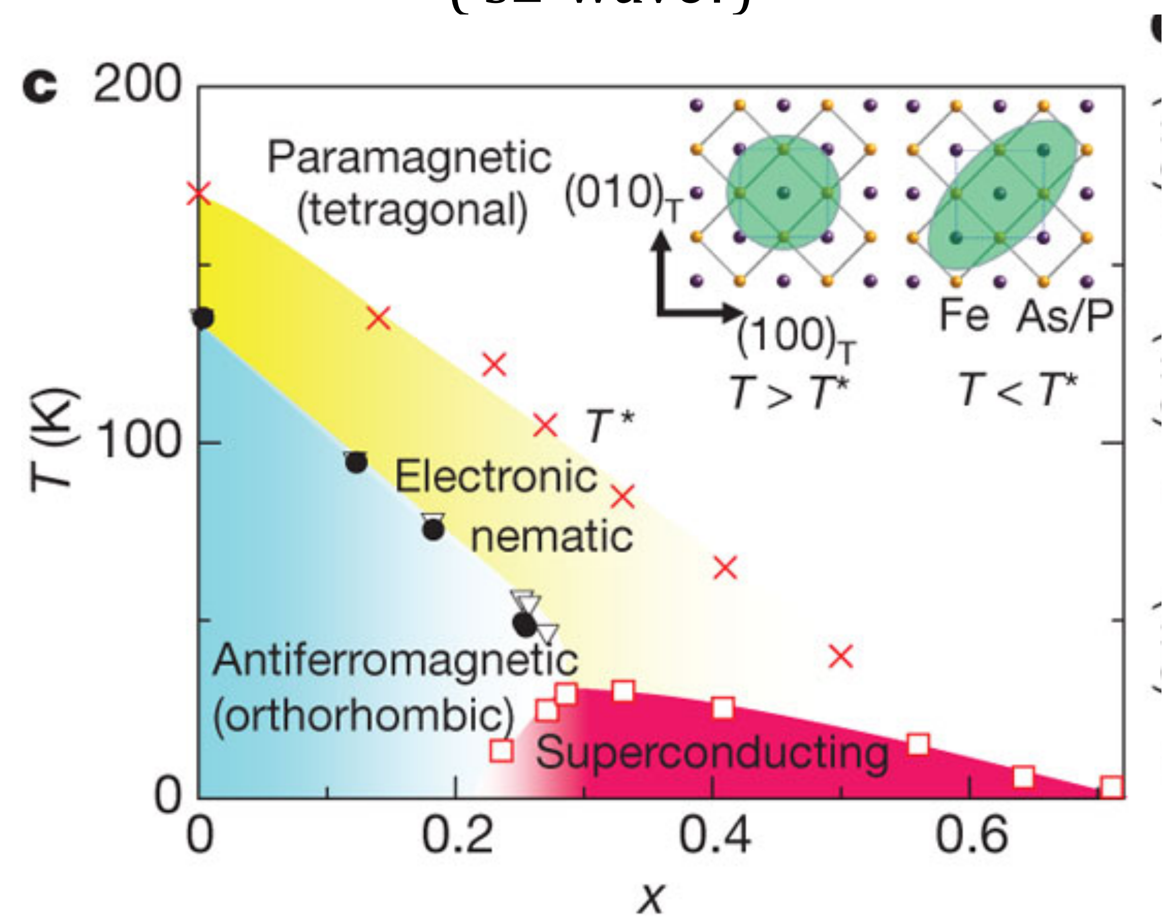
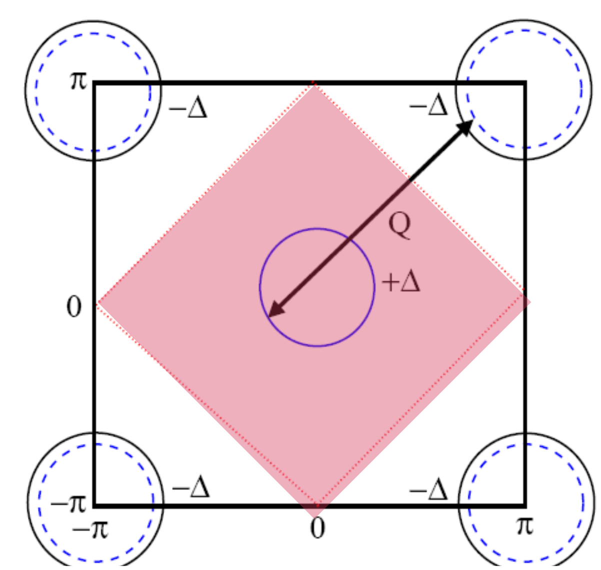
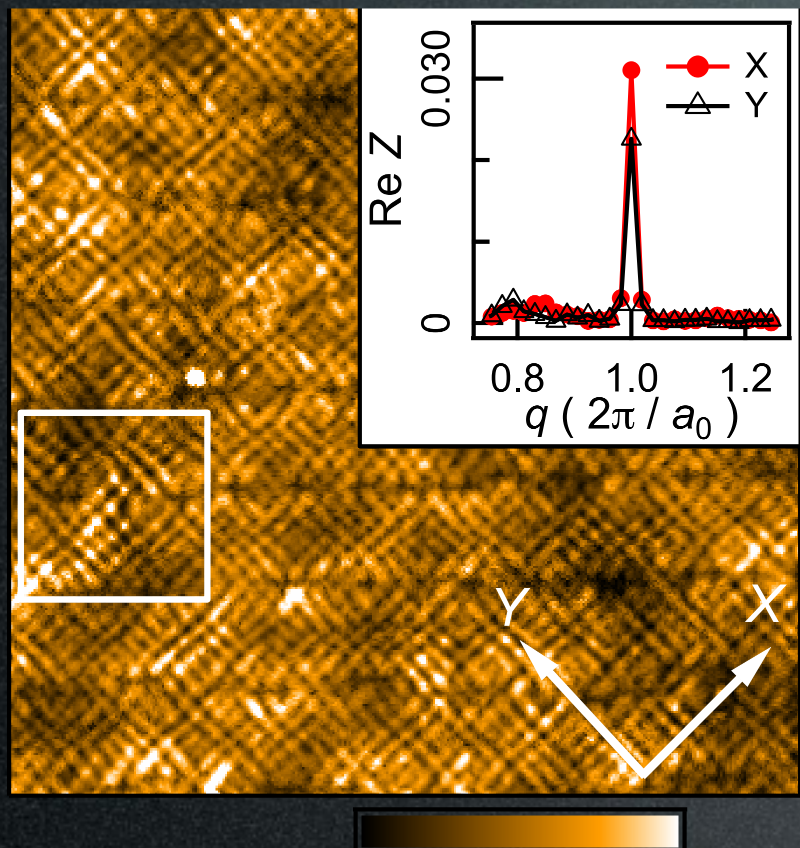




Recent Advances in High Res. Probes



20nm x 20nm

Y. Li "Unusual magnetic order in the pseudogap region of the superconductor HgBa2CuO41d"

Nature 455 372 2008

Jing Xia, "Polar Kerr-Effect Measurements of YBa2Cu3O6 x Superconductor: Evidence for Broken Symmetry near the Pseudogap Temperature"

PRL 100 127002 2008

M. J. Lawler "Intra-unit-cell electronic nematicity of the high-Tc copper-oxide pseudogap states"

Nature 466 347 2010

R. Daou "Broken rotational symmetry in the pseudogap phase of a high-Tc superconductor"

Nature 463 519 2010

S. De Almeida-Didry Evidence for intra-unit-cell magnetic order in Bi2Sr2CaCu2O8
PHYSICAL REVIEW B 86 020504(R) 2012

Tao Wu,"Magnetic-field-induced charge-stripe order in the high-temperature superconductor YBa2Cu3Oy"

Nature 477 191 2011

G. Ghiringhelli, “Long-Range Incommensurate Charge Fluctuations in (Y,Nd)Ba2Cu3O6+x”

Science 337 821 2012

J. Chang, "Direct observation of competition between superconductivity and charge density wave order in YBa2Cu3O6:67"

Nature Physics 8 871 2012

Recent Advances in Theory

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- New numerical approaches:
  Functional Renormalization Group

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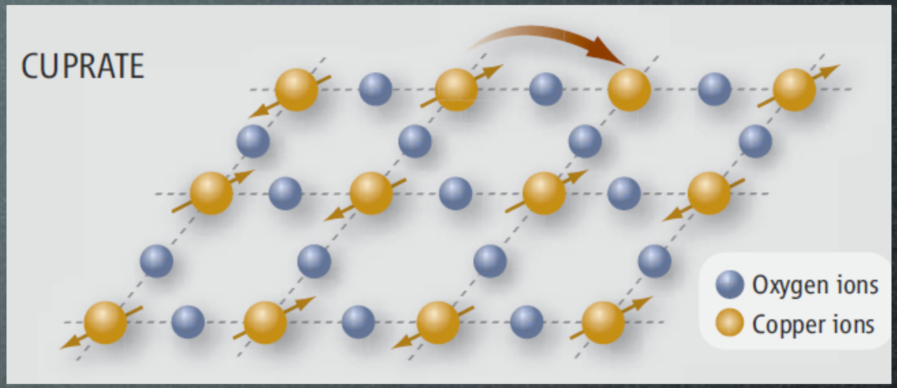
- Insight into the minimal model:
  the role of oxygen sites

Recent Advances in Theory

A Middle-Up/Down Approach

Recent Advances in Theory

Top-down:



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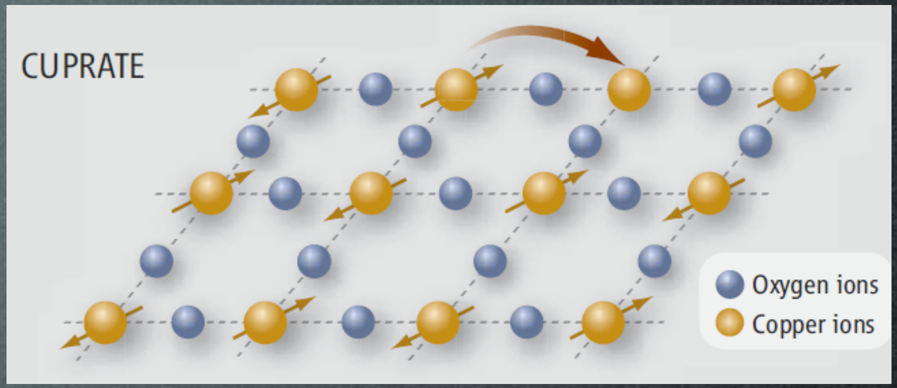

Bottom-up: Neutron Scattering ⟷ STM ⟷ ARPES

A Middle-Up/Down Approach

Recent Advances in Theory

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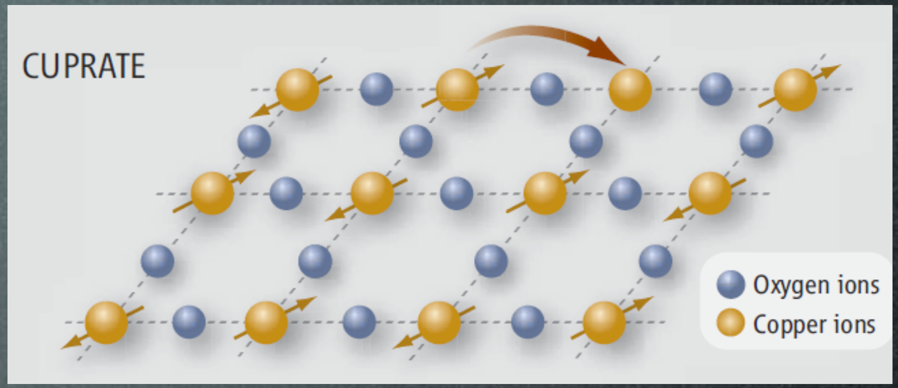


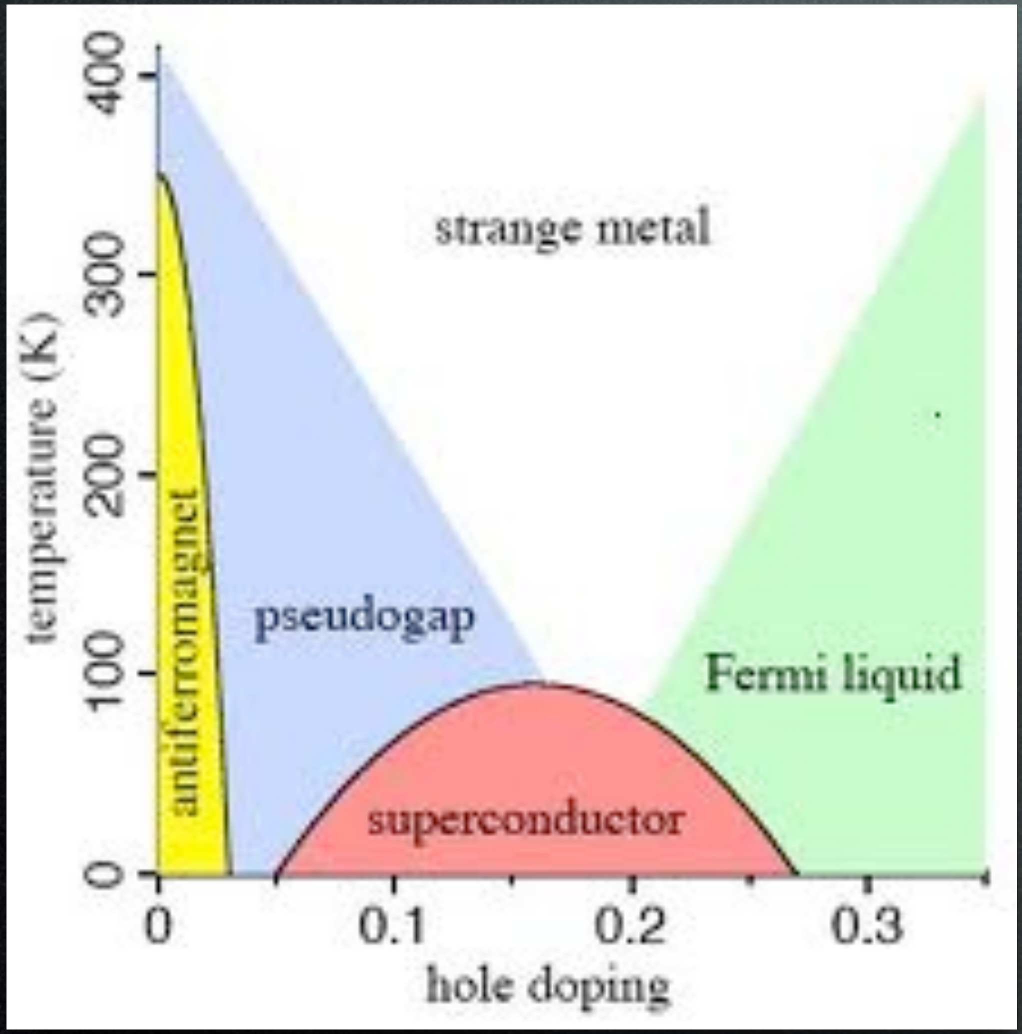
Middle-down/up: **Symmetry Principles**

Bottom-up: Neutron Scattering ↔ STM ↔ ARPES

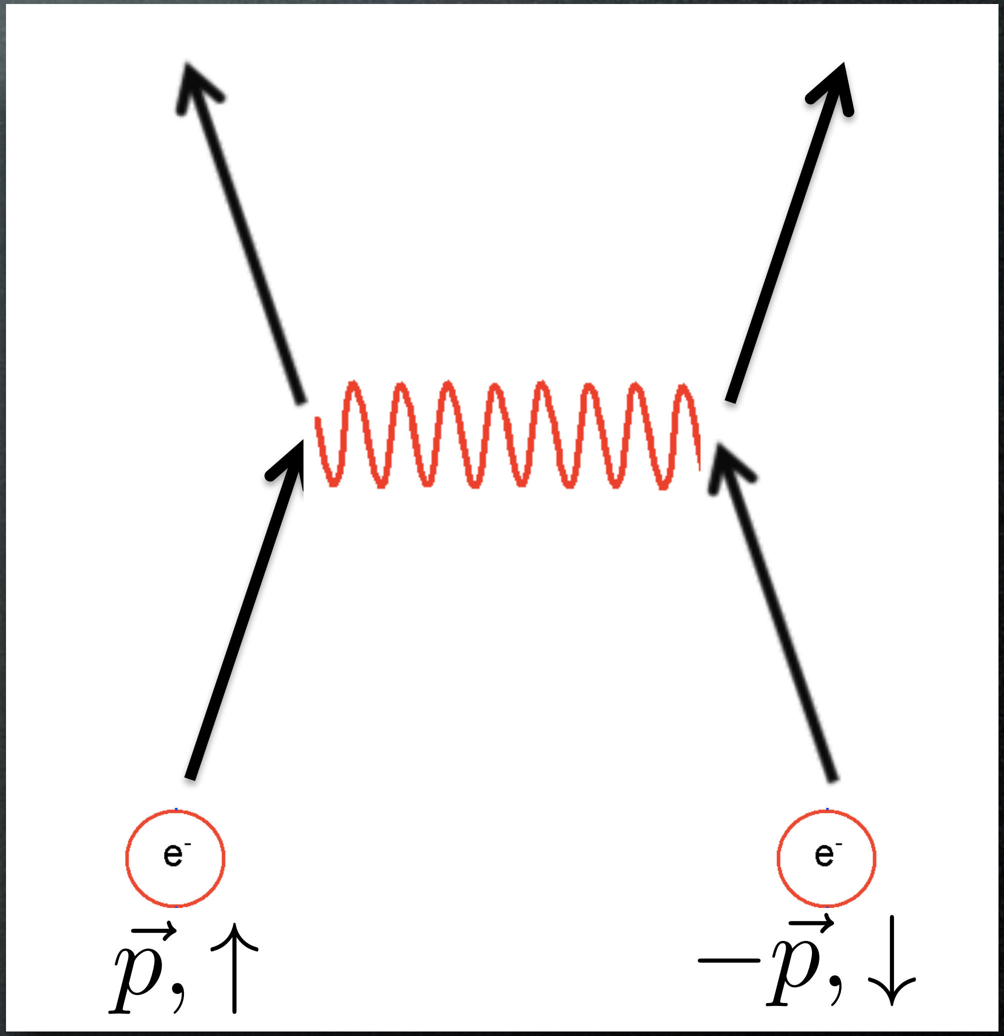
A Middle-Up/Down Approach

Key Questions in High-T_c Superconductivity:

The Phase Diagram?

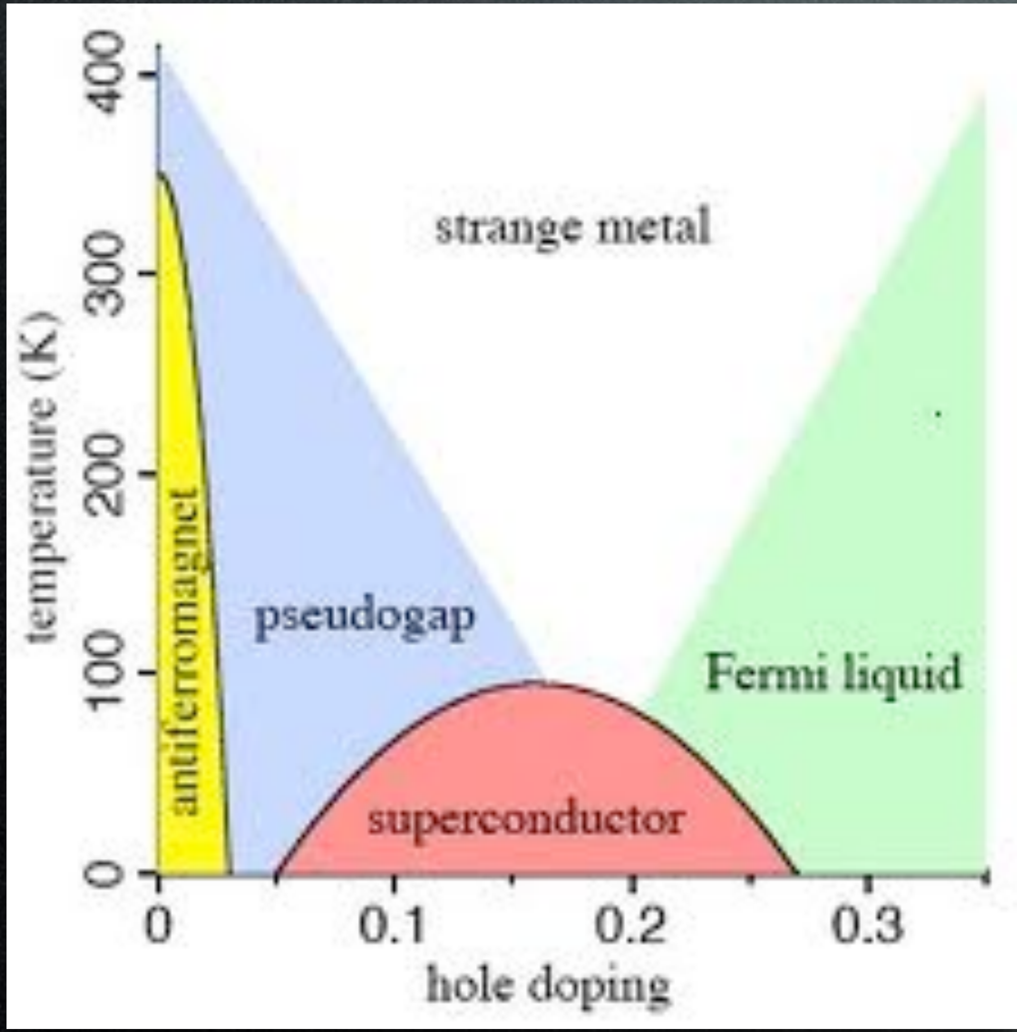


The Mechanism?

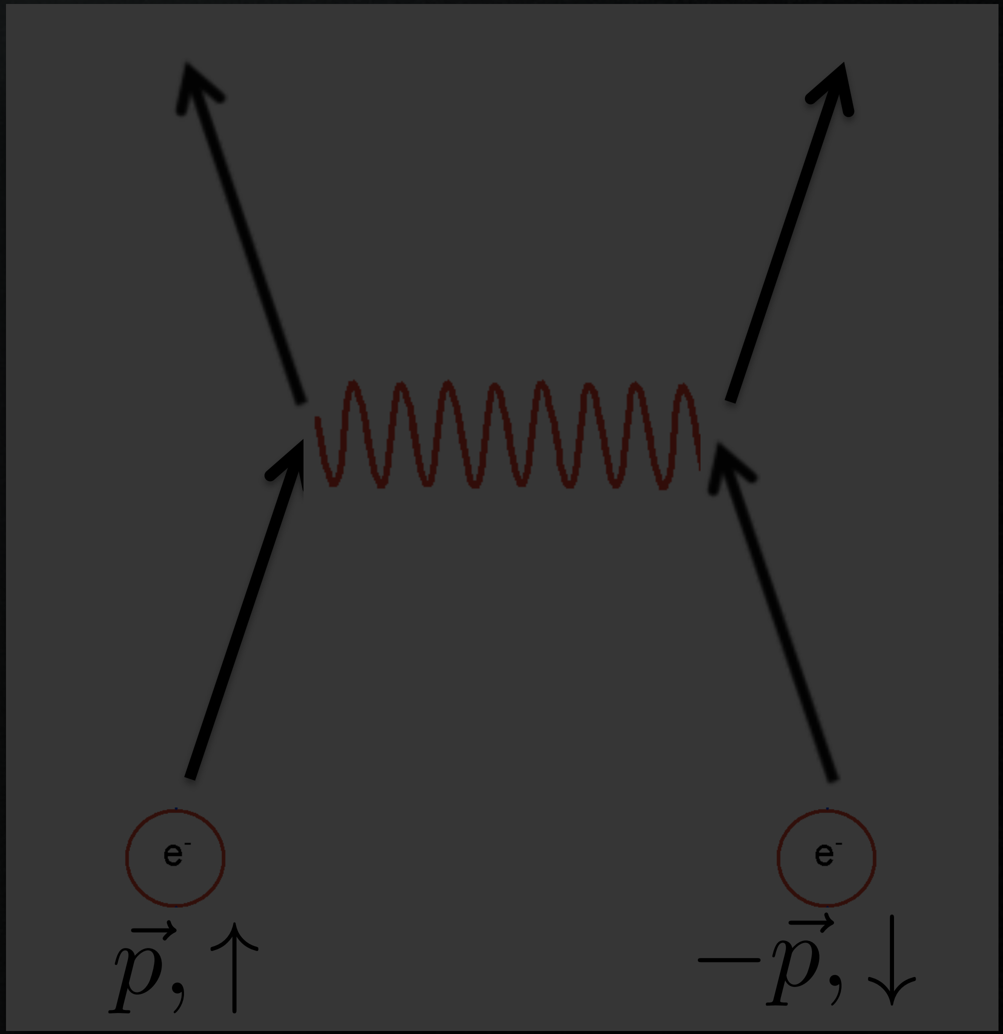


Key Questions in High-T_c Superconductivity:

The Phase Diagram?

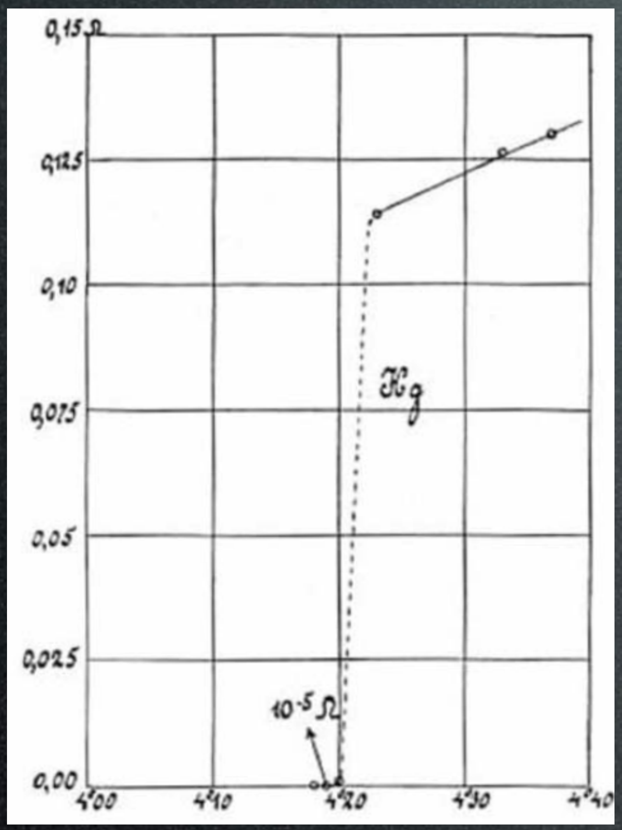


The Mechanism?



The Complex Phase Diagram

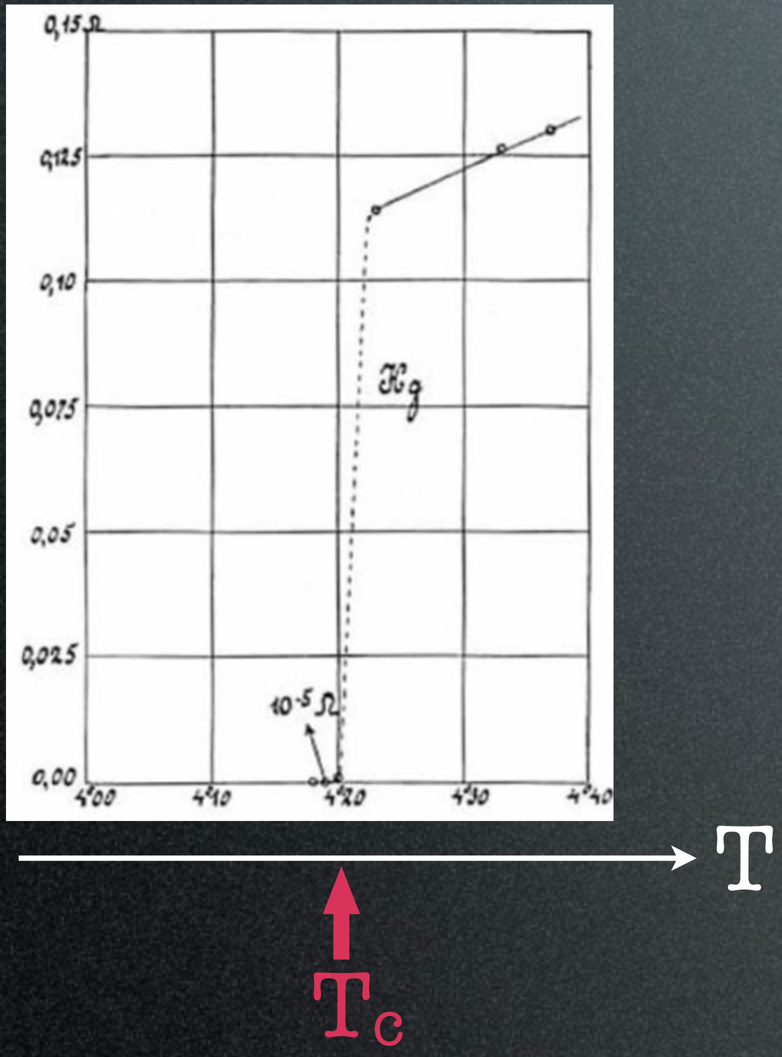
Simple PD of conventional SC



T

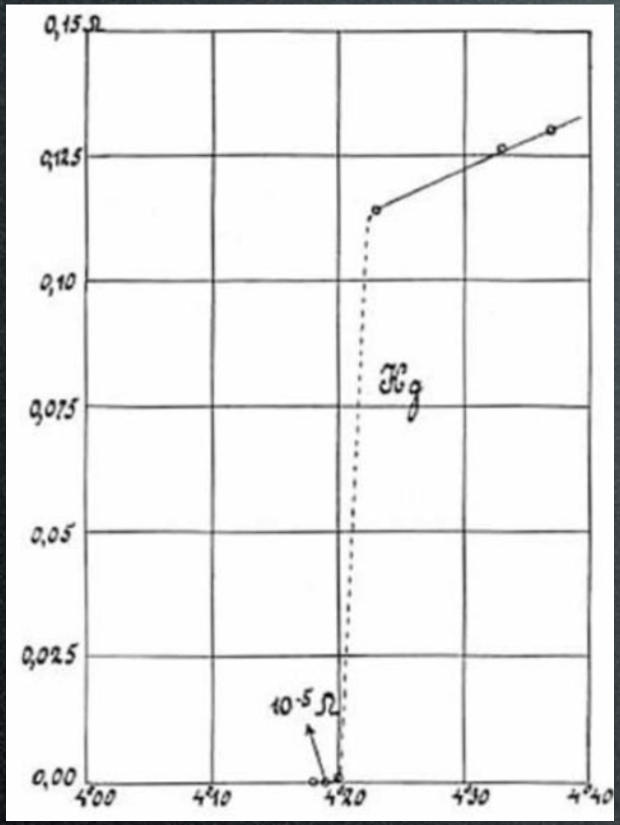
The Complex Phase Diagram

Simple PD of conventional SC



The Complex Phase Diagram

Simple PD of conventional SC



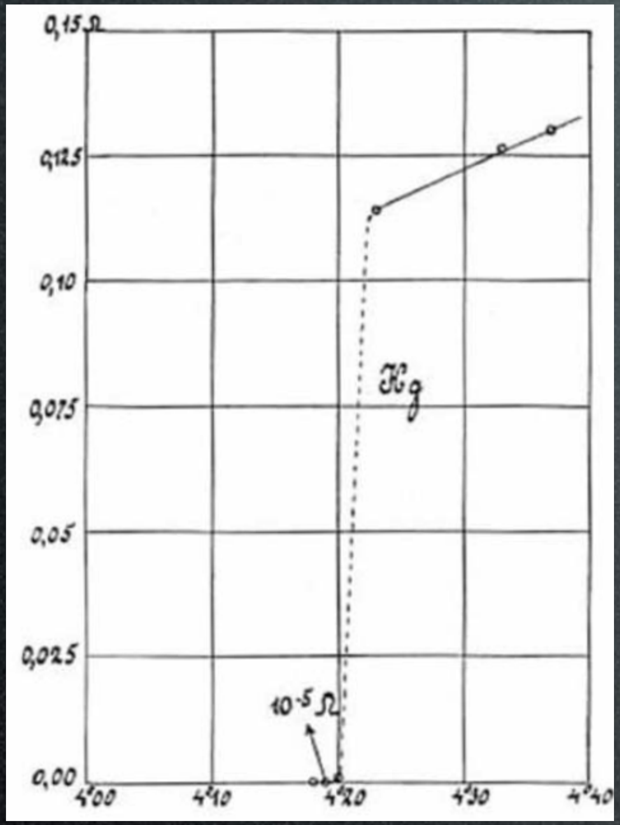
T

T_c

Fermi Liquid Metal

The Complex Phase Diagram

Simple PD of conventional SC



T

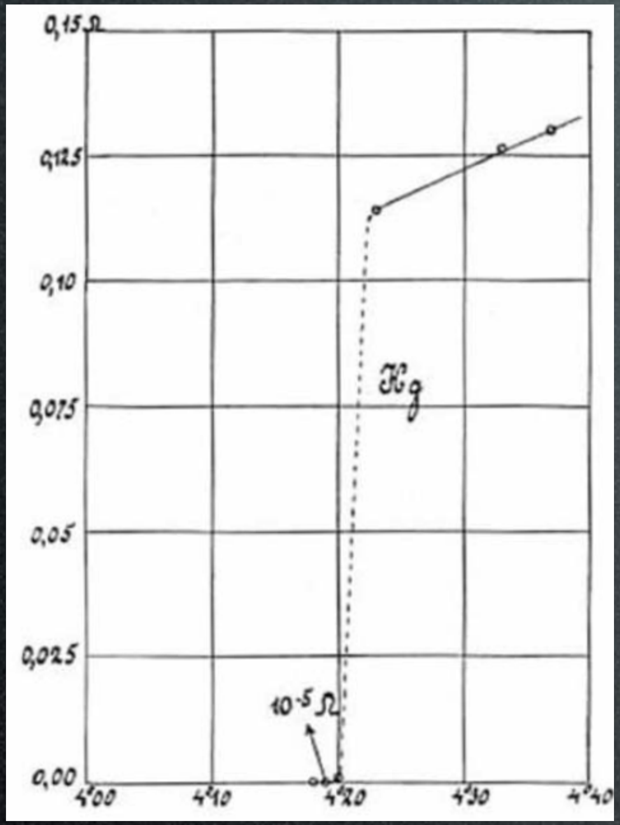
Superconductor

T_c

Fermi Liquid Metal

The Complex Phase Diagram

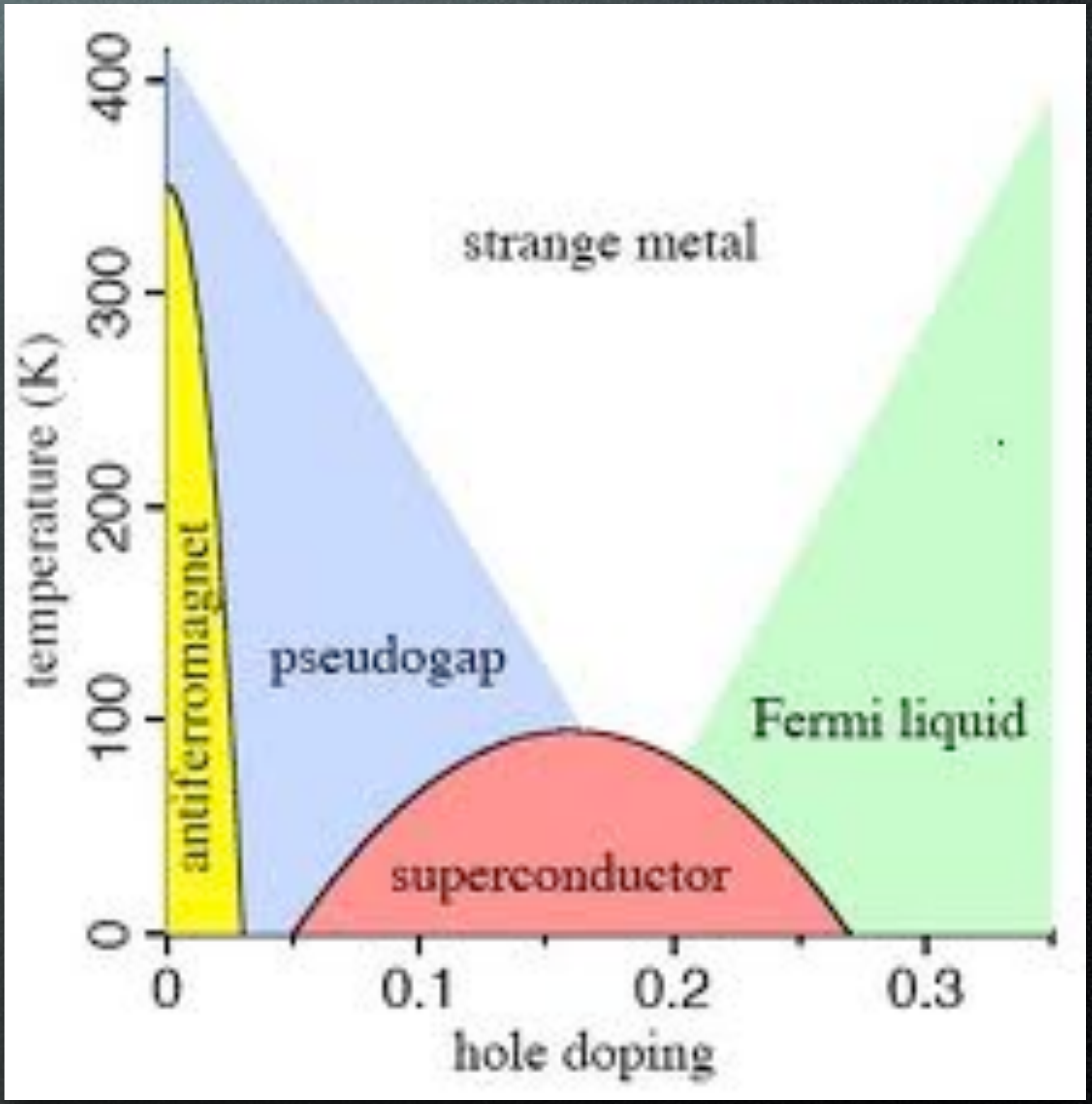
Simple PD of conventional SC



T

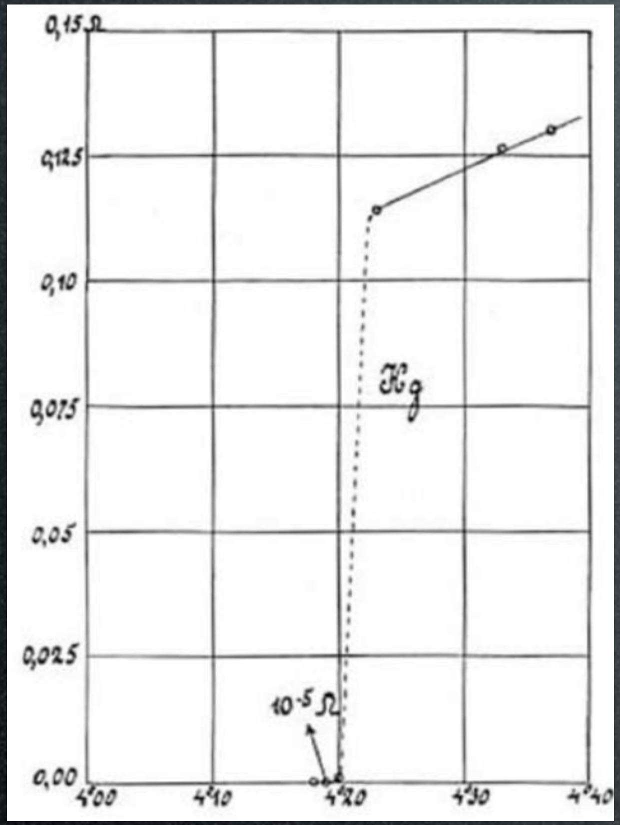
Superconductor T_c Fermi Liquid Metal

Complex PD of high T_c SC



The Complex Phase Diagram

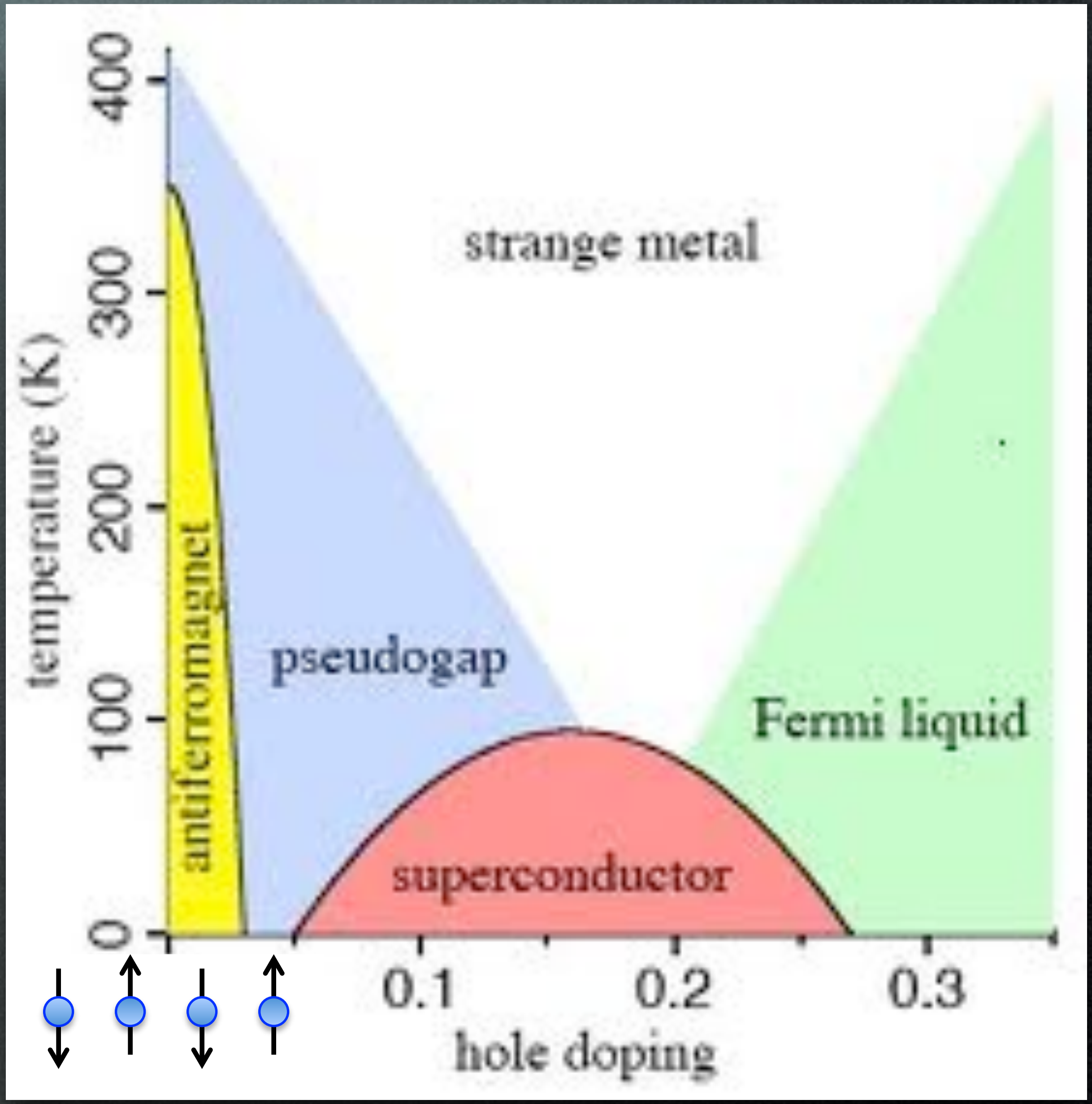
Simple PD of conventional SC



T

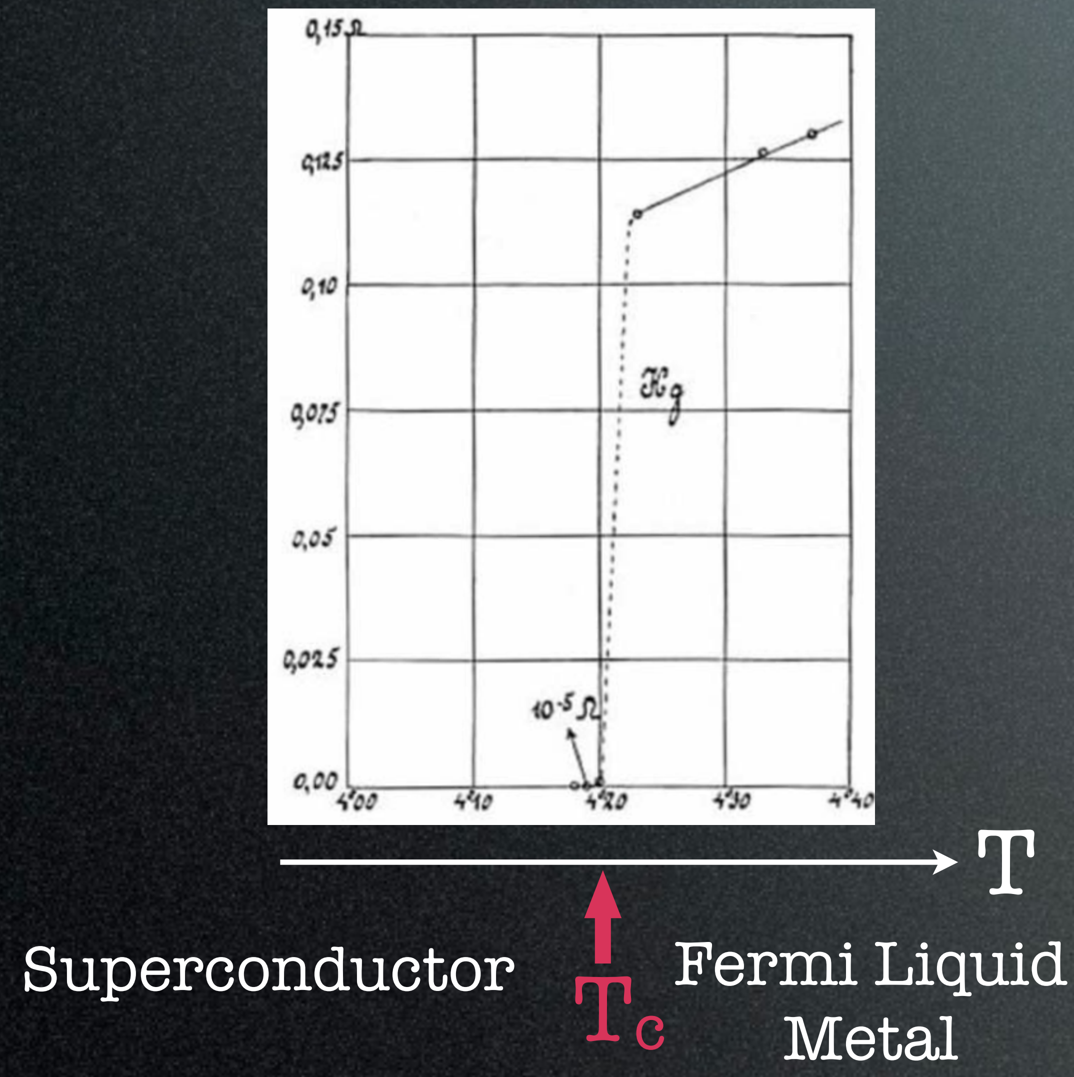
Superconductor T_c Fermi Liquid Metal

Complex PD of high T_c SC

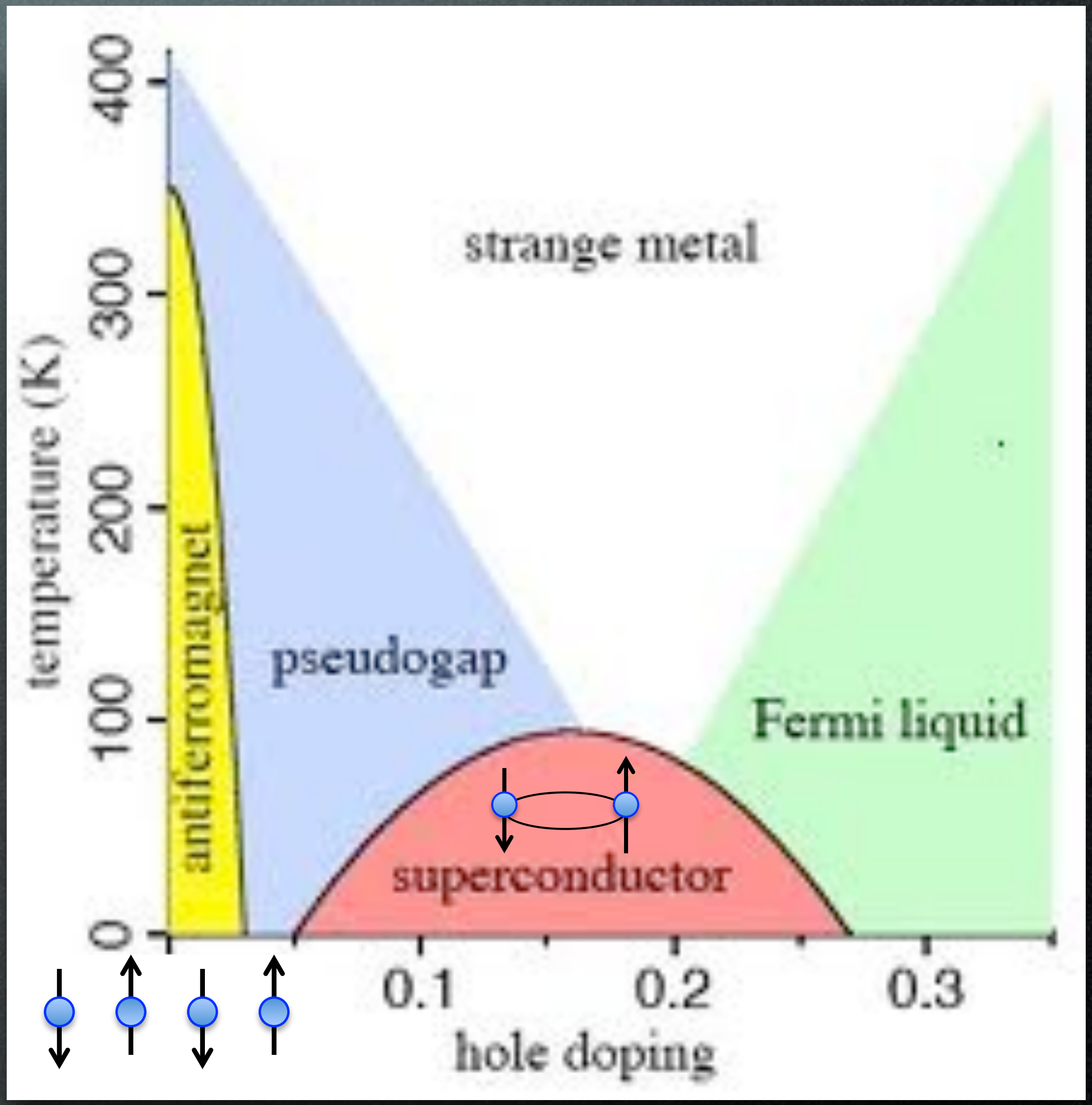


The Complex Phase Diagram

Simple PD of conventional SC

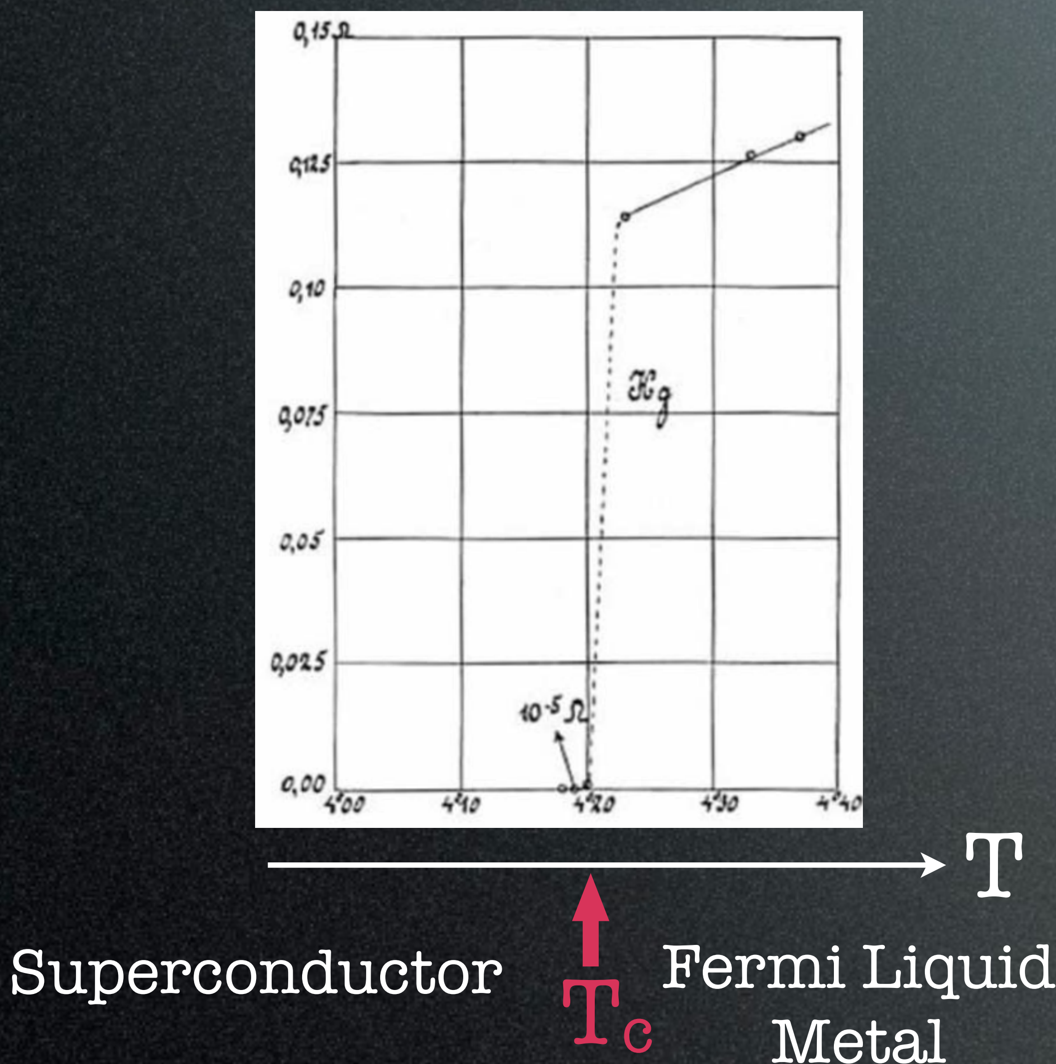


Complex PD of high T_c SC

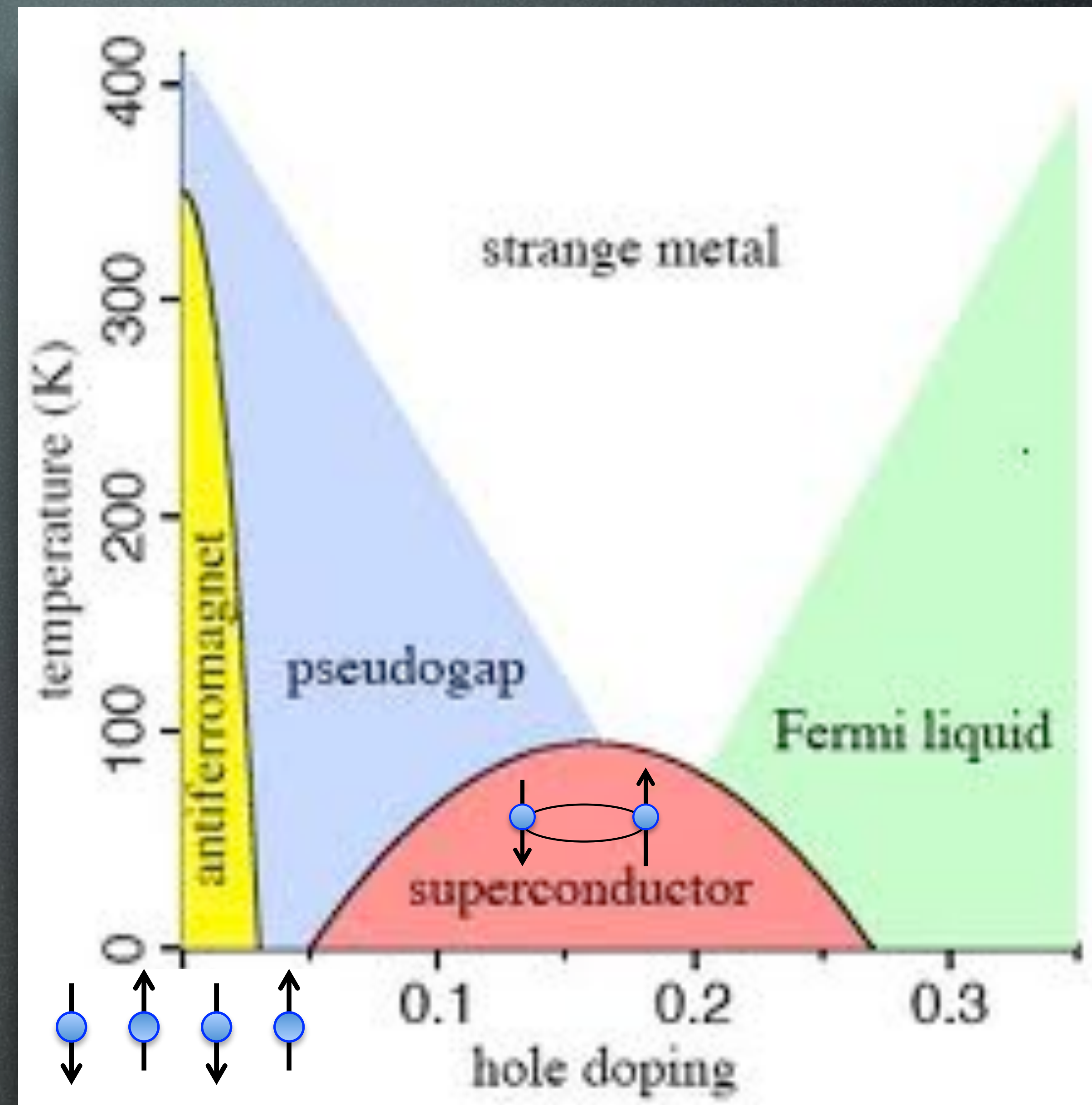


The Complex Phase Diagram

Simple PD of conventional SC



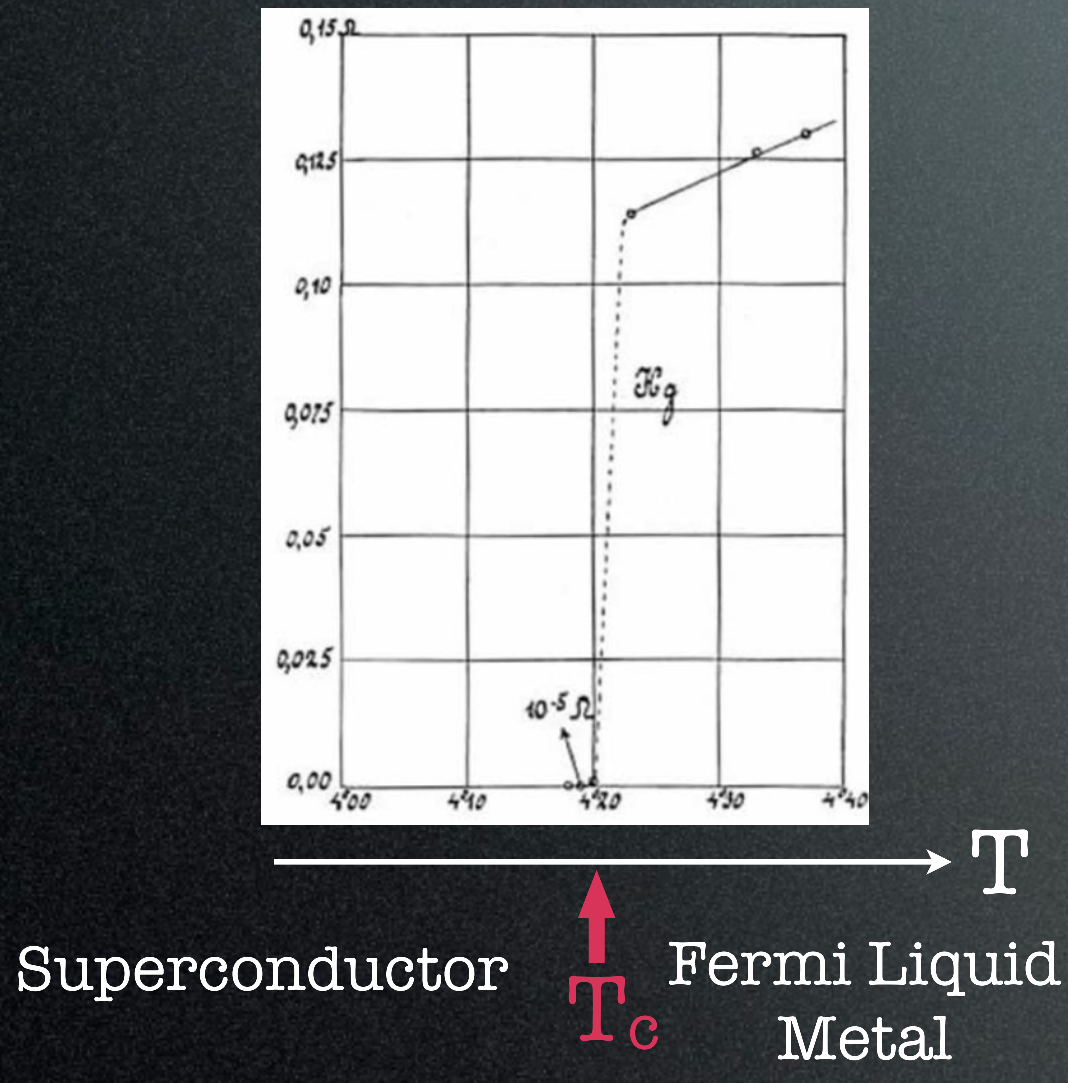
Complex PD of high T_c SC



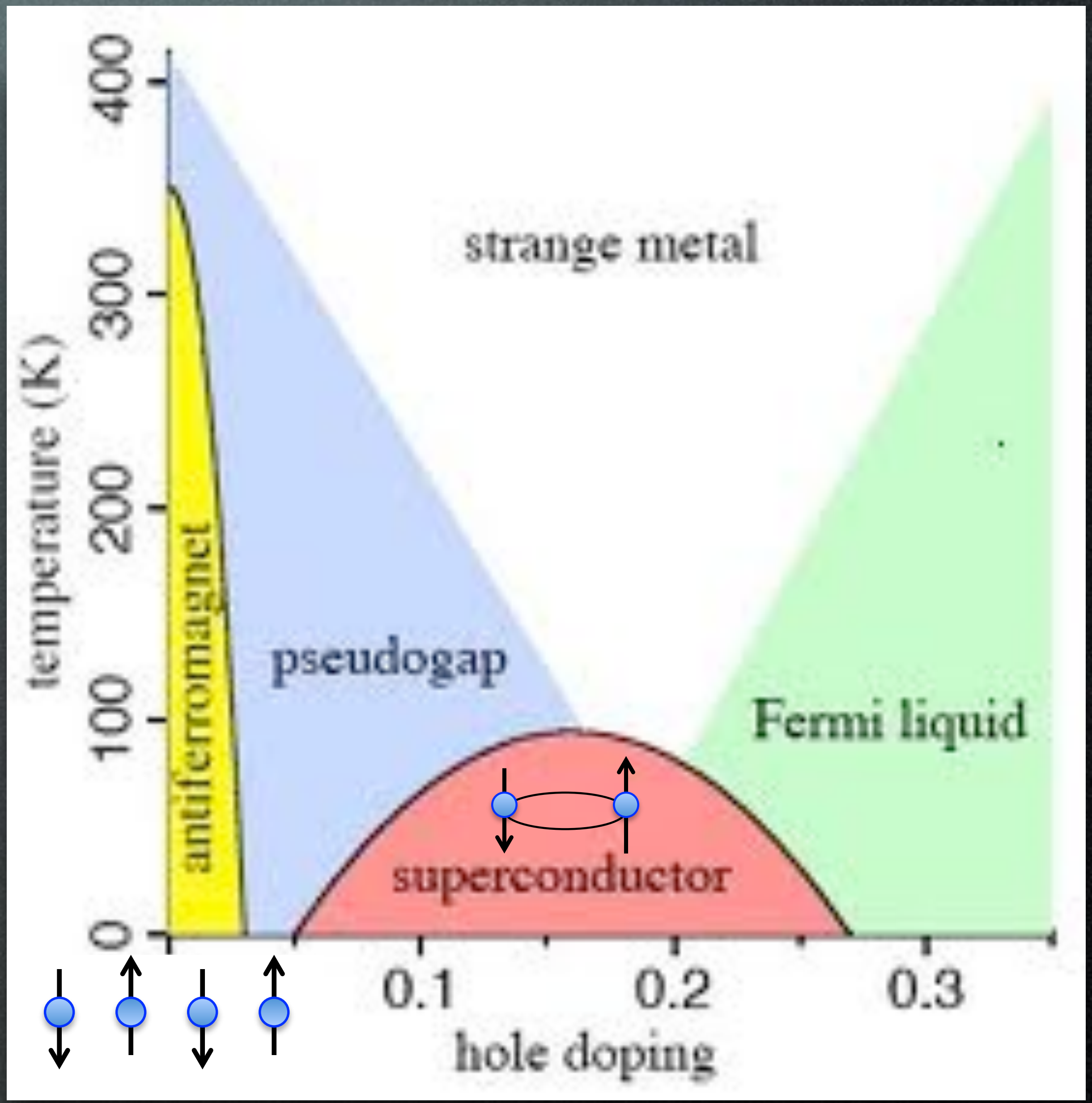
- Phases in between FL & MI

The Complex Phase Diagram

Simple PD of conventional SC



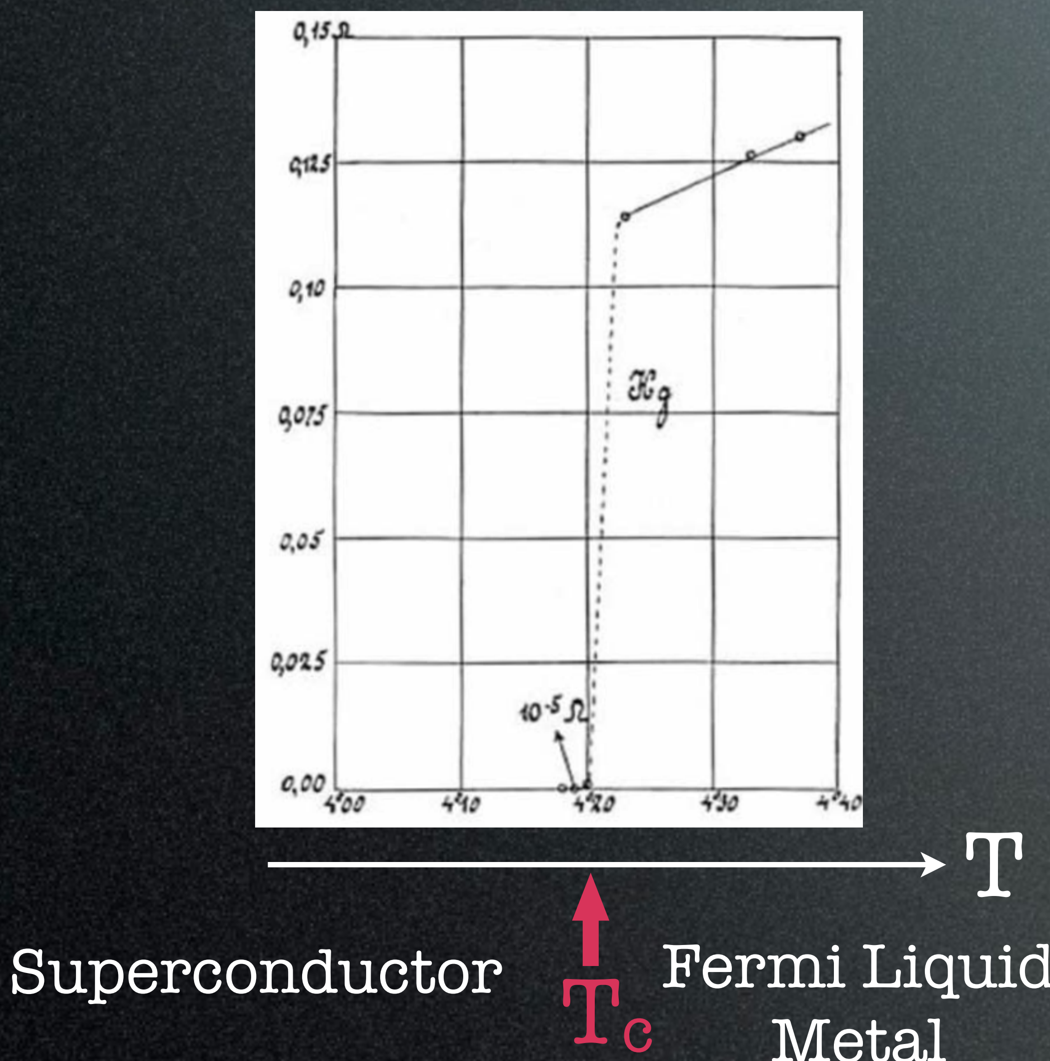
Complex PD of high T_c SC



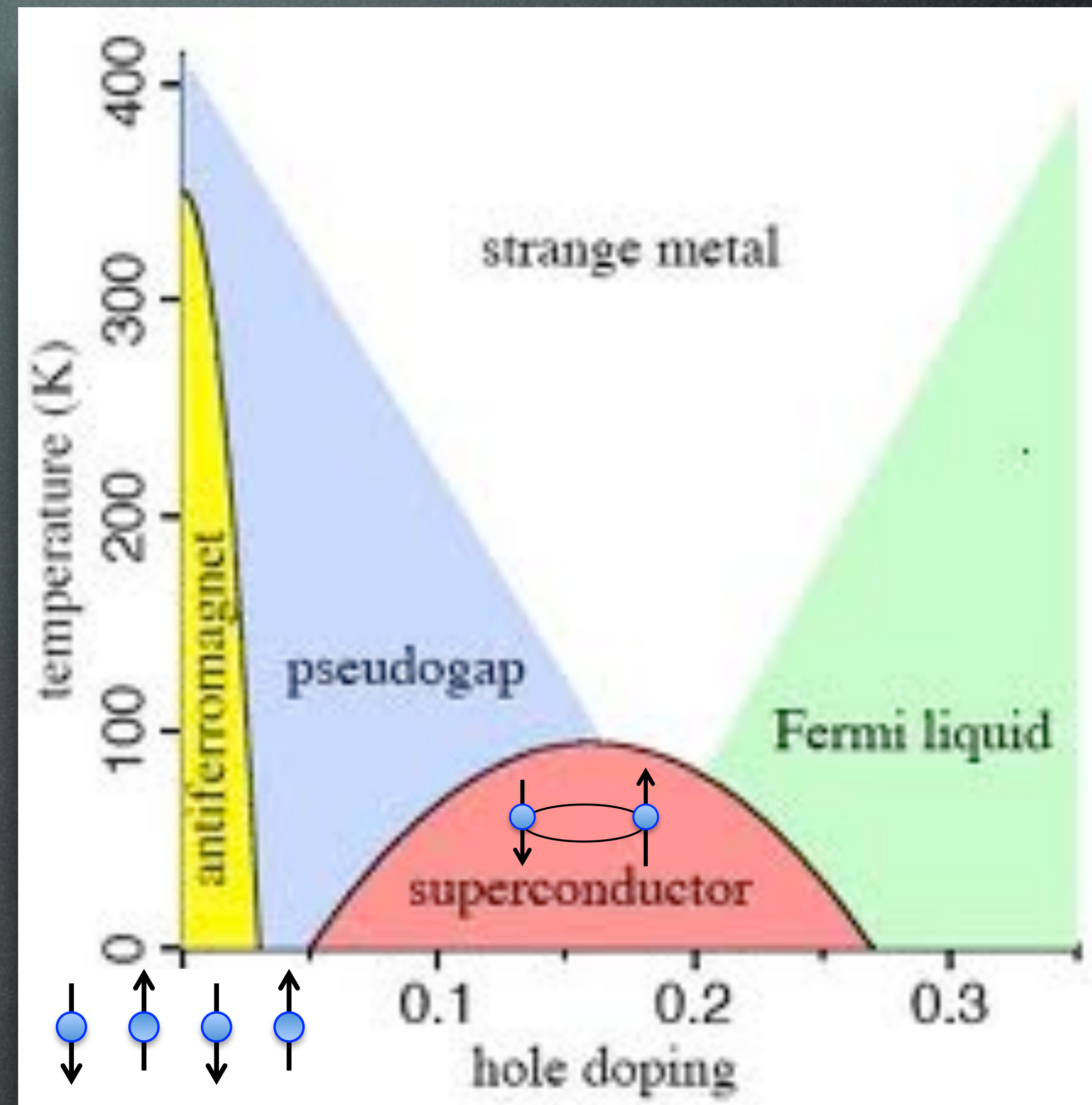
- Phases in between FL & MI
- Multiple "phases" at similar T

The Complex Phase Diagram

Simple PD of conventional SC



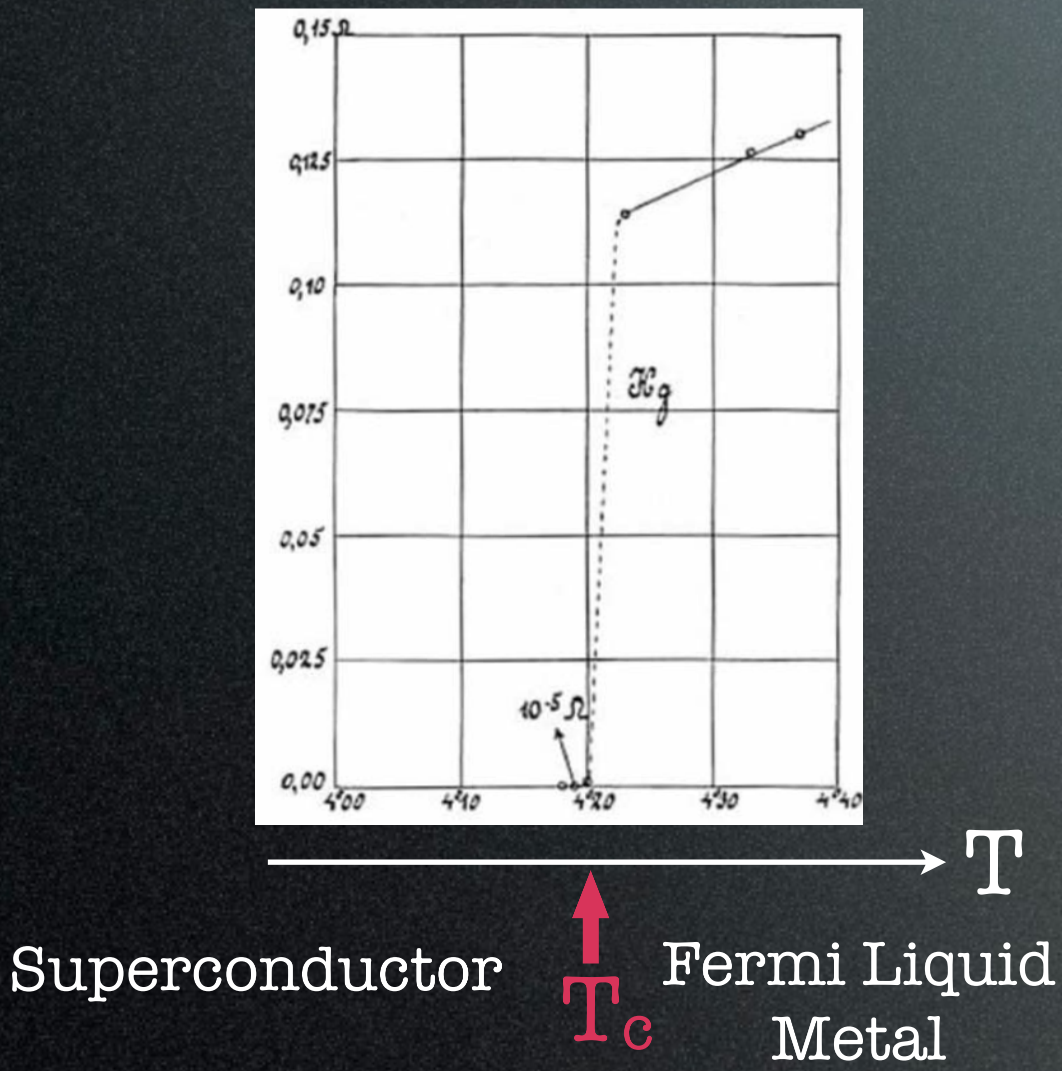
Complex PD of high T_c SC



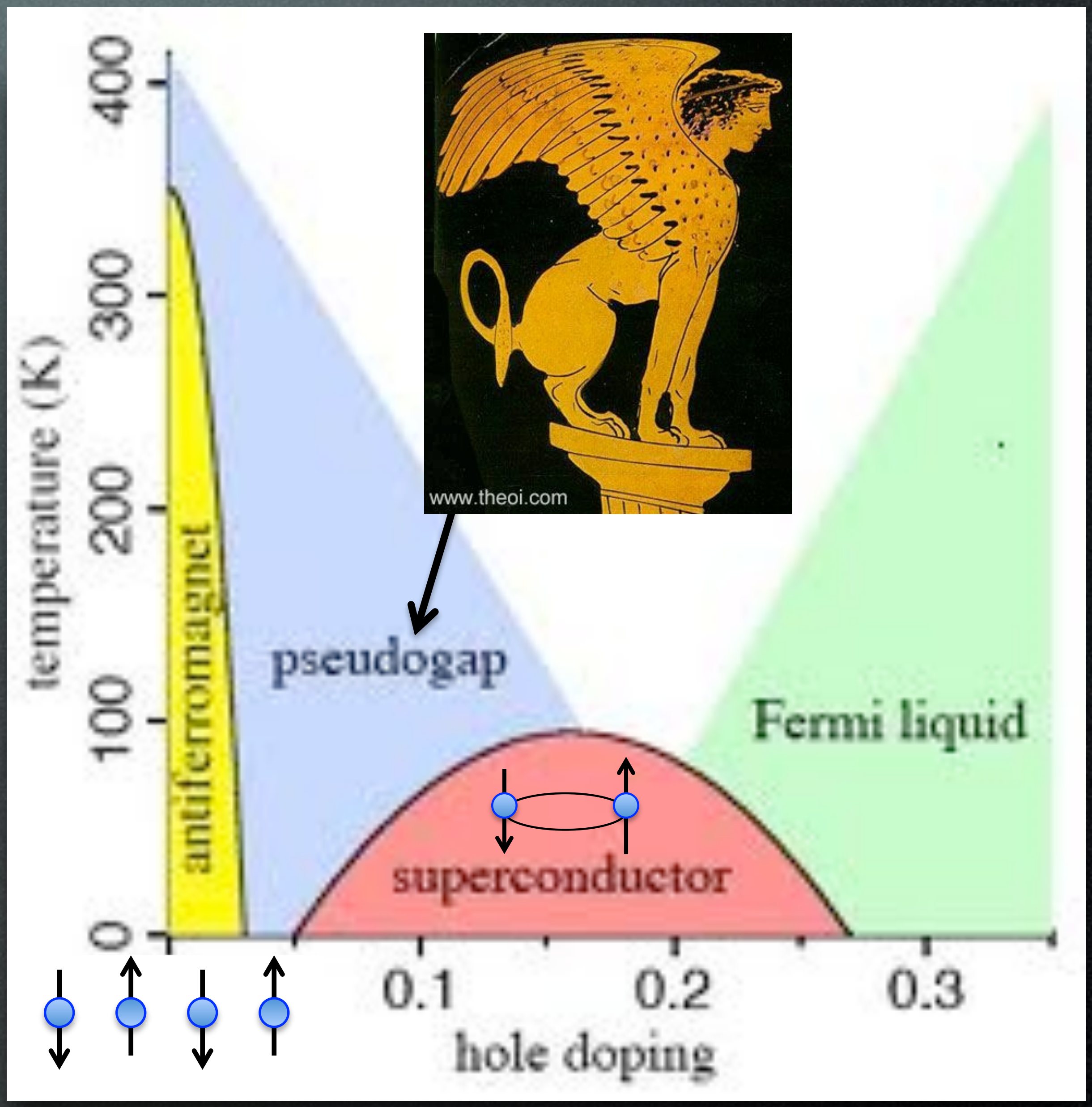
- Phases in between FL & MI
- Multiple "phases" at similar T
- Unidentifiable regions

The Complex Phase Diagram

Simple PD of conventional SC



Complex PD of high T_c SC



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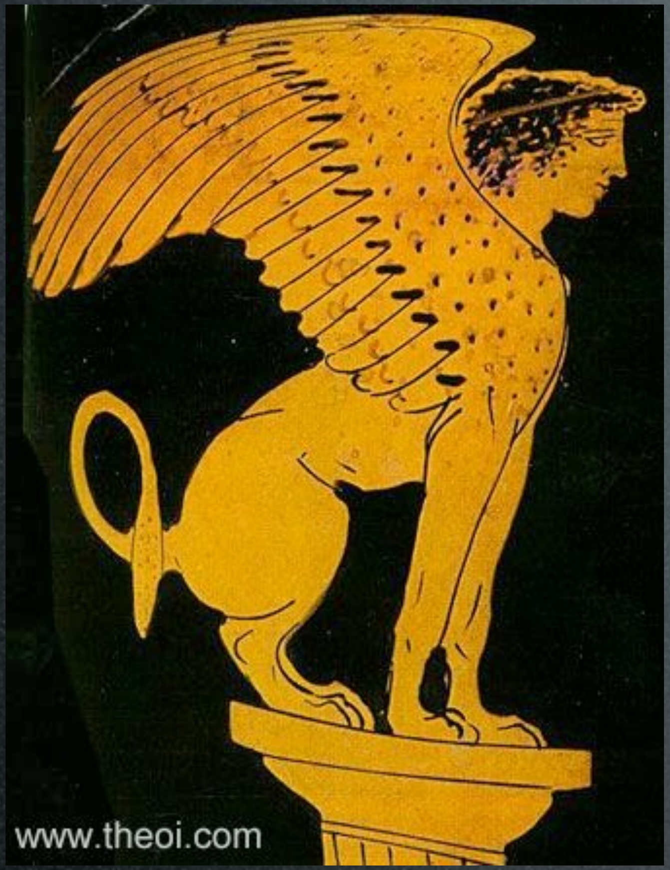
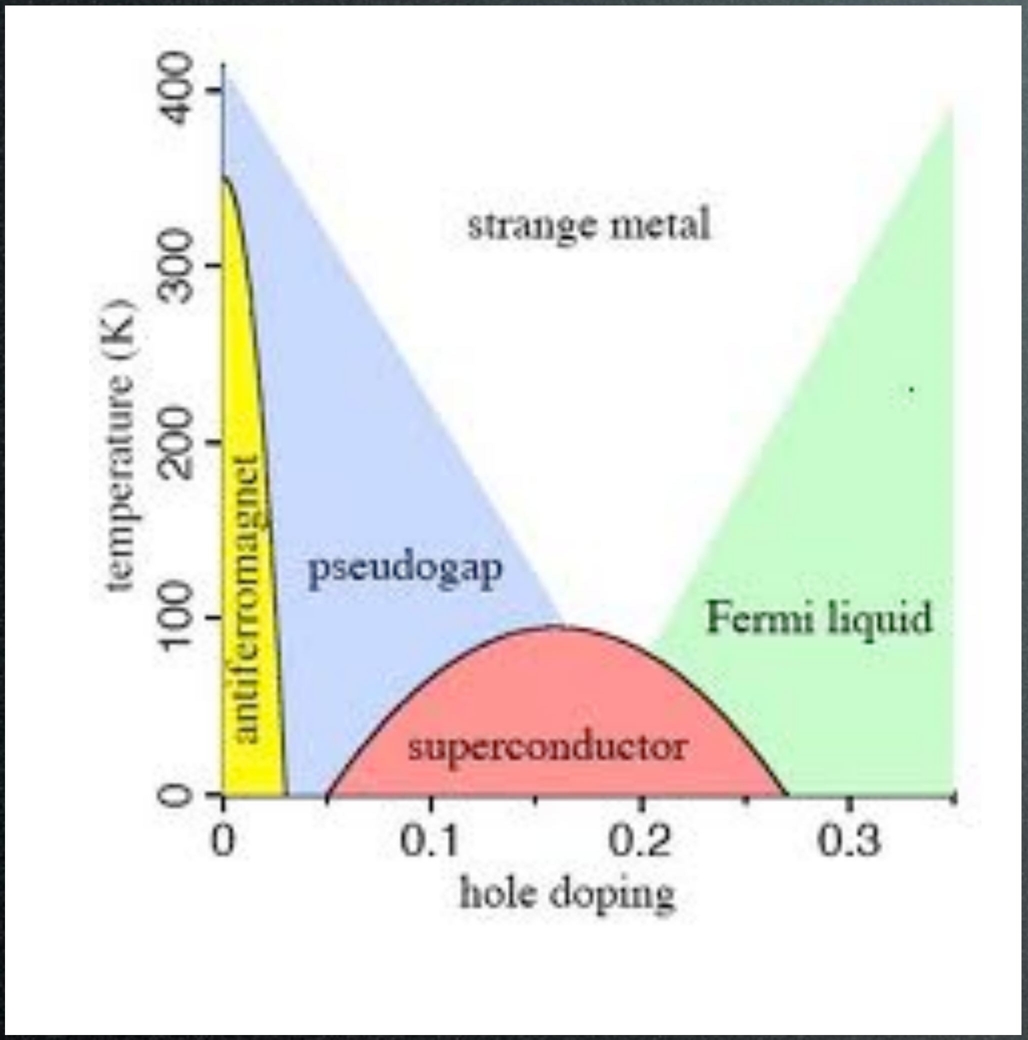
- Multiple "phases" at similar T
- Unidentifiable regions

Riddles

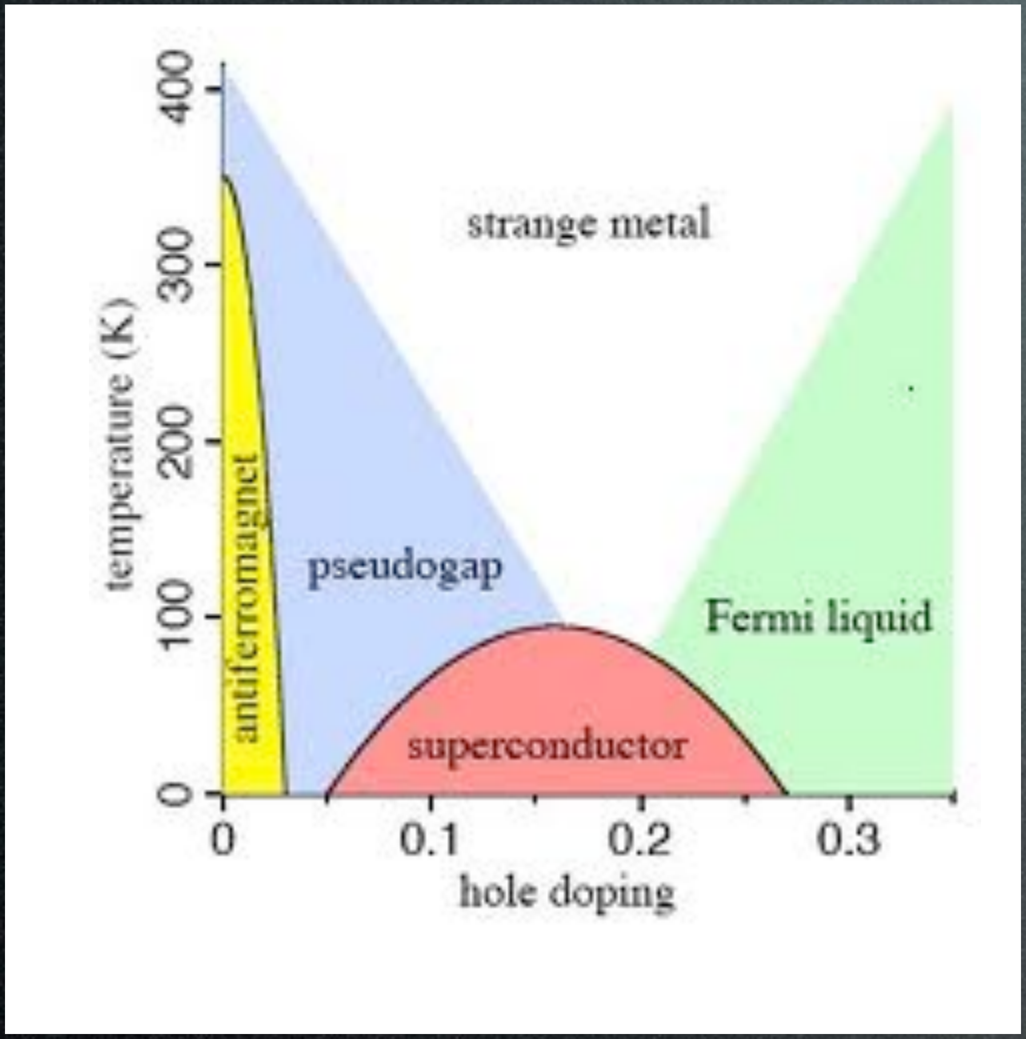


Riddles of Pseudo Gap



AF: Antiferromagnet
SC: Superconductor
PG: Pseudogap
HTS: Hight temperature Superconductor

Riddles of Pseudo Gap



- Cross-over or Phase transition?

AF: Antiferromagnet
SC: Superconductor
PG: Pseudogap
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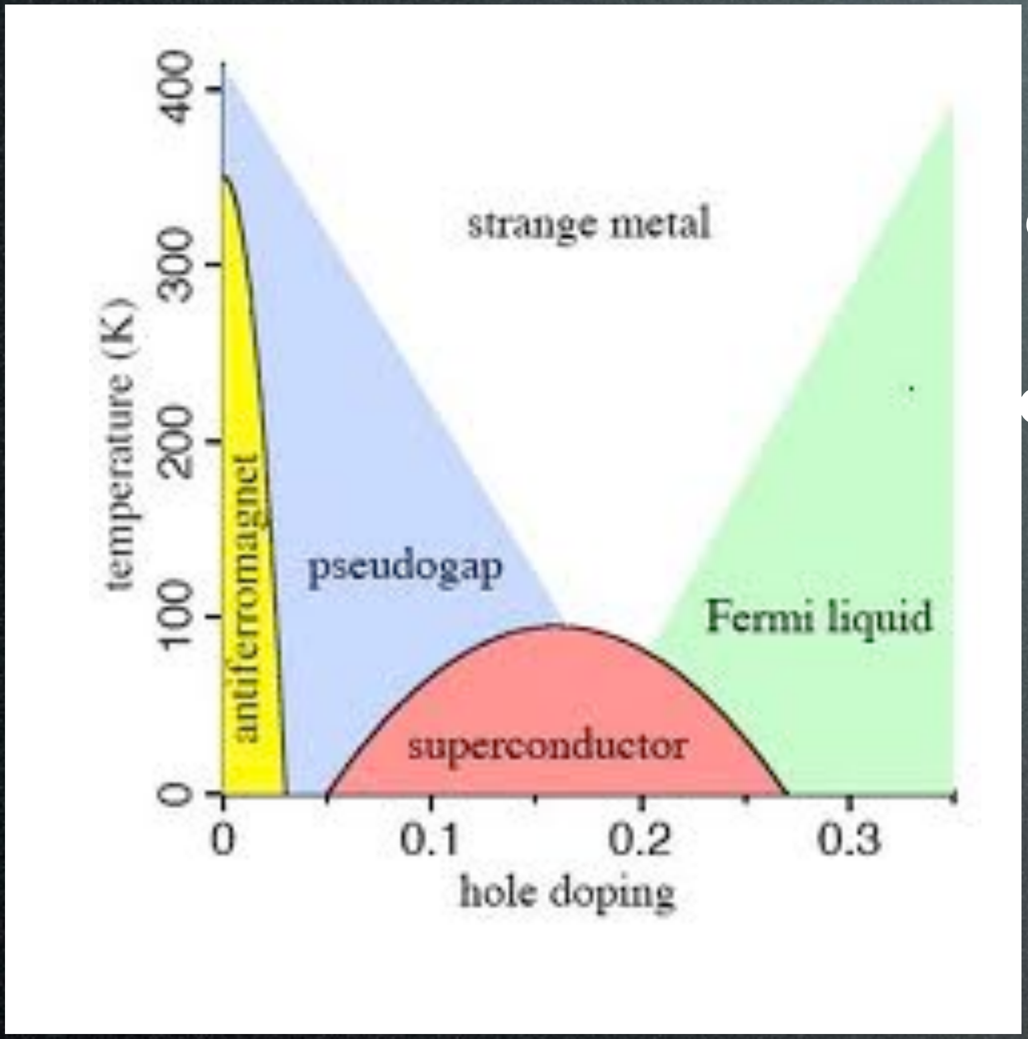
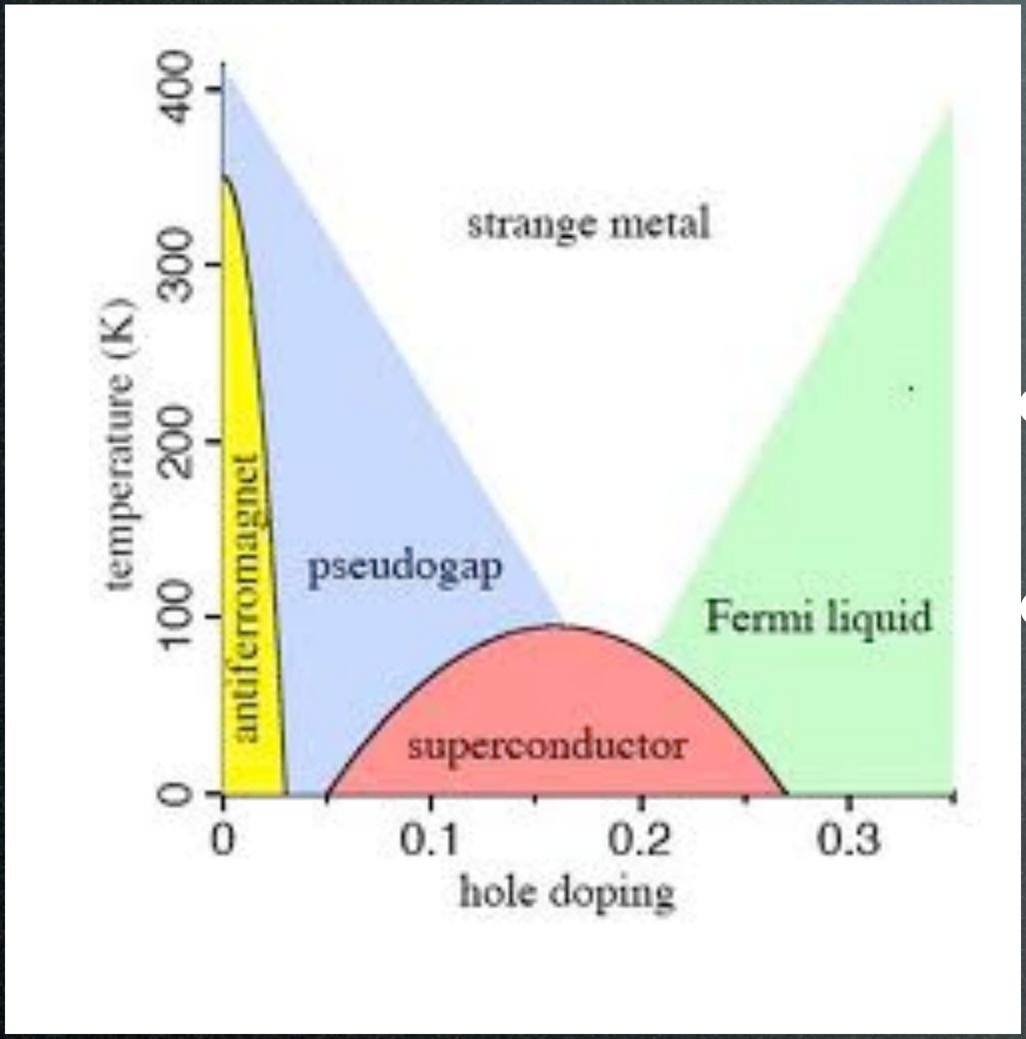
Riddles of Pseudo Gap



- Cross-over or Phase transition?
- Symmetry breaking?

AF: Antiferromagnet
SC: Superconductor
PG: Pseudogap
HTS: Hight temperature Superconductor

Riddles of Pseudo Gap



- Cross-over or Phase transition?
- Symmetry breaking?
- What are broken symmetries?

AF: Antiferromagnet
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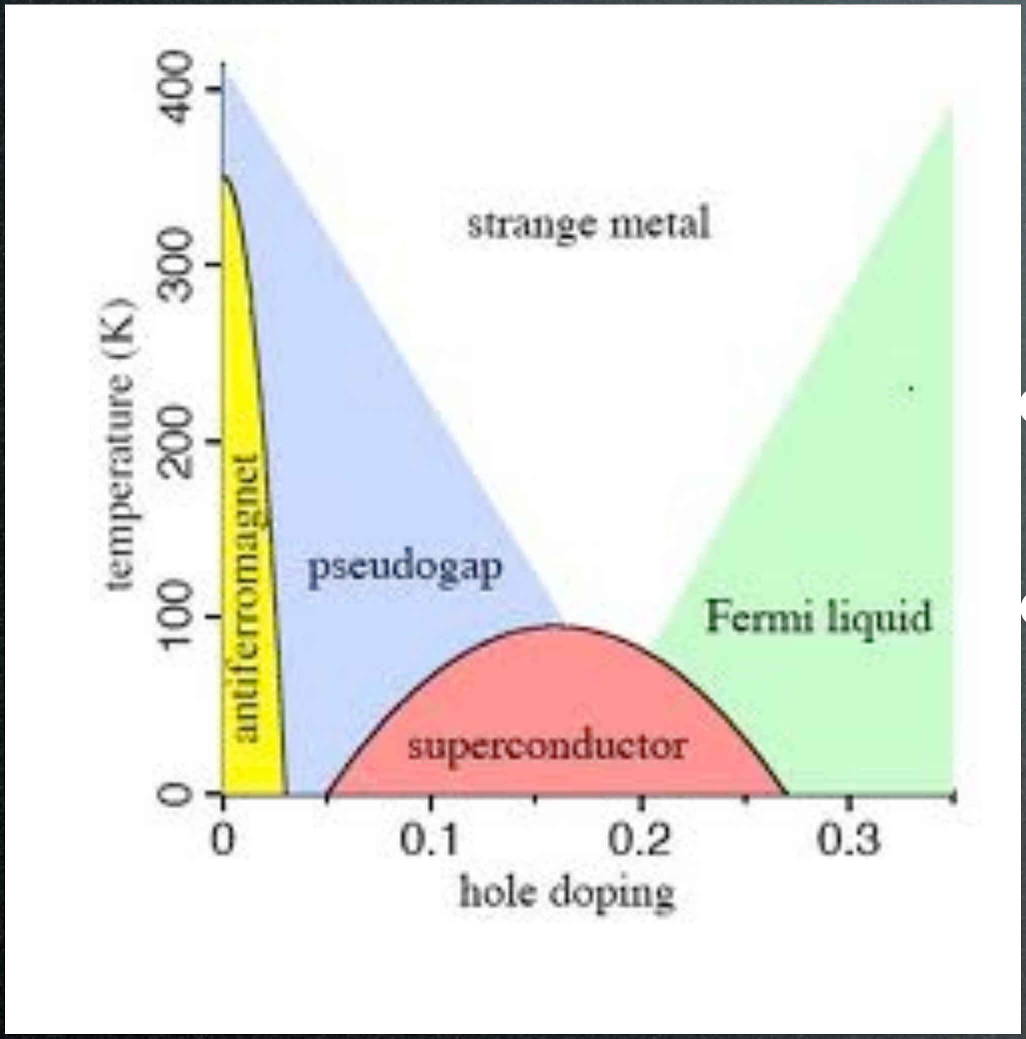
Riddles of Pseudo Gap



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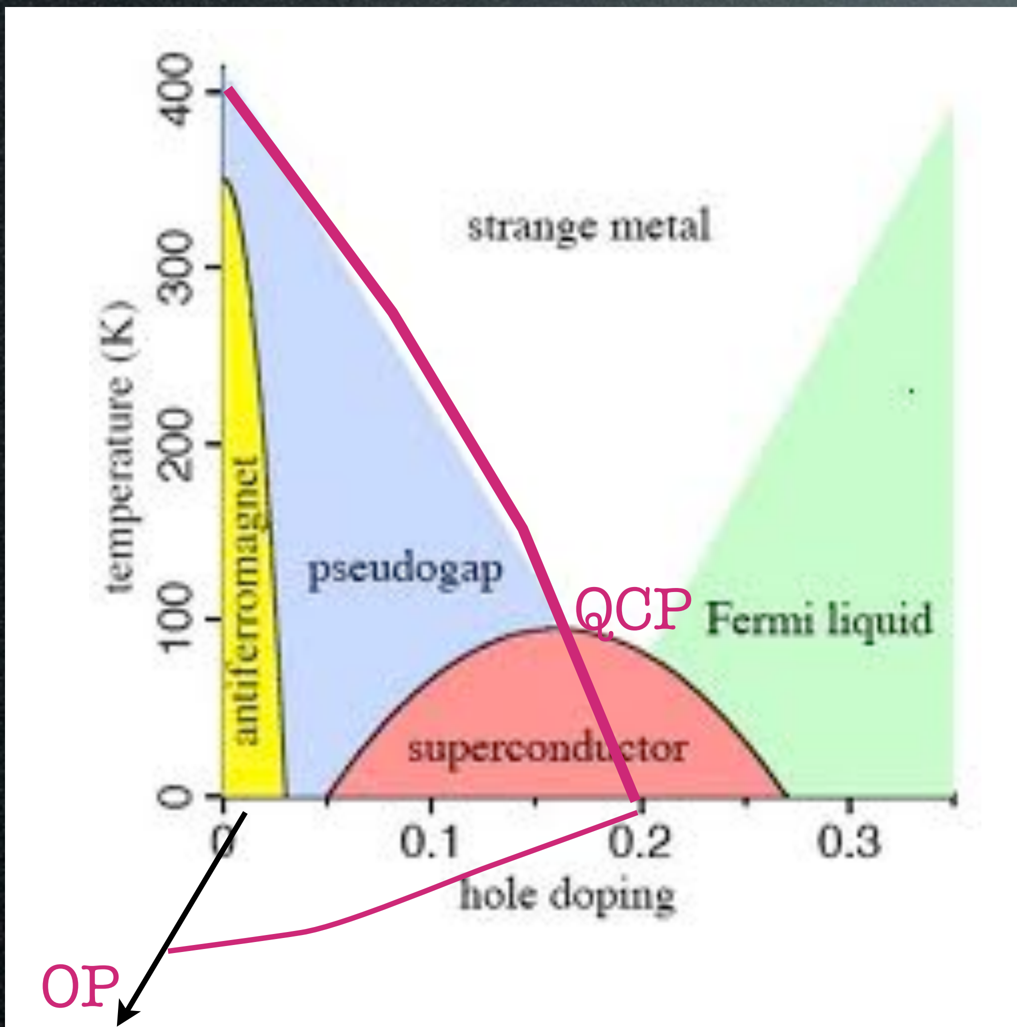
➡ Challenge:

1) Define and detect order parameter

AF: Antiferromagnet
SC: Superconductor
PG: Pseudogap
HTS: Hight temperature Superconductor

Riddles of Pseudo Gap



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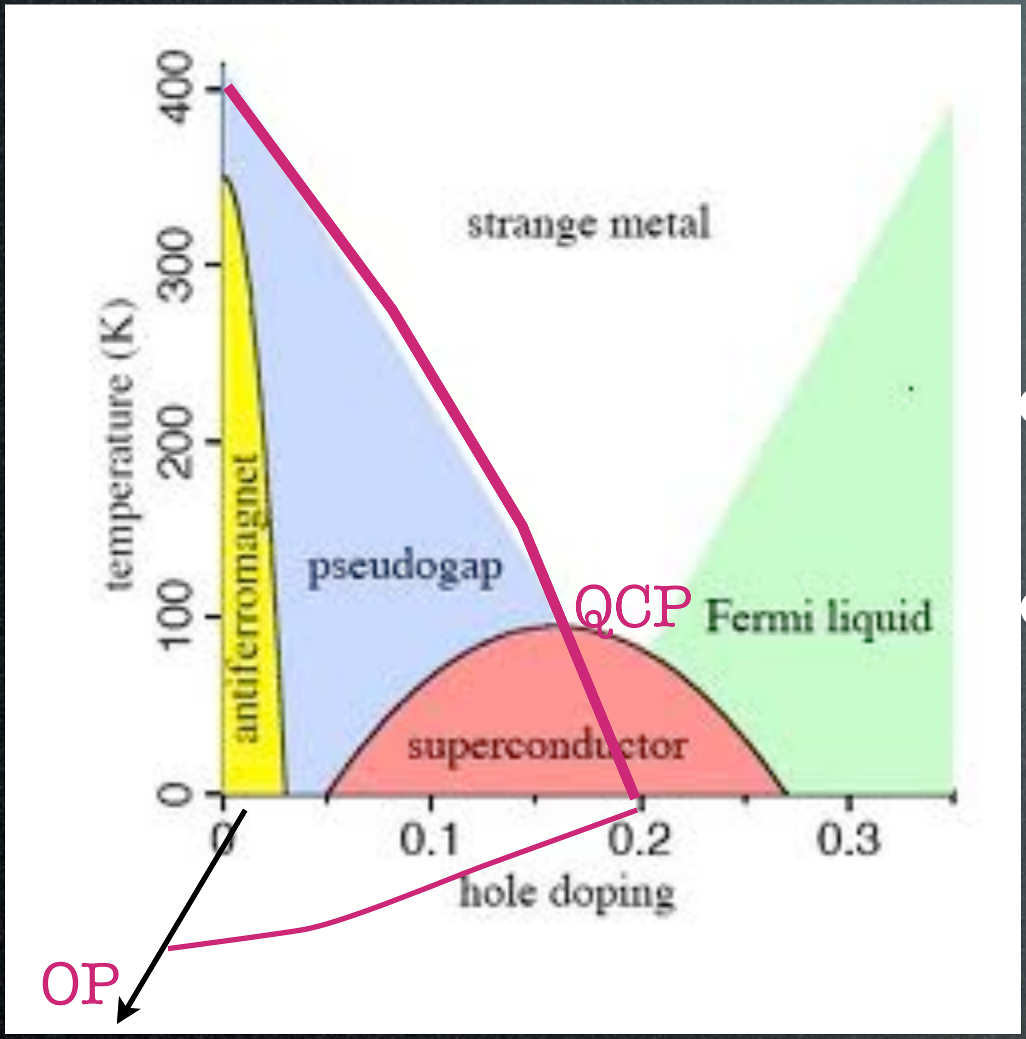
Riddles of Pseudo Gap



- Cross-over or Phase transition?
- Symmetry breaking?
- What are broken symmetries?

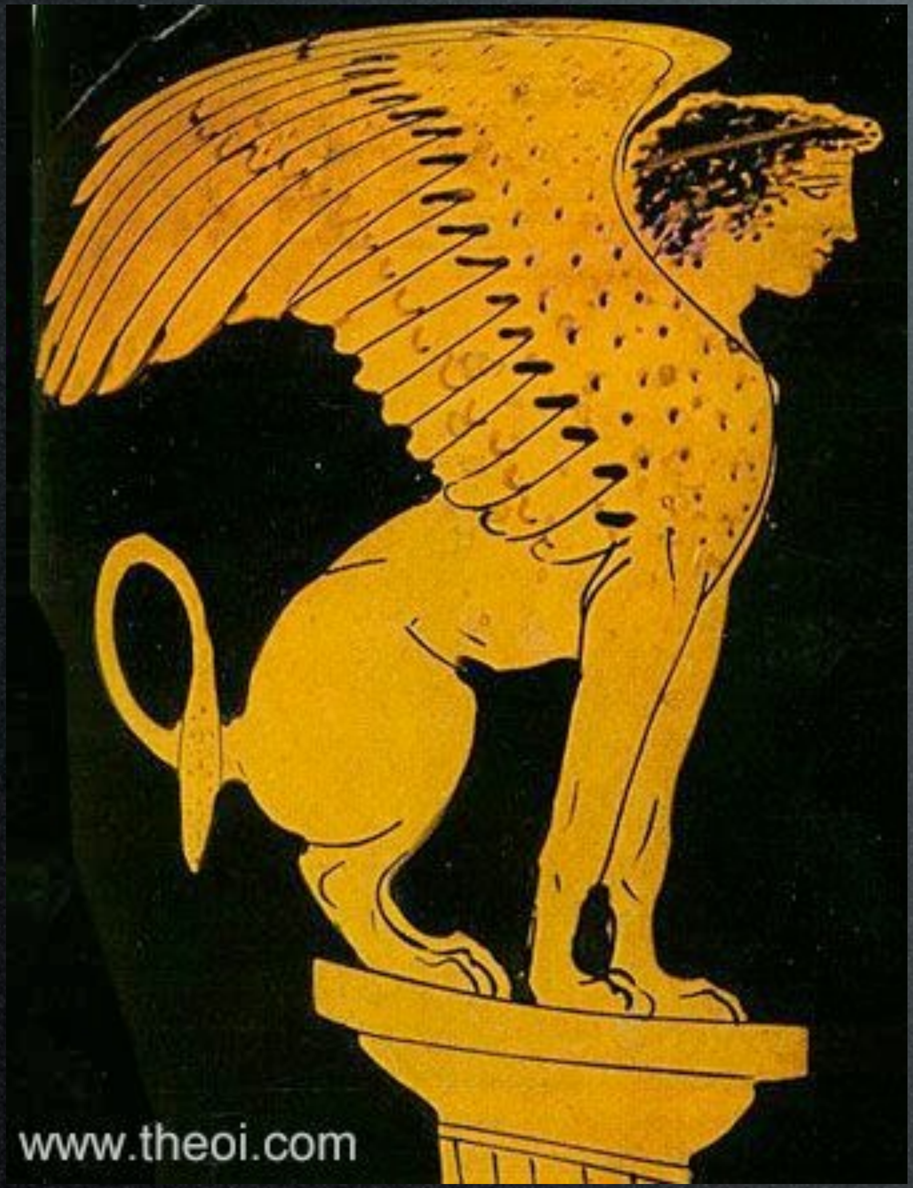
➡ Challenge:

1) Define and detect order parameter

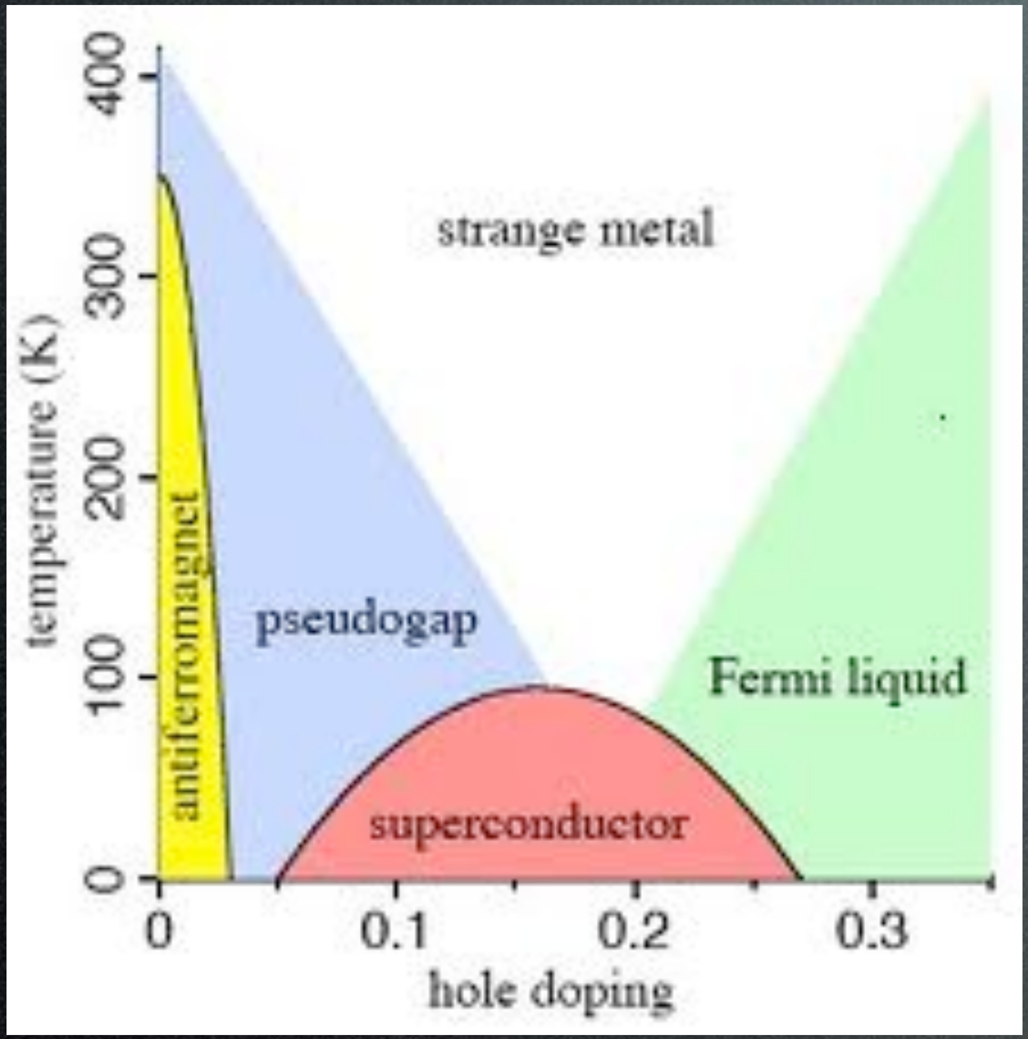
2) Locate the Quantum Critical Point (QCP)

AF: Antiferromagnet
SC: Superconductor
PG: Pseudogap
HTS: Hight temperature Superconductor

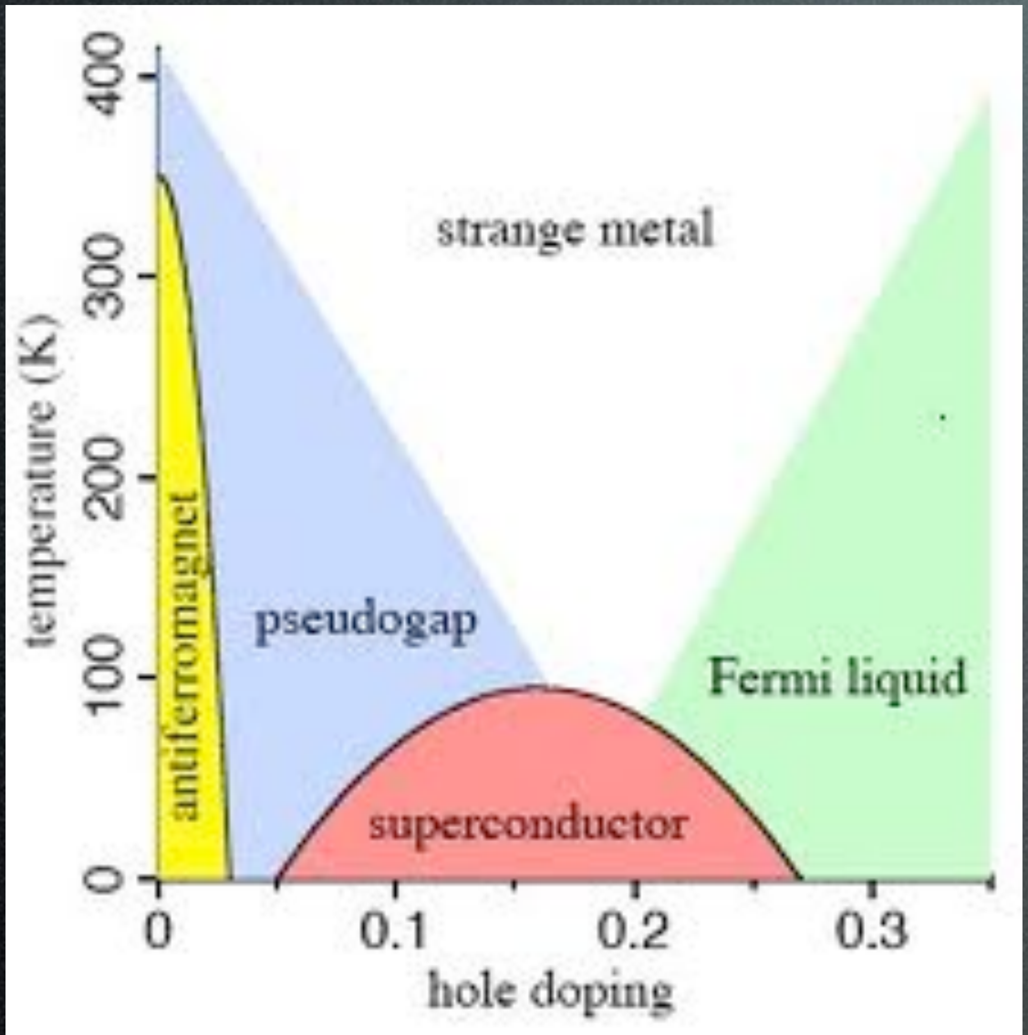
Riddles of Sphinx



Riddles of Pseudogap



Riddles of Pseudogap



Y. Li "Unusual magnetic order in the pseudogap region of the superconductor HgBa2CuO41d”

Nature 455 372 2008

Jing Xia, "Polar Kerr-Effect Measurements of YBa2Cu3O6 x Superconductor: Evidence for Broken Symmetry near the Pseudogap Temperature"

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PHYSICAL REVIEW B 86 020504(R) 2012

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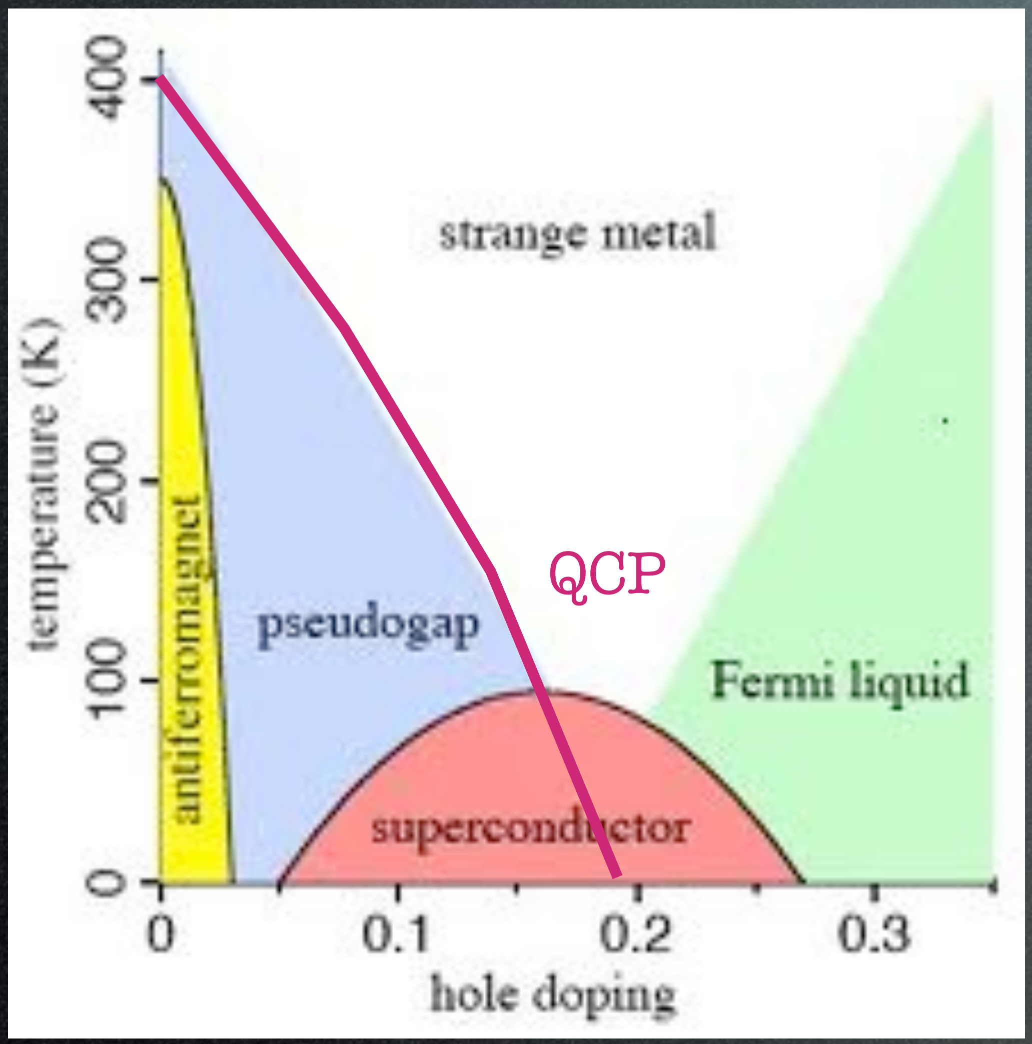

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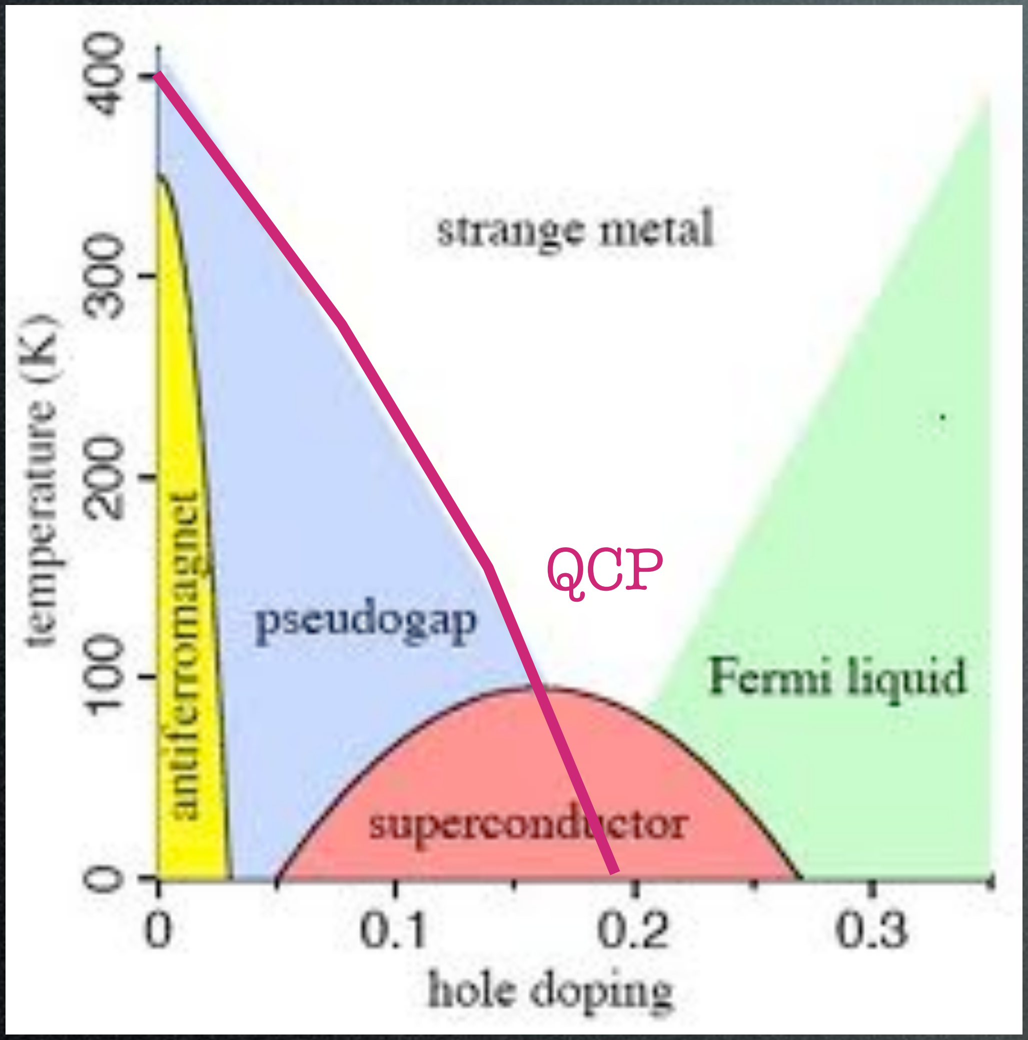
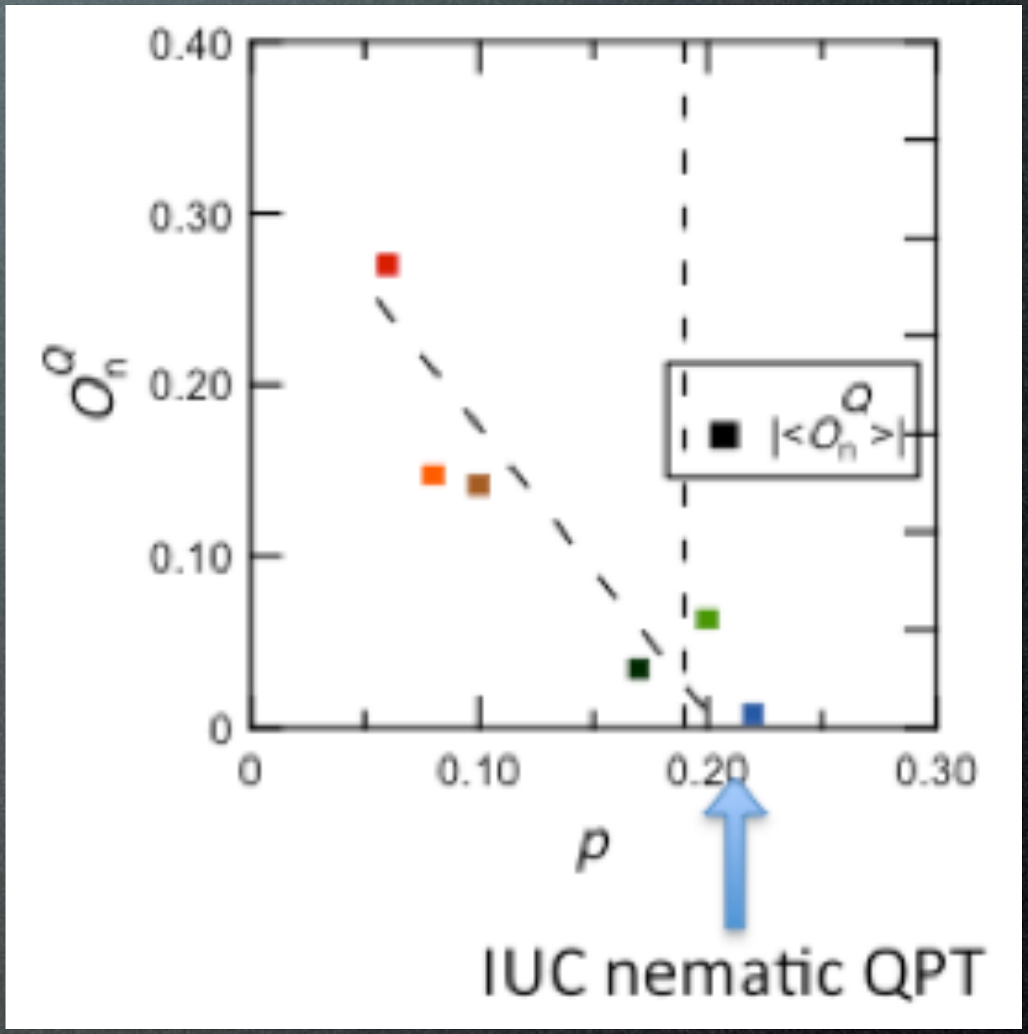
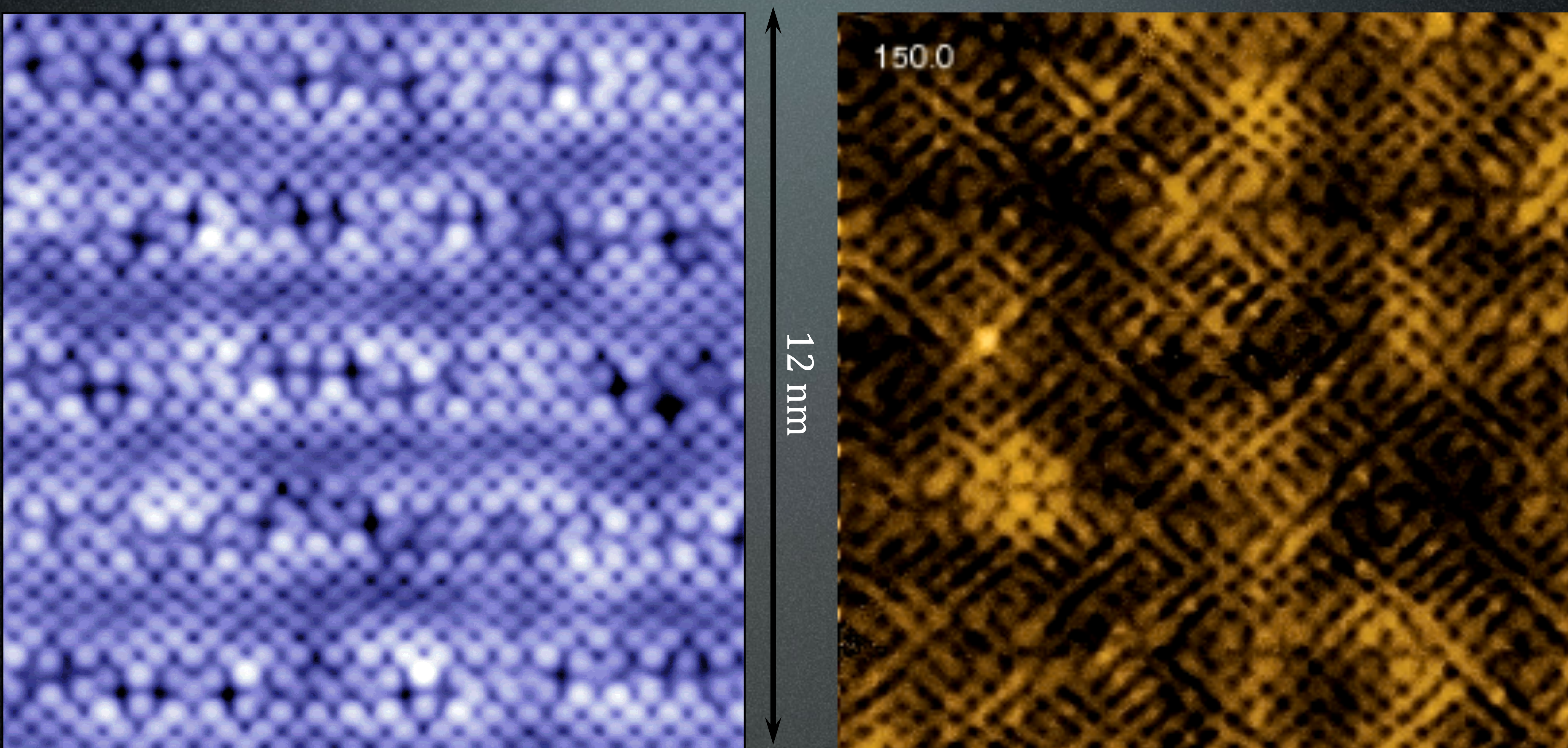




K. Fujita et al, submitted to Science (2014)

Visualize Broken-Symmetry States

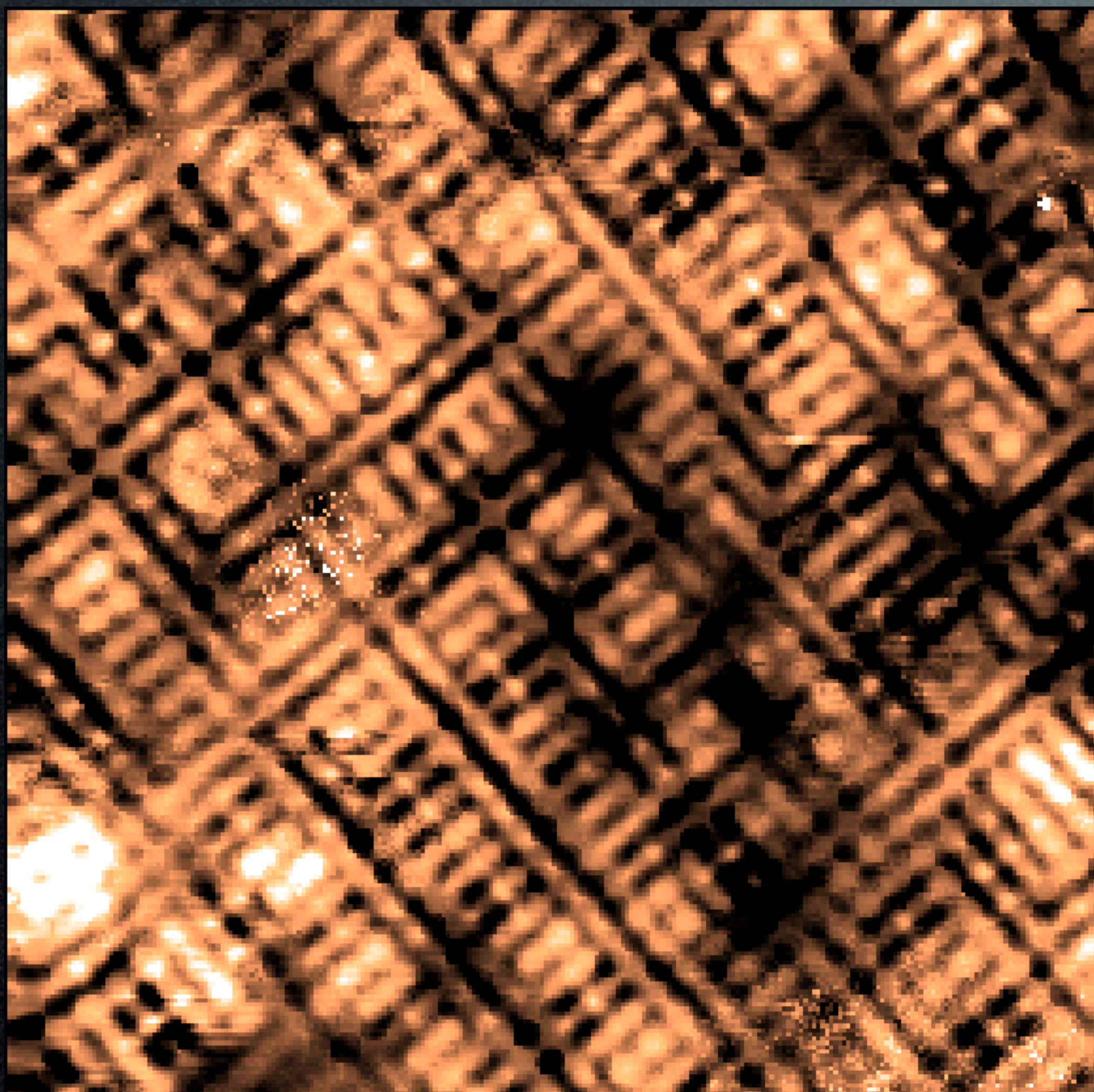
Science 315, 1380 (2007)



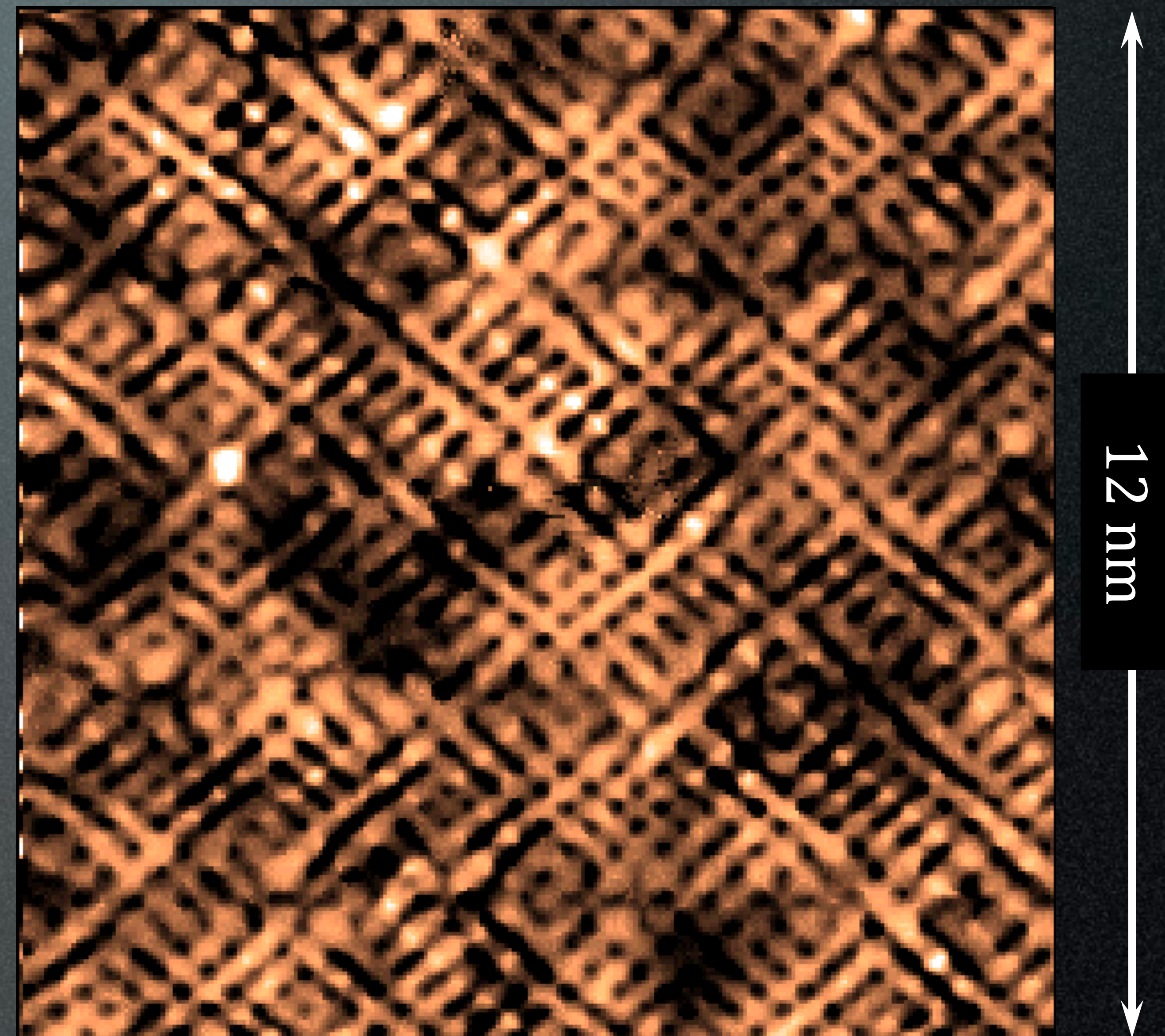
$Bi_{2.2}Sr_{1.8}(Ca,Dy)Cu_2O_y$

Not due to surface /crystal symmetry / dopant disorder etc

Science 315, 1380 (2007)



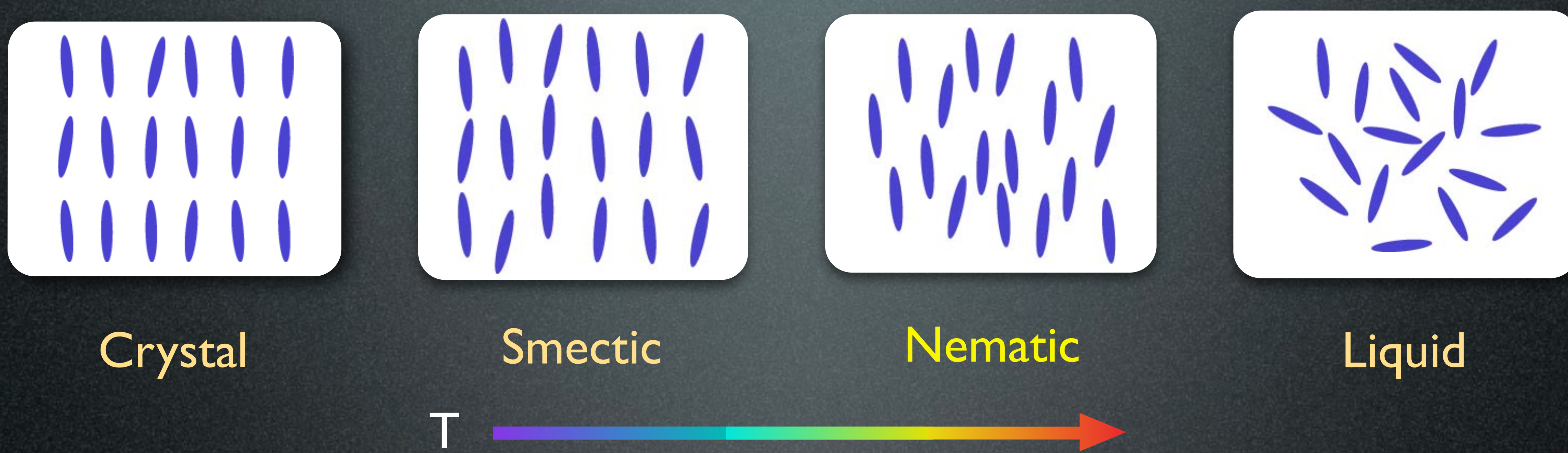
$Ca_{1.90}Na_{0.10}CuO_2Cl_2$



$Bi_{2.2}Sr_{1.8}Ca_{0.8}Dy_{0.2}Cu_2O_y$

Symmetry Based Perspective

Analogy different phases of rod-like polymers



Symmetry Based Perspective

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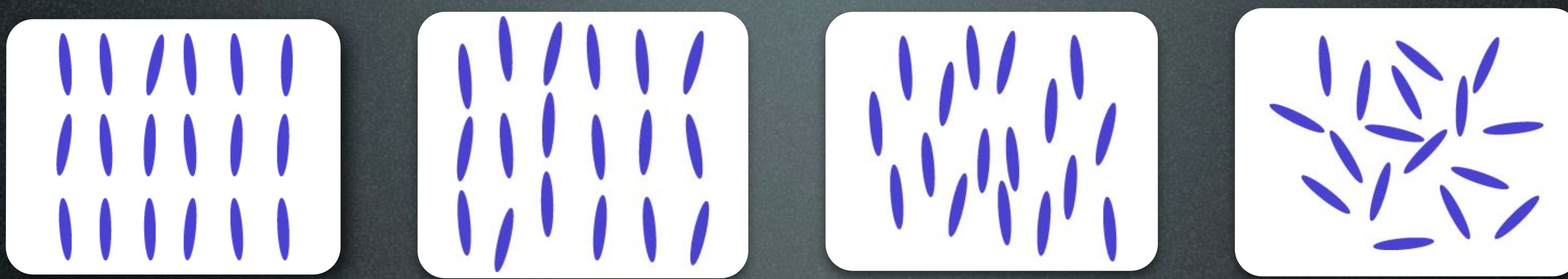
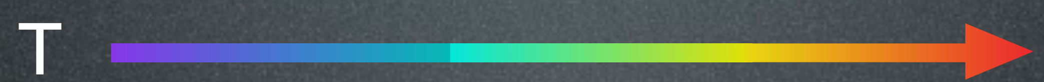


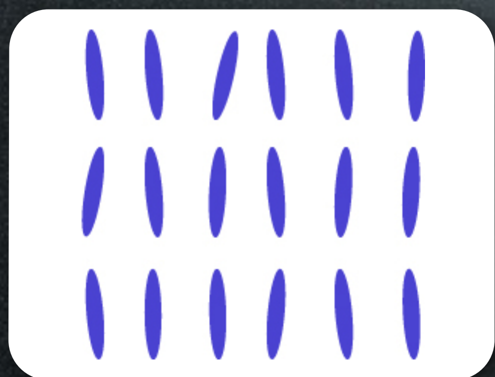
Crystal Smectic Nematic Liquid



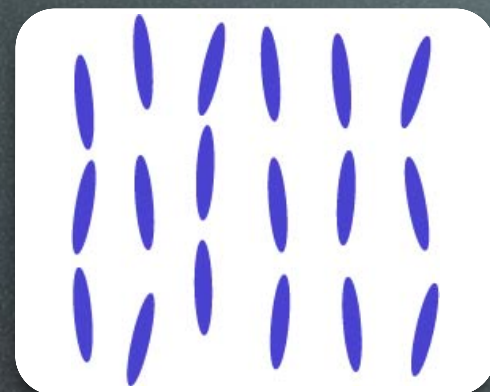
$\hat{T}_a, \hat{T}_b, \hat{R}$

Symmetry Based Perspective

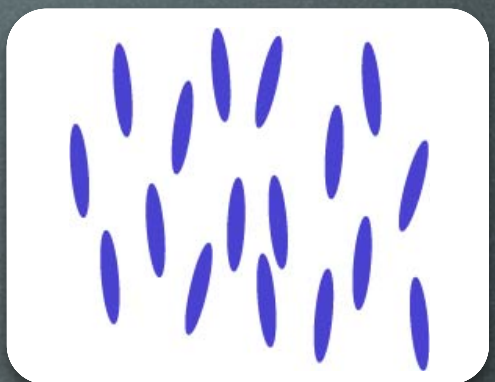
Analogy different phases of rod-like polymers



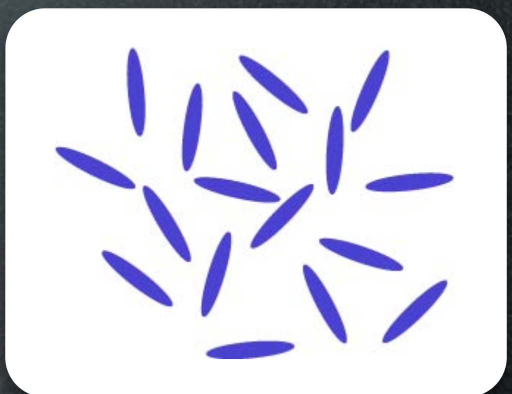
Crystal



Smectic



Nematic



Liquid

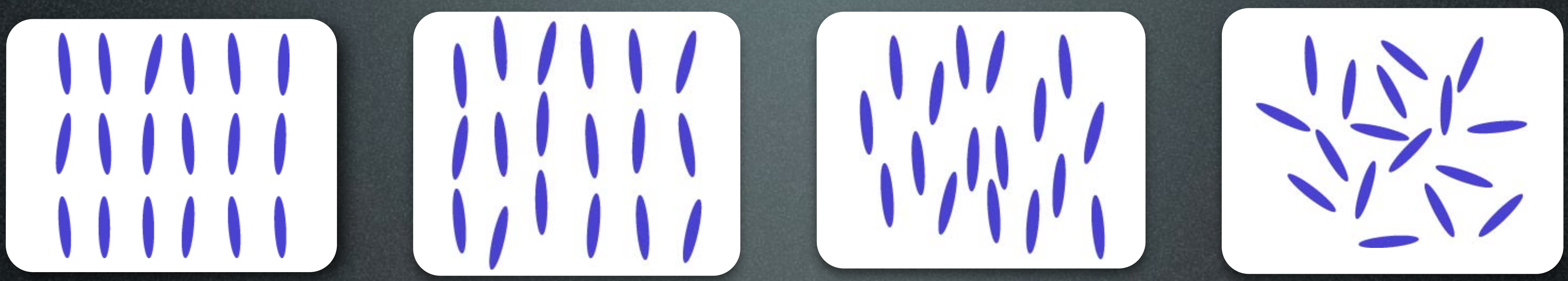
T

$\hat{T}_a, \hat{T}_b, \hat{R}$

$\hat{T}_a, \hat{R}$

Symmetry Based Perspective

Analogy different phases of rod-like polymers



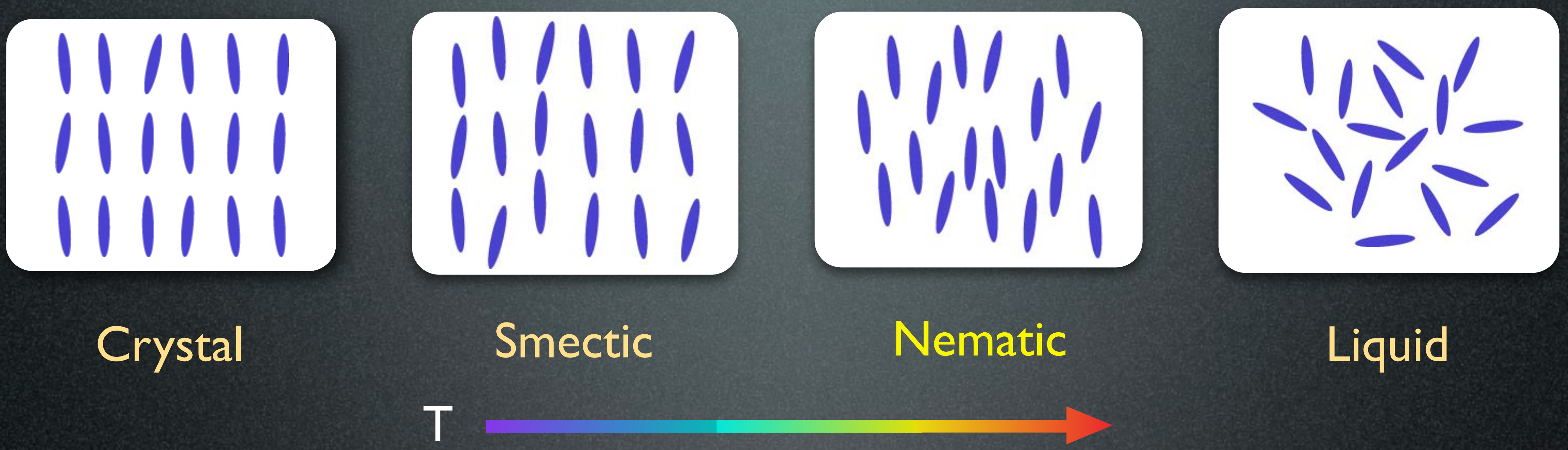
Crystal — Smectic — Nematic — Liquid

T →

$\hat{T}_a, \hat{T}_b, \hat{R}$ — $\hat{T}_a, \hat{R}$ — $\hat{R}$

Symmetry Based Perspective : ELC

Analogy different phases of rod-like polymers

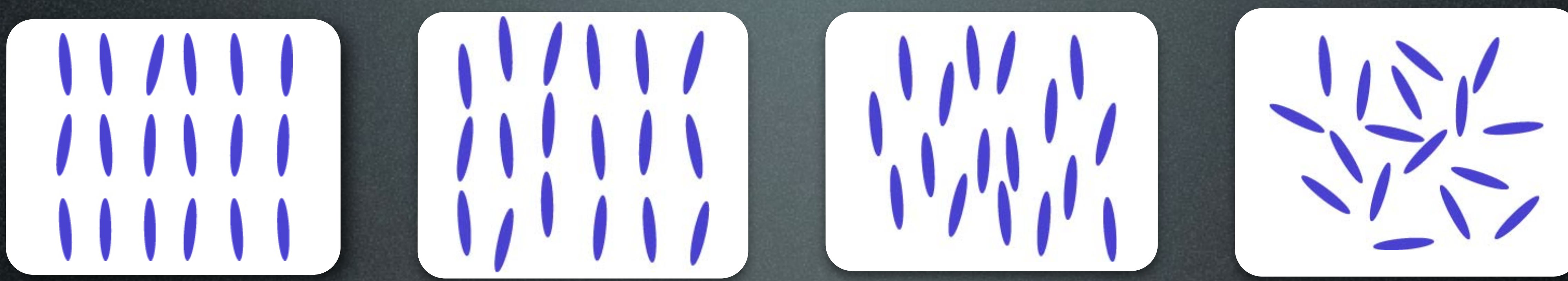


$\hat{T}_a, \hat{T}_b, \hat{R}$ $\hat{T}_a, \hat{R}$ $\hat{R}$

Electronic
Analogue
?

Symmetry Based Perspective : ELC

Analogy different phases of rod-like polymers

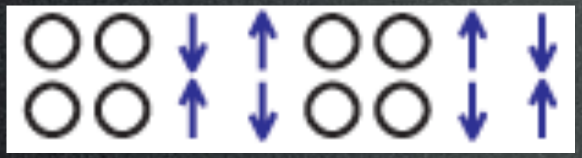


Crystal   Smectic   Nematic   Liquid

T →

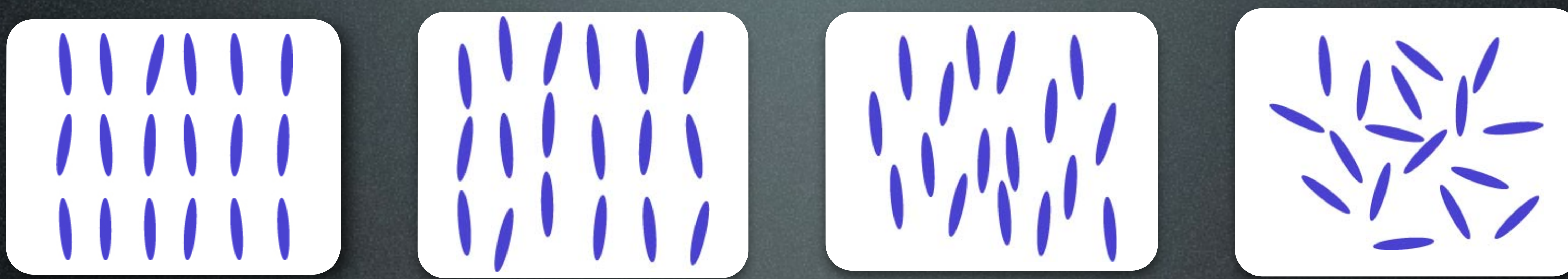
$\hat{T}_a, \hat{T}_b, \hat{R}$ $\hat{T}_a, \hat{R}$ $\hat{R}$

Electronic
Analogue
?



Symmetry Based Perspective : ELC

Analogy different phases of rod-like polymers

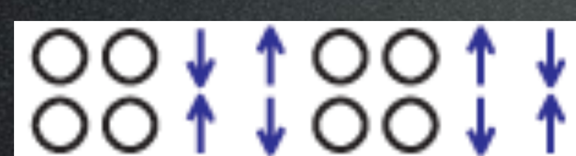


Crystal | Smectic | Nematic | Liquid

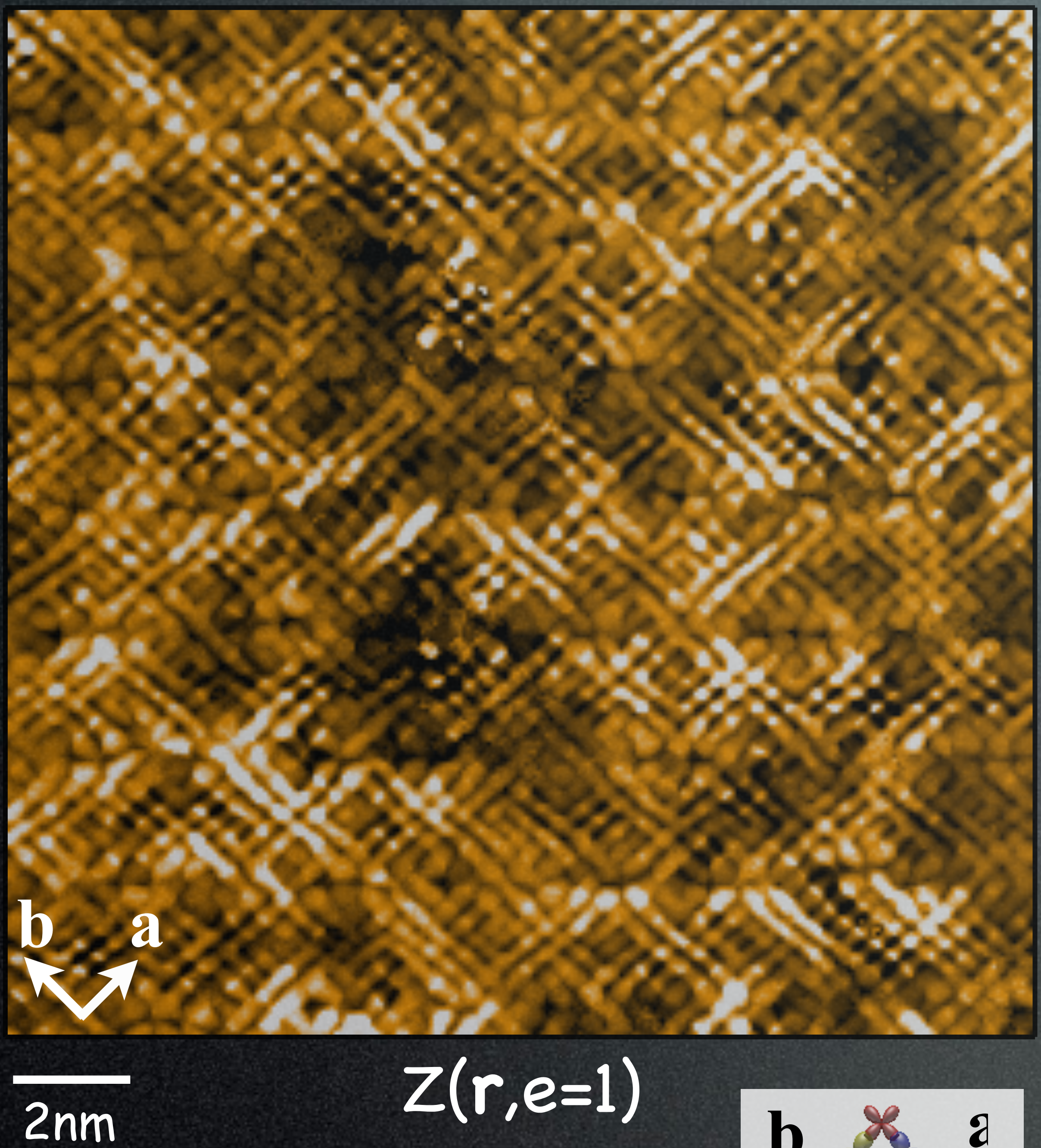
T →

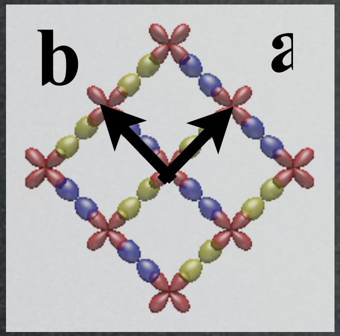
$\hat{T}_a, \hat{T}_b, \hat{R}$ | $\hat{T}_a, \hat{R}$ | $\hat{R}$

Electronic Analogue ?



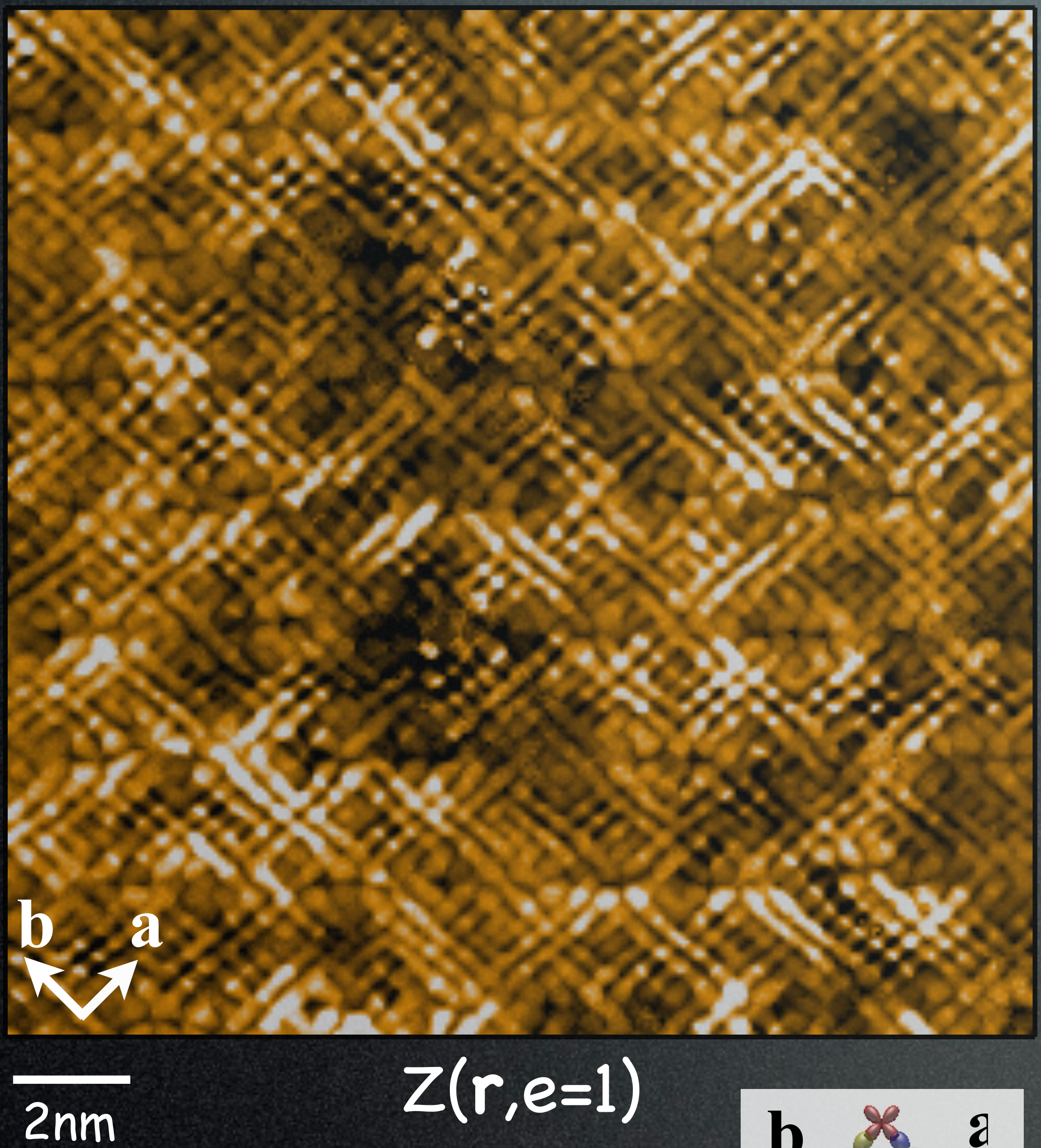
?



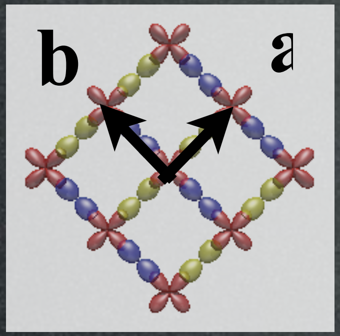


Position space

Separate Broken Symmetries?: Use distinct Fourier Components



Position space



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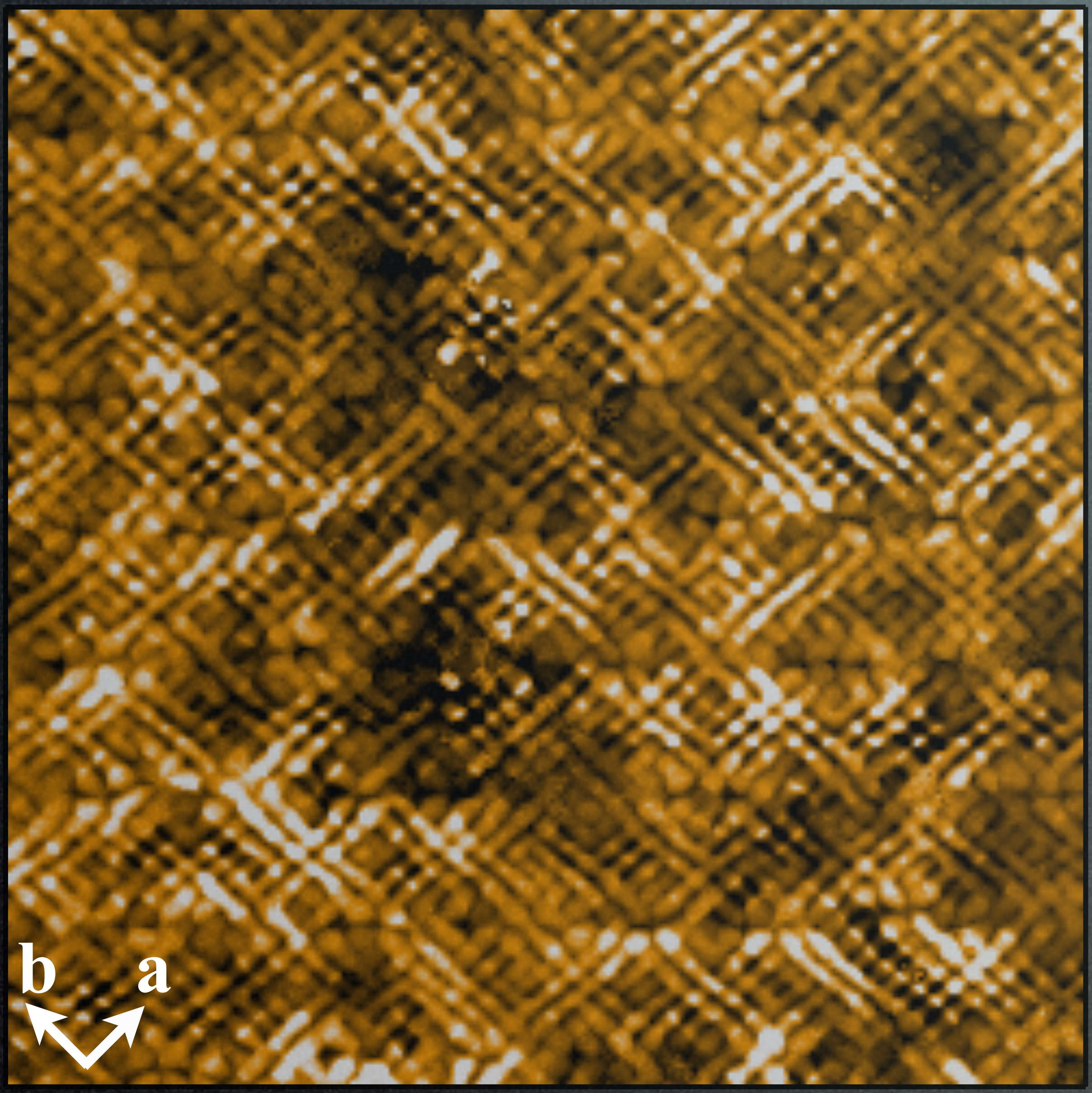
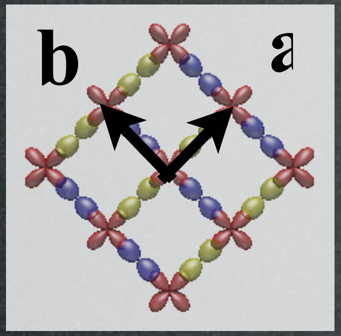


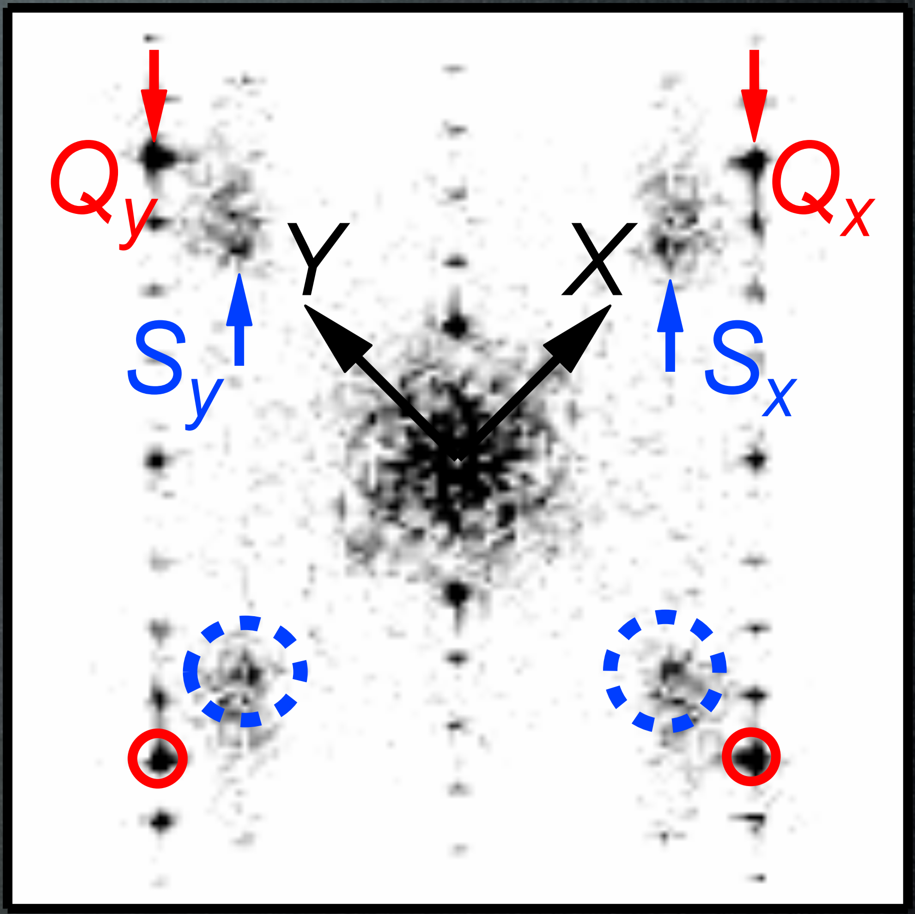
2nm

Z(**r**,e=1)

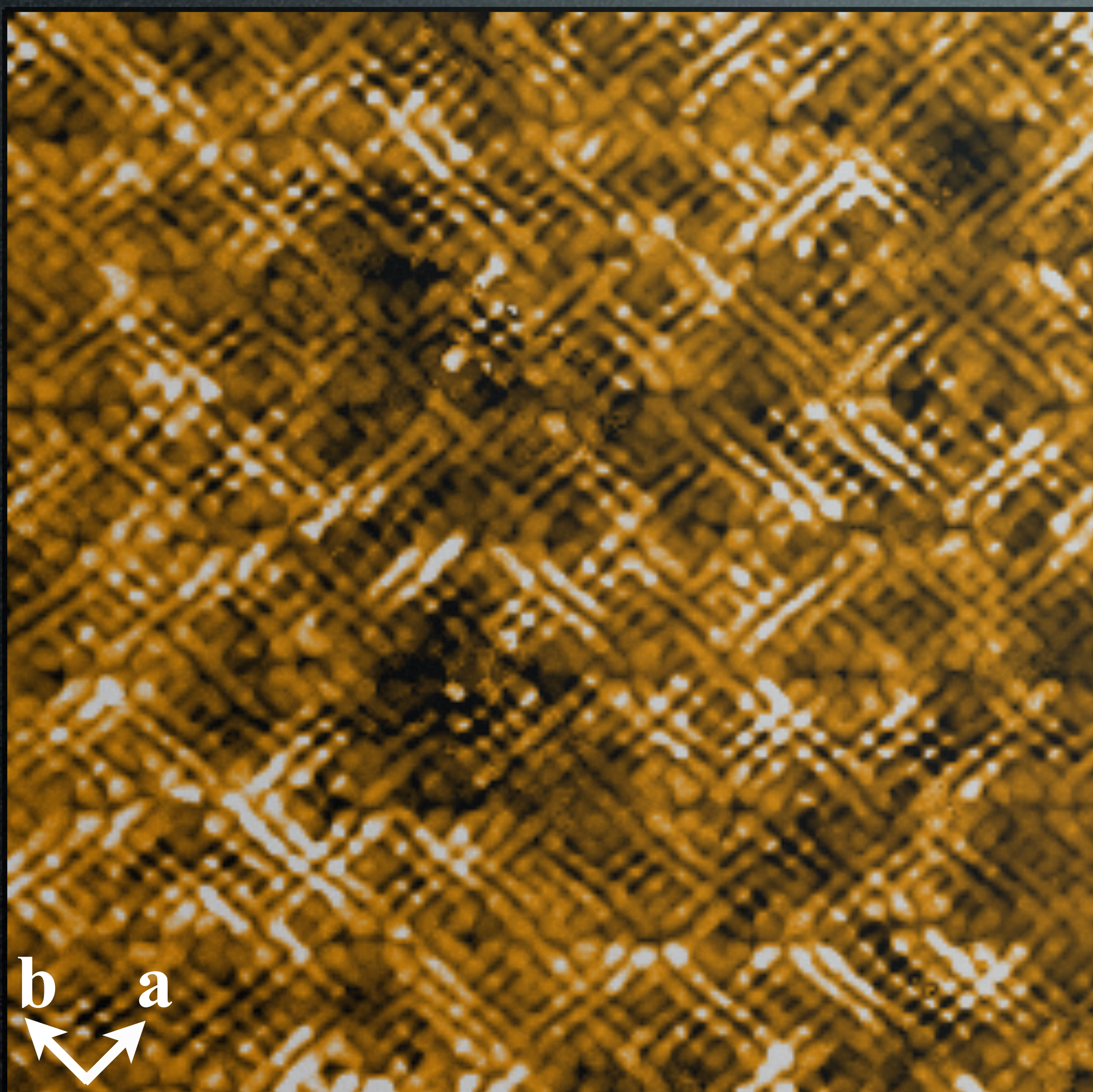
Position space



Fourier space



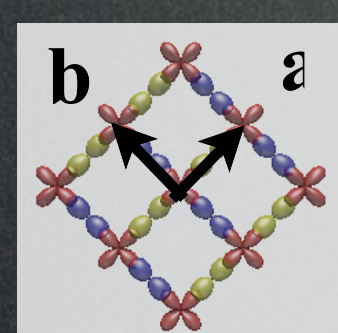
Separate Broken Symmetries?: Use distinct Fourier Components



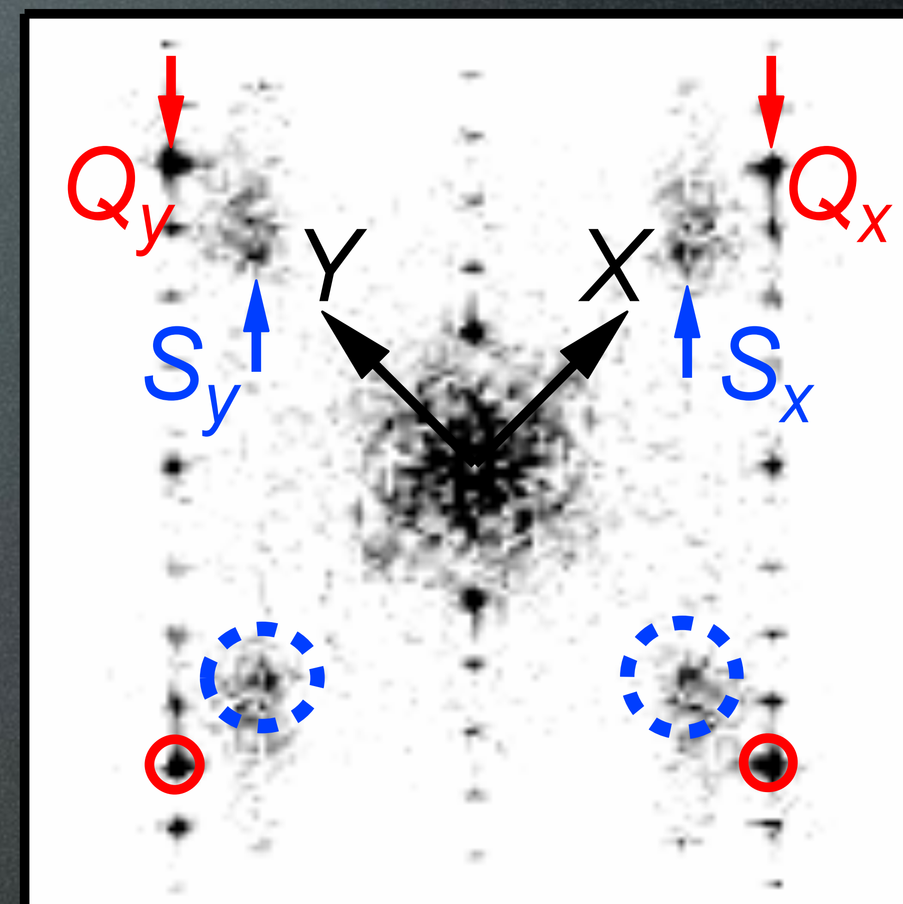
2nm

$Z(\mathbf{r}, e=1)$

Position space



Fourier space



IUC order: Q_x & Q_y?

$\hat{T}_a, \hat{T}_b$ breaking:

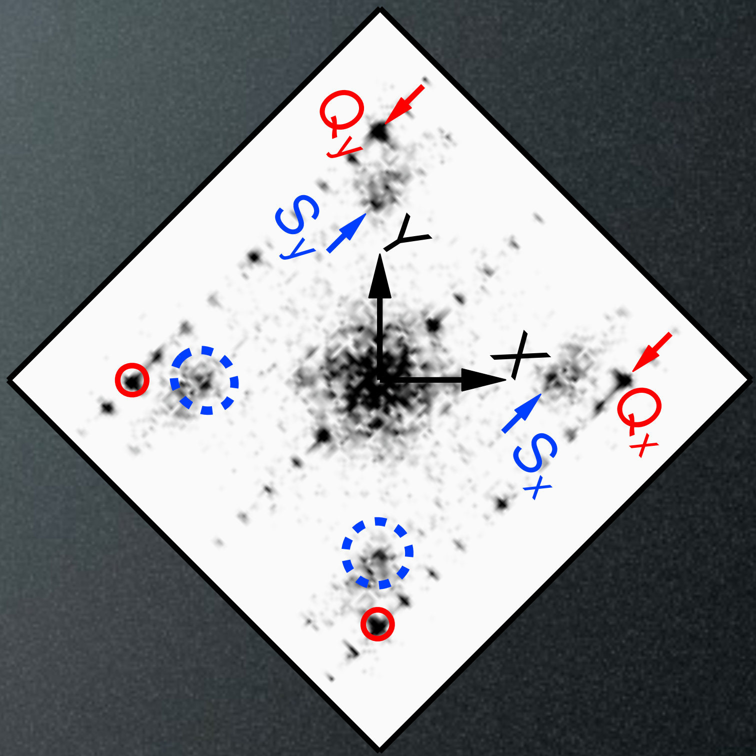
S_x & S_y?

$\overleftrightarrow{Q_x}$ vs $\overleftrightarrow{Q_y}$

- For any local map $M(\vec{r})$
- Bragg peak

$$\tilde{M}(\vec{Q}_x) = \frac{1}{\sqrt{N}} \sum_{\vec{R},\vec{d}} M(\vec{R}+\vec{d}) e^{-i\vec{Q}_x\cdot\vec{d}}$$

$$\vec{Q}_x = (2\pi/a, 0)$$



M.J. Lawler et al Nature 2010

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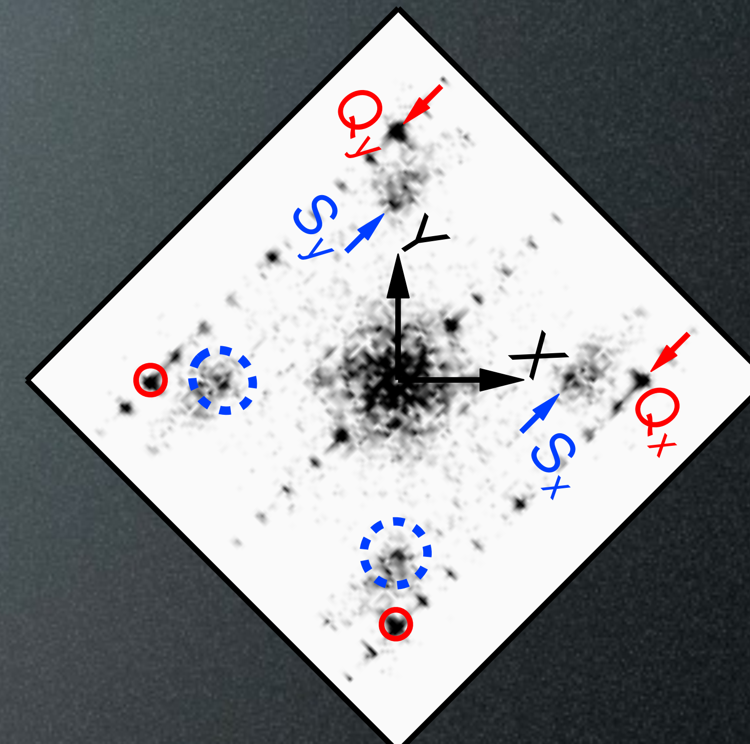


- Nematic OP

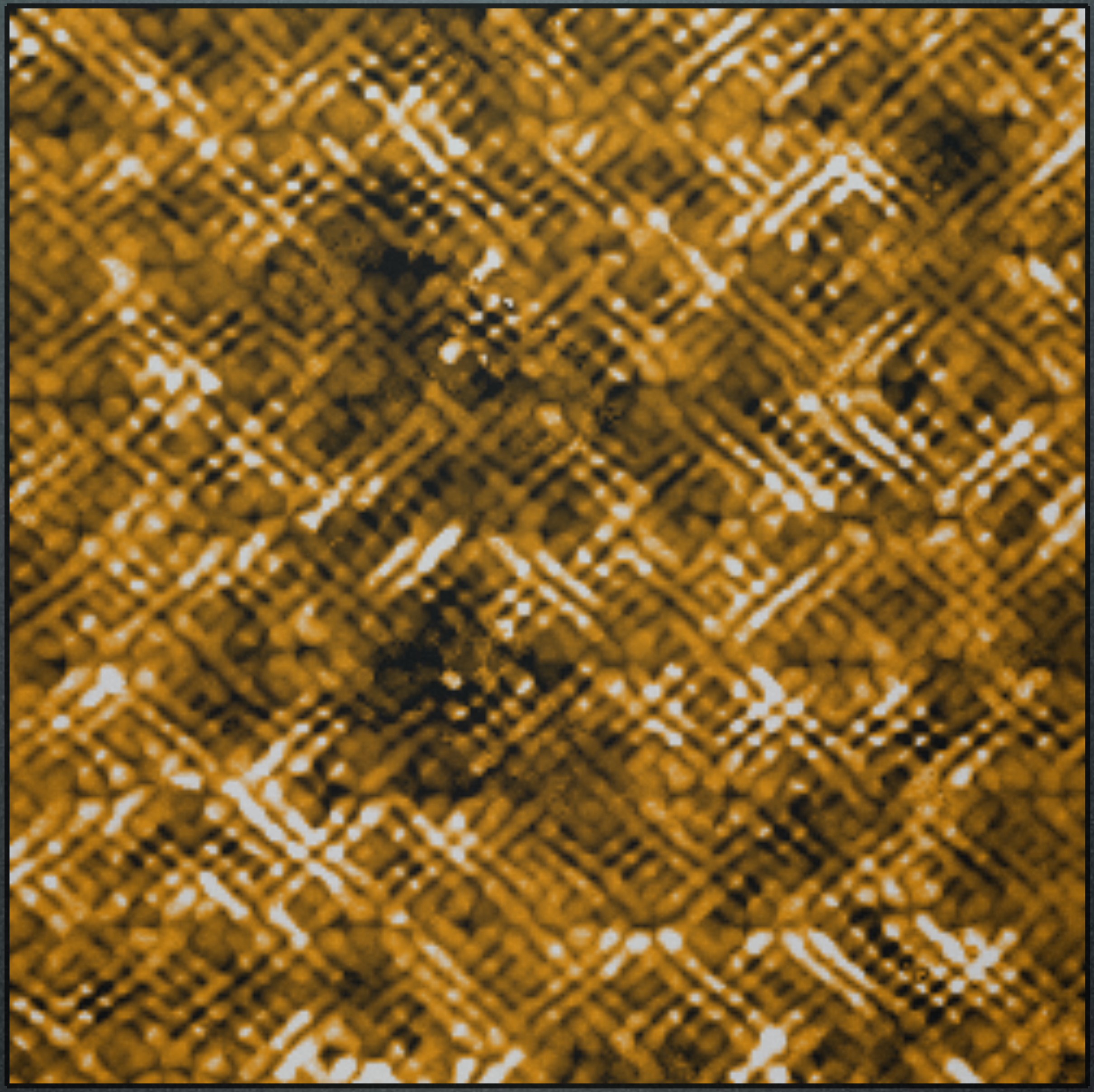
$$\begin{aligned} \mathcal{O}_N[M] &= \tfrac{1}{2}\left[\tilde{M}(\vec{Q}_y)-\tilde{M}(\vec{Q}_x)+\tilde{M}(-\vec{Q}_y)-\tilde{M}(-\vec{Q}_x)\right] \\ &= \mathrm{Re}\tilde{M}(\vec{Q}_y) - \mathrm{Re}\tilde{M}(\vec{Q}_x) \end{aligned}$$

➡Measures C_4 breaking

➡Preserves lattice translation

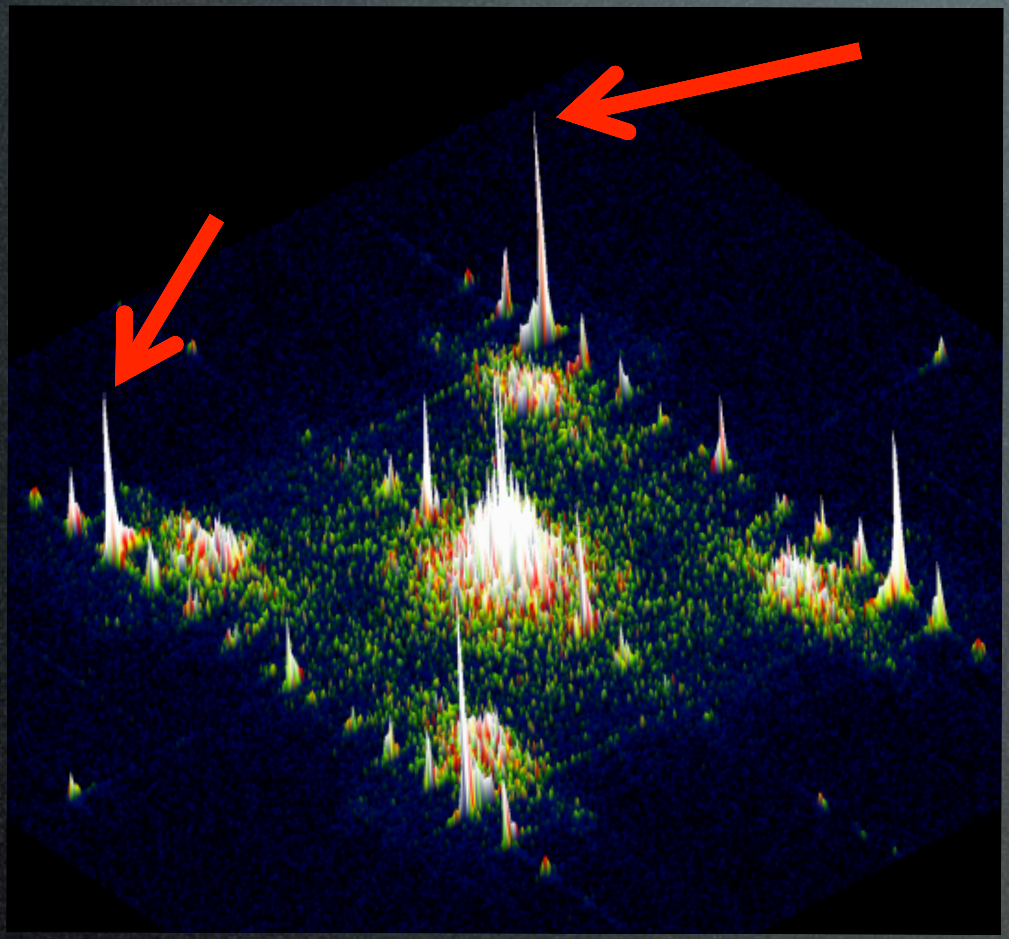
M.J. Lawler et al Nature 2010

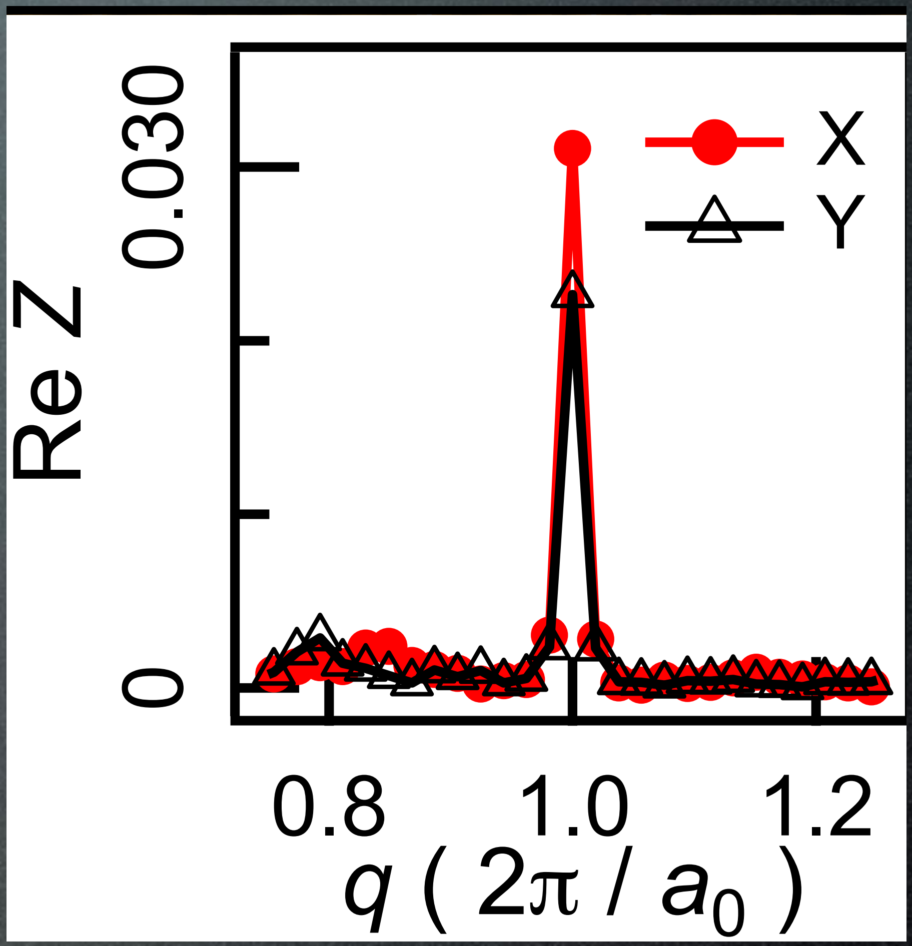
Bragg Peaks



IUC Nematic in BSCCO

Bragg Peaks





IUC Nematic in BSCCO

$\mathcal{O}_N$ intra-unit-cell structure

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$$\tilde{Z}(\vec{Q}_x) = \bar{Z}_{\mathrm{Cu}} - \bar{Z}_{\mathrm{O}_x} + \bar{Z}_{\mathrm{O}_y}, \tilde{Z}(\vec{Q}_y) = \bar{Z}_{\mathrm{Cu}} + \bar{Z}_{\mathrm{O}_x} - \bar{Z}_{\mathrm{O}_y}$$

$$\mathcal{O}_N \propto (\bar{Z}_{O_x} - \bar{Z}_{O_y})$$ M.J. Lawler et al, Nature 2010

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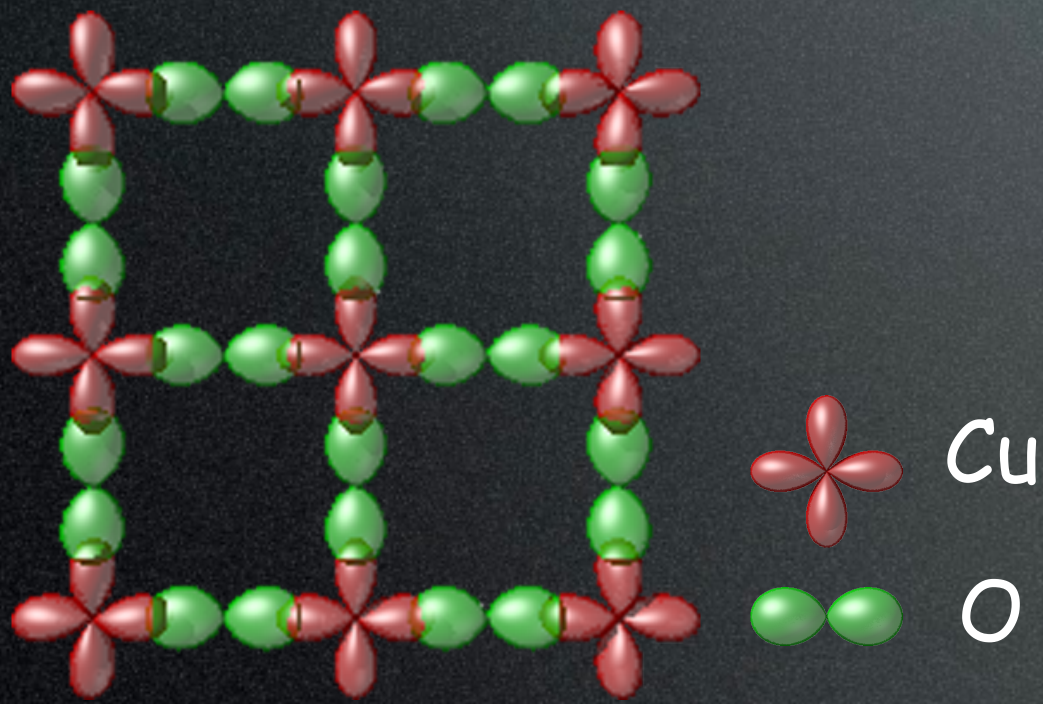
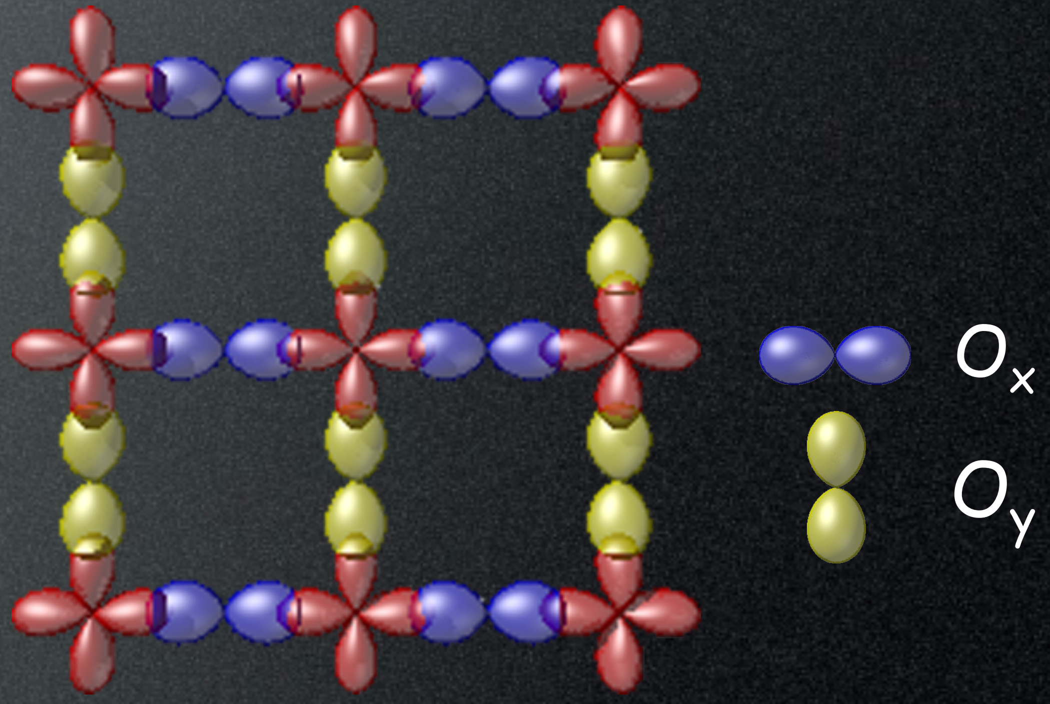
➡ Intra-unitcell pattern including O sites



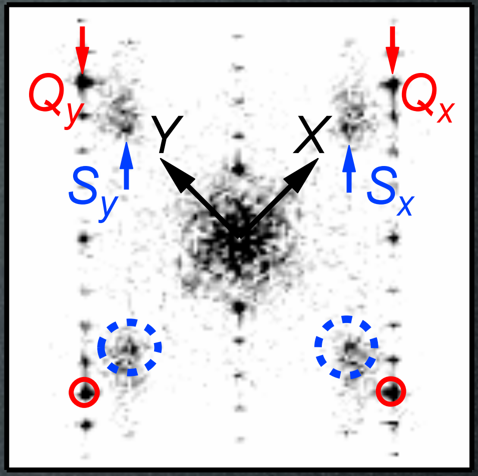
CuO_2 plane



Intra unitcell Nematic:
$C_4 \Rightarrow C_2$

Local version of Nematic OP $\mathcal{O}_N(\vec{x})$

- How strongly do each point $\vec{x}$ contribute to a Q space peak $\tilde{M}(\vec{Q})$?



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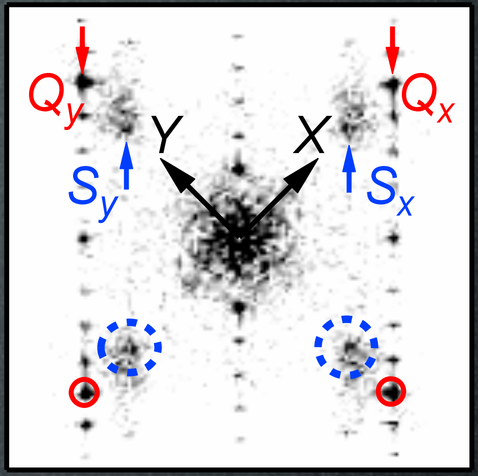

$$\tilde{M}(\vec{Q},\vec{x}) = \text{low pass}_\Lambda\left[M(\vec{x})e^{i\vec{Q}\cdot\vec{x}}\right]$$

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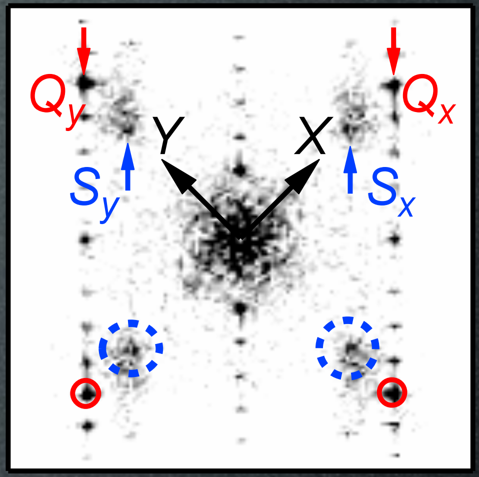

$$\tilde{M}(\vec{Q},\vec{x}) = \text{low pass}_\Lambda \left[M(\vec{x}) e^{i\vec{Q}\cdot\vec{x}} \right]$$

- Local order parameter:

$$\mathcal{O}_N[M](\vec{x}) = \frac{1}{2}\left[\tilde{M}(\vec{Q}_y,\vec{y}) - \tilde{M}(\vec{Q}_x,\vec{x}) + \tilde{M}(-\vec{Q}_y,\vec{x}) - \tilde{M}(-\vec{Q}_x,\vec{x})\right]$$

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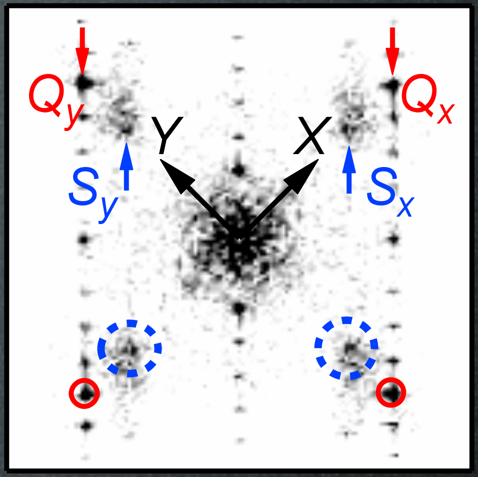

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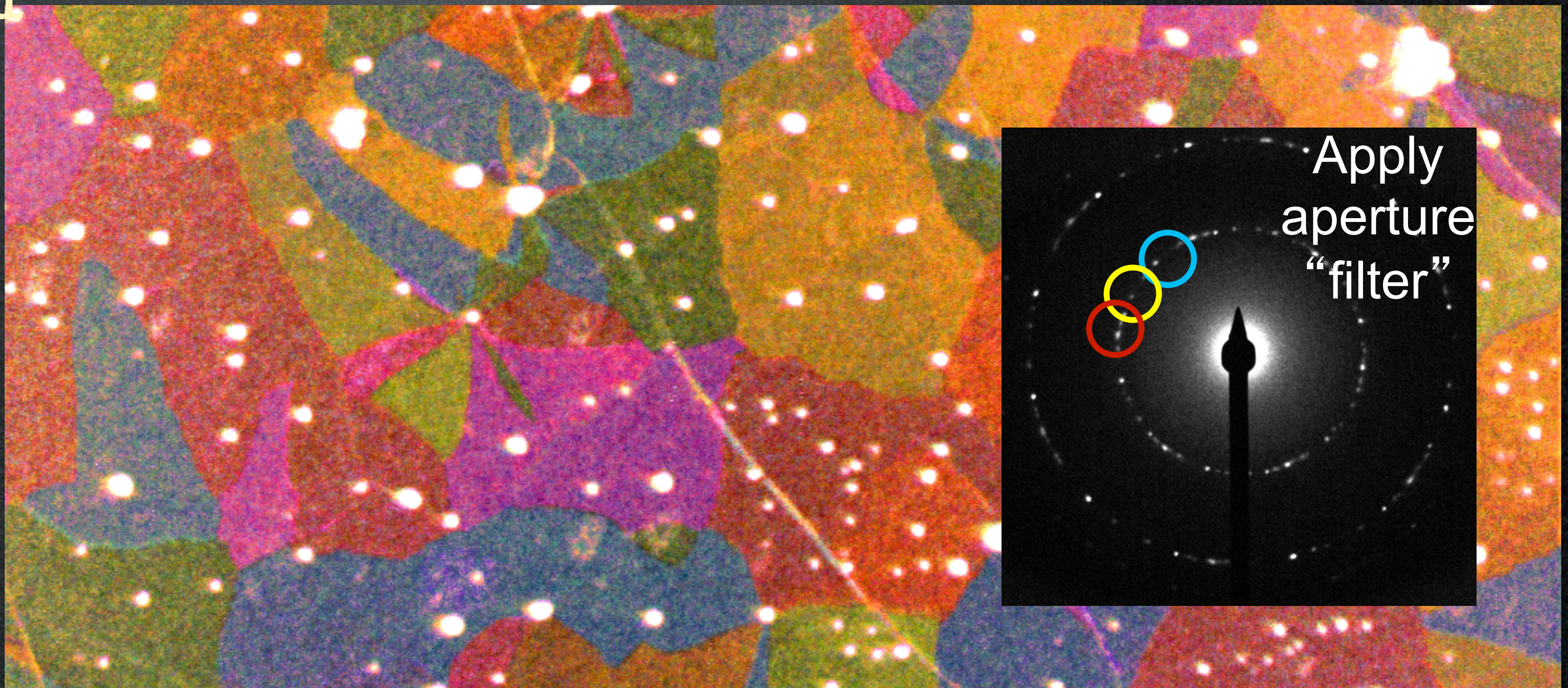
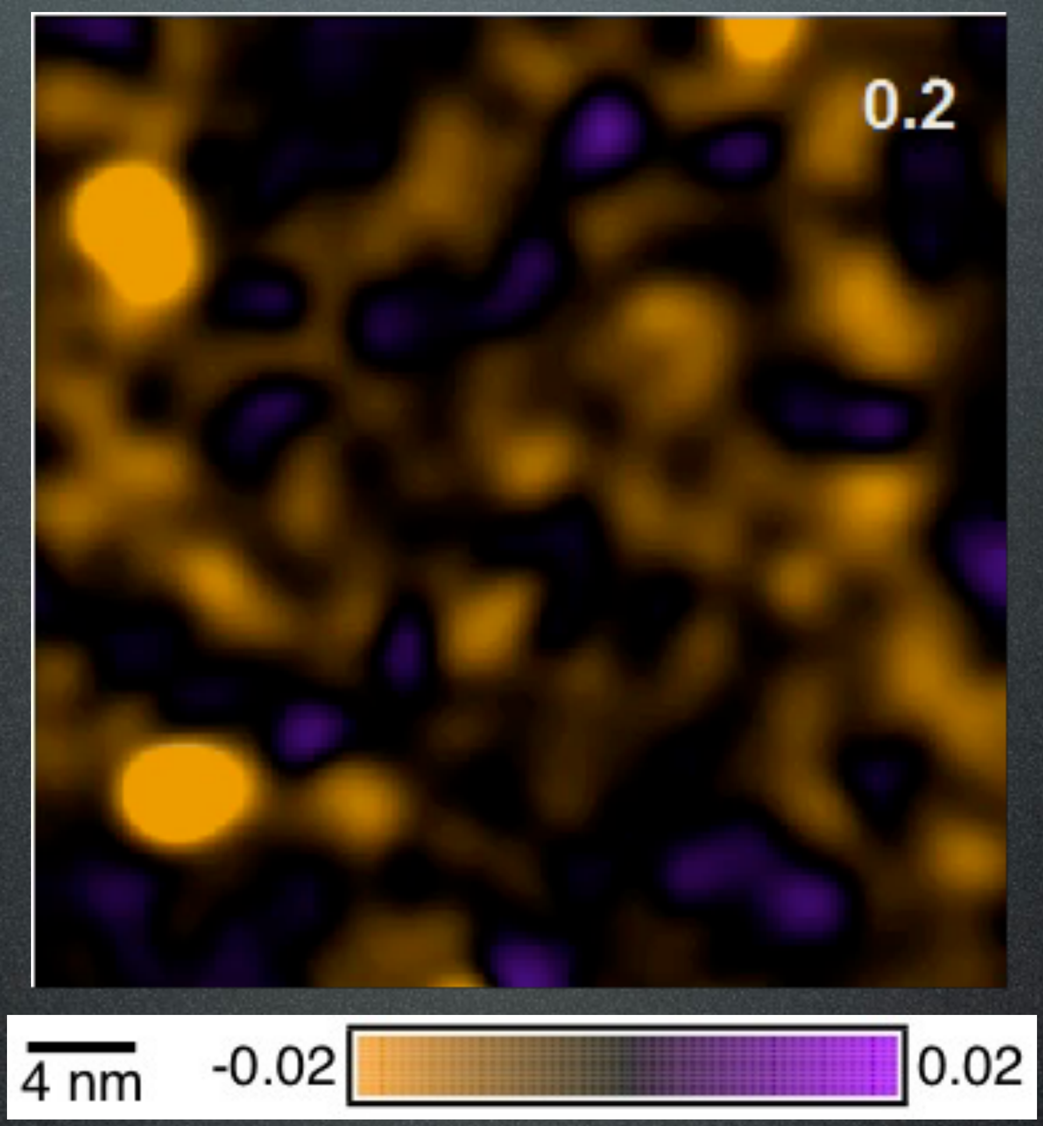
- ala TEM on graphene [Huang et al, Nature 2011]



$\vec{Q} = 0$ Nematic Order

- Shift Q_x, Q_y to origin

- Low pass filter (long distance physics)



Lawler, Fujita et al, Nature 2010

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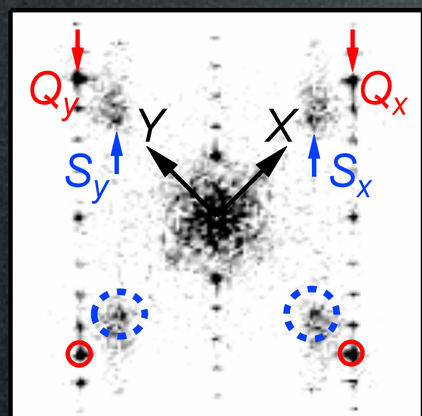

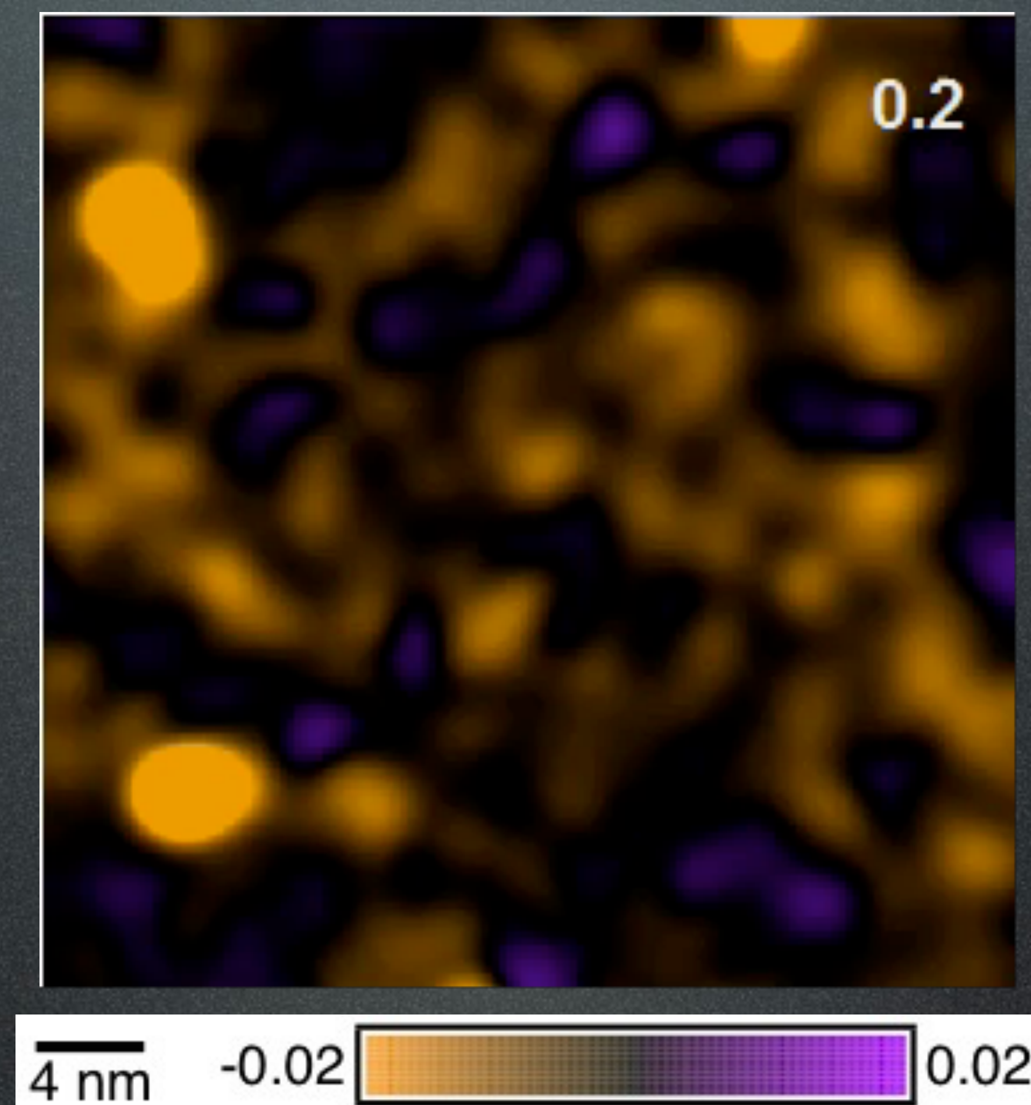

Lawler, Fujita et al, Nature 2010

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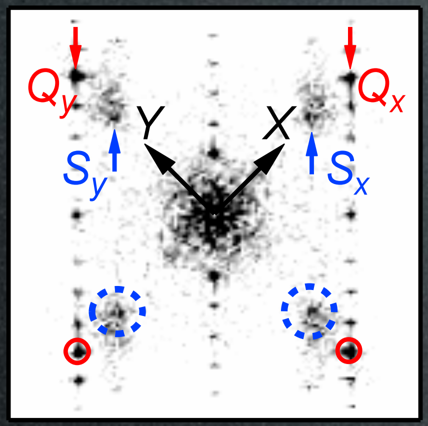
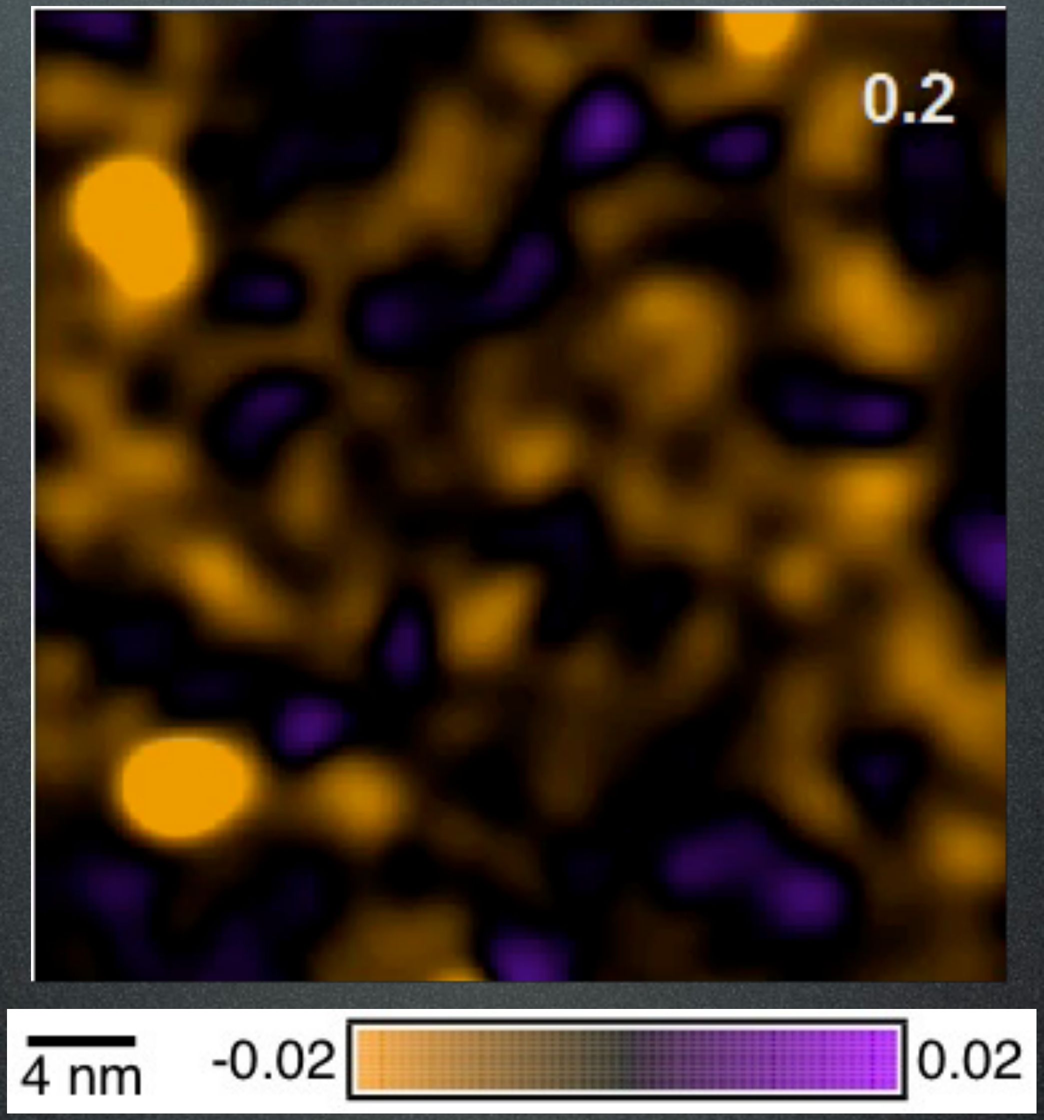


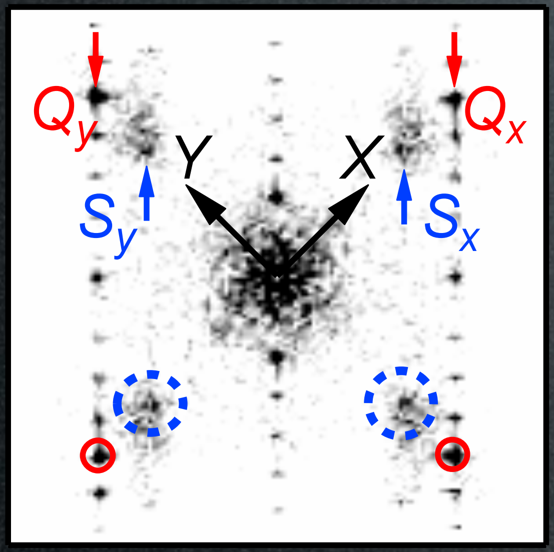


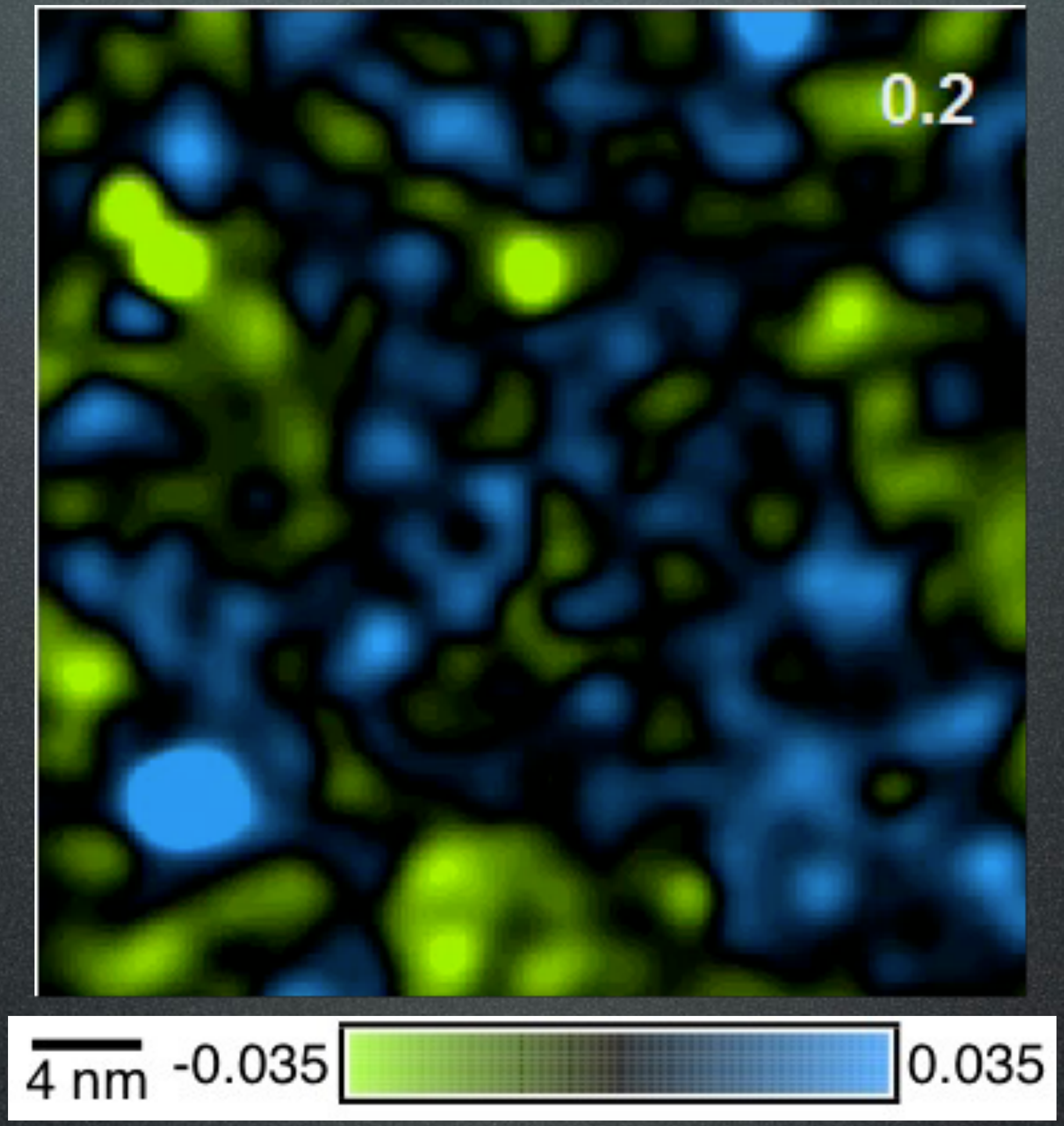
Orders near pseudogap energy scale

Lawler, Fujita et al, Nature 2010

$\vec{Q} \neq 0$ Smectic domains

- Shift S_x, S_y to origin ("tune to the channel")
- Low pass filter (long distance physics)





Lawler, Fujita et al, Nature 2010

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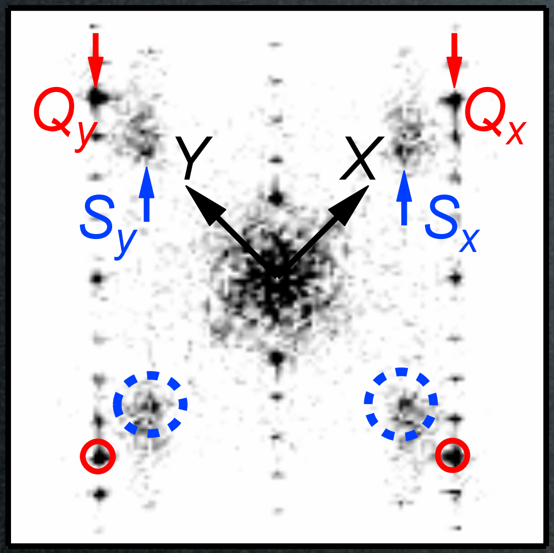

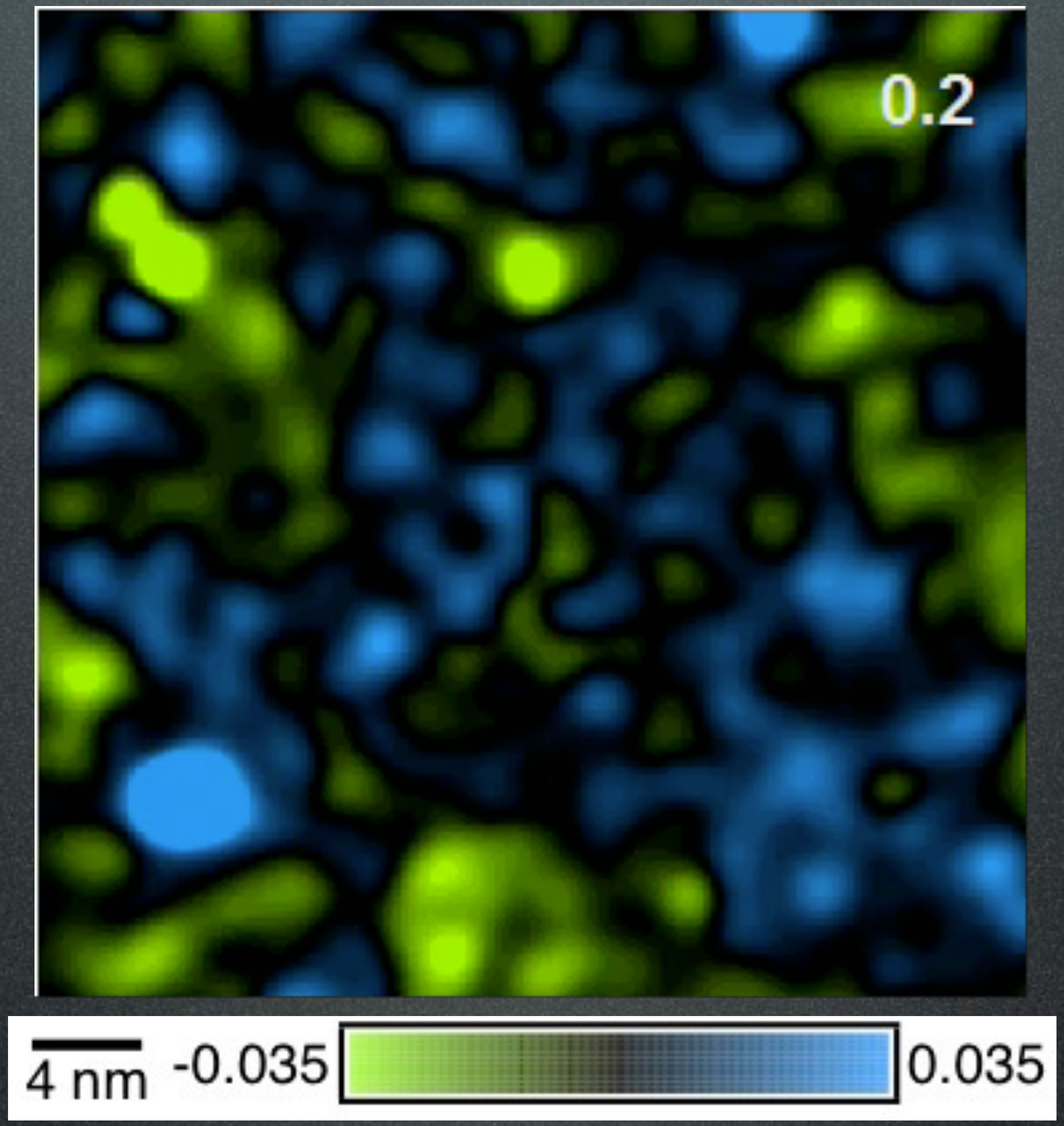

Lawler, Fujita et al, Nature 2010

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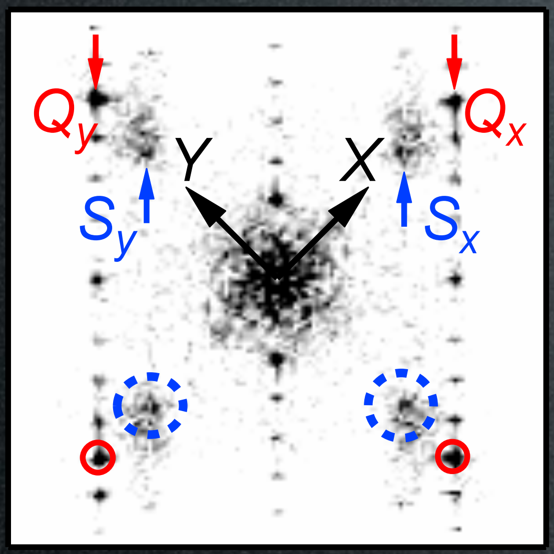
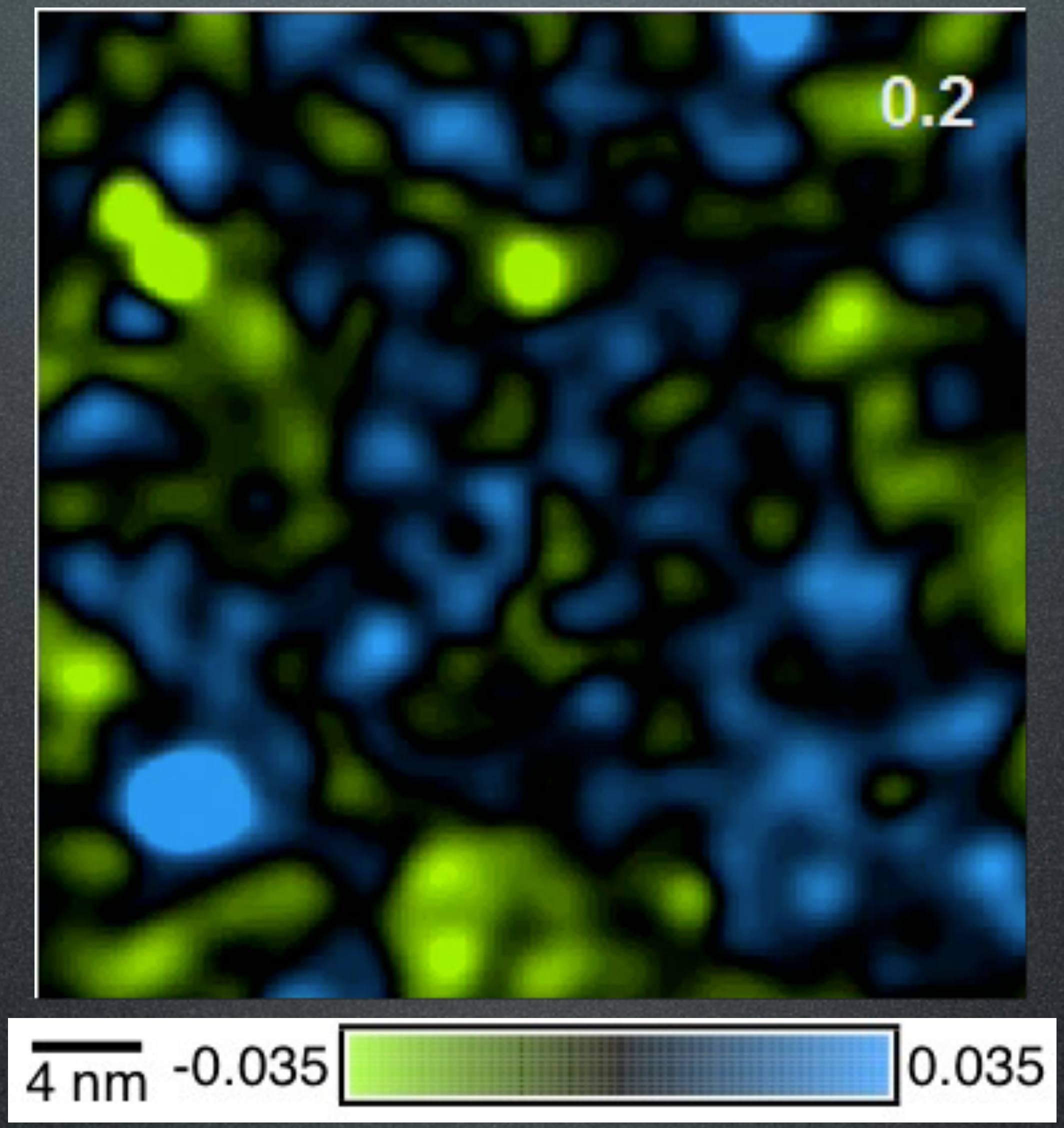




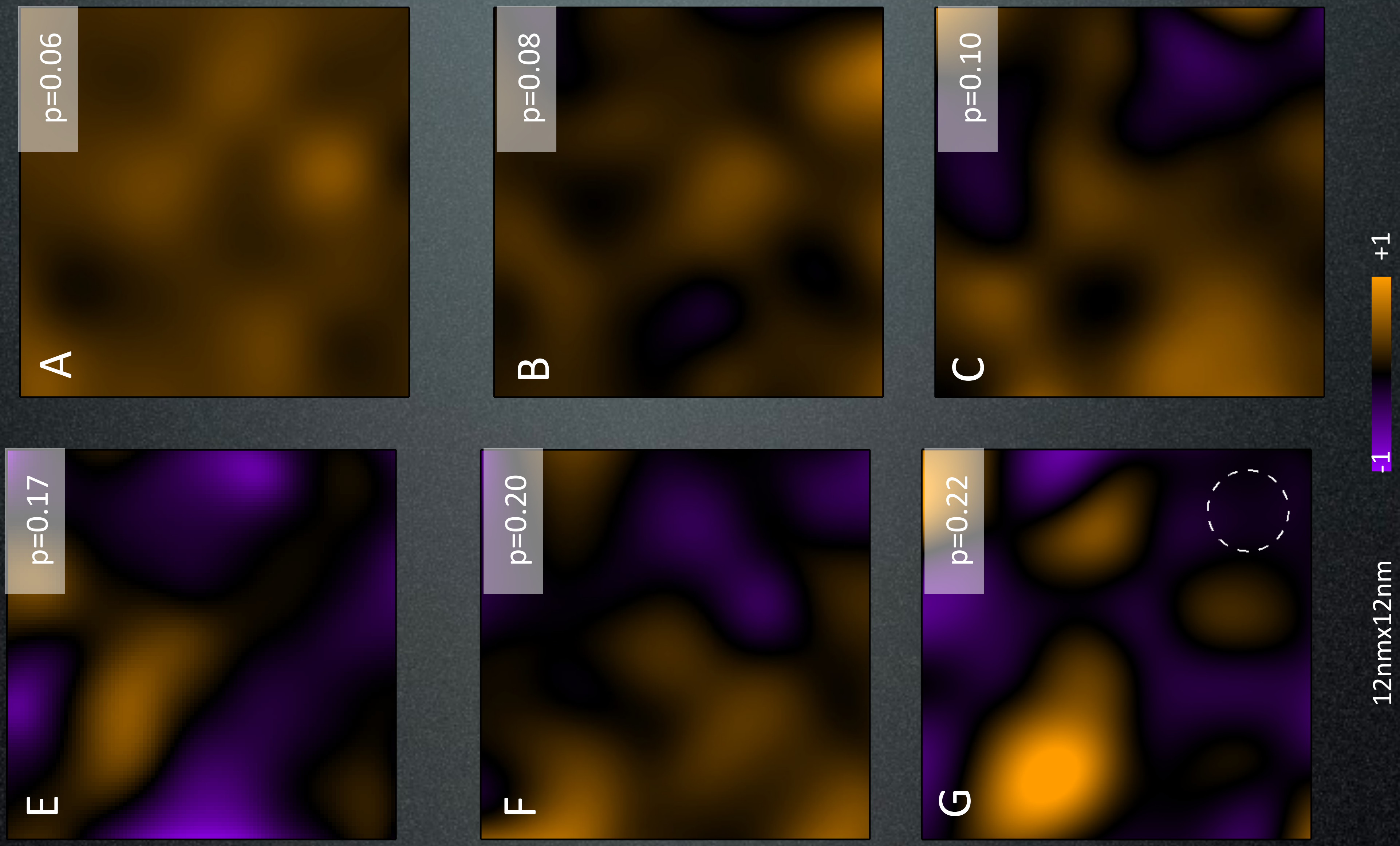
Lawler, Fujita et al, Nature 2010

Severely fluctuating in space at all energies

:Consistent with previous studies

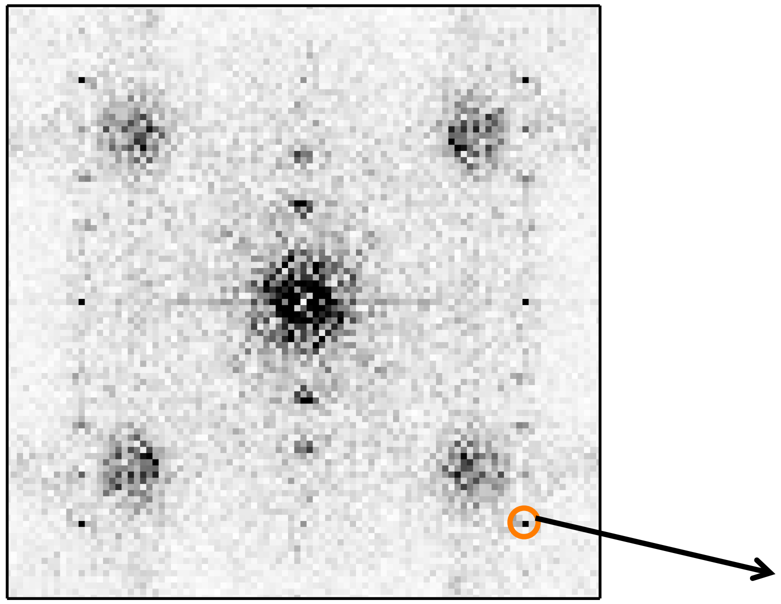
Howald et al (2003) Kohsaka et al (2008) Robertson et. al. (2006) Del Meastro et. al. (2006)

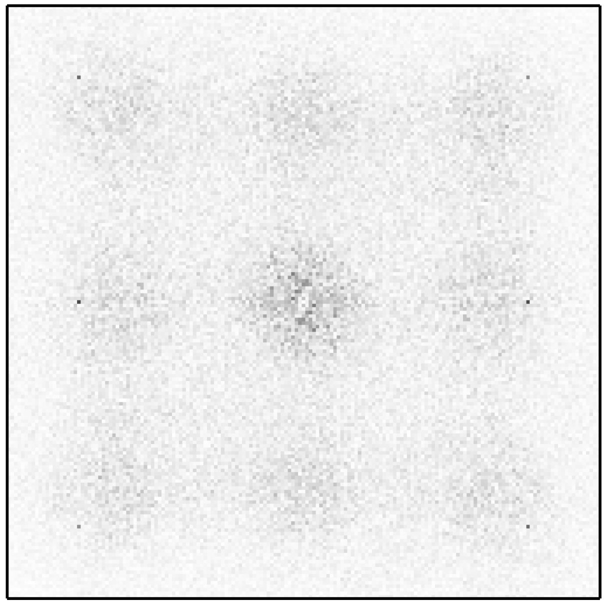
DOPING DEPENDENCE OF Q=0 SYMMETRY BREAKING



K. Fujita *et al* (2013)

Doping Dependence of Q=0 IUC Nematic





K. Fujita et al, Science (2014)

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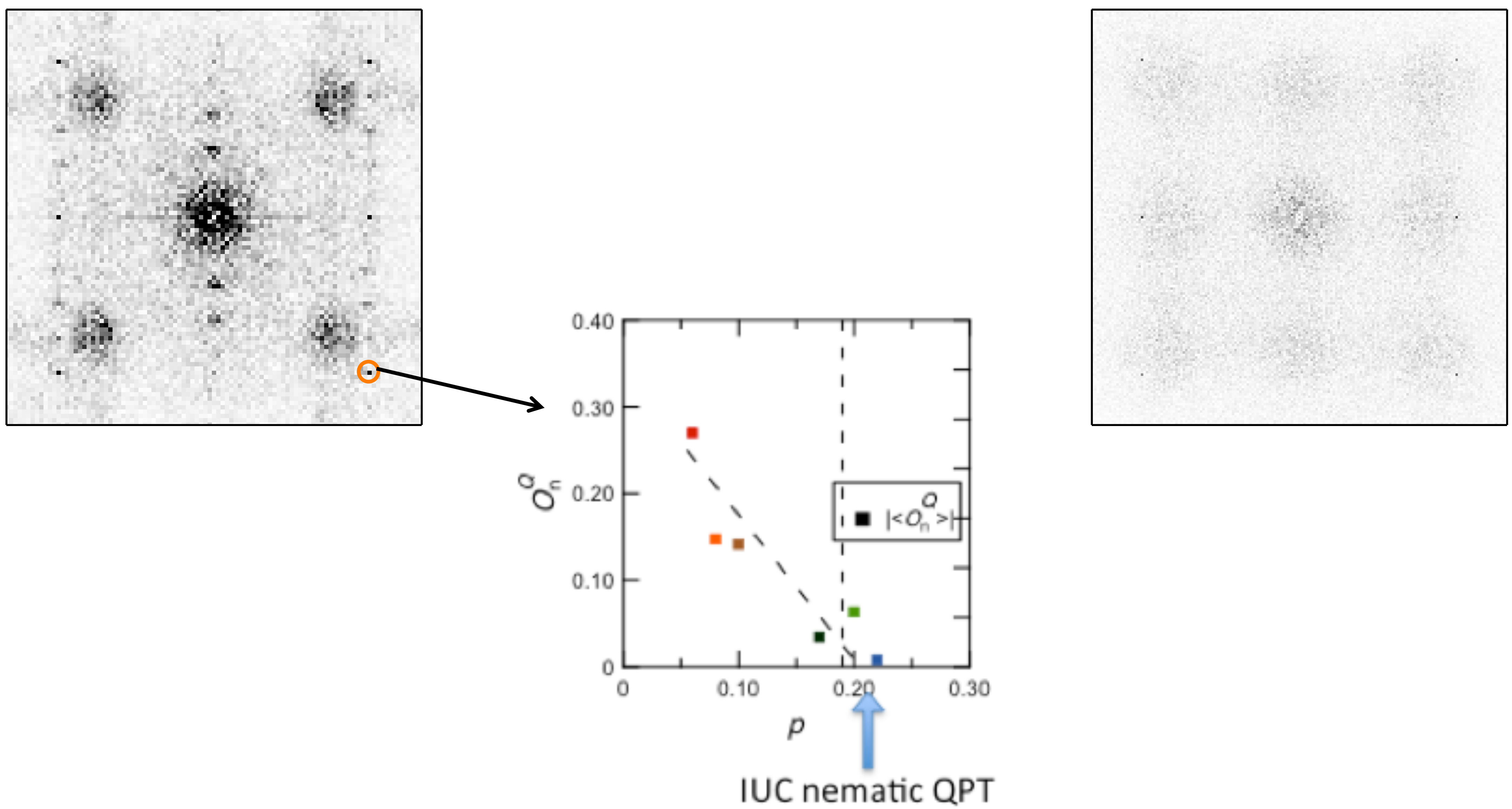
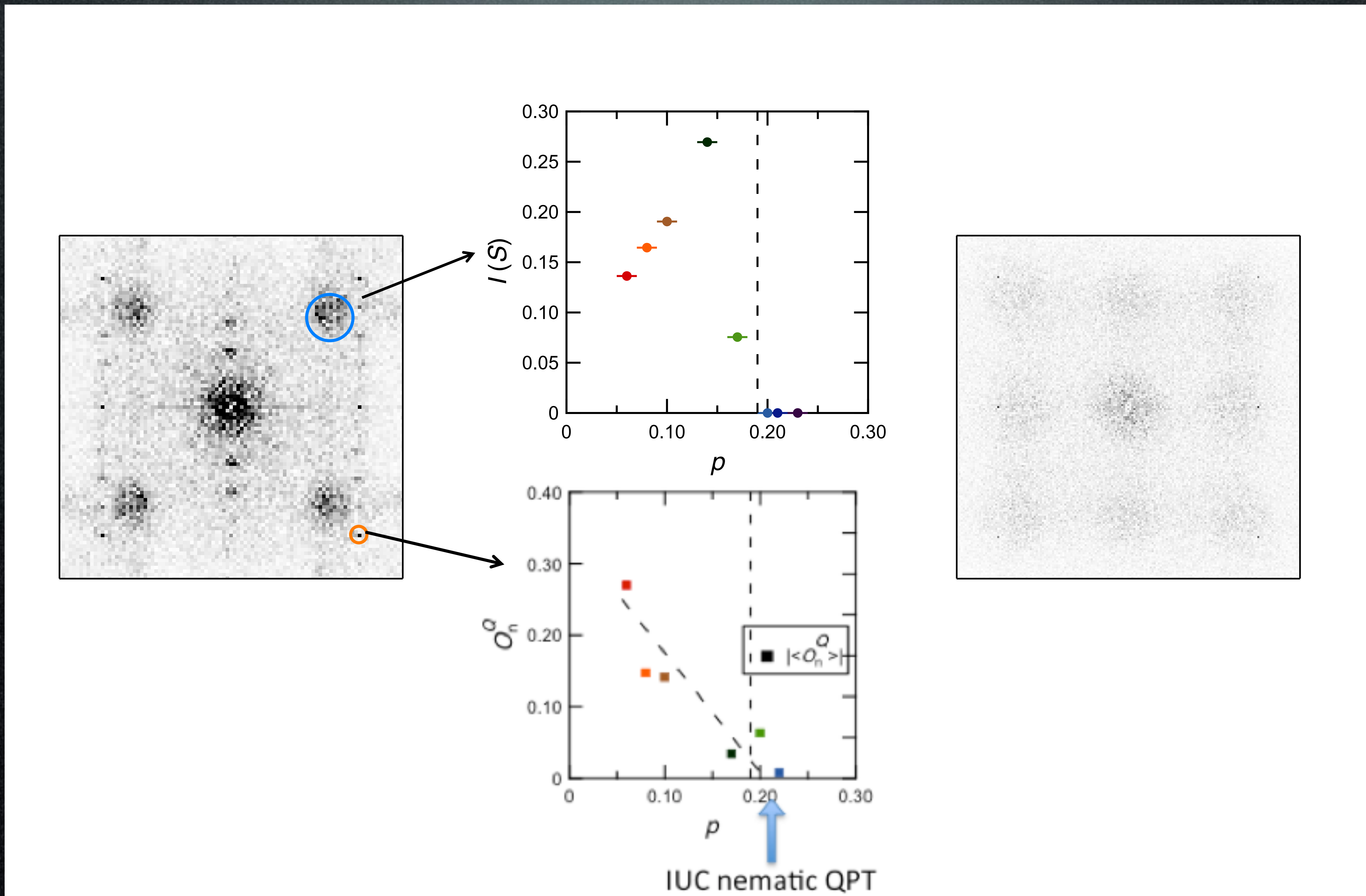


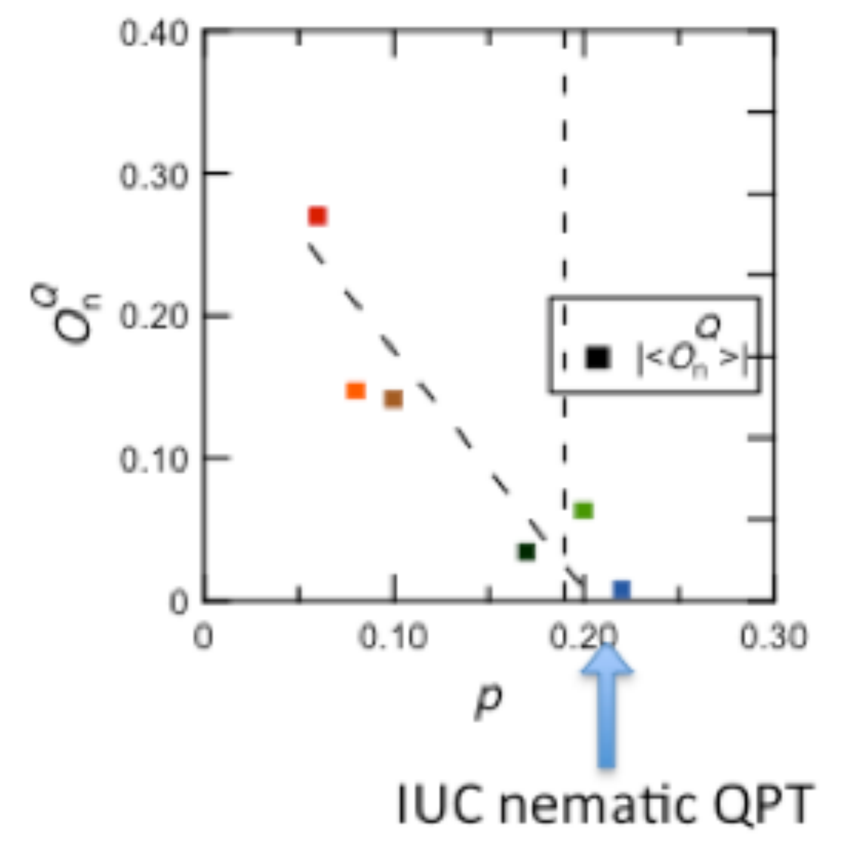
K. Fujita et al, Science (2014)

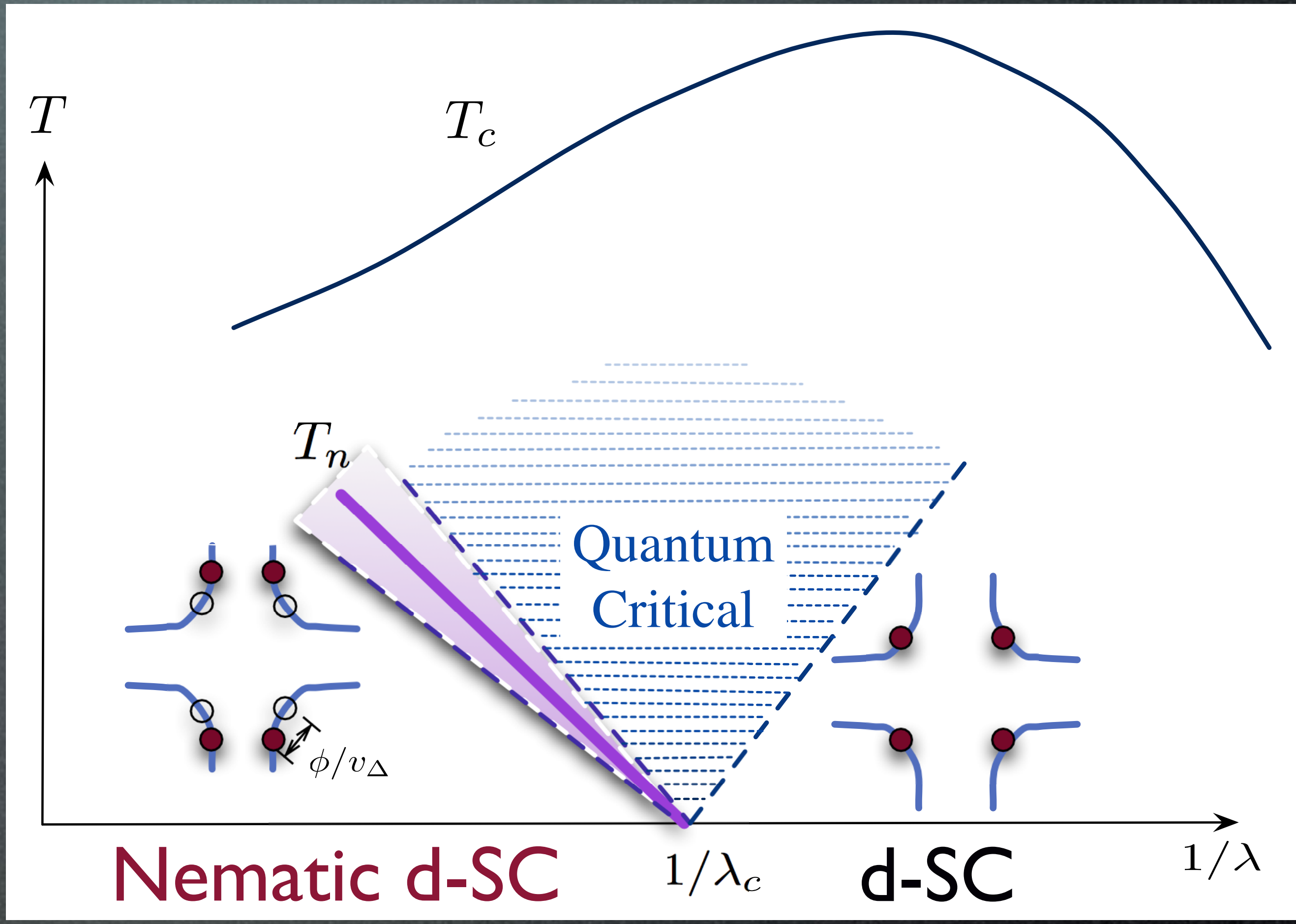
Doping Dependence of Q=0 and Q≠0 Symmetry Breaking



K. Fujita et al, Science (2014)

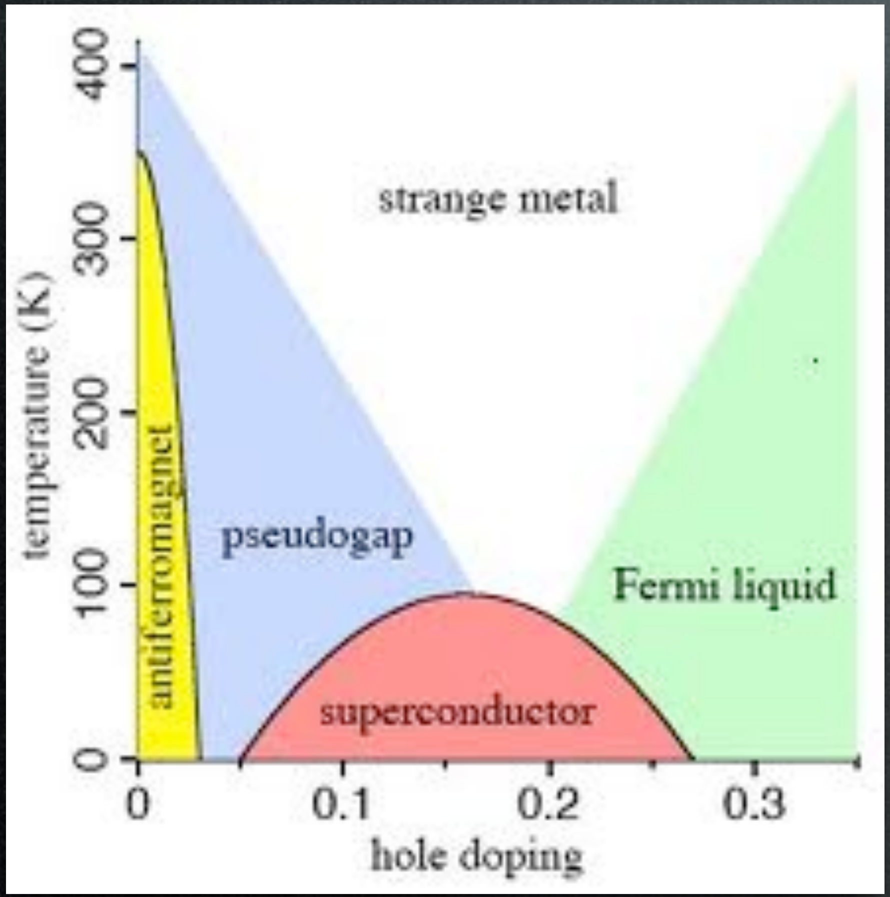
Earlier study of Nematic quantum criticality





Kim et. al., PRB **77**, 184514 (2008)

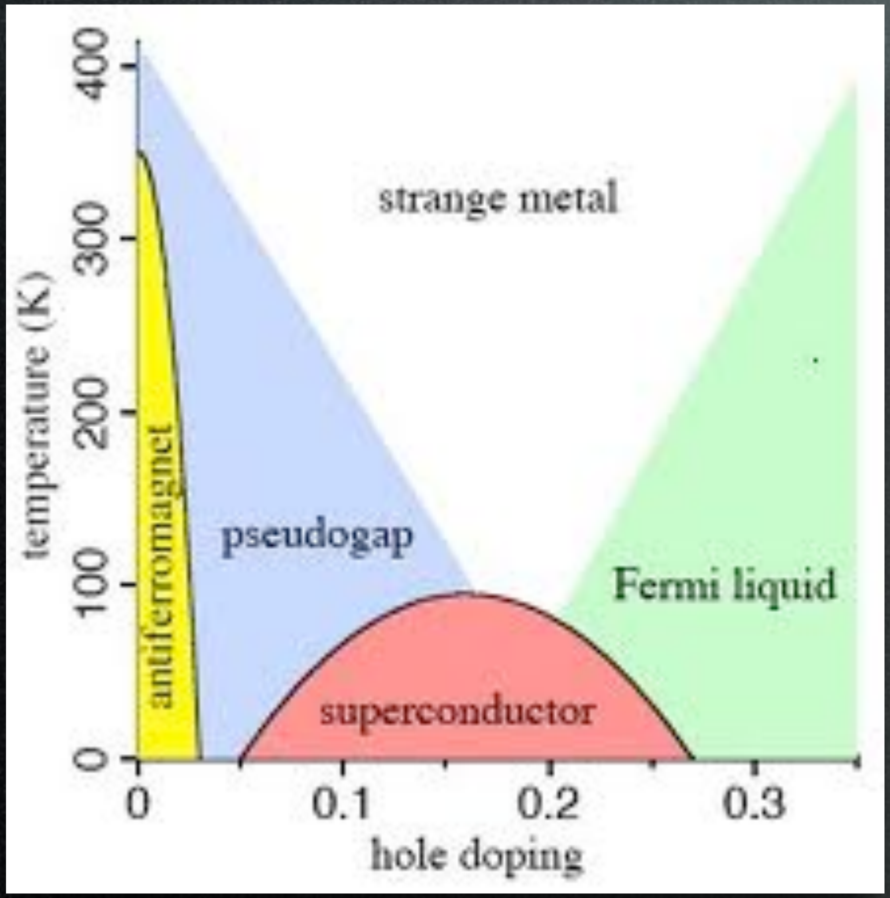
The Phase Diagram, summary



Lawler et al, Nature 2010
Fujita et al, Science 2014

The Phase Diagram, summary

- **Long-range IUC symmetry breaking** in STM data of pseudogap states



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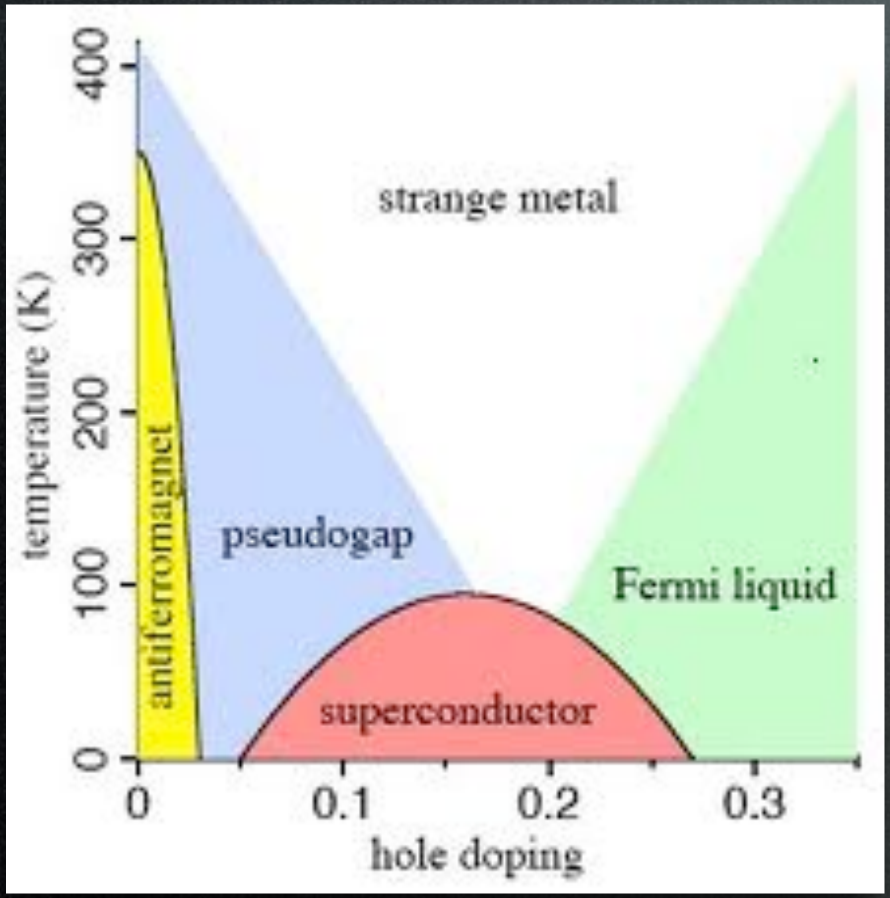

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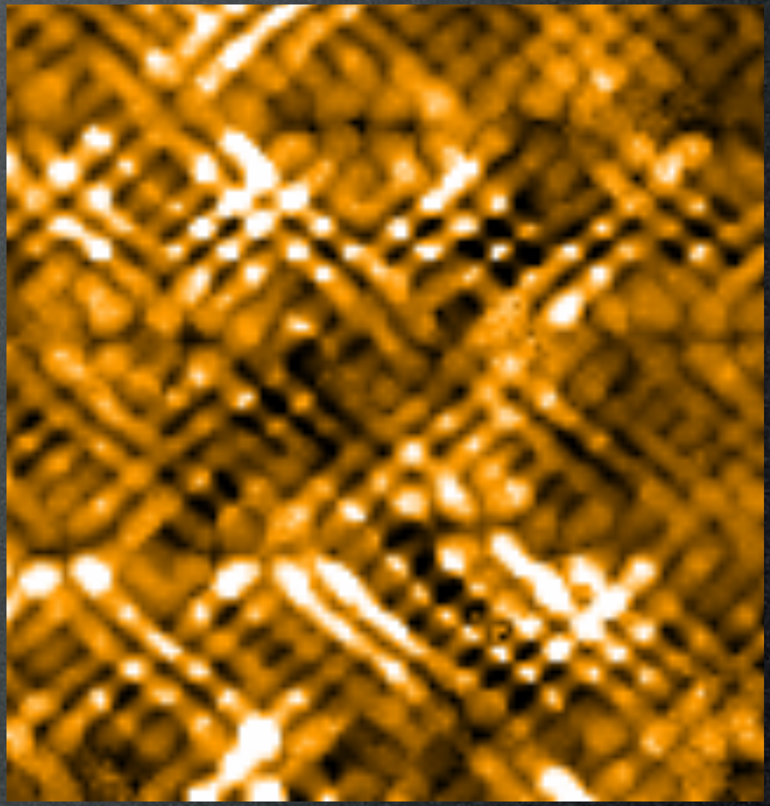

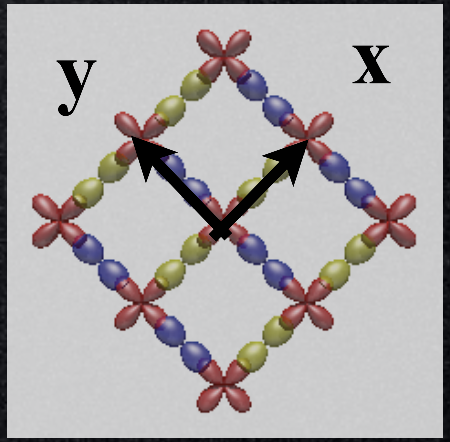

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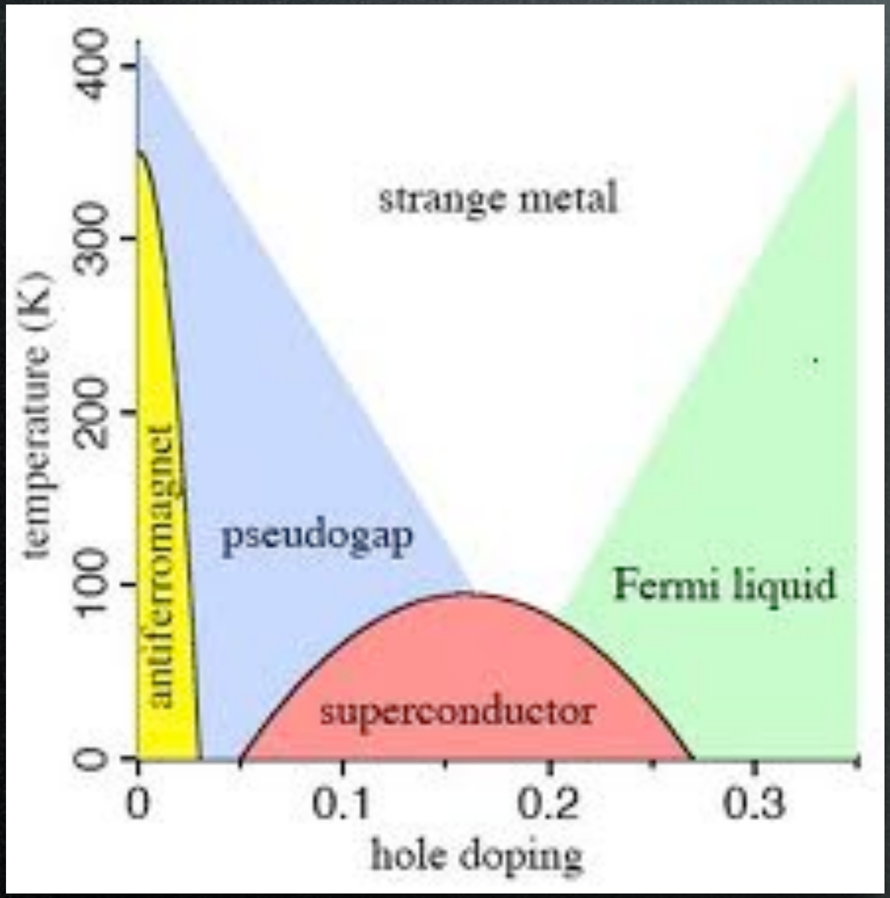

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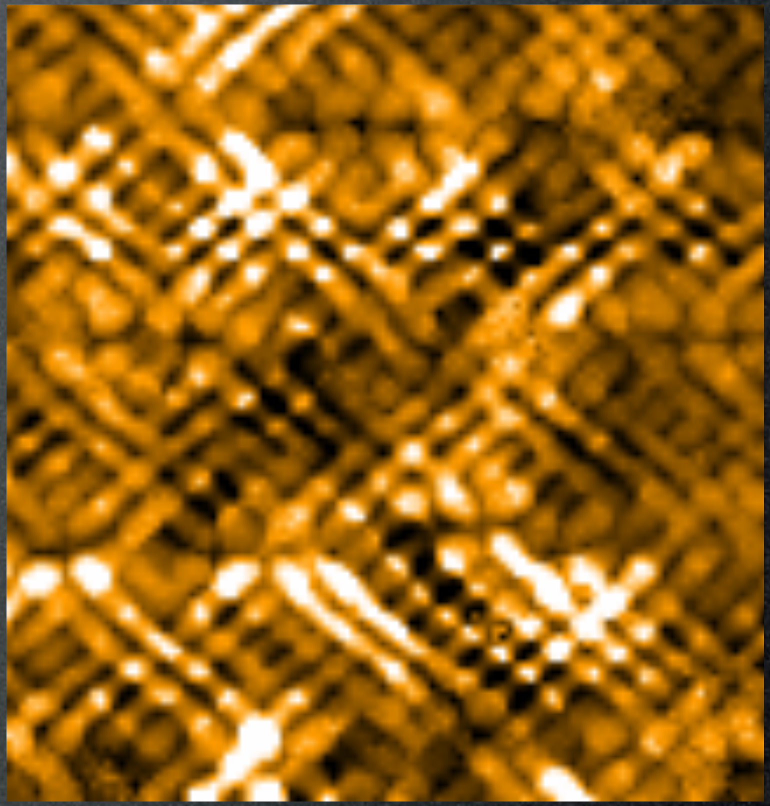

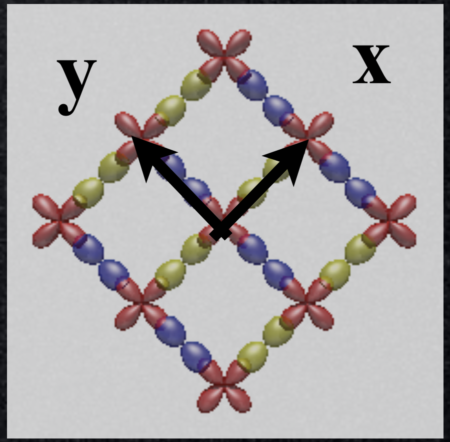

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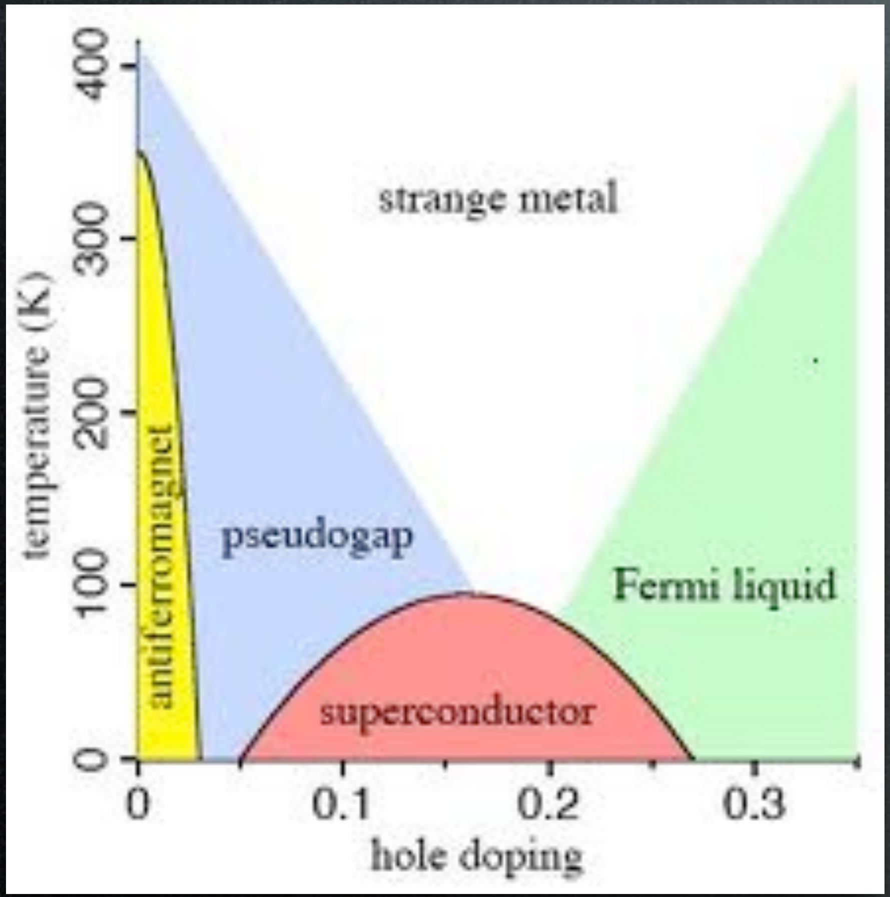

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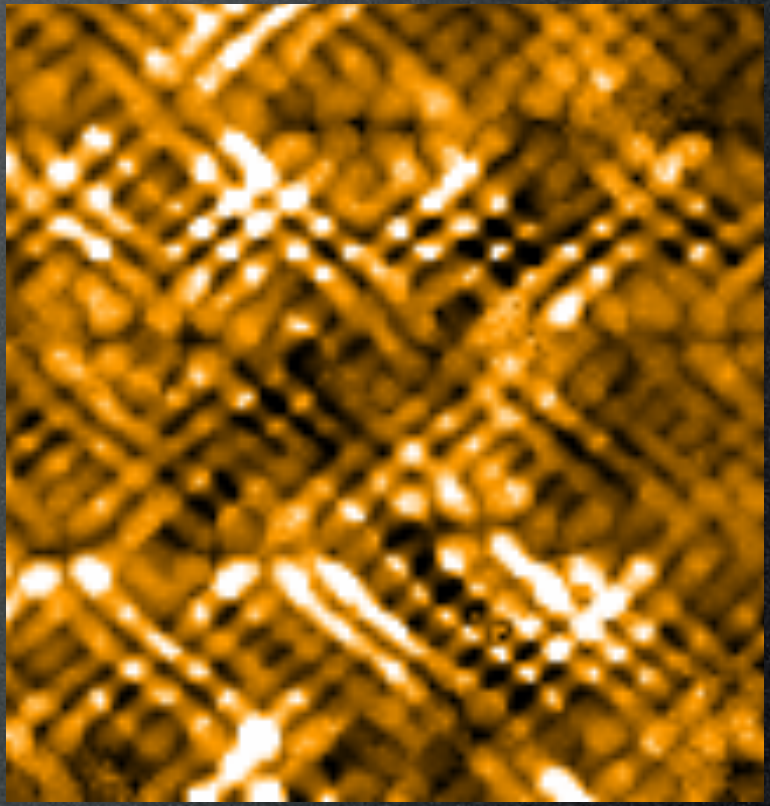

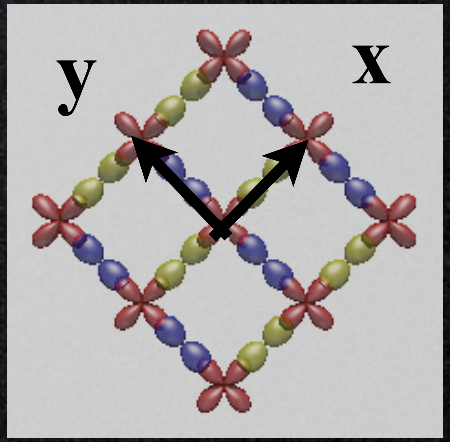

Lawler et al, Nature 2010
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➡ **Nematic QCP**

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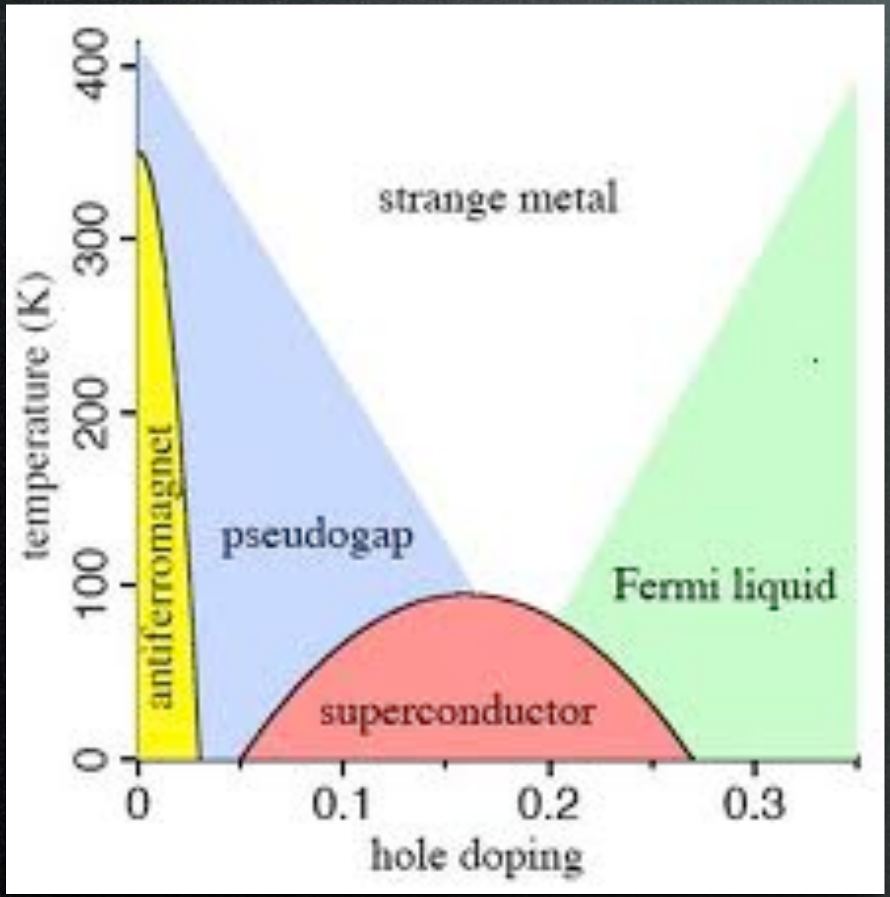

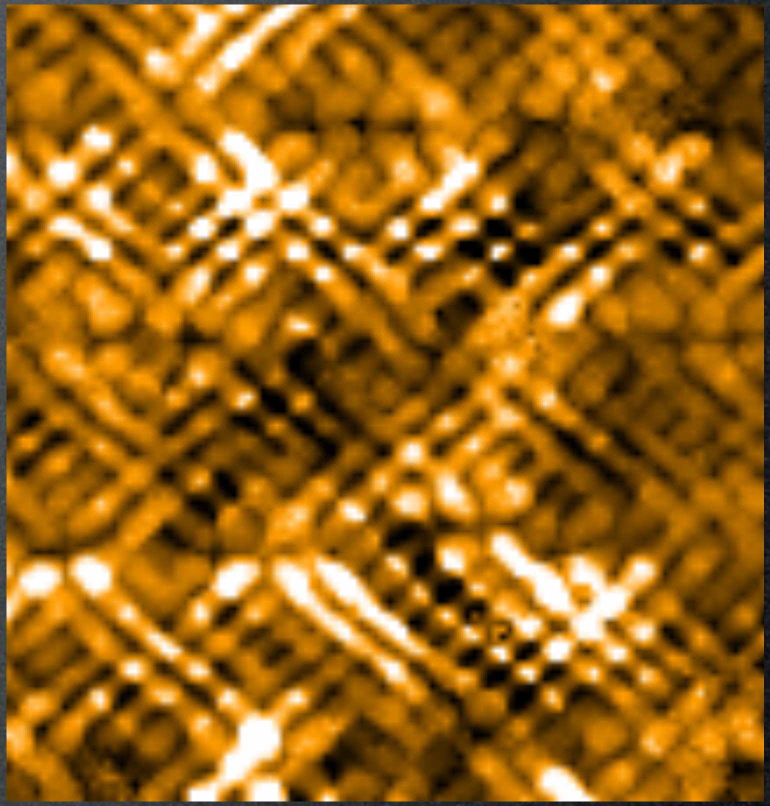

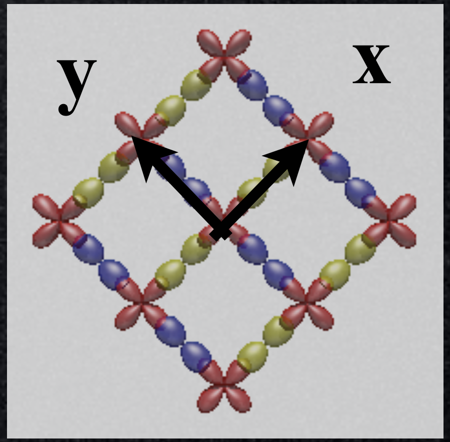

Lawler et al, Nature 2010
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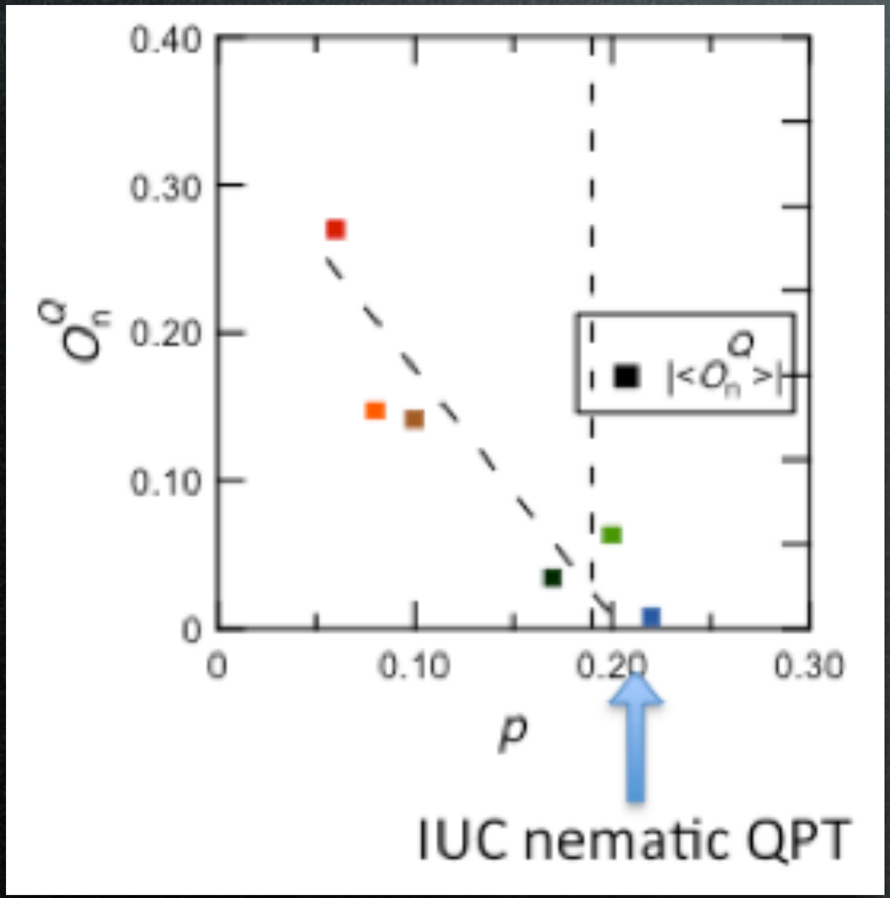

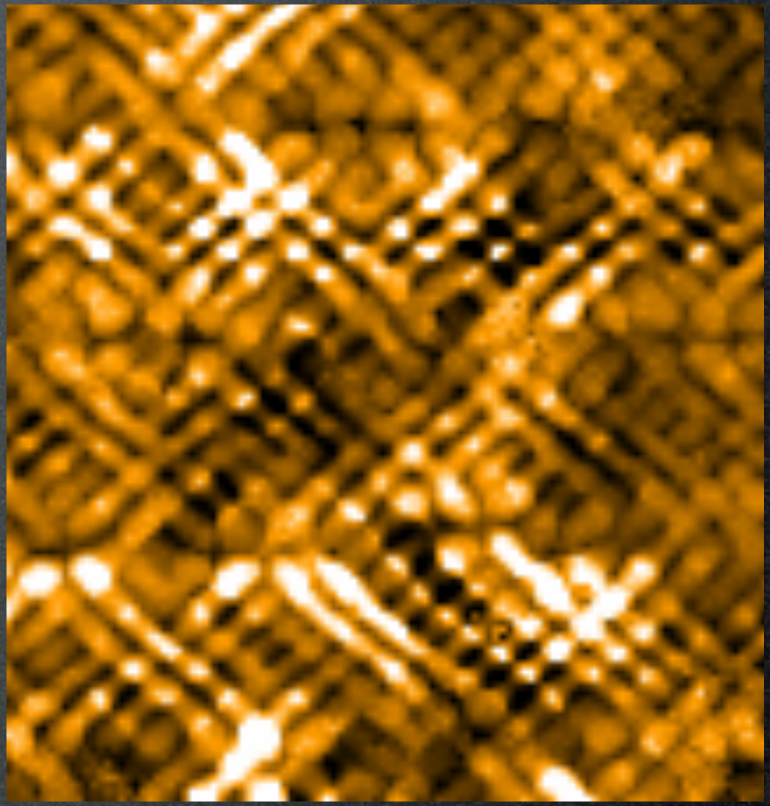

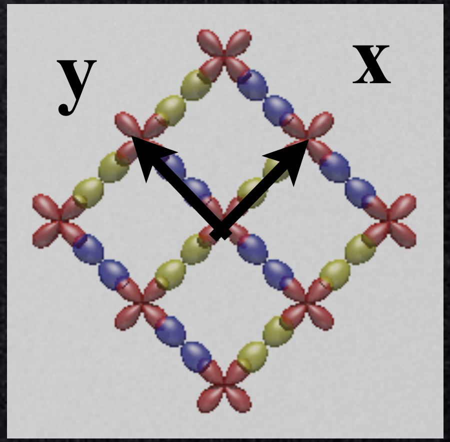

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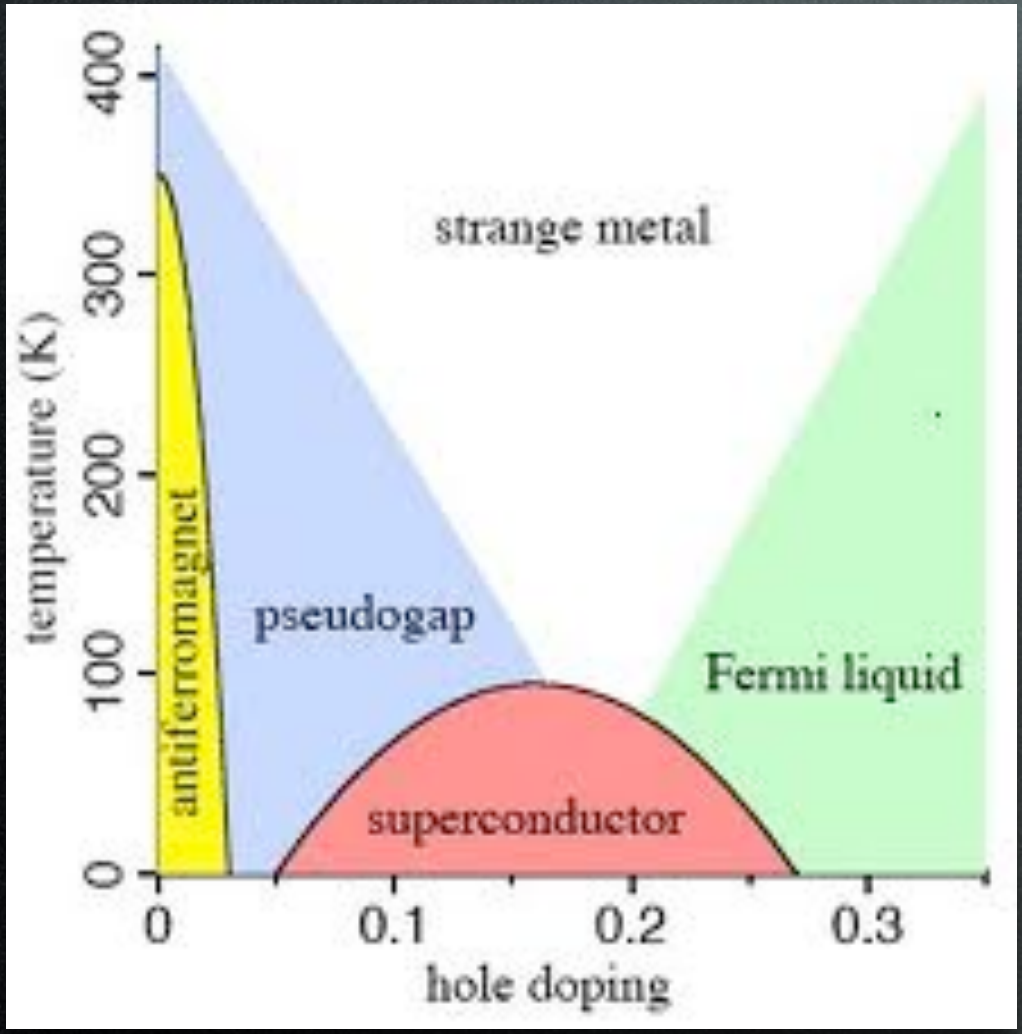
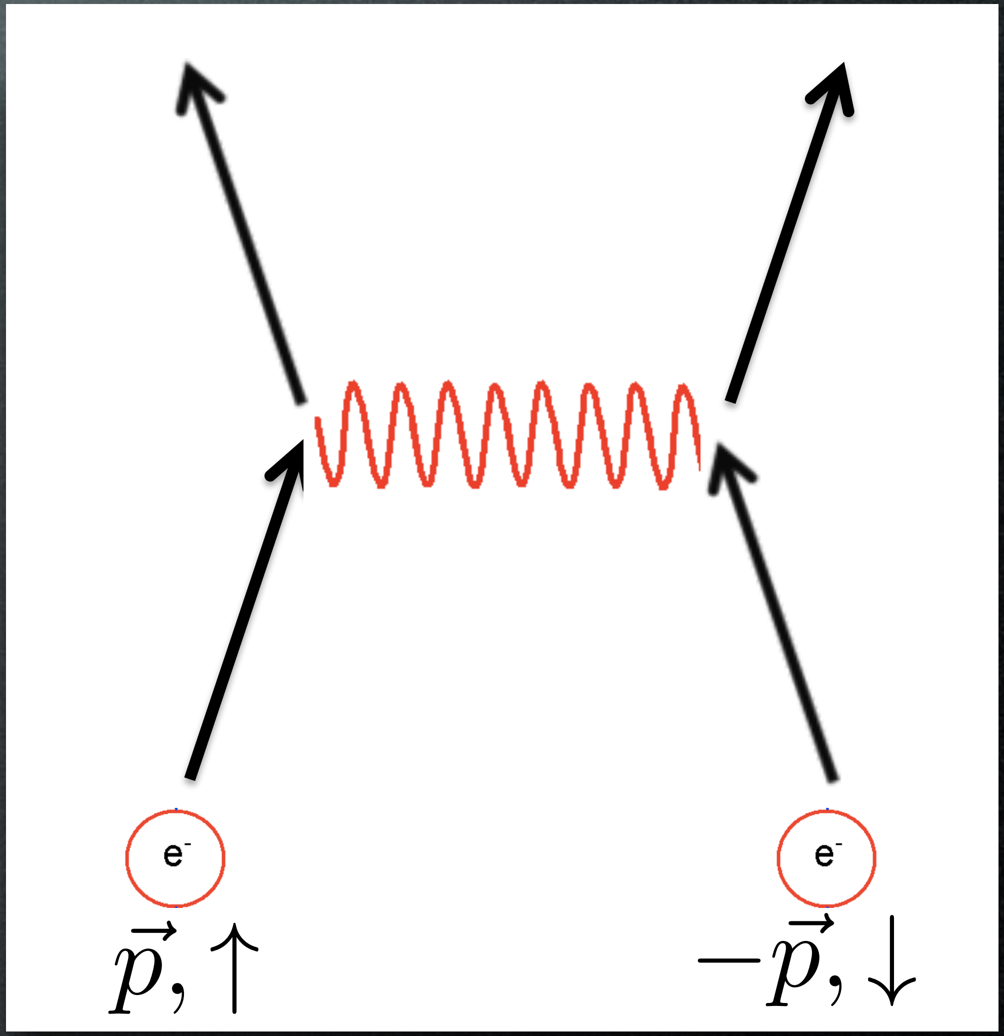
Key Questions in High-T_c Superconductivity:

The Phase Diagram?

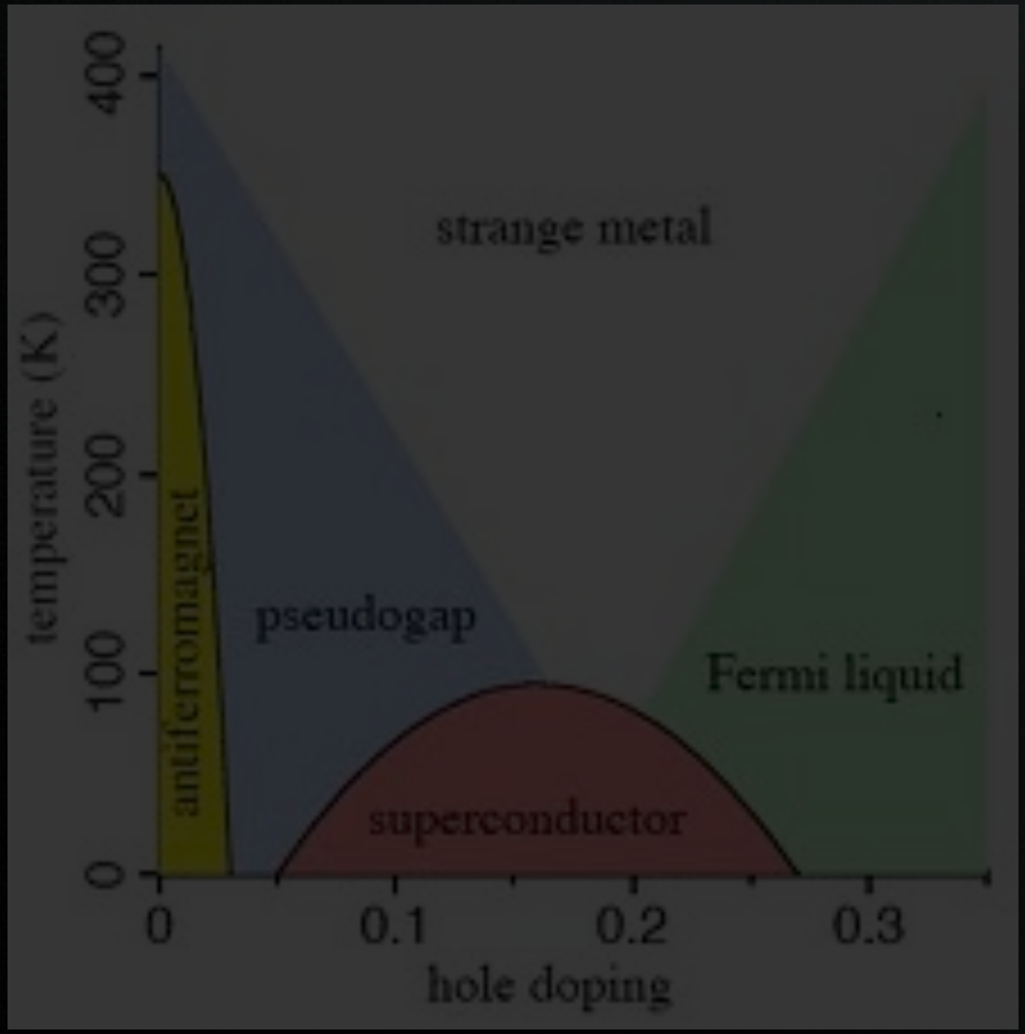


The Mechanism?

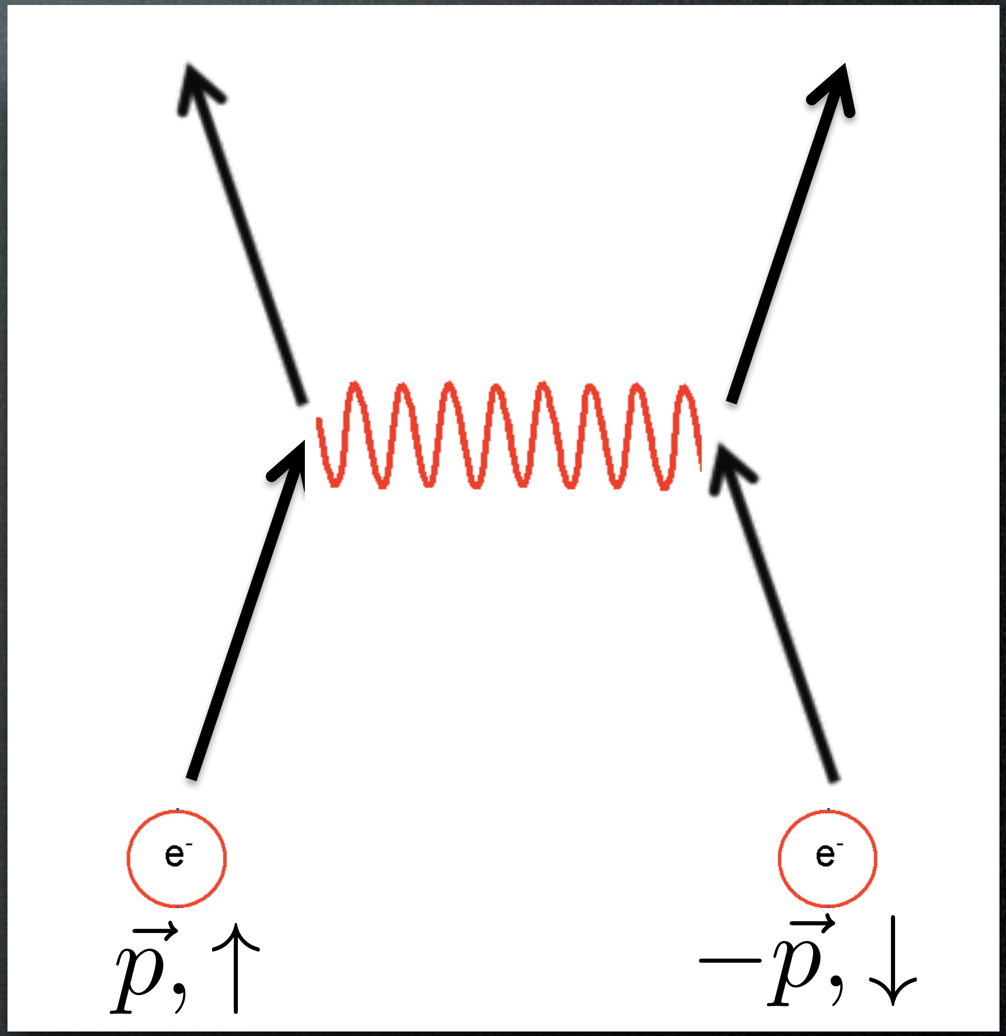


Key Questions in High-T_c Superconductivity:

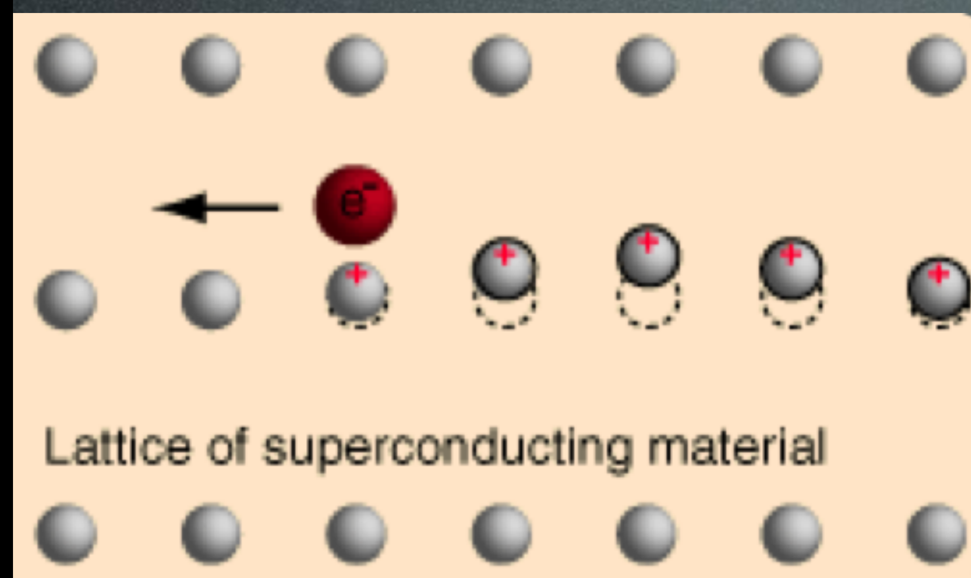
The Phase Diagram?



The Mechanism?



Electron-phonon coupling in BCS-SC?



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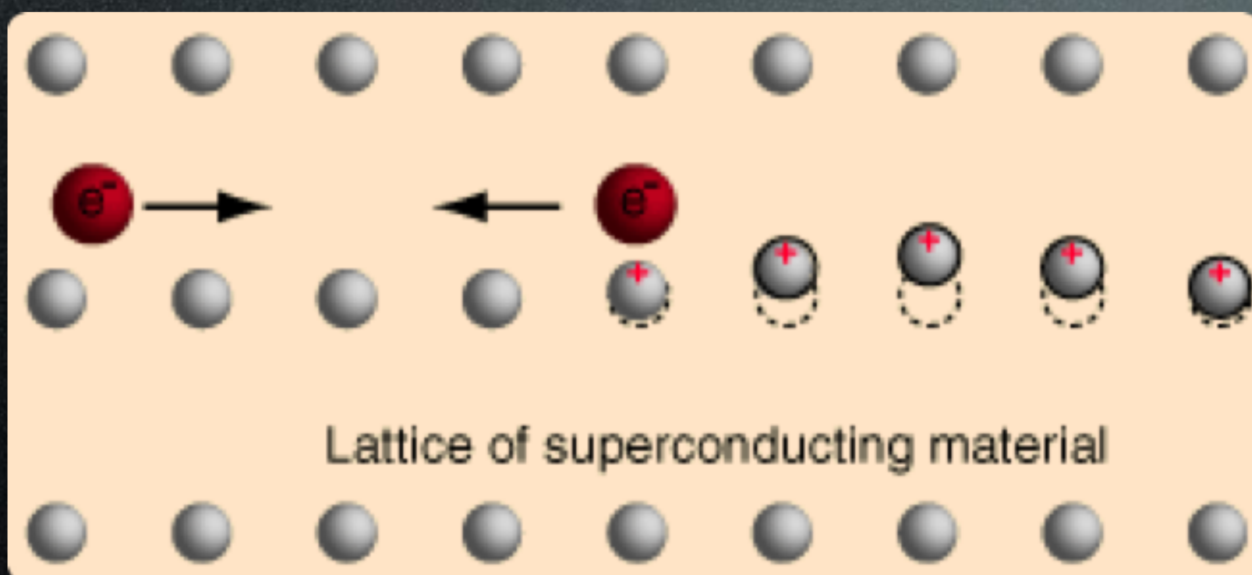

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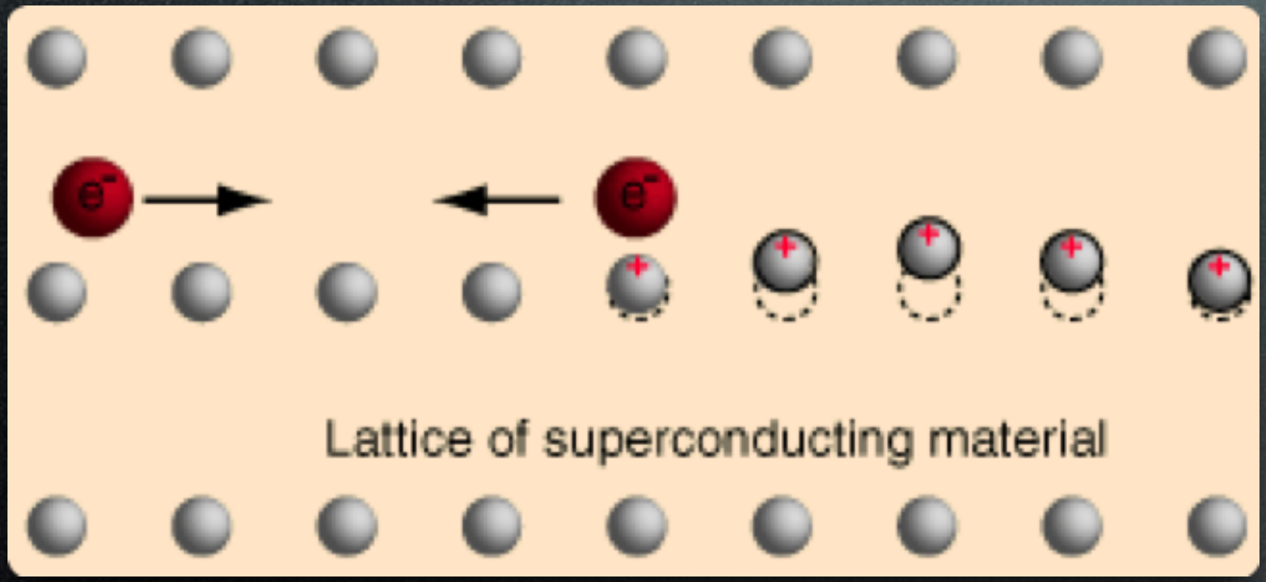
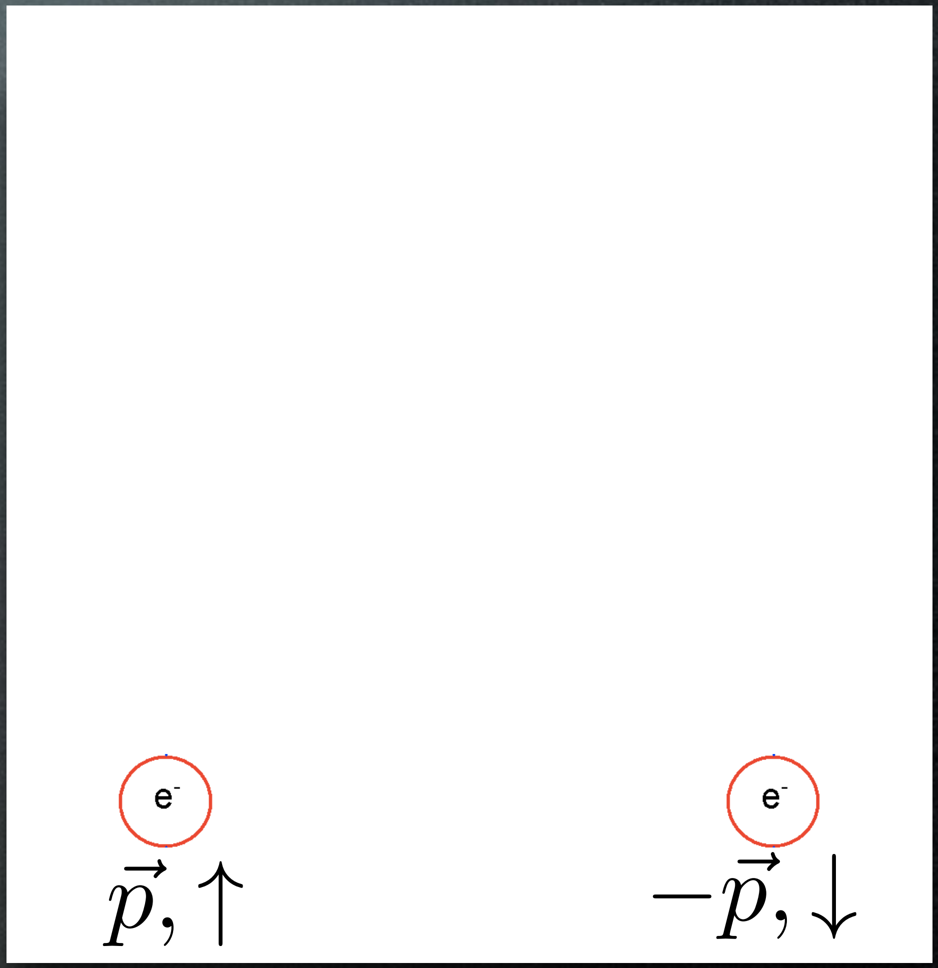
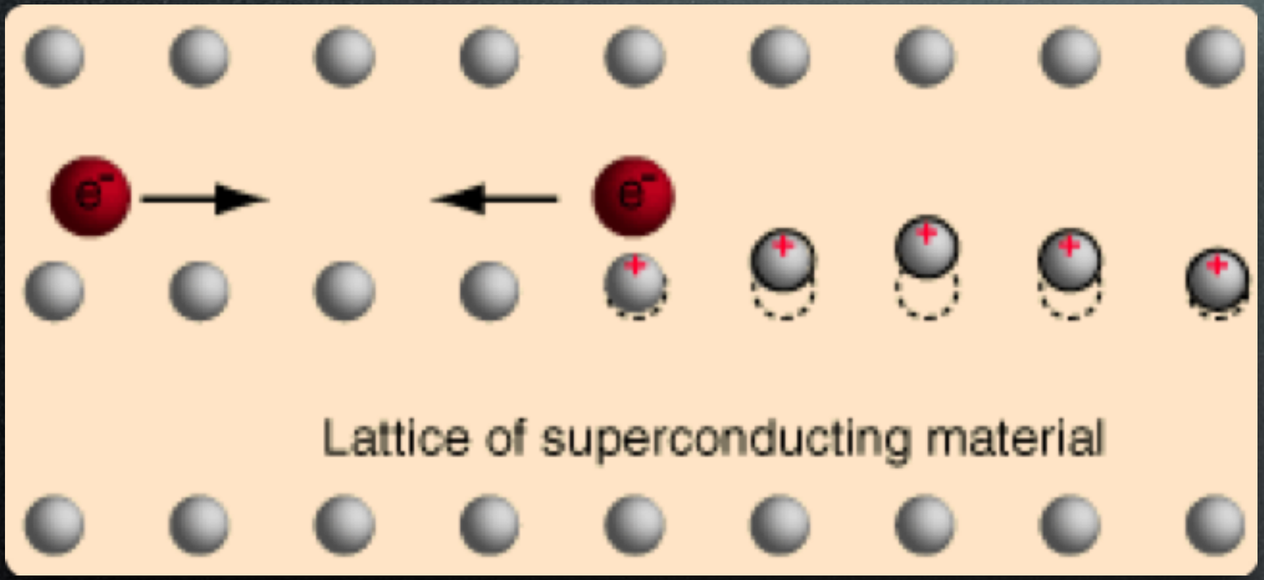
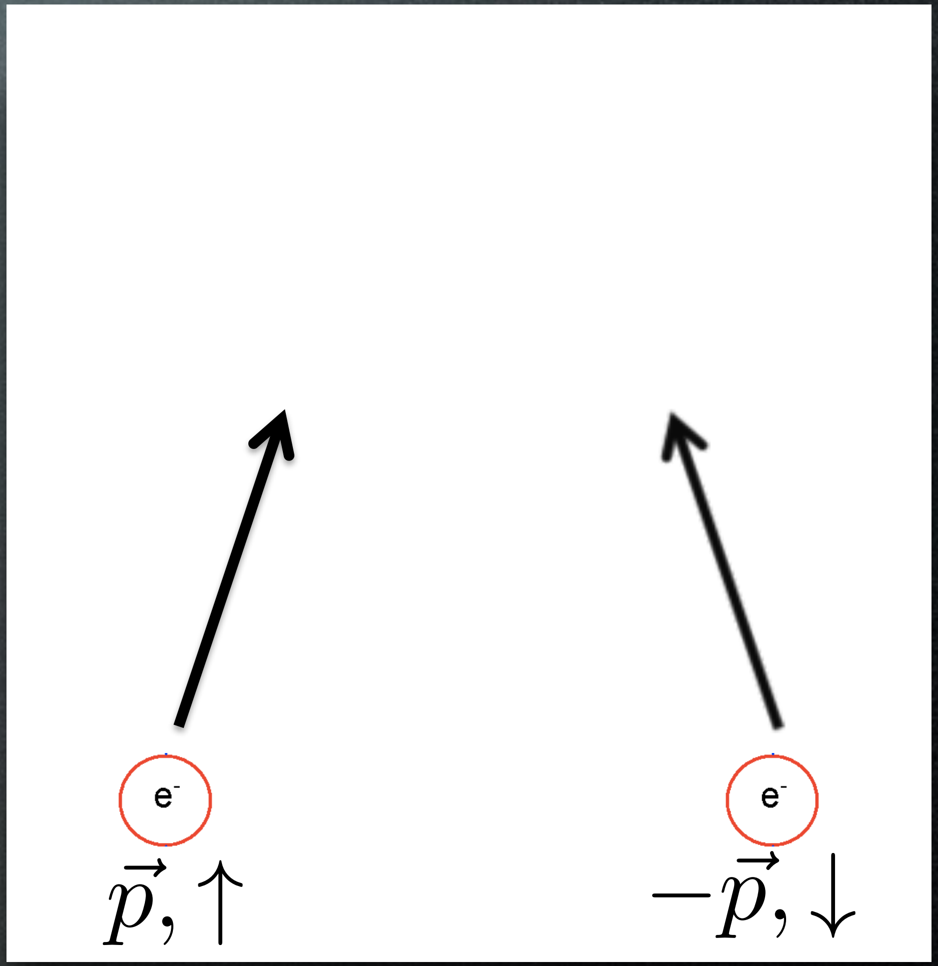


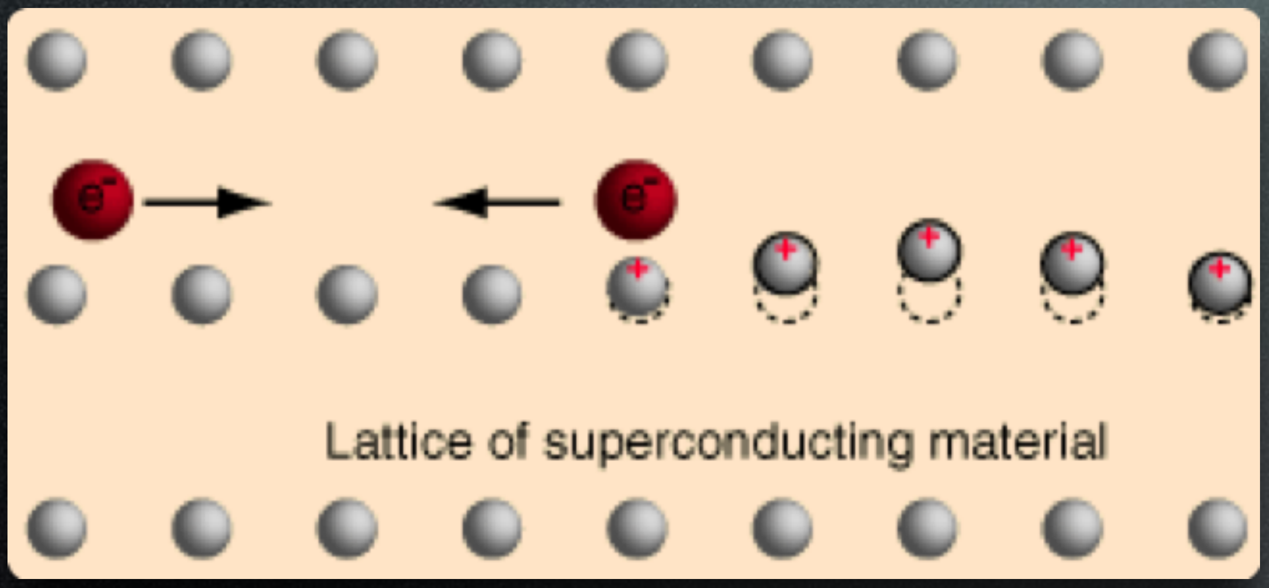


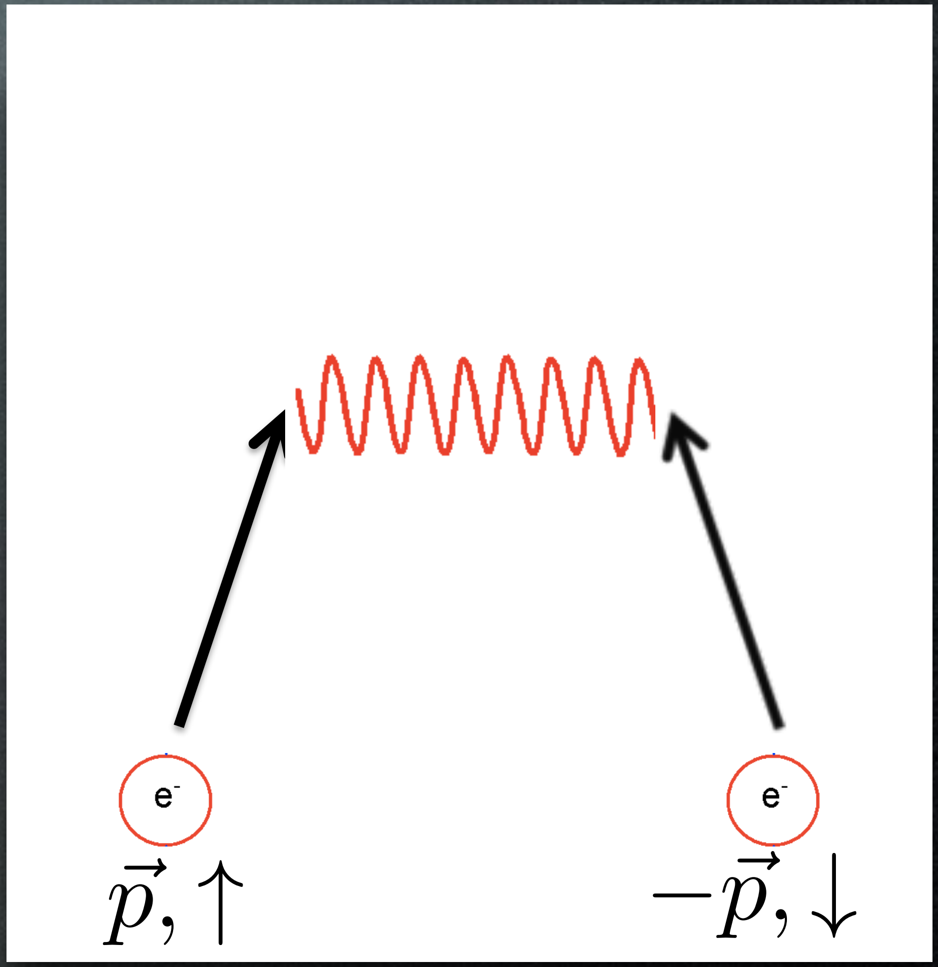
Electron-phonon coupling in BCS-SC?



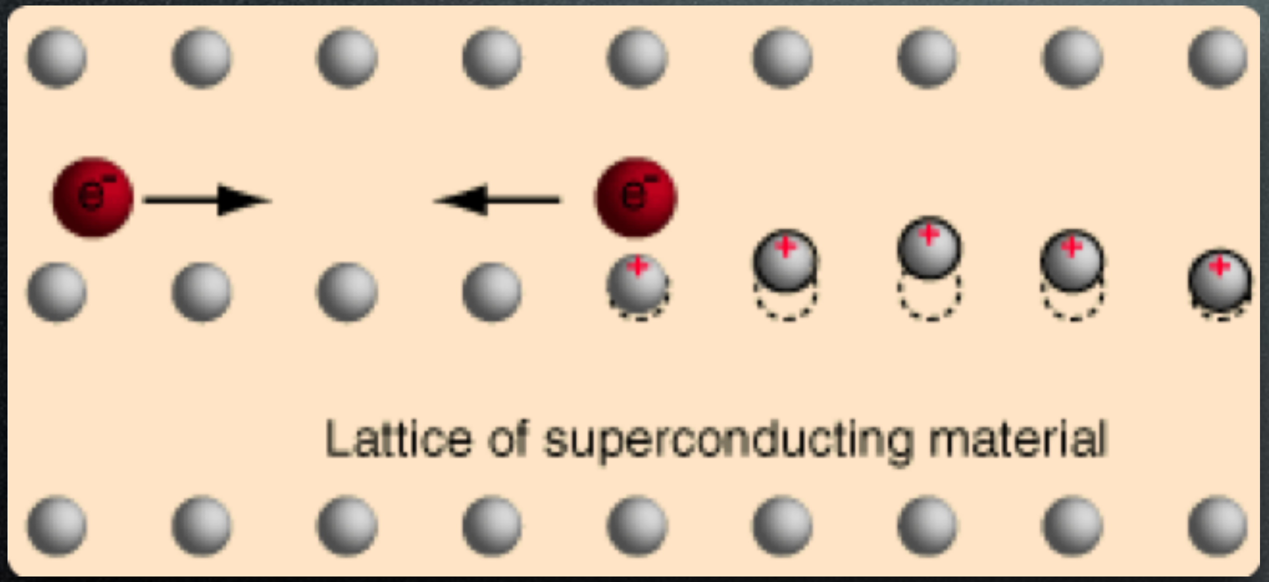


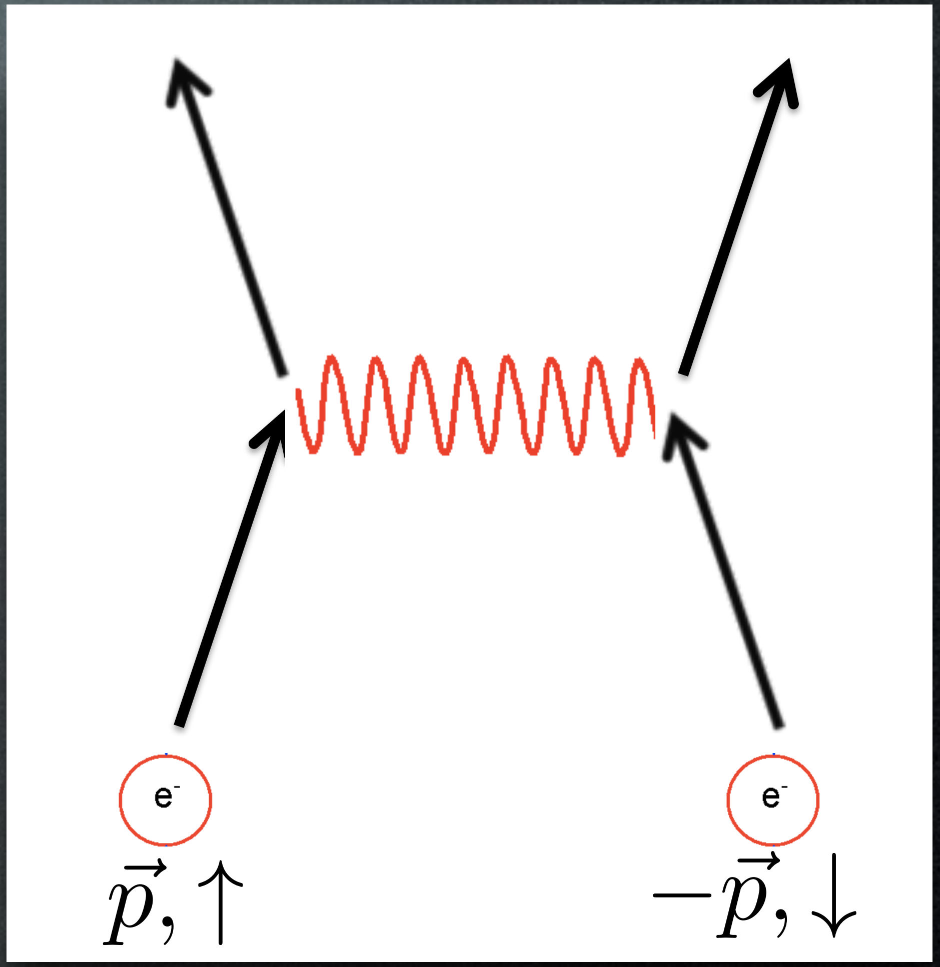
Electron-phonon coupling in BCS-SC?



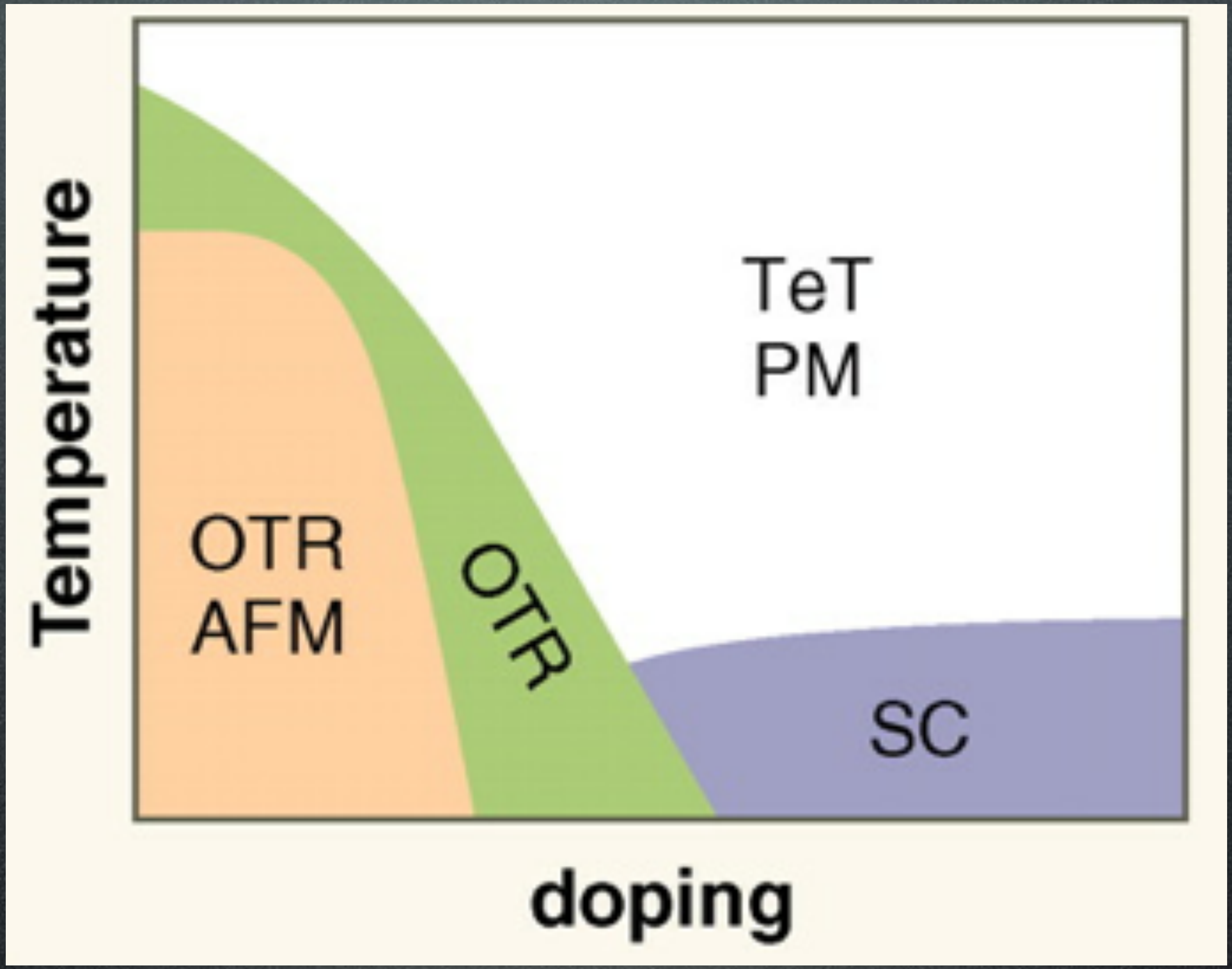


Electron-phonon coupling in BCS-SC?





Pairing Mechanism of FeSC?

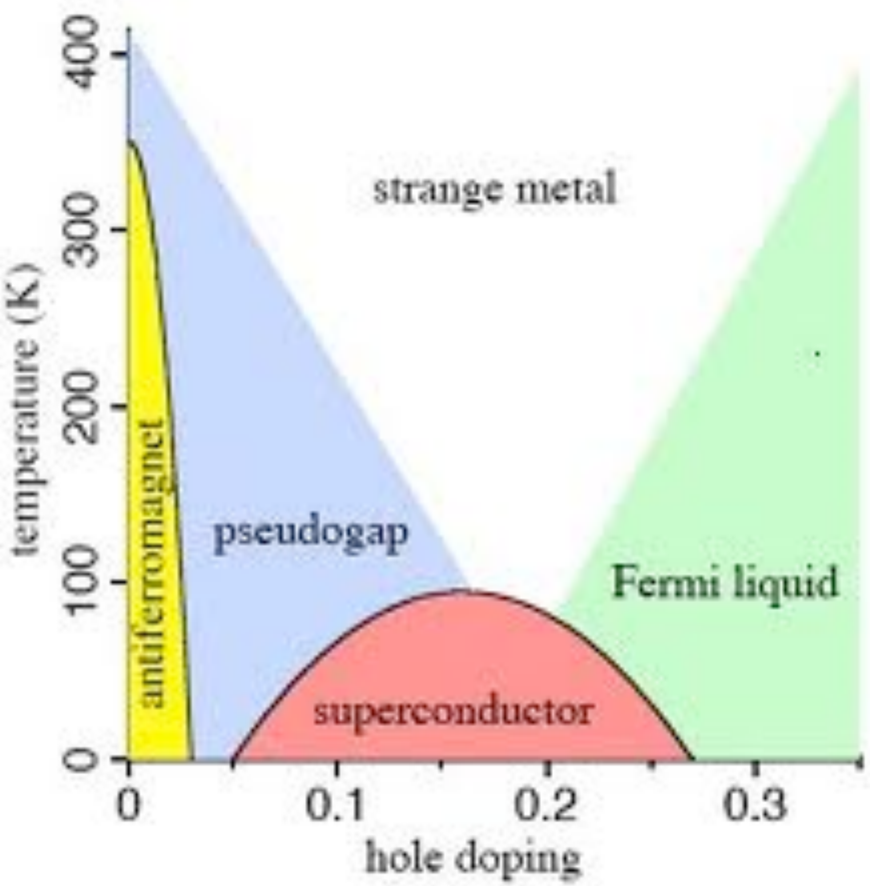


Wang & Lee, 2011

- Structural / magnetic transition near SC
  ⇒ Is it boson-mediated superconductivity?

Copper-oxide vs Iron-pnictide

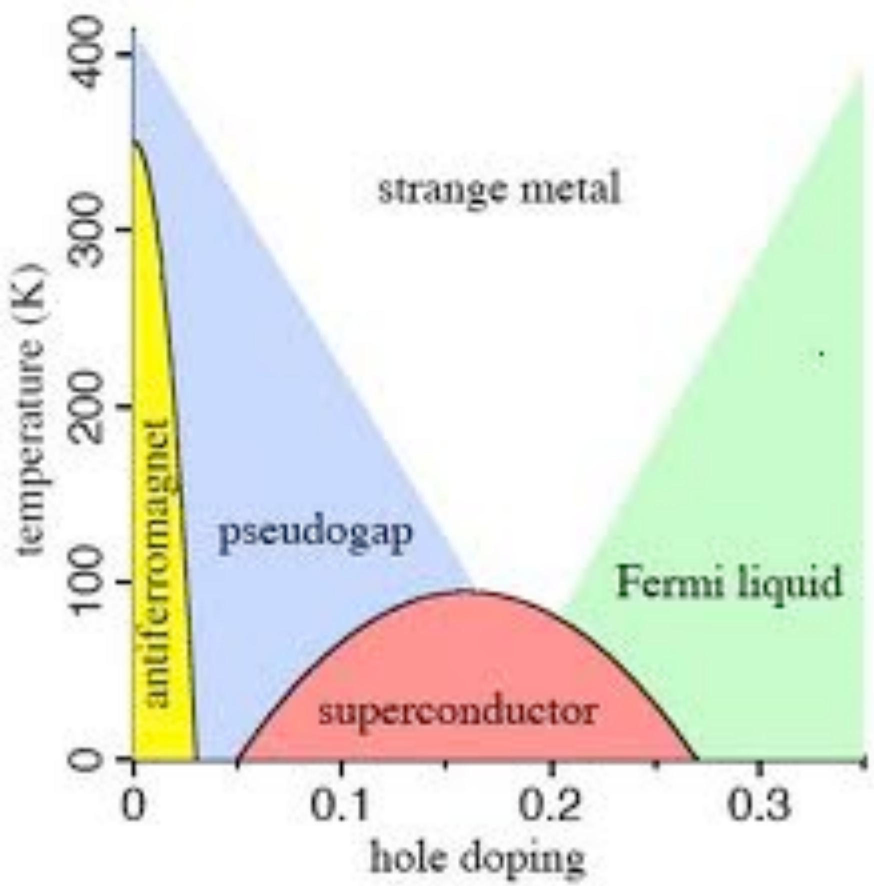
Copper-oxide
(d-wave)



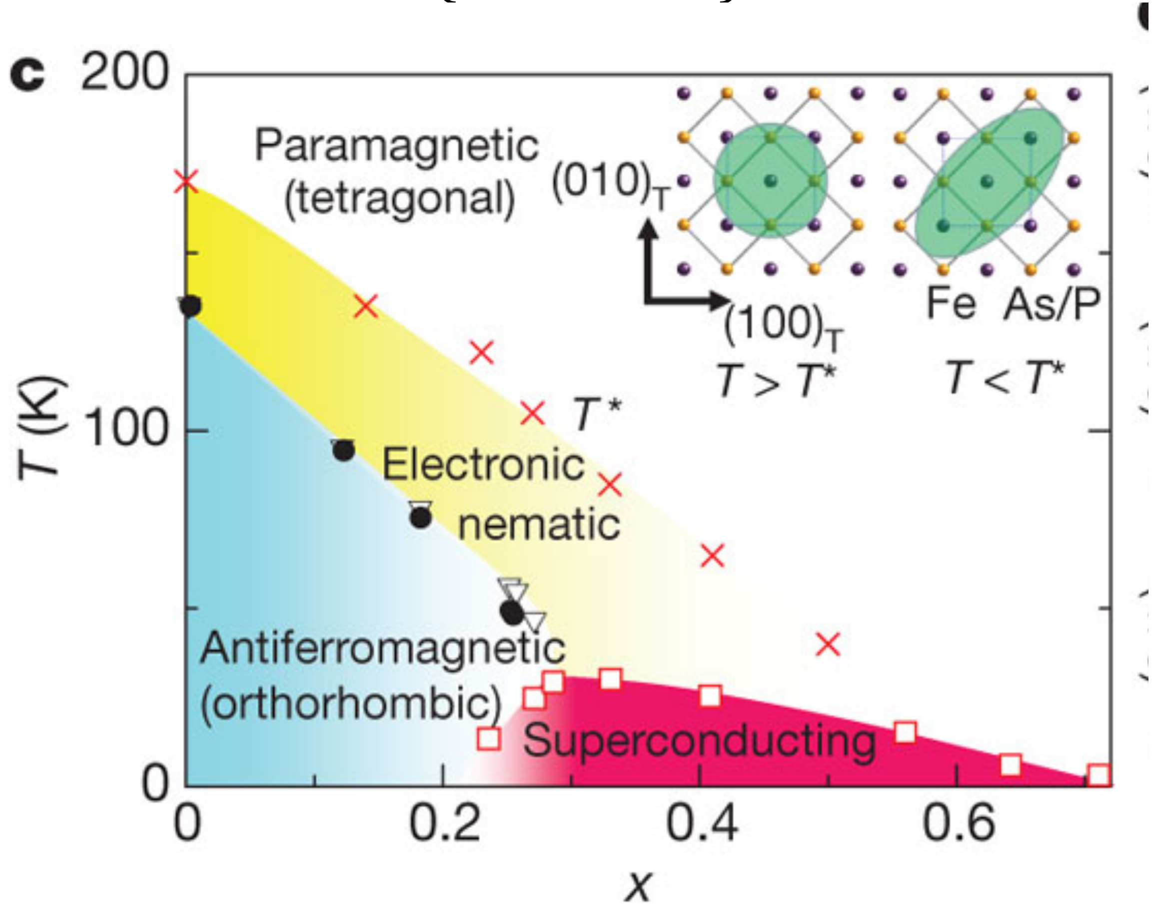
Iron-pnictide
(s±-wave?)

Copper-oxide vs Iron-pnictide

Copper-oxide
(d-wave)



Iron-pnictide
(s±-wave?)



Copper-oxide vs Iron-pnictide

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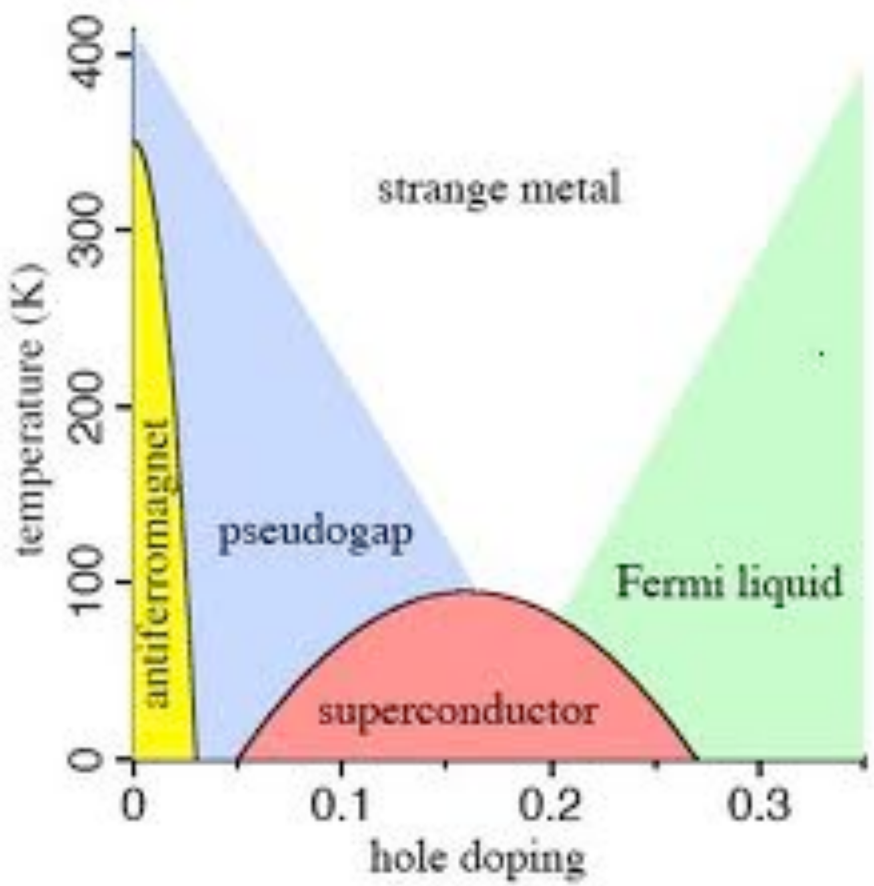

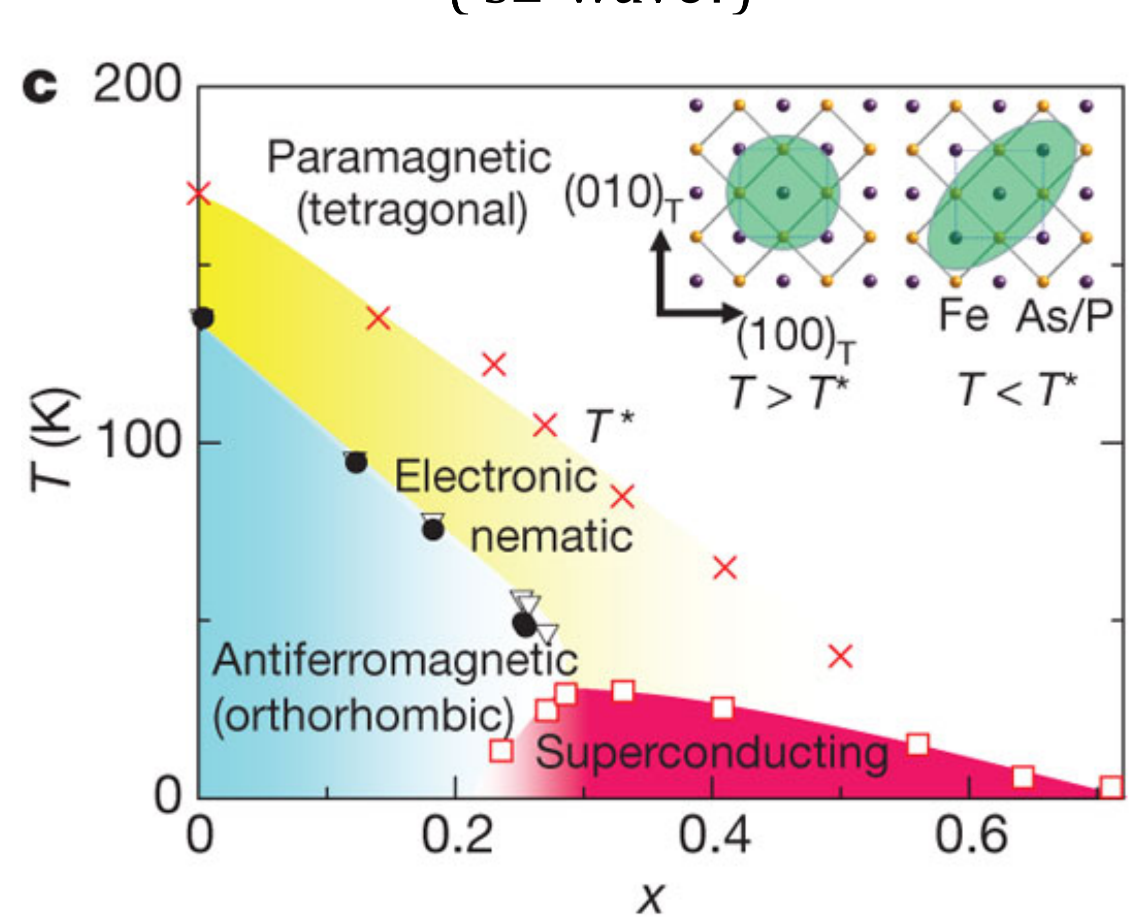

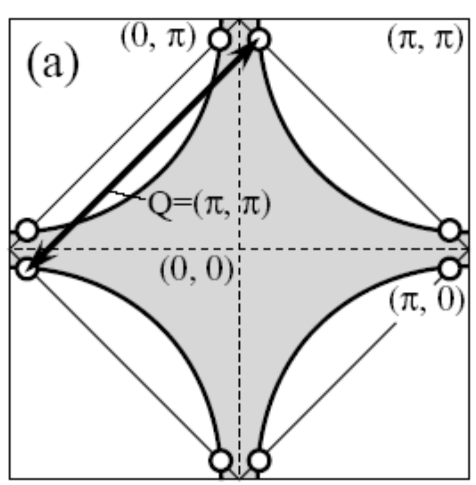

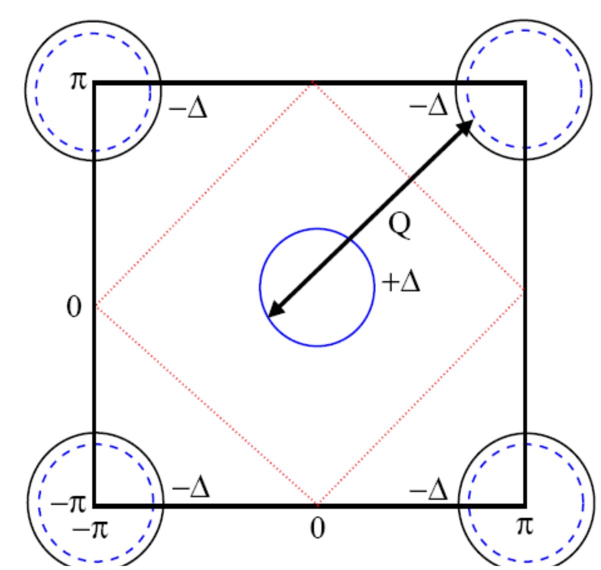

Copper-oxide vs Iron-pnictide

Copper-oxide
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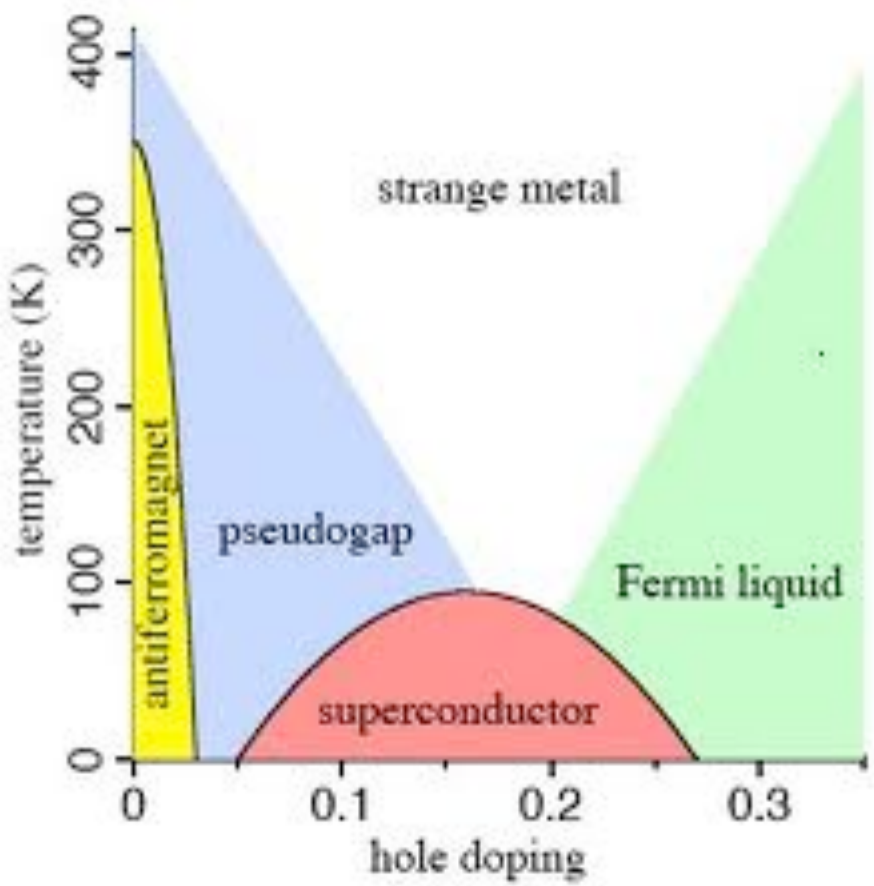
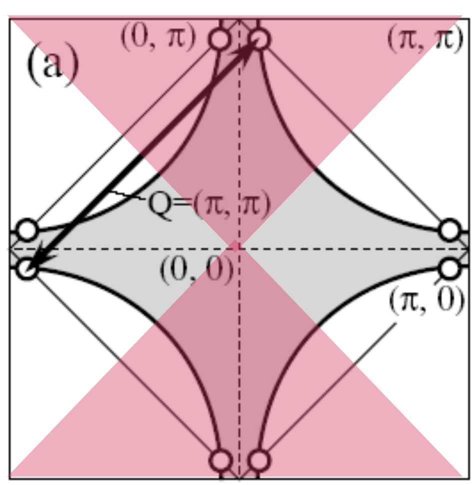
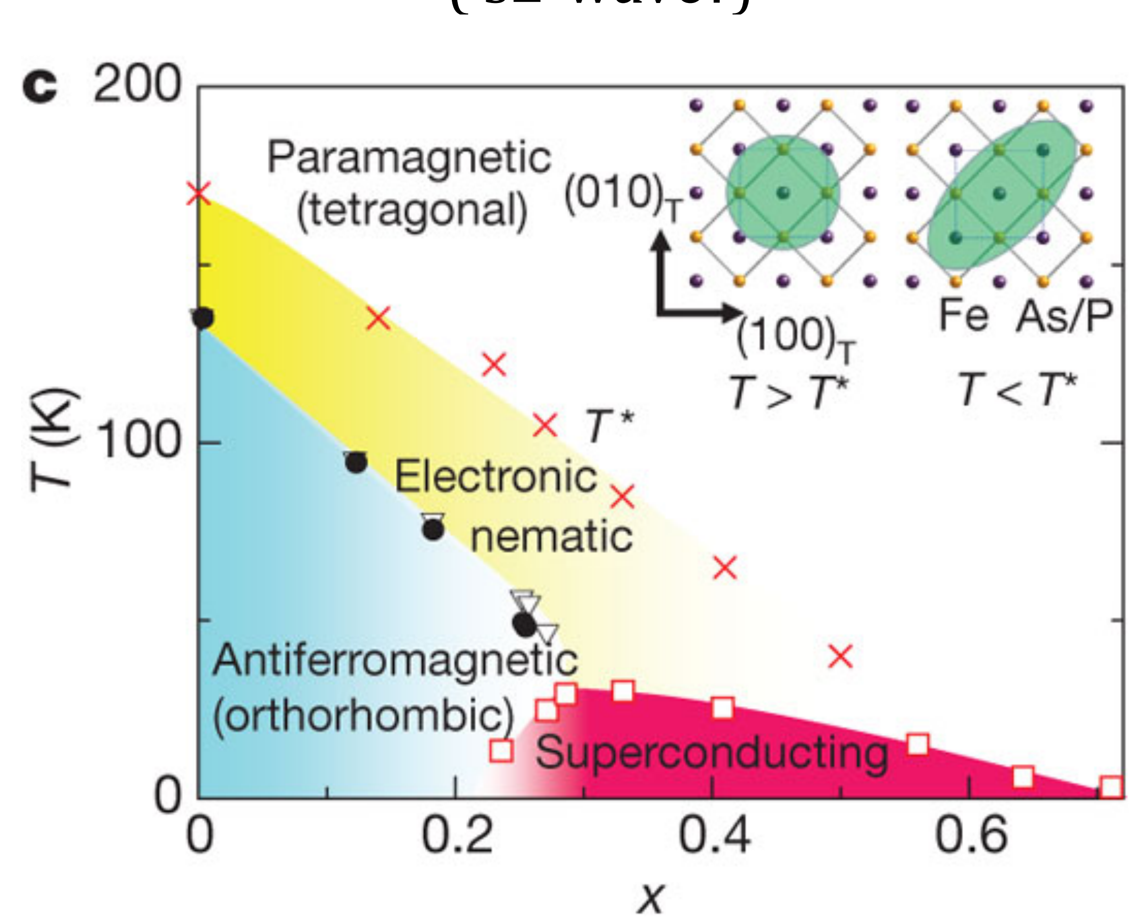
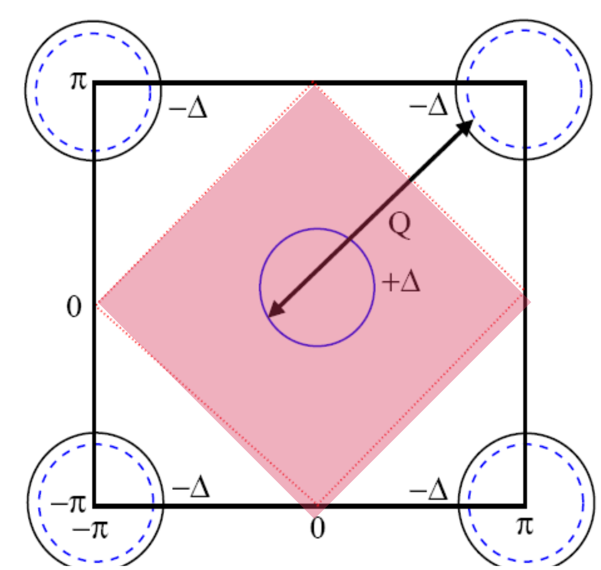




Iron-pnictide
(s±-wave?)





Three step approach

Three step approach

1. Identify suspects

Three step approach

1. Identify suspects
2. Gather evidence

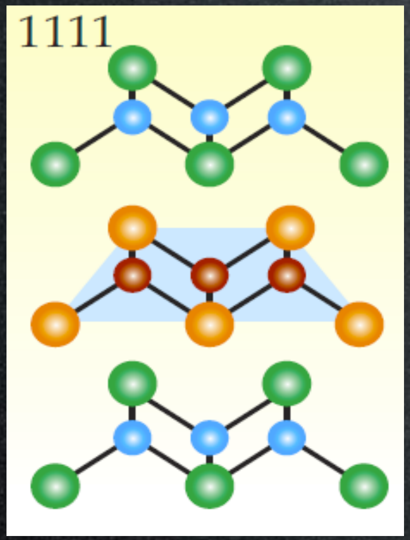
Three step approach

1. Identify suspects
2. Gather evidence
3. Match evidence to a suspect

LiFeAs

SmFeAsO

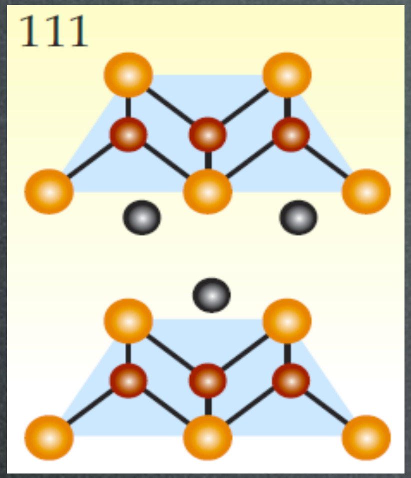
"1111"



Highest T_C~56K

LiFeAs

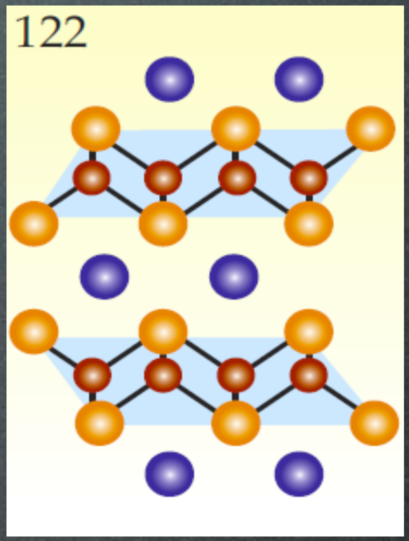
"111"



Highest T_C~18K

$BaFe_2As_2$

"122"

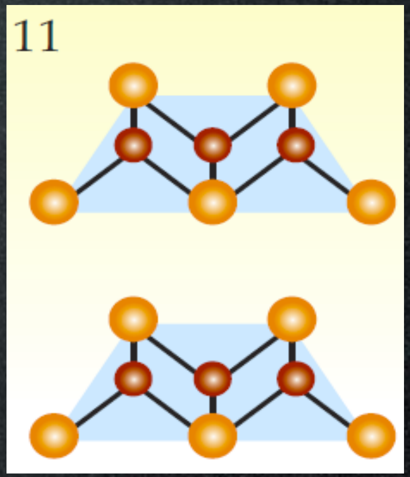


Highest T_C~38K

$Ca_{0.86}Pr_{0.14}Fe_2As_2$, T_C~45K

FeSe

"11"



Highest T_C~15K

T_C~36.7K at 8.9GPa

Why LiFeAs?

Why LiFeAs?

- Neutral cleave plane

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- Detailed knowledge of electronic structure

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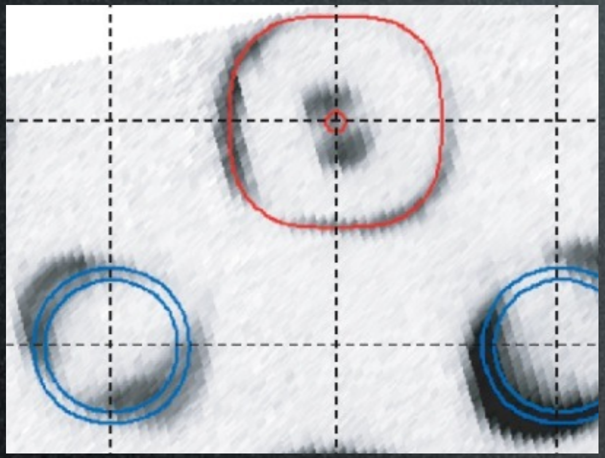

ARPES
Knolle *et al.* 2012

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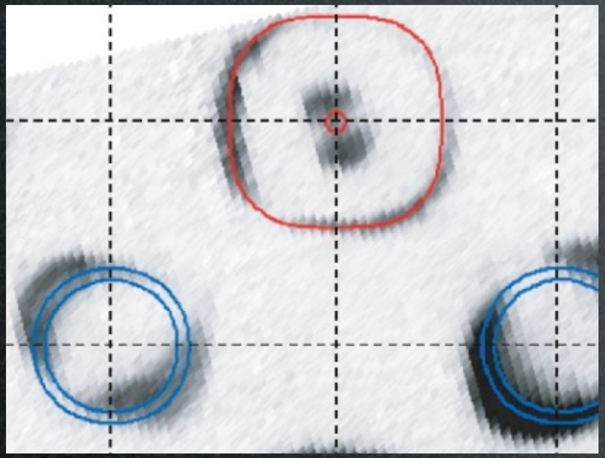

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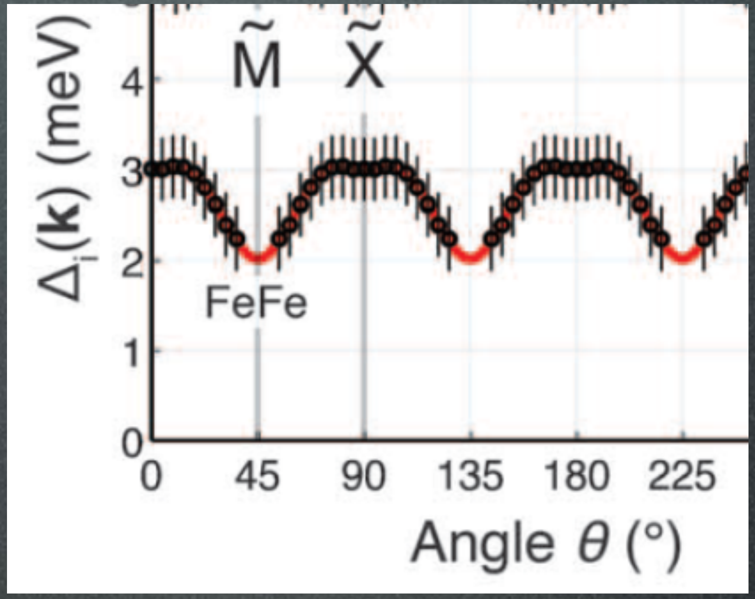

STM
Allan & Rost *et al.* 2012

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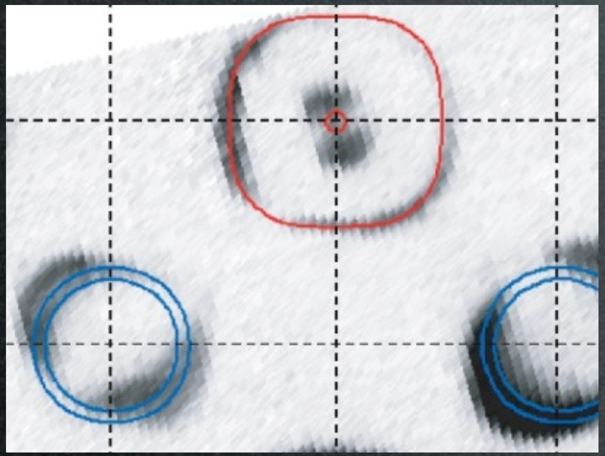

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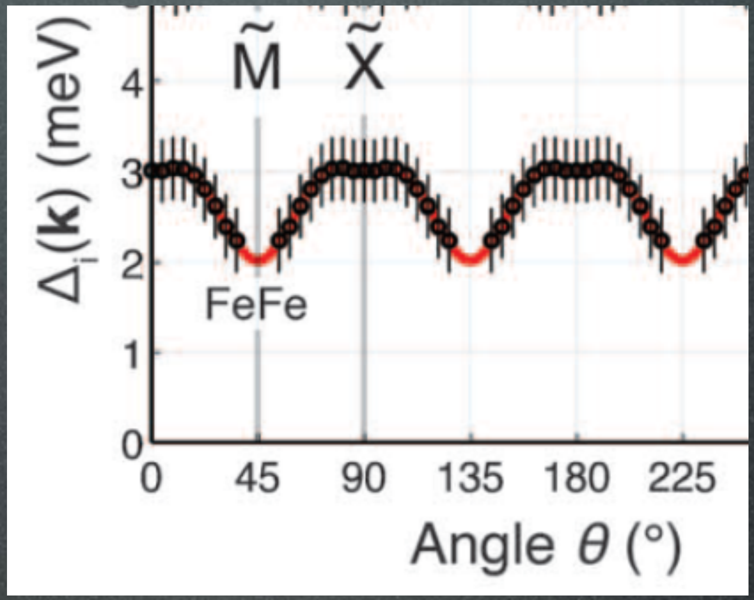

STM
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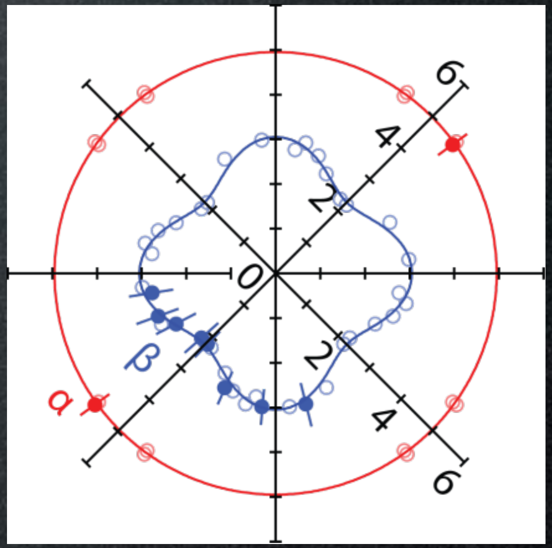

ARPES
Umezawa *et al.* 2012

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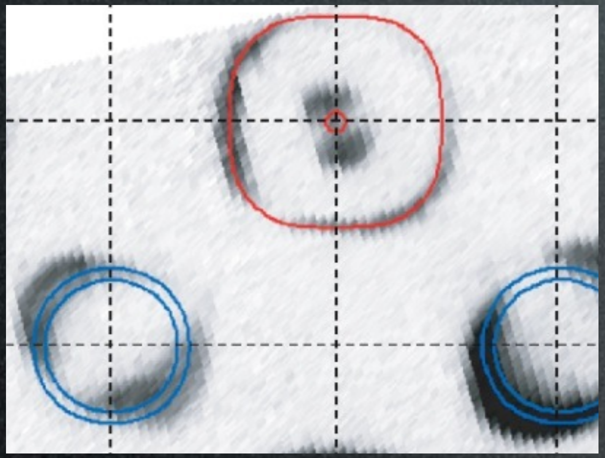

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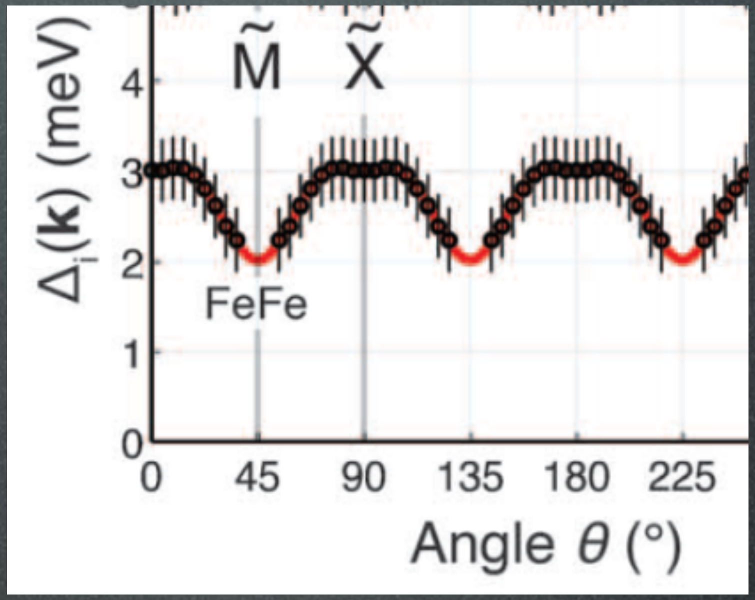

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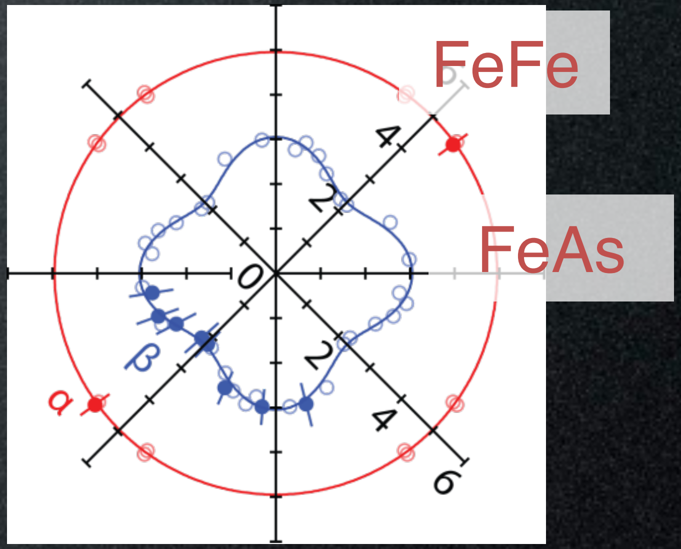

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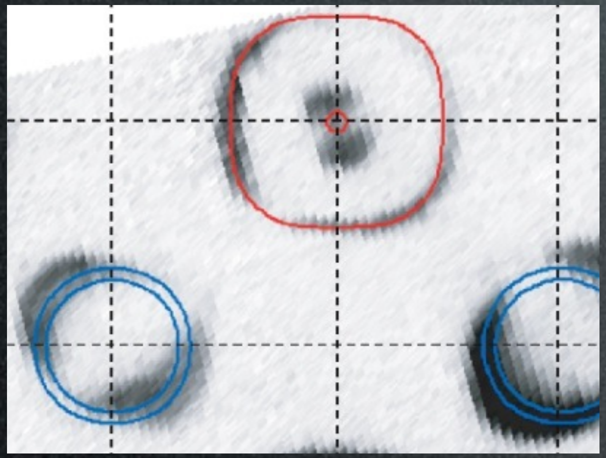

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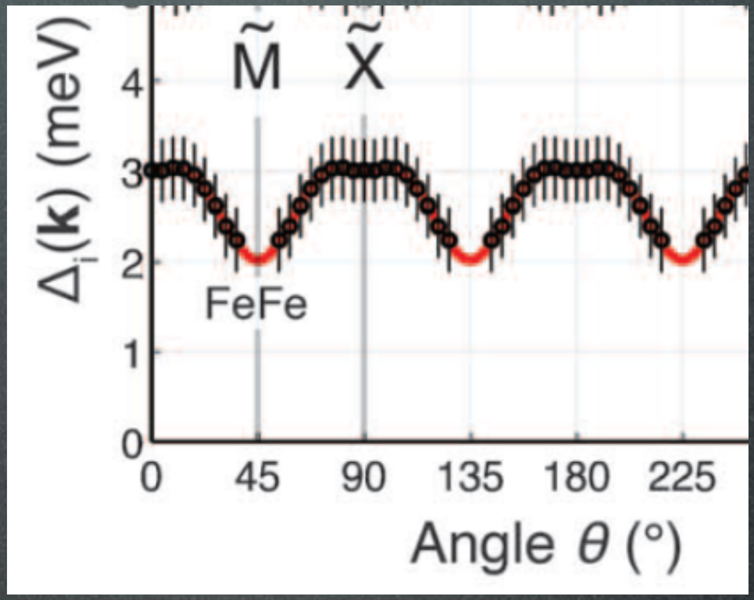

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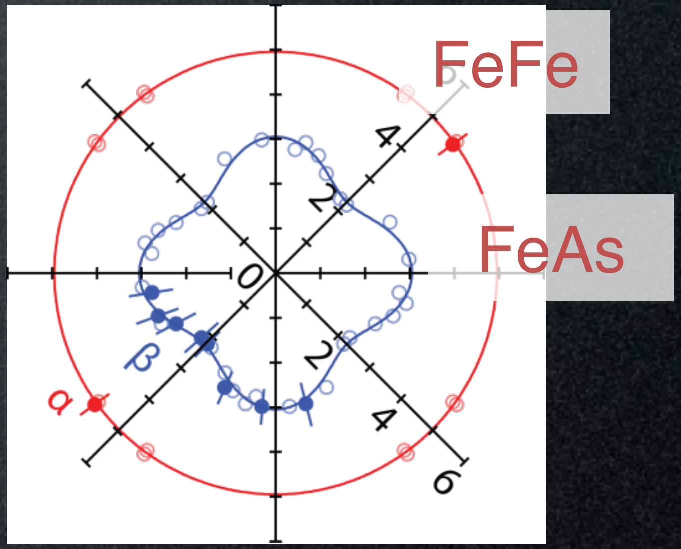


ARPES
Umezawa *et al.* 2012

- Large hole pocket (γ) with a single orbital character d_{xy}

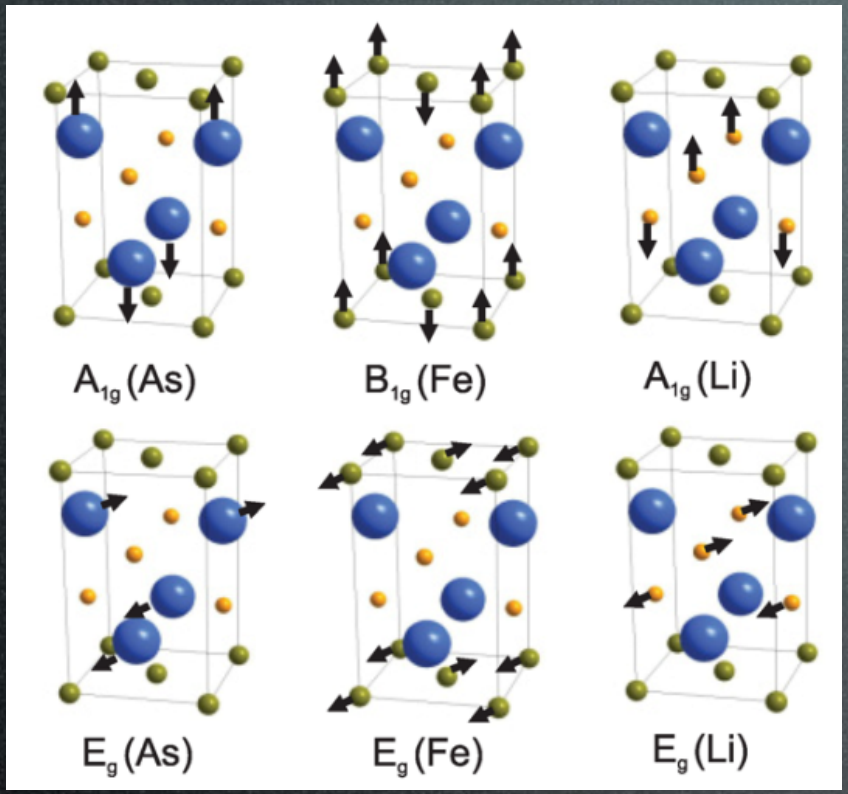
1. Identify suspects

Bosons suspects in LiFeAs

- Fe E_g optical phonon
  - argued to induce orbital fluctuation
  - Ω=15meV (Raman, DFT)

Bosons suspects in LiFeAs

Phonons



Raman
Um *et al.* 2012

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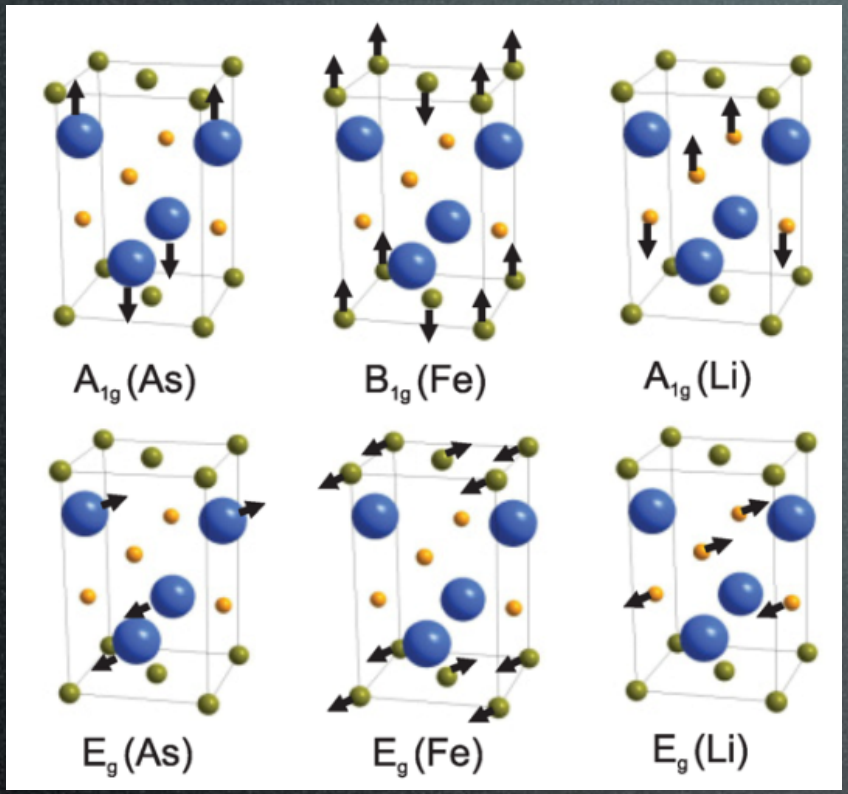

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Spin Fluctuation

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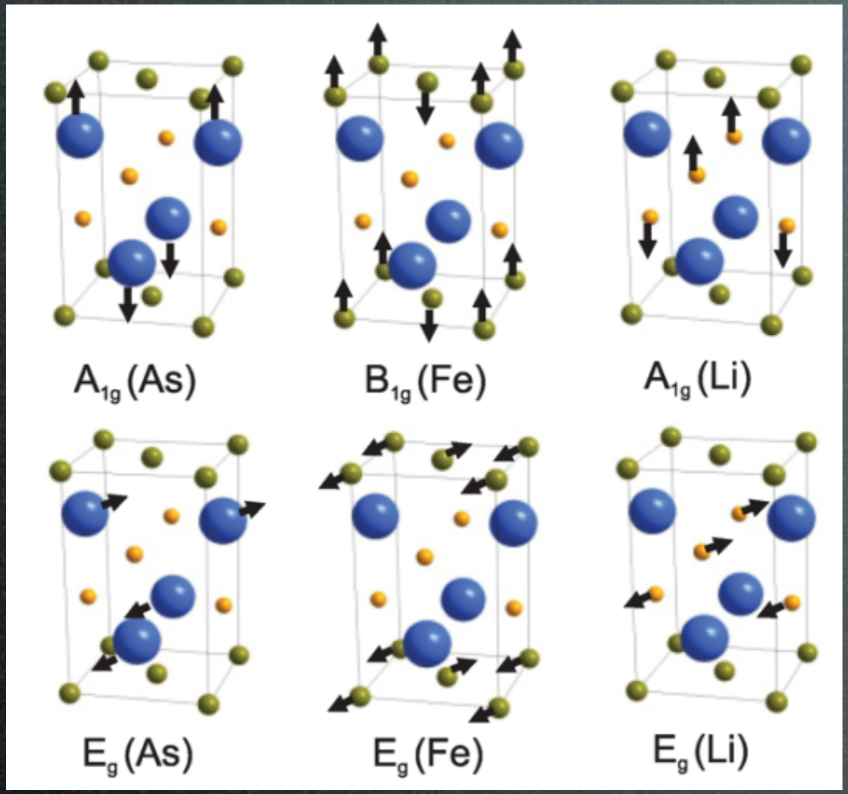
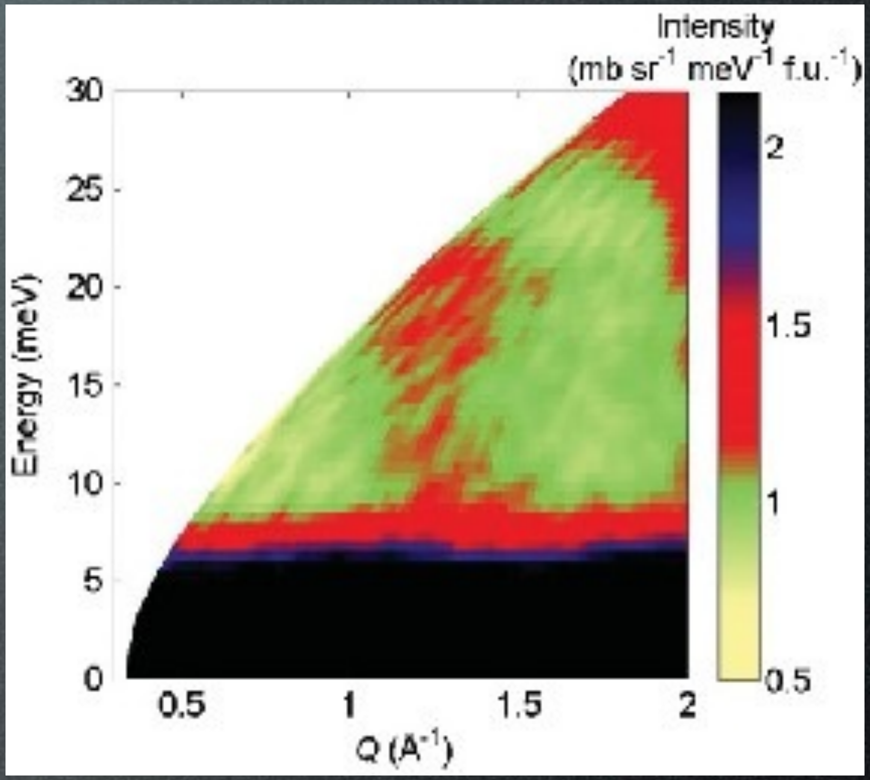
Phonons



Raman
Um *et al.* 2012

Spin Fluctuation



Inelastic Neutron
Taylor *et al.* 2011

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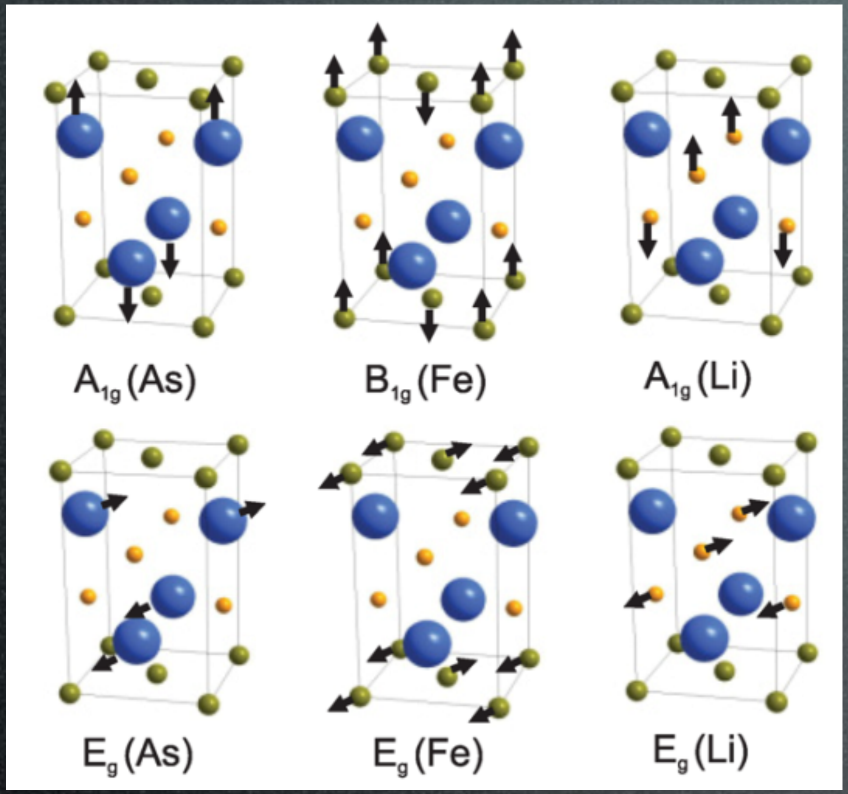

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Um *et al.* 2012

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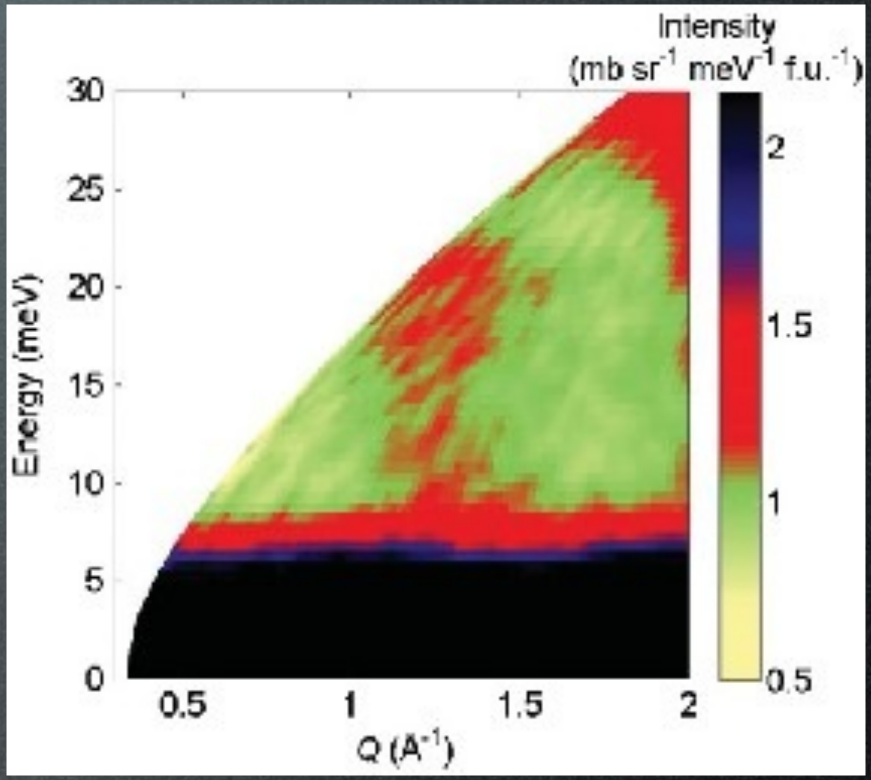
Spin Fluctuation



Inelastic Neutron
Taylor *et al.* 2011

- Resonant mode centered at Q=(π, π) (AFSF)
  - Ω=6meV

2. Gather evidence

Scanning Tunneling Spectroscopy
Quasiparticle Interference

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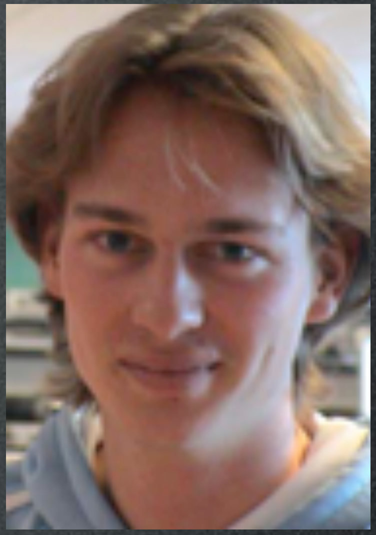
Scanning Tunneling Spectroscopy
Quasiparticle Interference

Milan P. Allan

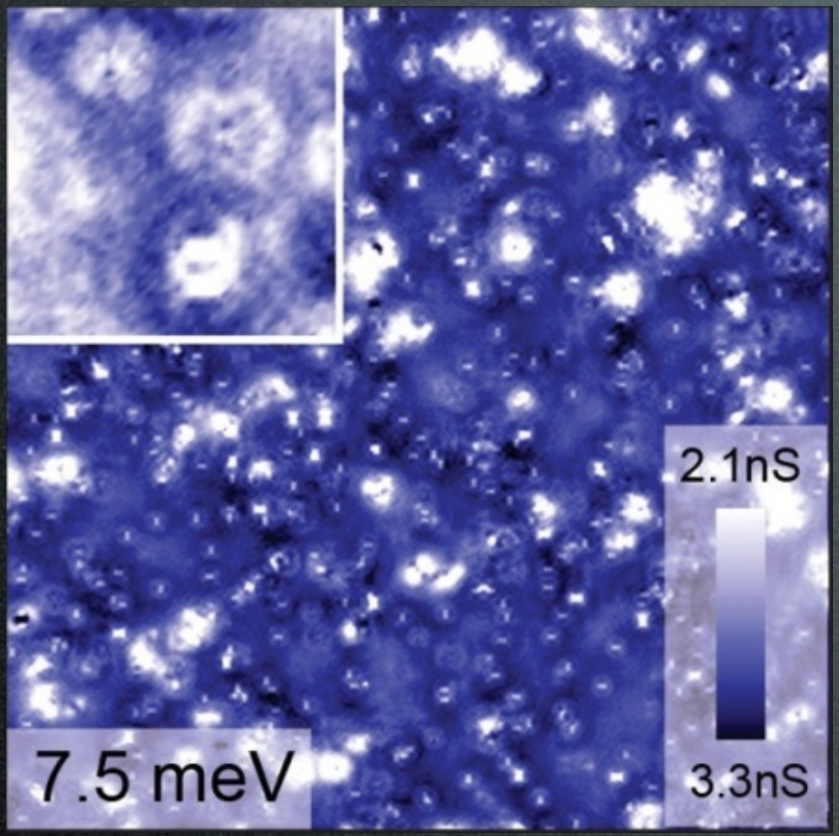
Andreas W. Rost



Freek Massee

J.C. Davis

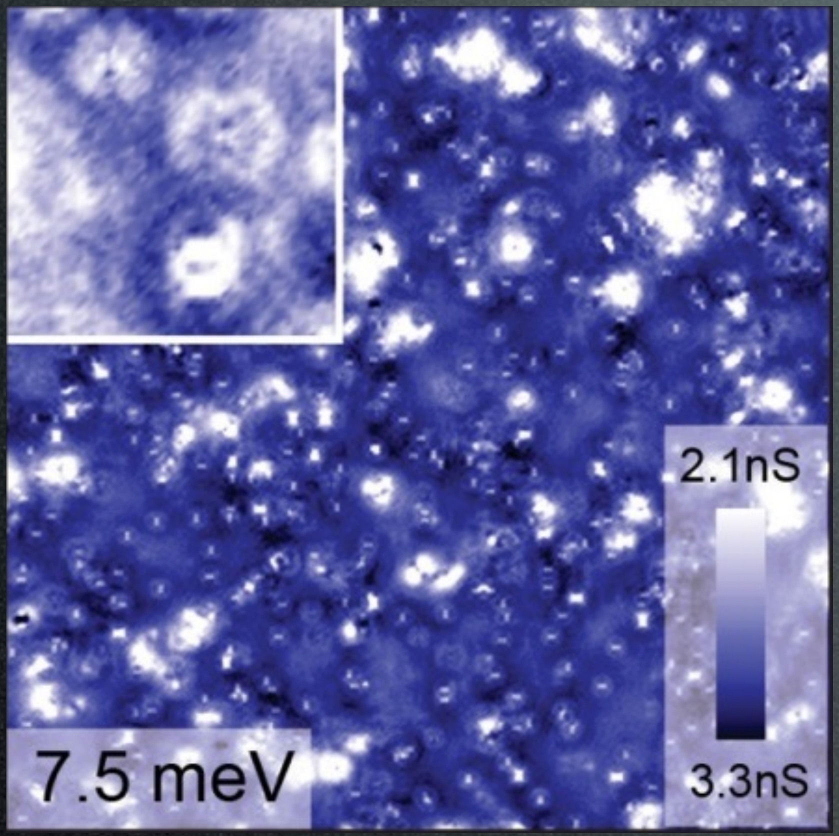
Scanning Tunneling Spectroscopy



$g(\mathbf{r}, \omega)$

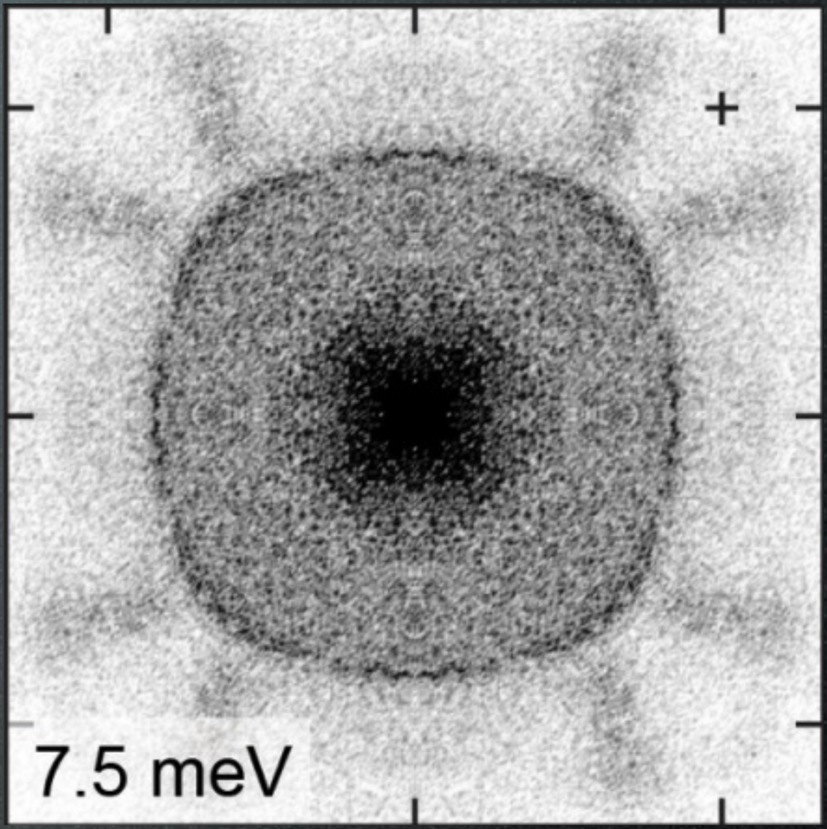
$$g(\mathbf{r}, \omega = eV) \equiv \frac{\mathrm{d}I}{\mathrm{d}V}(\mathbf{r}, V)$$

Quasiparticle Interference



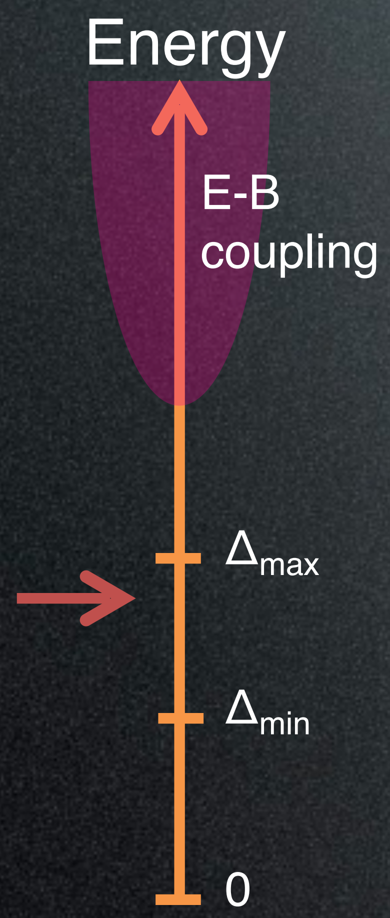
$g(\mathbf{r}, \omega)$

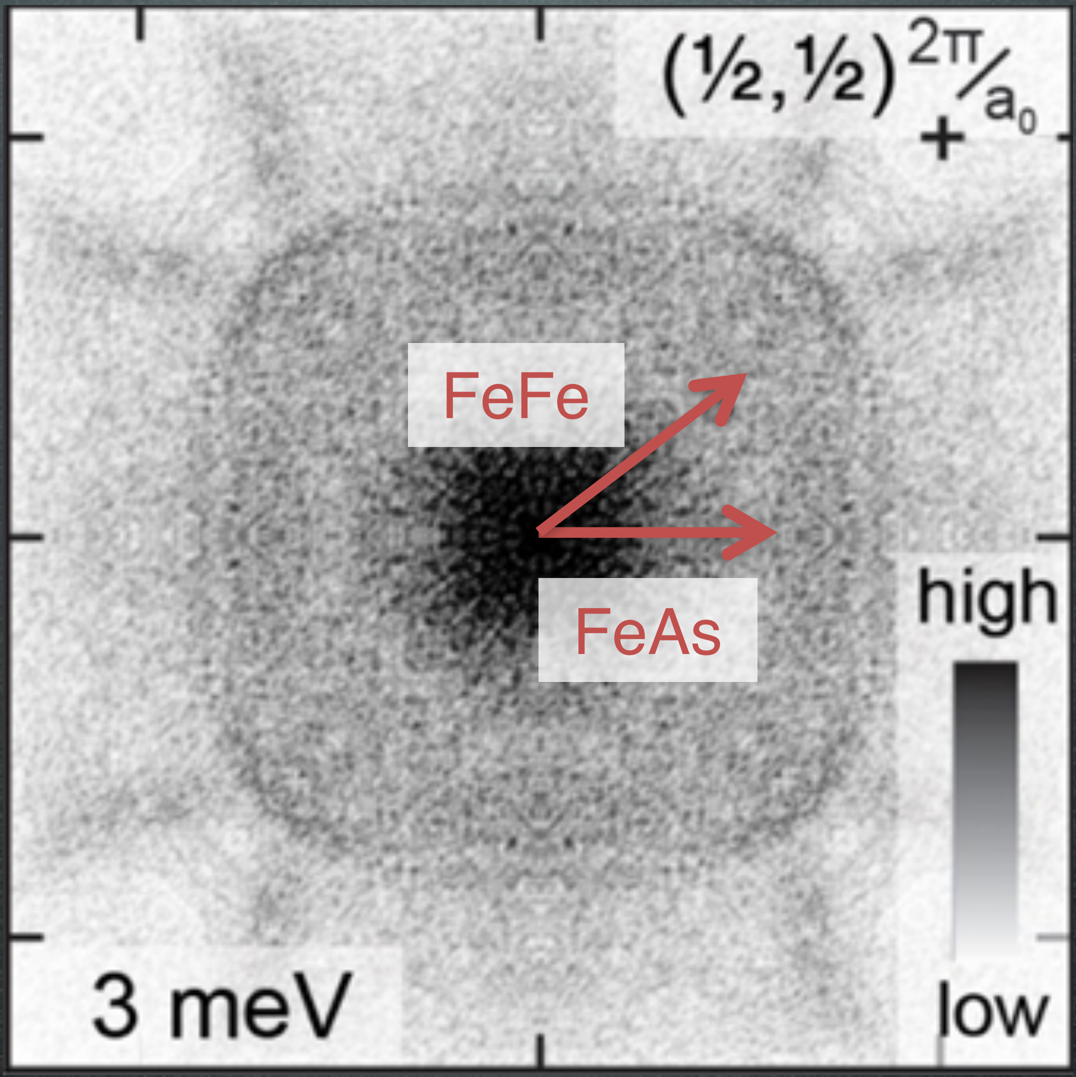
Fourier Transform



$g(\mathbf{q}, \omega)$

Energy dependent anisotropy





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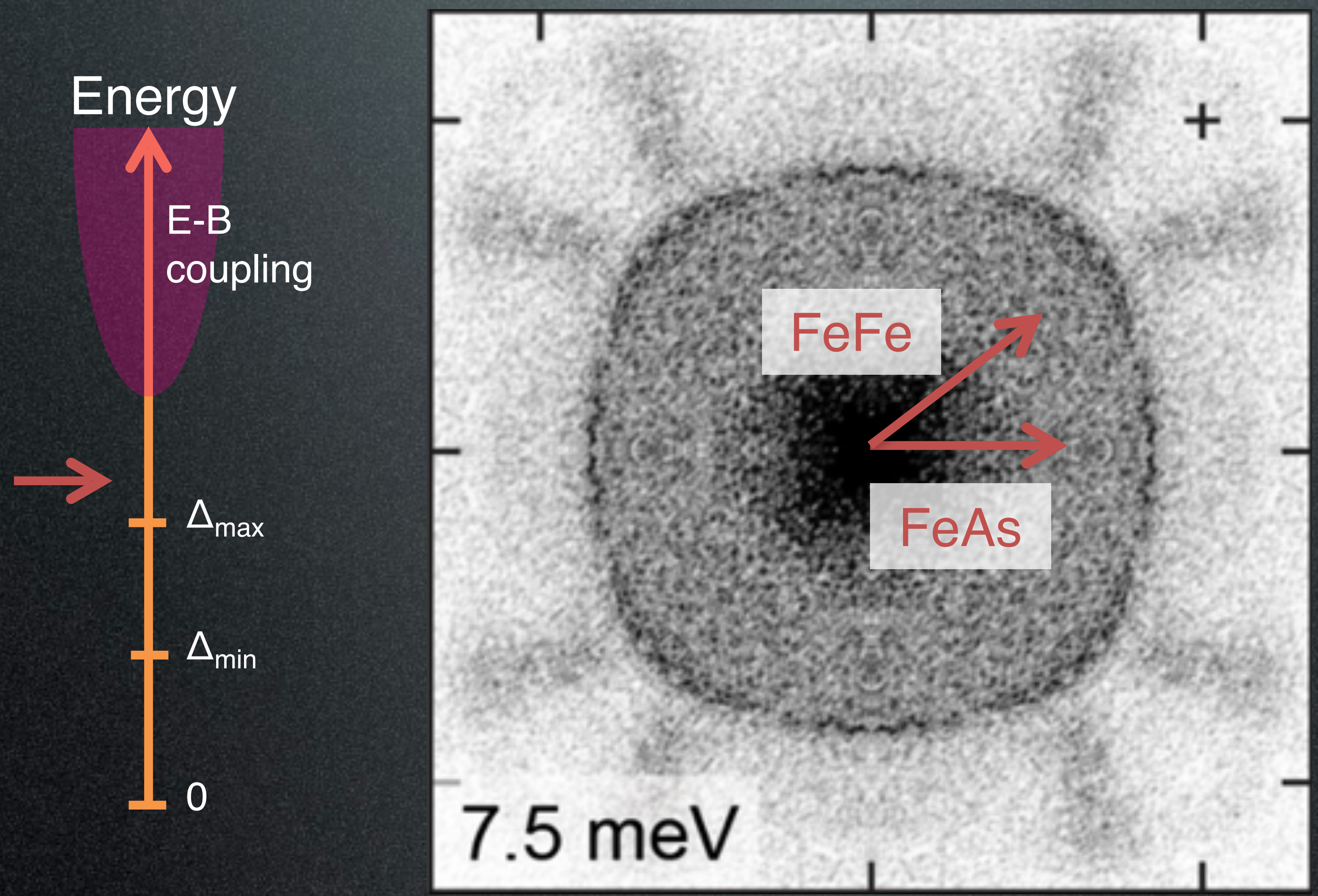

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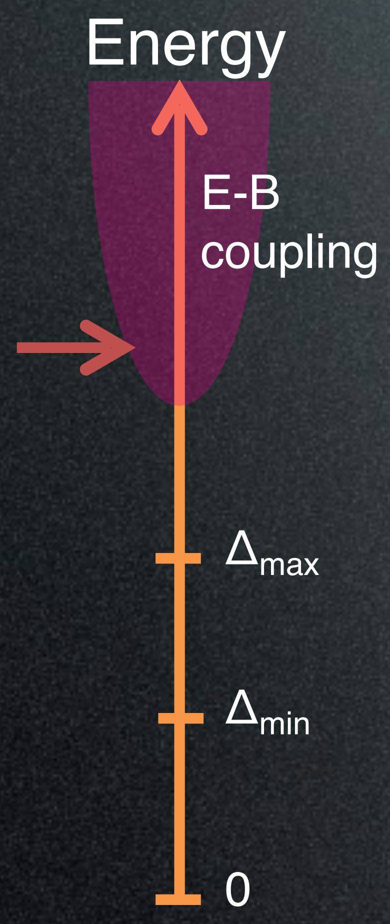

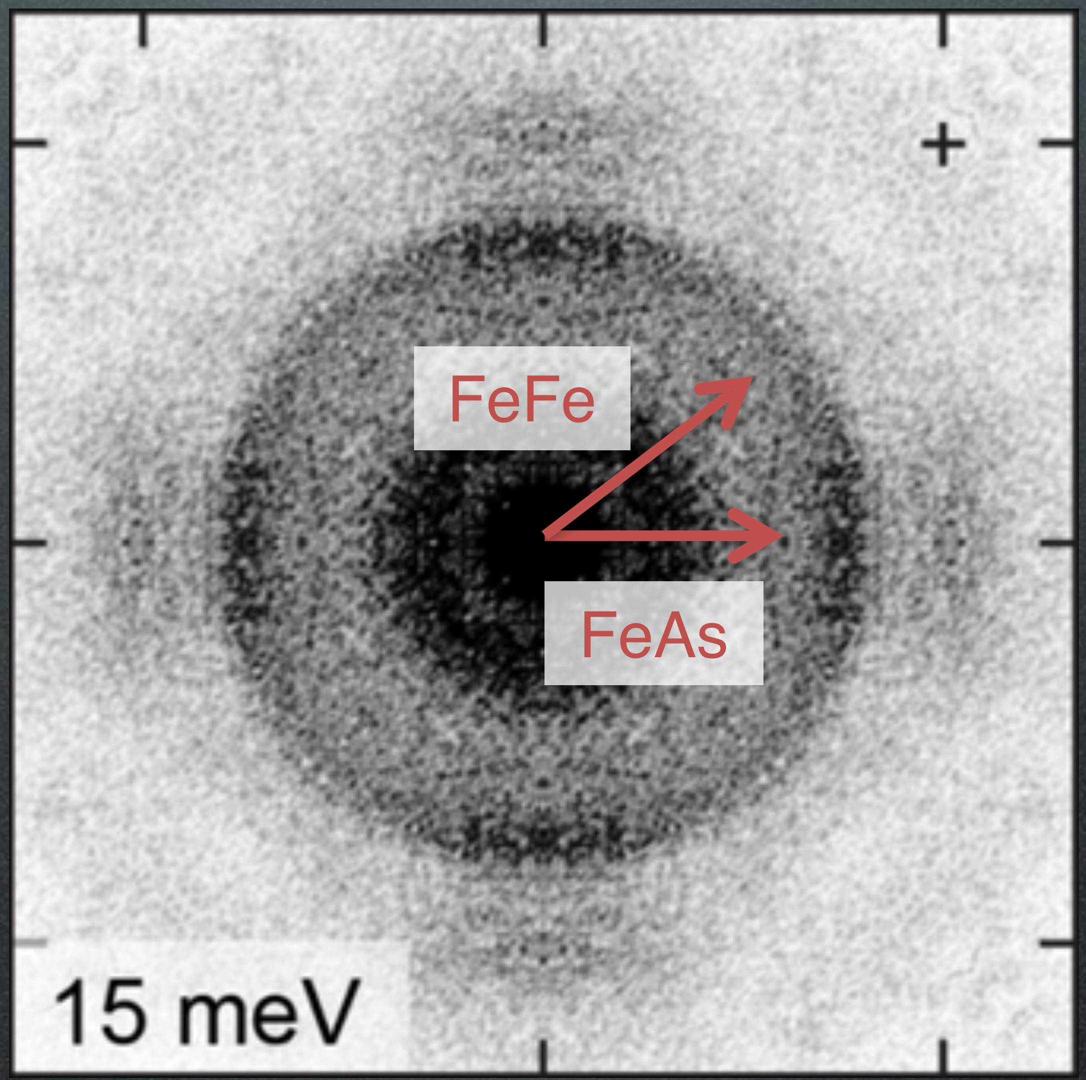

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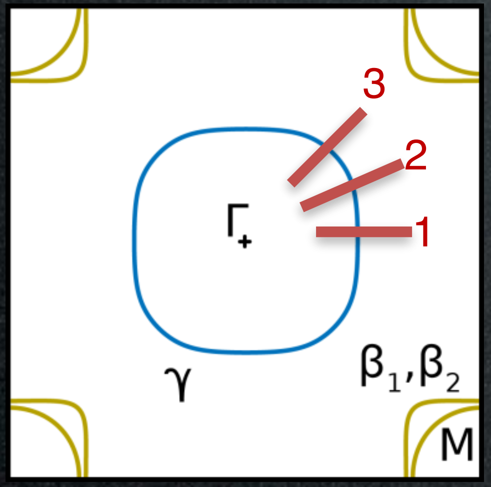
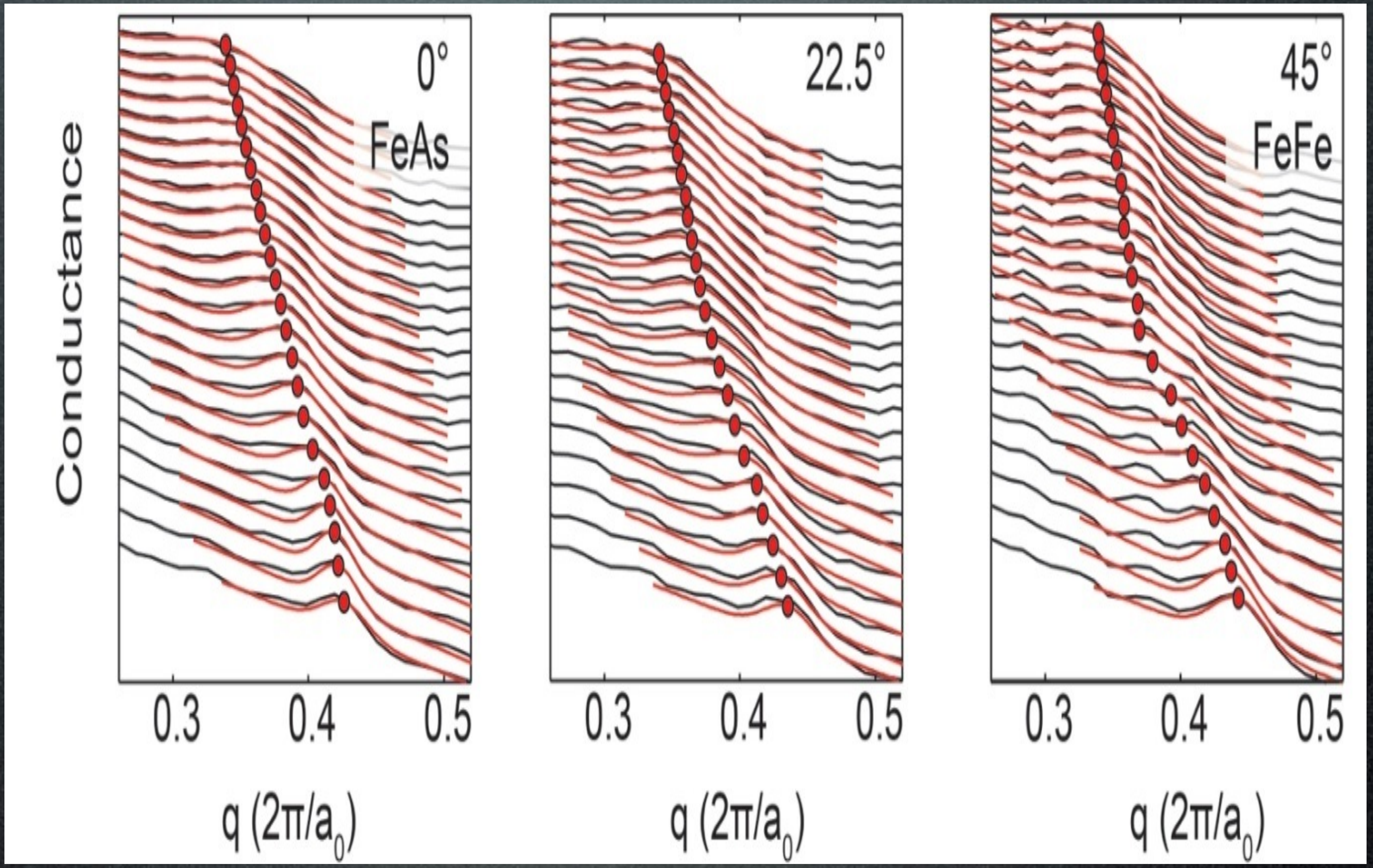




3. Match evidence to a suspect

Electron Self Energy

Kyungmin Lee

Mark Fischer

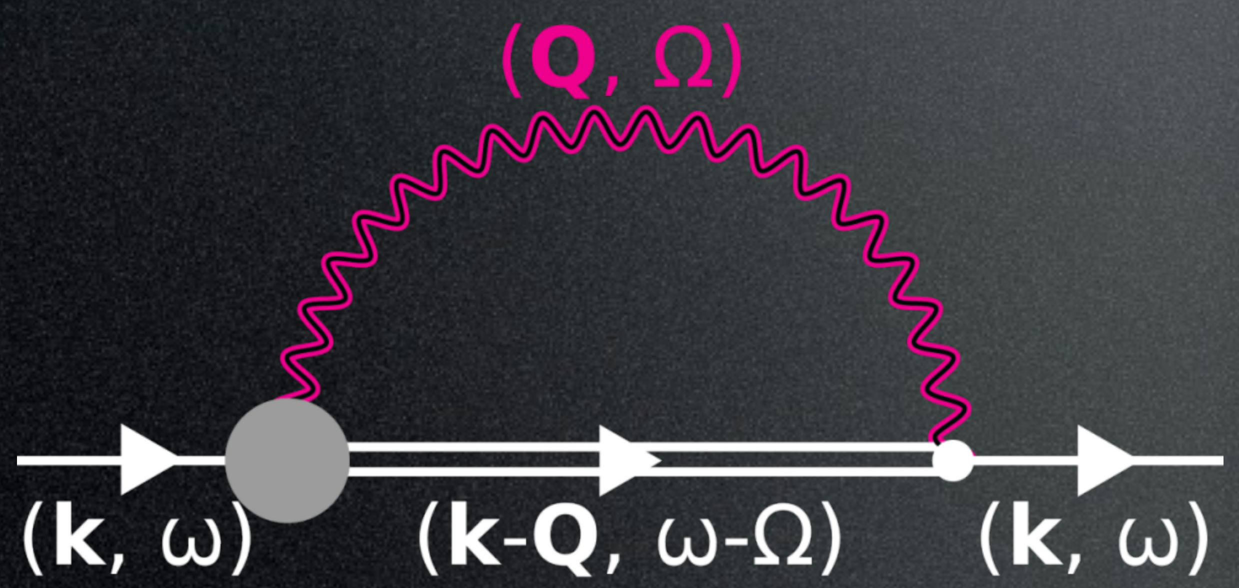
Self-Energy

Electron Self Energy

- Self energy captures electron-boson coupling

$$\hat{G}^{-1}(\mathbf{k},\omega) = \hat{G}_0^{-1}(\mathbf{k},\omega) - \hat{\Sigma}(\mathbf{k},\omega)$$

- ReΣ : change in dispersion
- ImΣ : broadening



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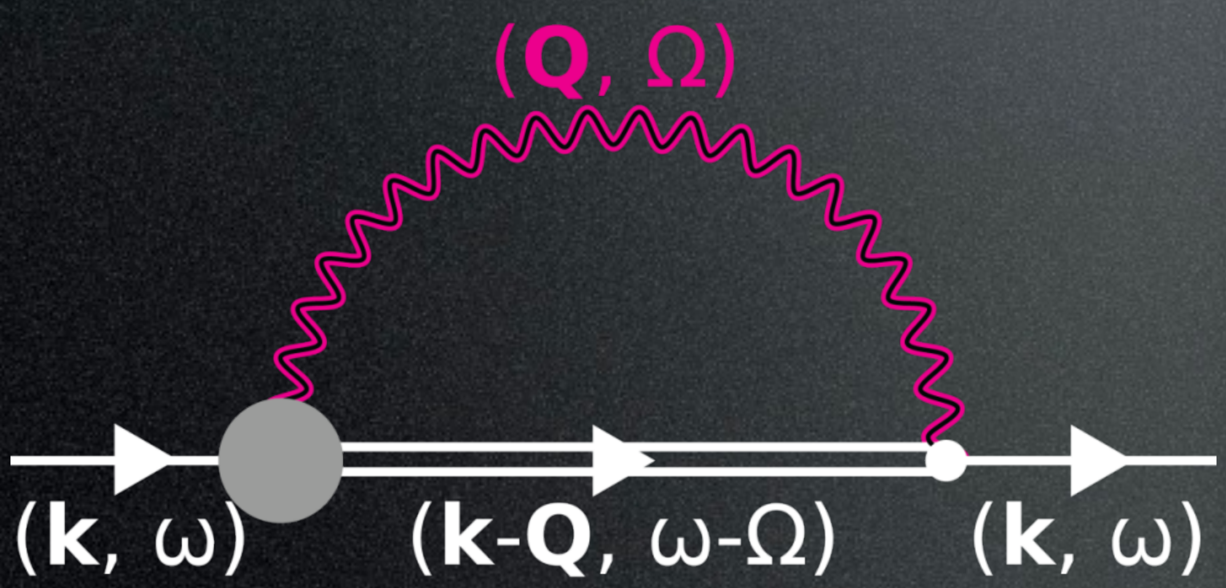

Three moving parts

Electron Self Energy

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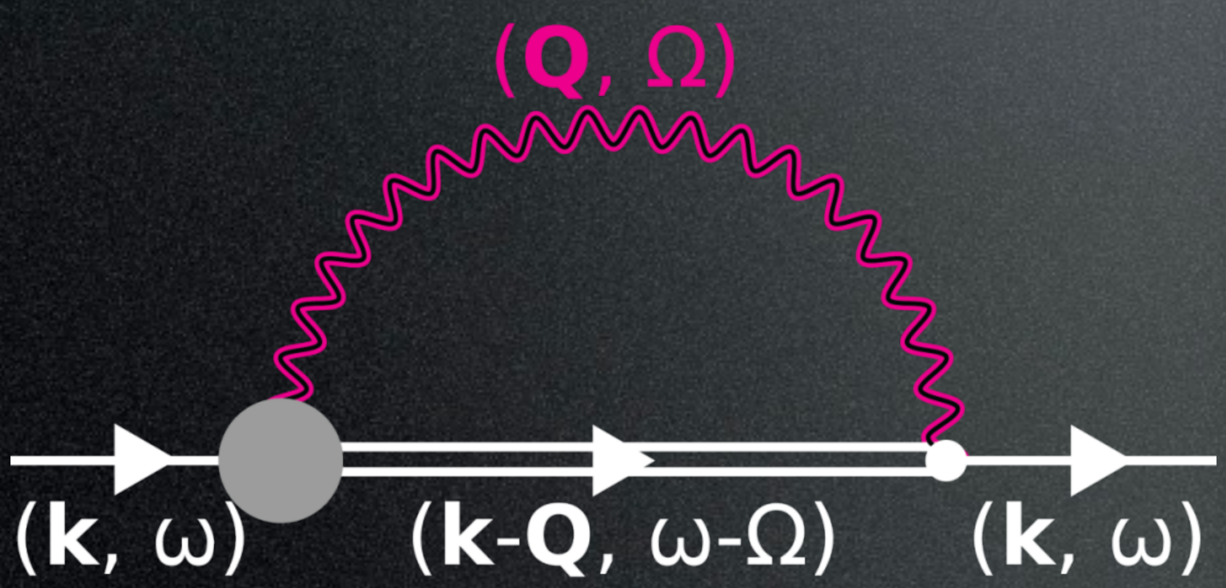

Three moving parts

- Fermion propagator

Electron Self Energy

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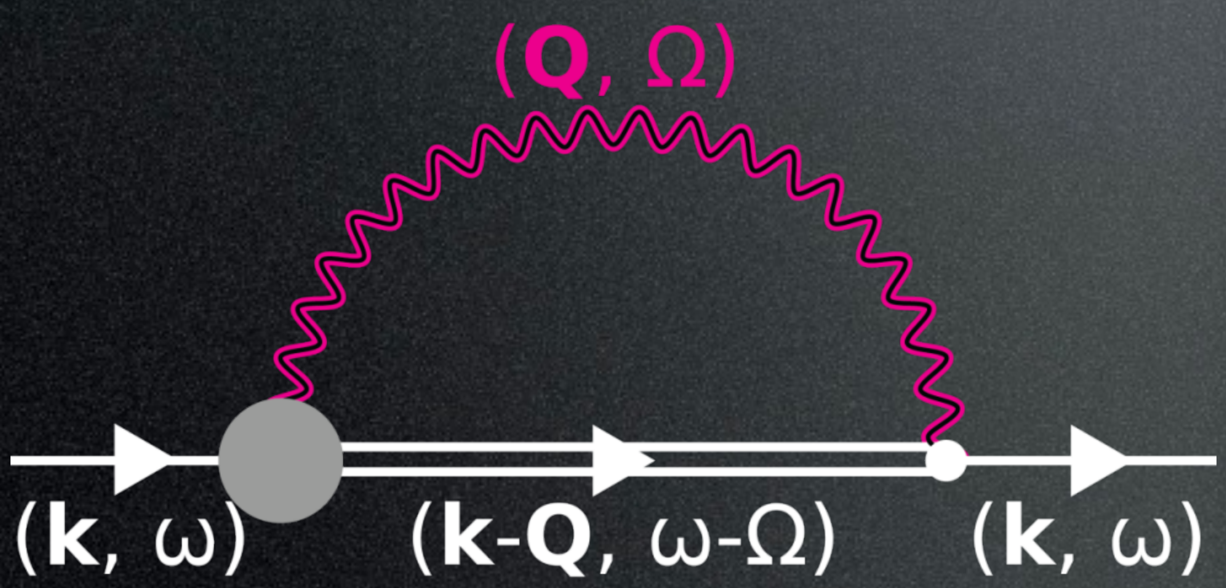


Three moving parts

- Fermion propagator
- Boson propagator

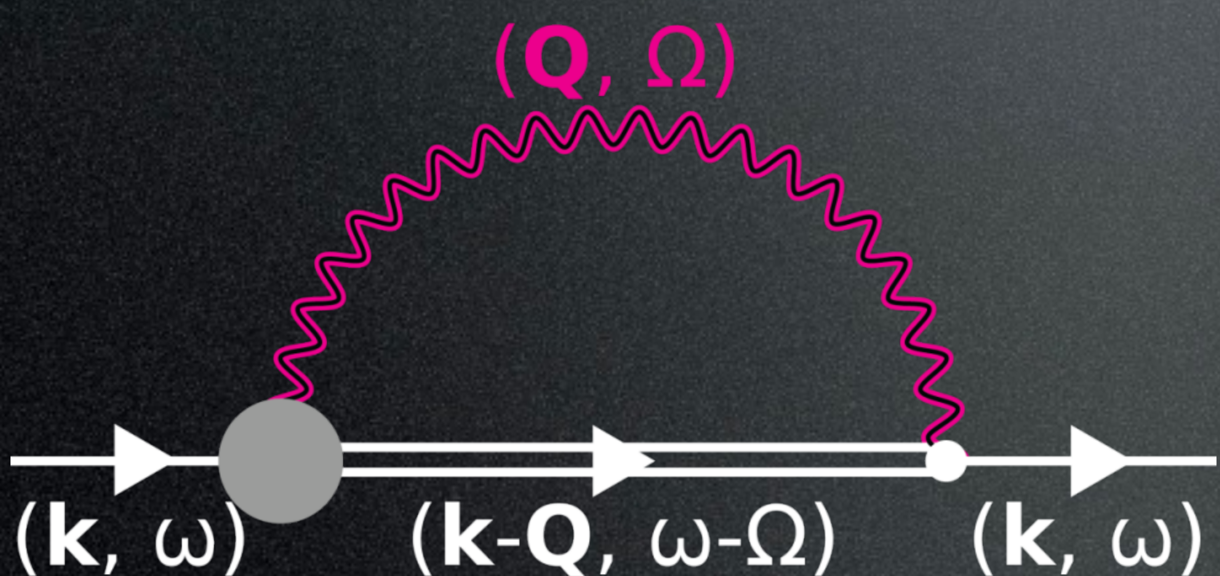
Electron Self Energy

- Self energy captures electron-boson coupling

$$\hat{G}^{-1}(\mathbf{k},\omega) = \hat{G}_0^{-1}(\mathbf{k},\omega) - \hat{\Sigma}(\mathbf{k},\omega)$$

- ReΣ : change in dispersion

- ImΣ : broadening

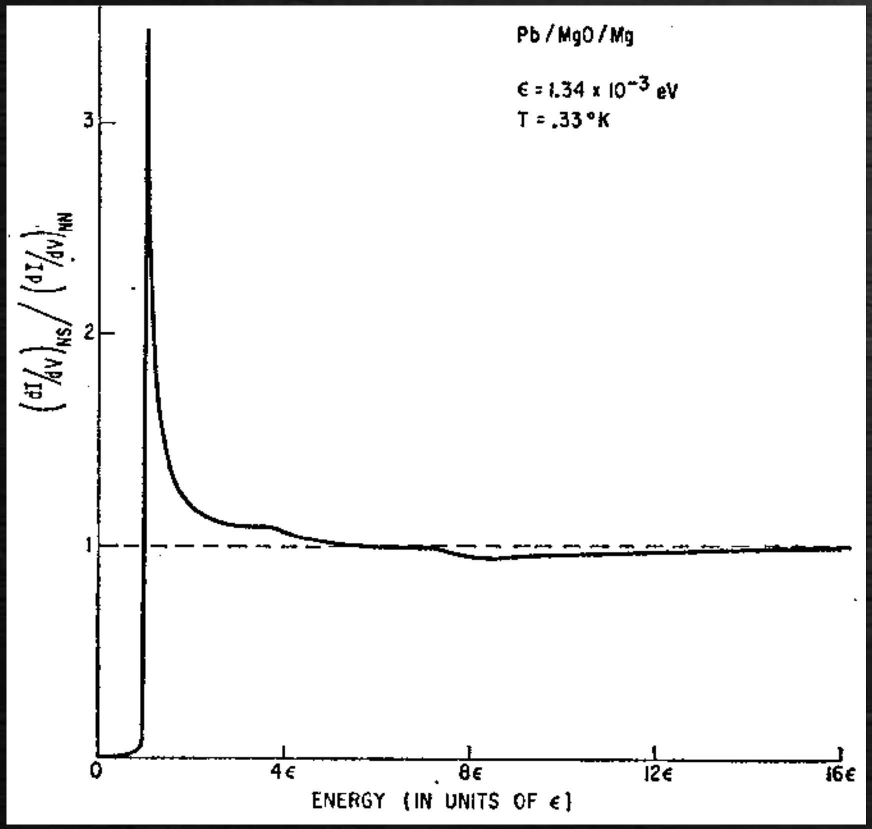


<u>Three moving parts</u>

- Fermion propagator
- Boson propagator
- Coupling vertex

Classic Example: Pb

- Tunneling experiment
  - Superconducting Pb
  - Signature of electron-phonon coupling

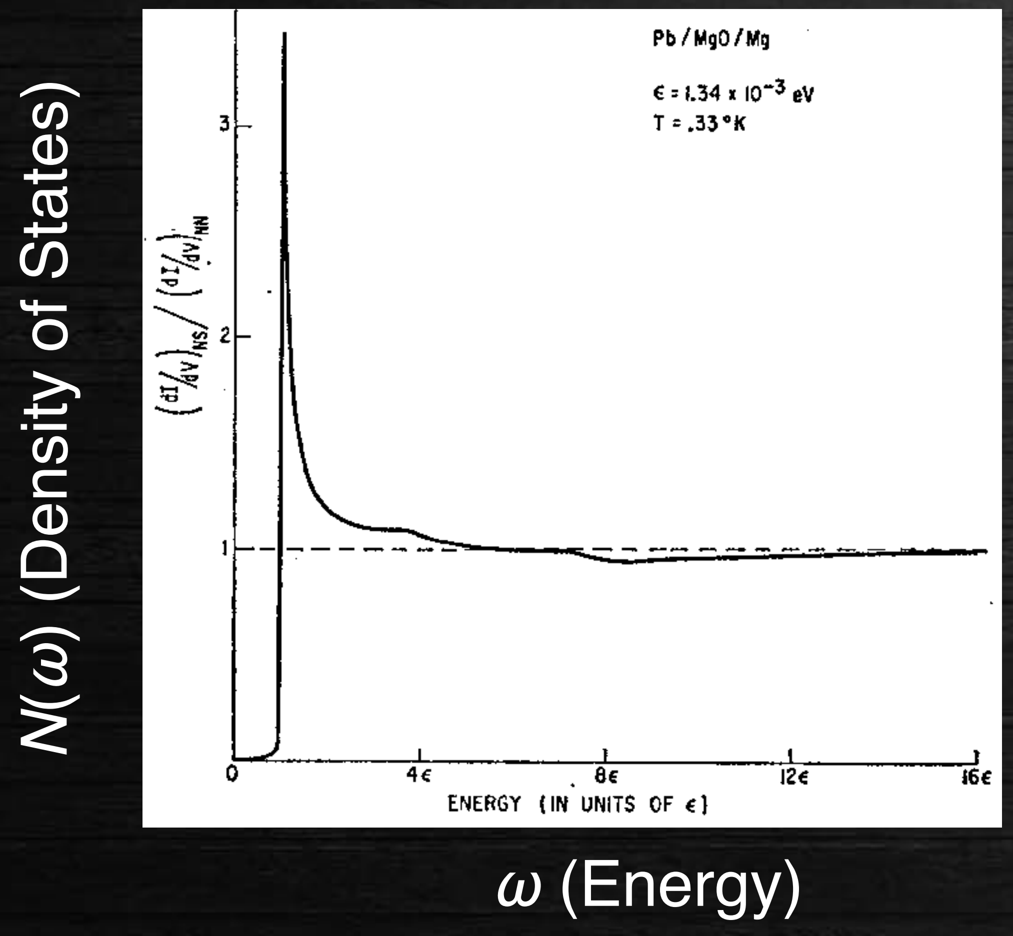


$N(\omega)$ (Density of States)

ω (Energy)

Classic Example: Pb

- Tunneling experiment
  - Superconducting Pb
  - Signature of electron-phonon coupling
- Migdal-Eliashberg,



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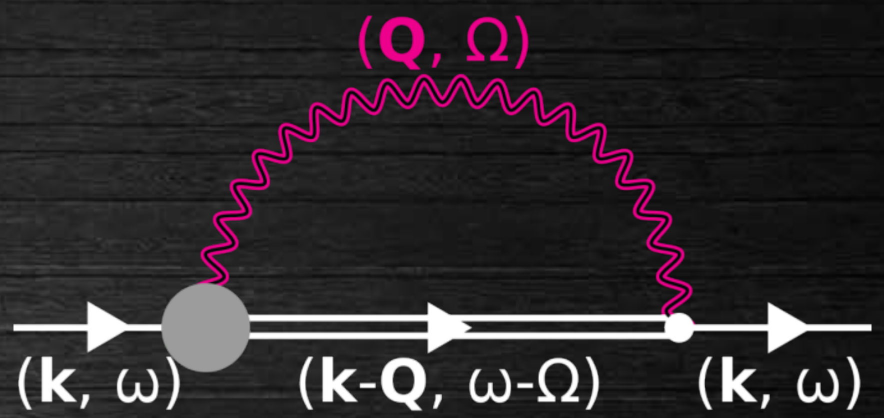

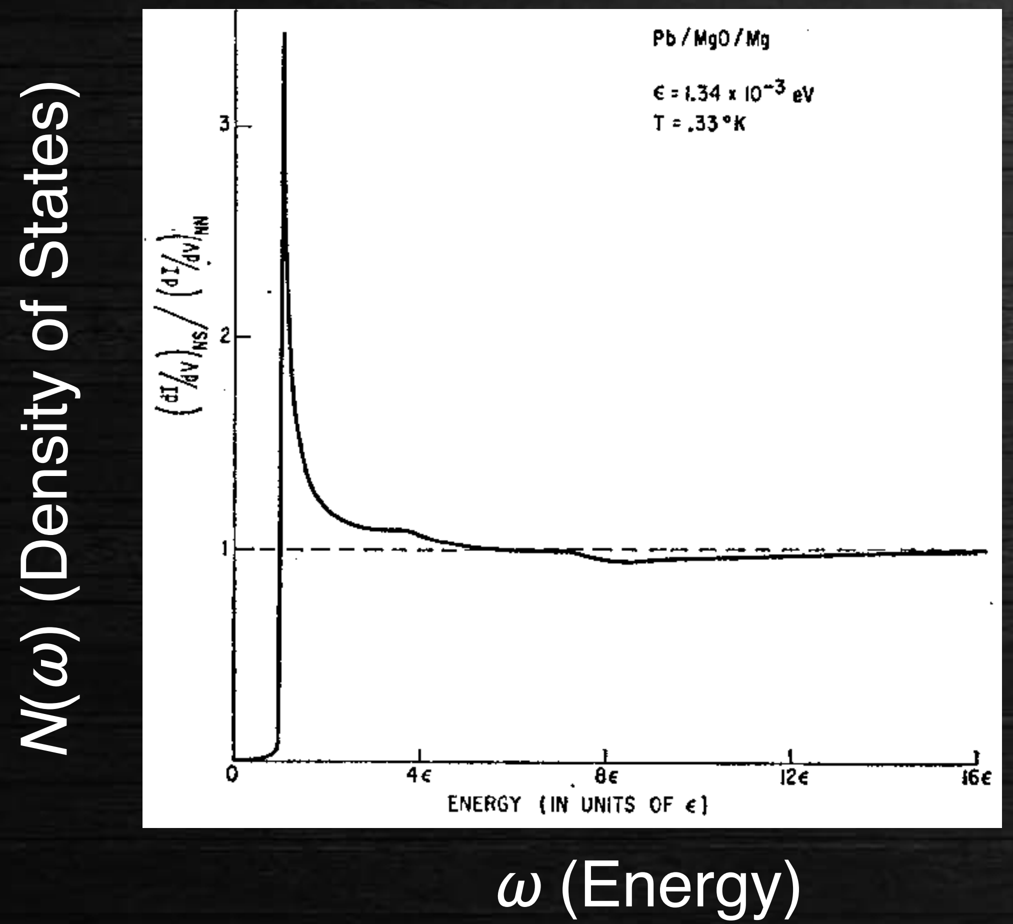

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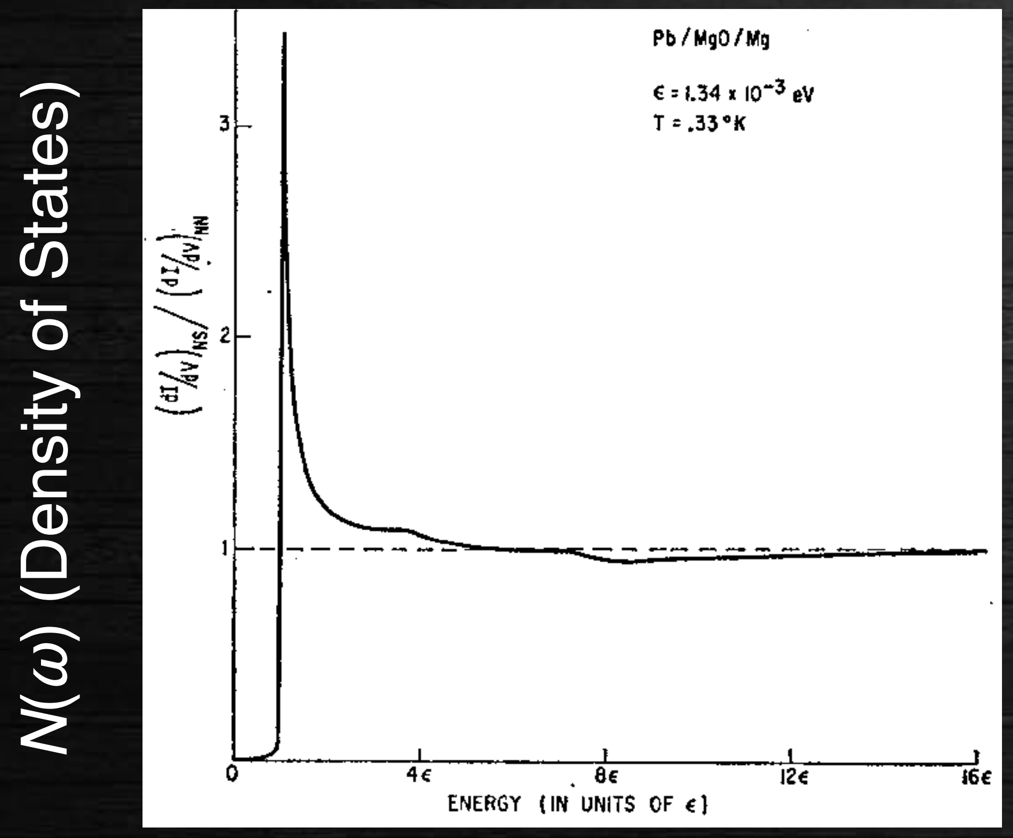

ω (Energy)

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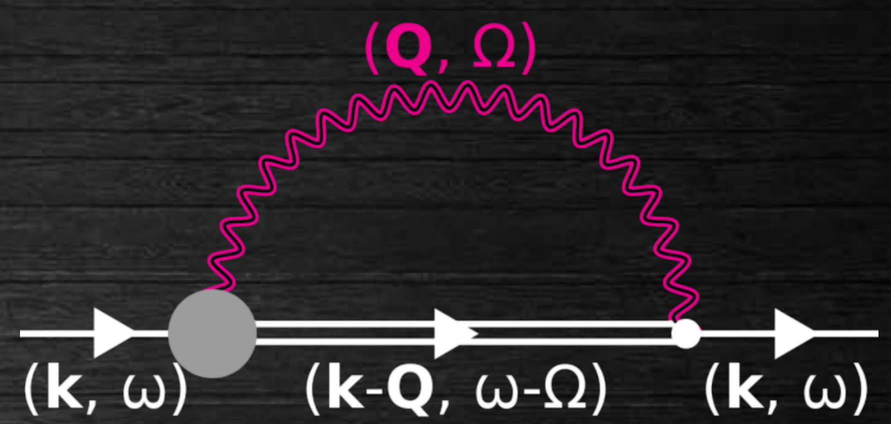


1. Start from Fermi liquid
2. Compute self energy to all orders, ignoring vertex correction

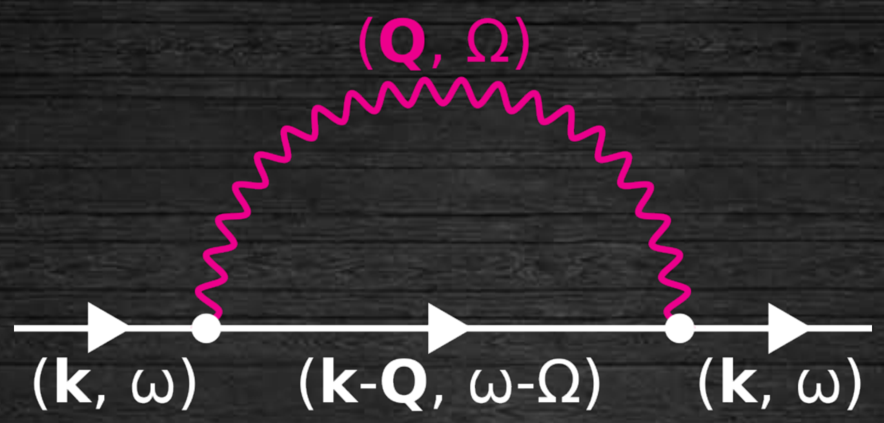
→ Boson coupling produces both SC and high energy fingerprint

Challenges

- No separation of scales for spin fluctuation
  → Vertex correction cannot be ignored

- Multiple bands
  (5 Fe3d-orbitals)

Perturbative Self Energy

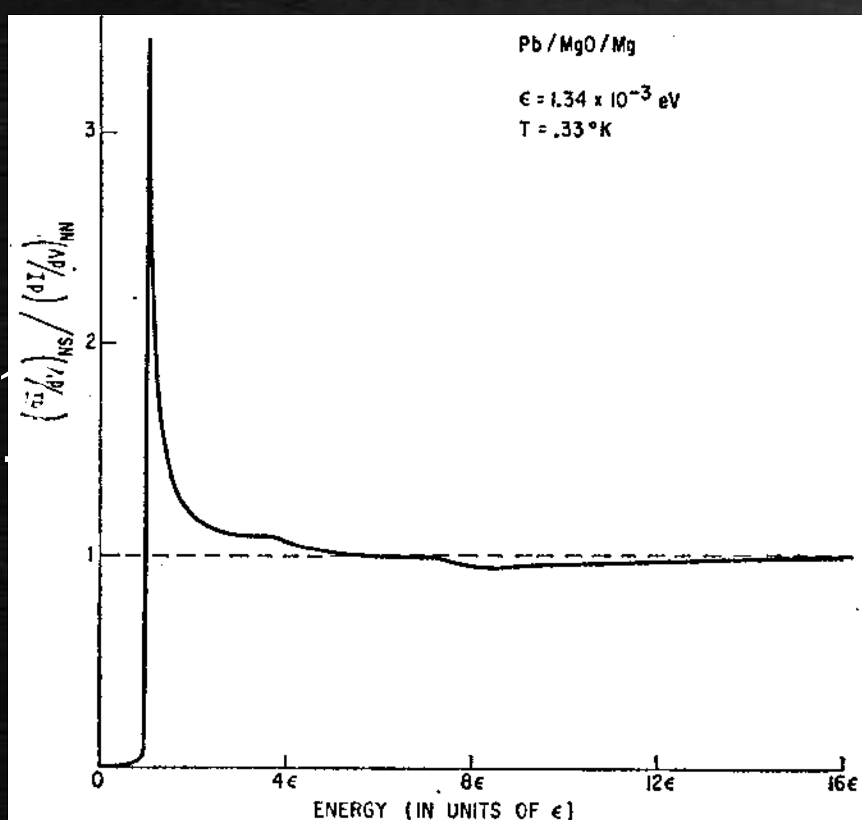


1. Start from experimentally measured gap (BdG)
2. Compute lowest order self energy

→ Boson coupling produces high energy fingerprint

Classic Example: Pb

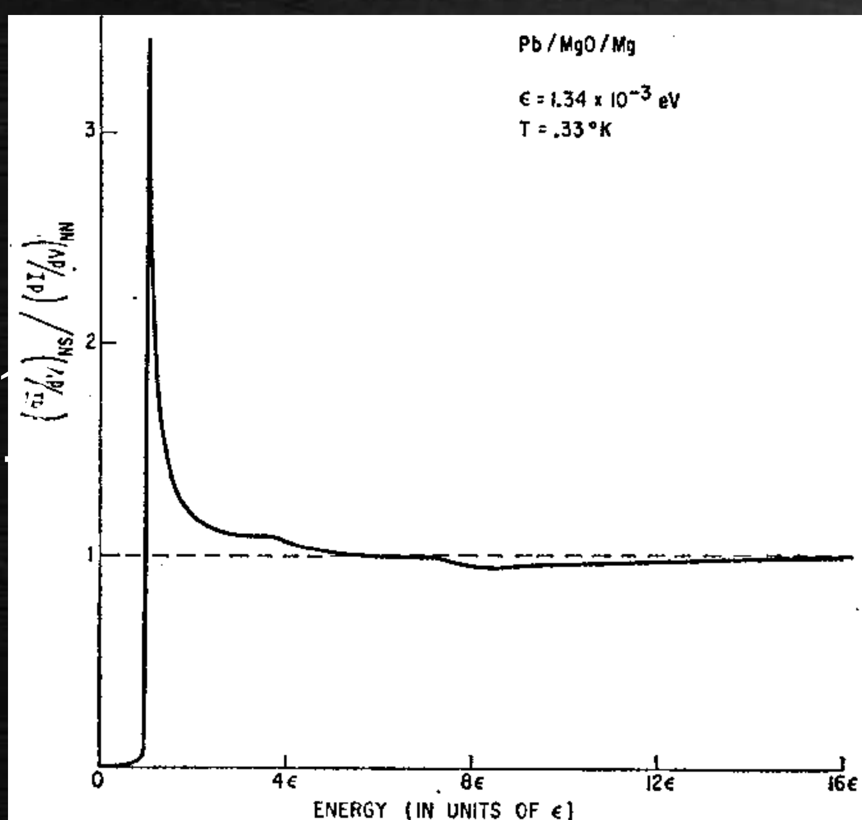
- Tunneling
  - Superconducting Pb
  - Signature of electron-phonon coupling



ω (Energy)

Classic Example: Pb

- Tunneling
  - Superconducting Pb
  - Signature of electron-phonon coupling
- BdG + perturbative S.E.
  - Circular FS + S-wave Δ
  - Einstein phonon Ω
  - Reproduces deviation from BCS (mean field)



ω (Energy)

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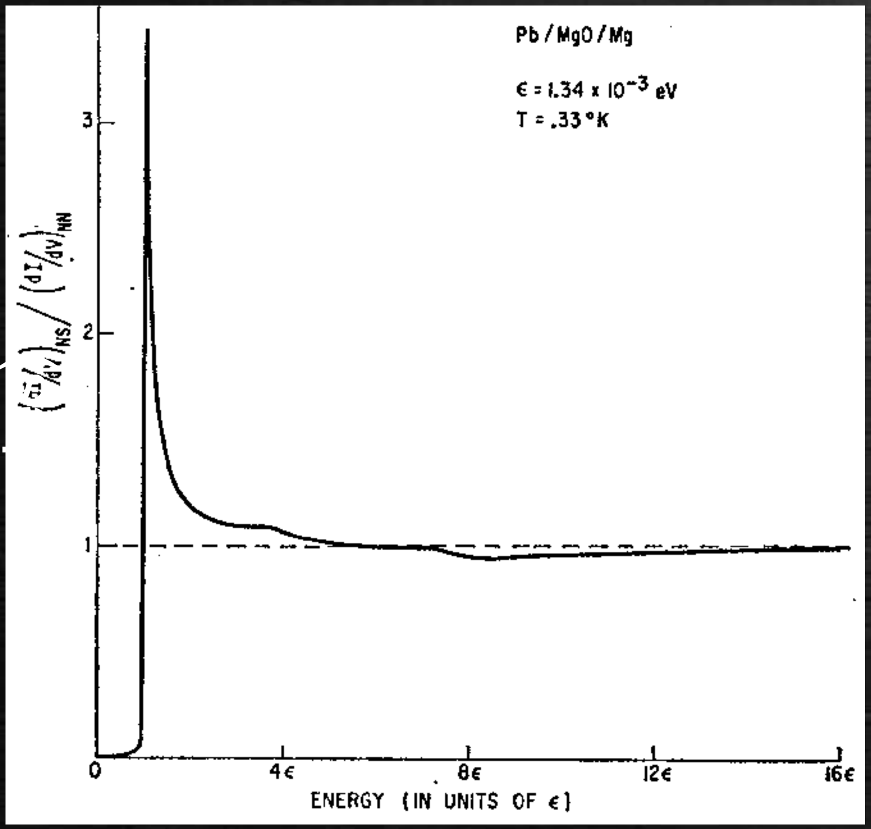

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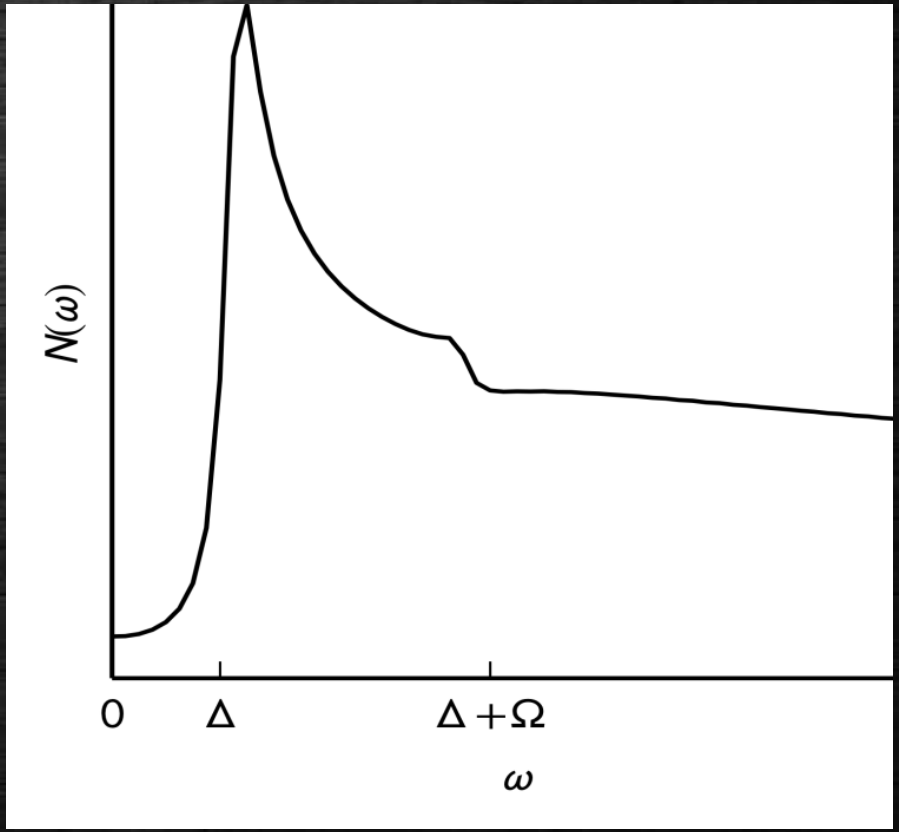

What about cuprate?

PHYSICAL REVIEW B **69**, 094523 (2004)

Effect of an electron-phonon interaction on the one-electron spectral weight of a *d*-wave superconductor

A. W. Sandvik,[1,2,*] D. J. Scalapino,[2,†] and N. E. Bickers[3,‡]
[1]*Department of Physics, Åbo Akademi University, Porthansgatan 3, FIN-20500 Turku, Finland*
[2]*Department of Physics, University of California, Santa Barbara, California 93106-9530, USA*
[3]*Department of Physics, University of Southern California, Los Angeles, California 90089-0484, USA*
(Received 5 September 2003; published 30 March 2004)

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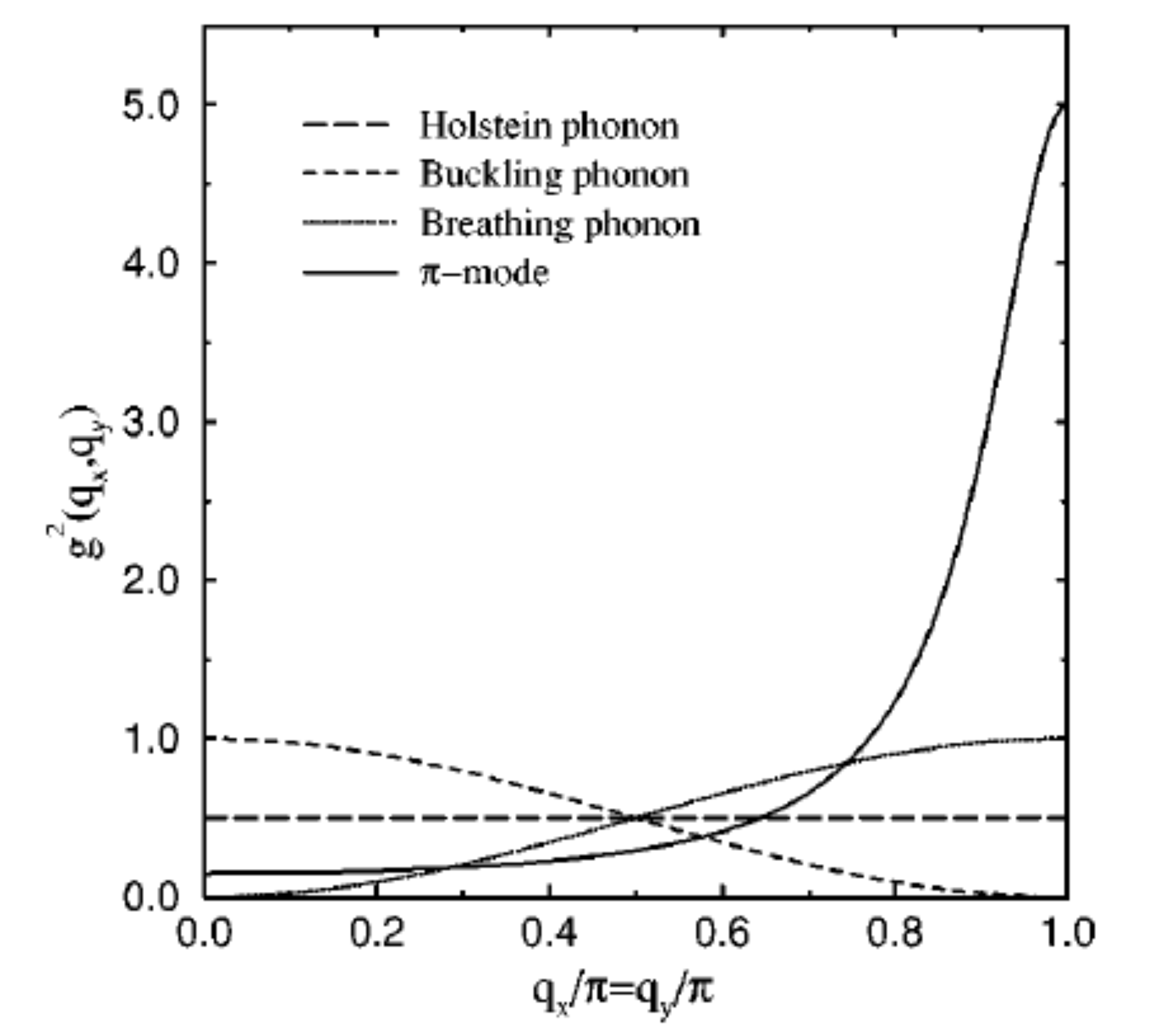

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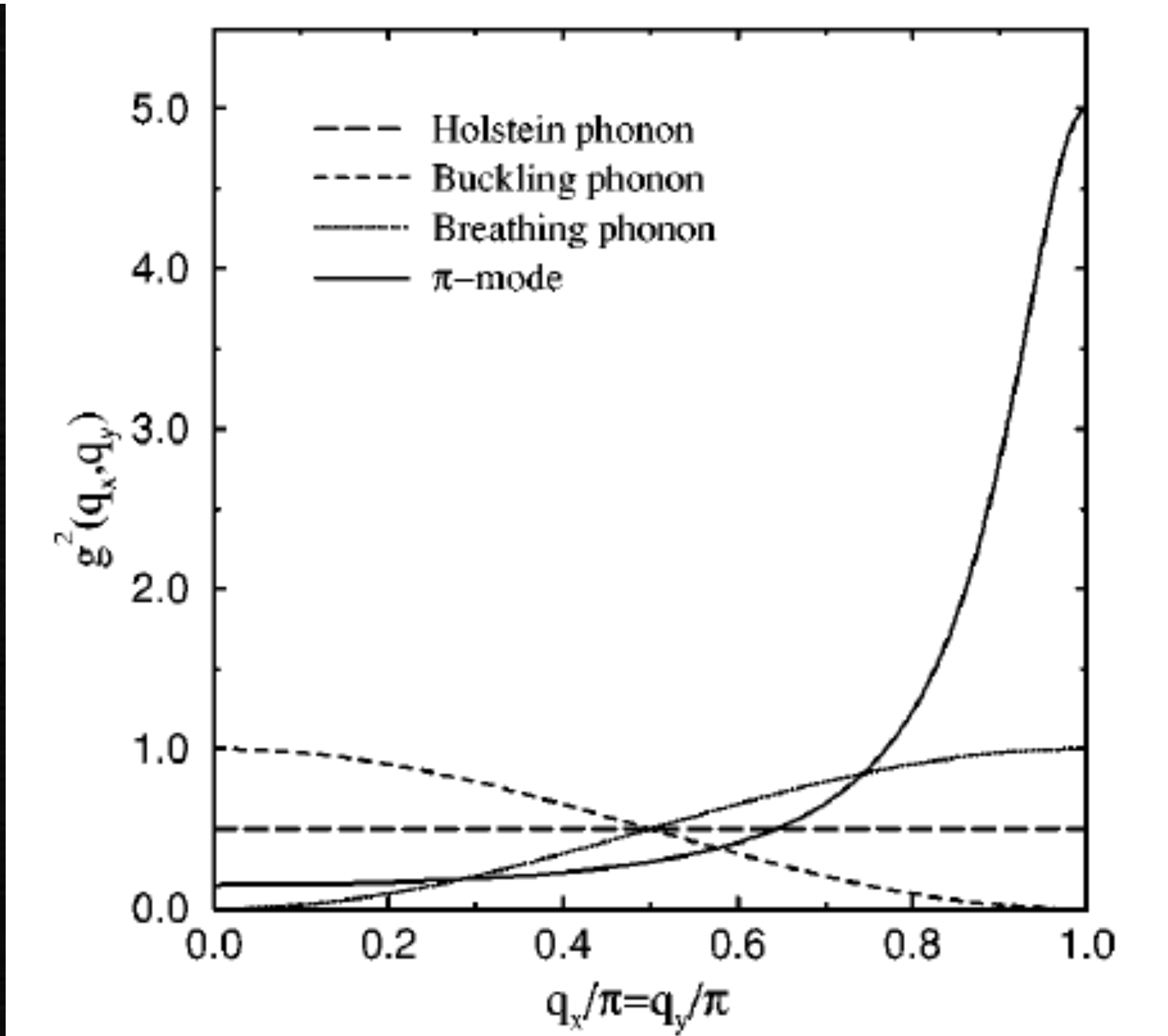
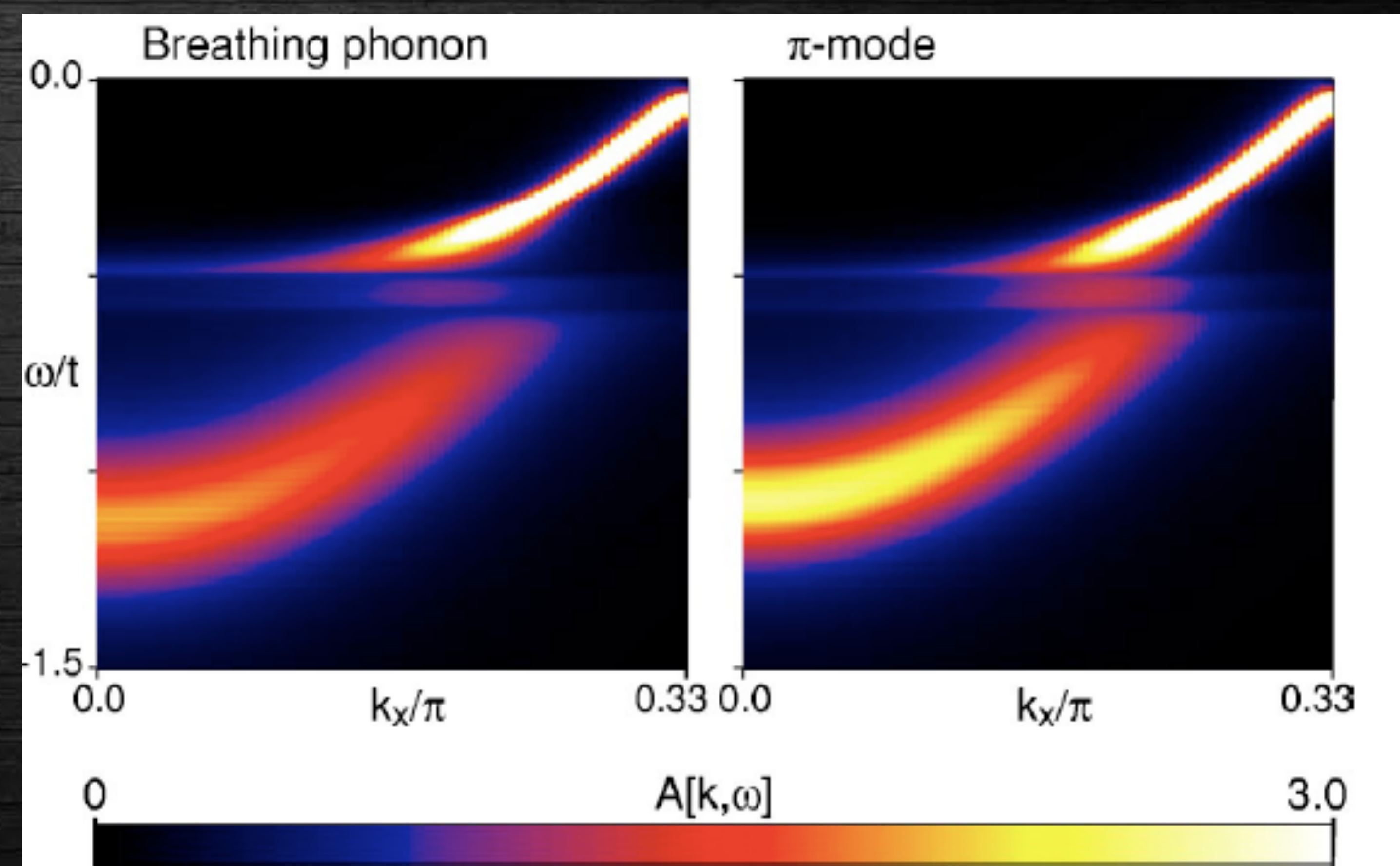
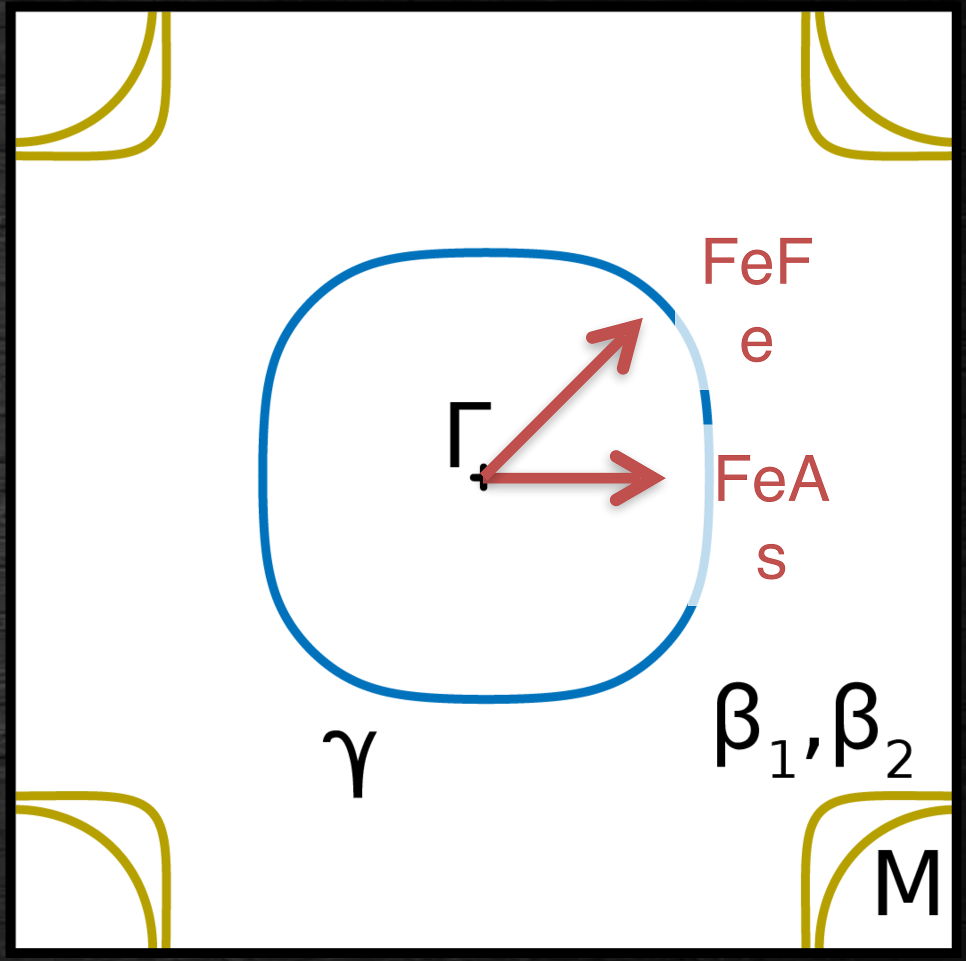




Model Electronic Structure of LiFeAs

- Three band model
  - Electron pockets (β_1,β_2) around M
  - Large hole pocket (γ) around Γ with uniform orbital character (d_{xy})



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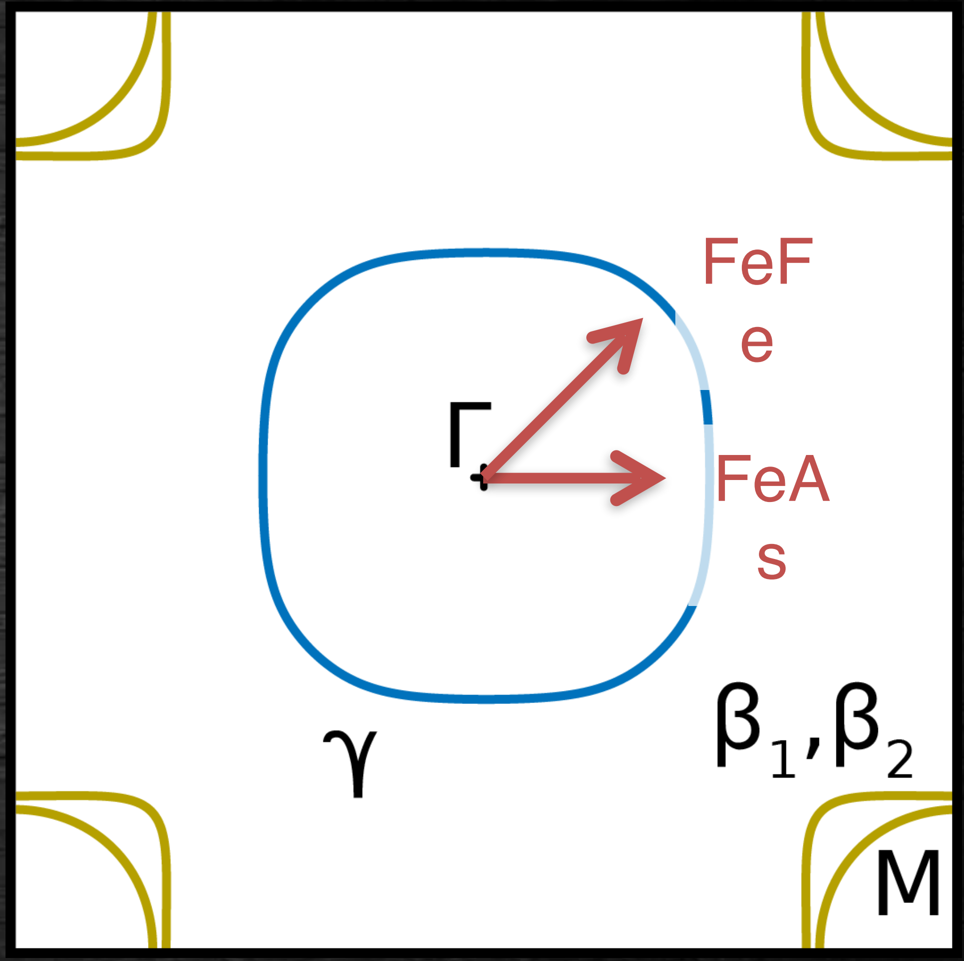
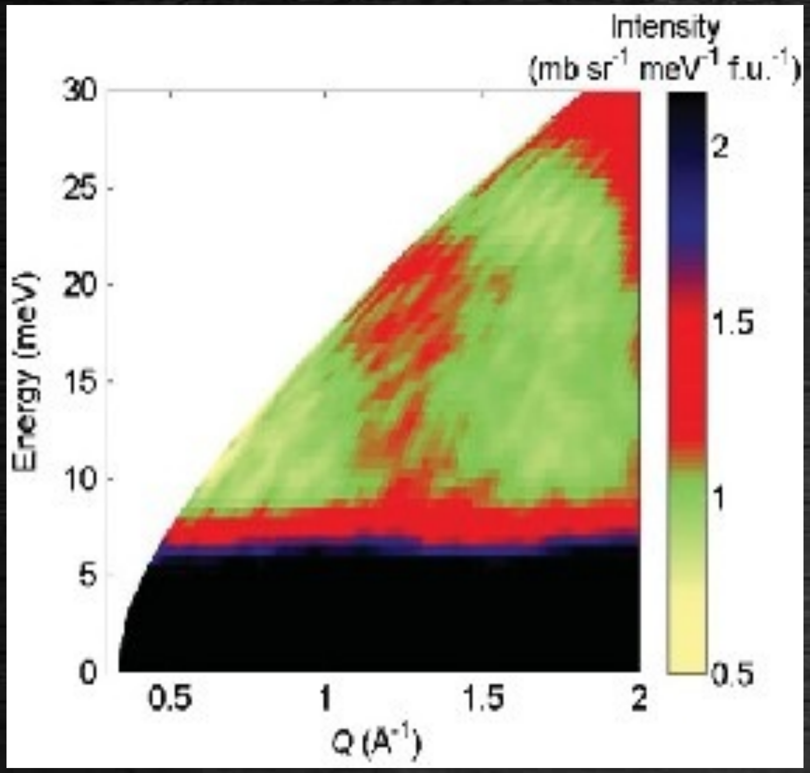
- Experimentally measured Superconducting gap



Model for AF Spin Fluctuation



Taylor *et al.* 2011

- Peaked at $Q=(\pi, \pi)$ with energy $\Omega=6$meV

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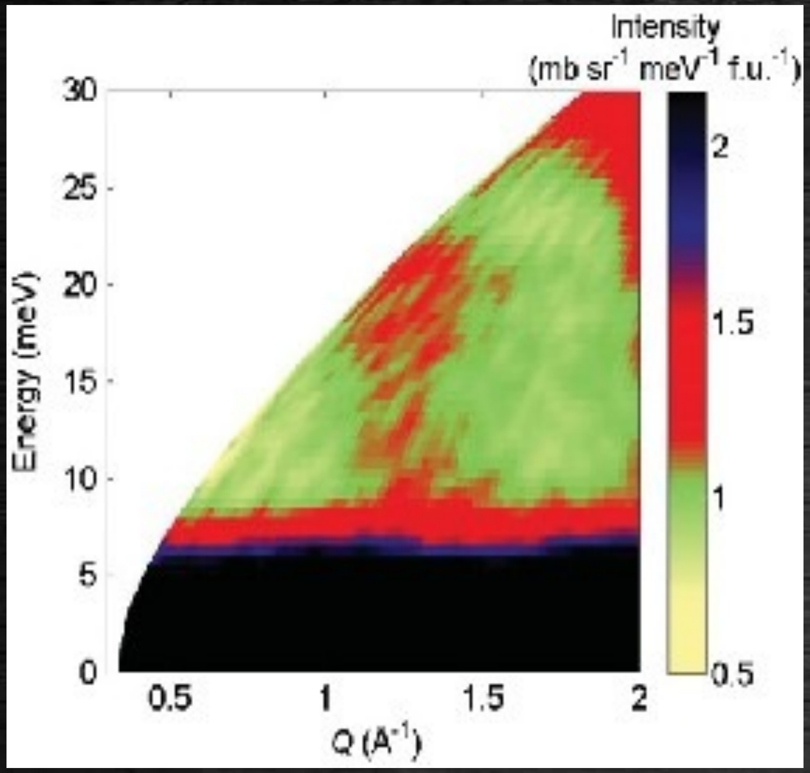

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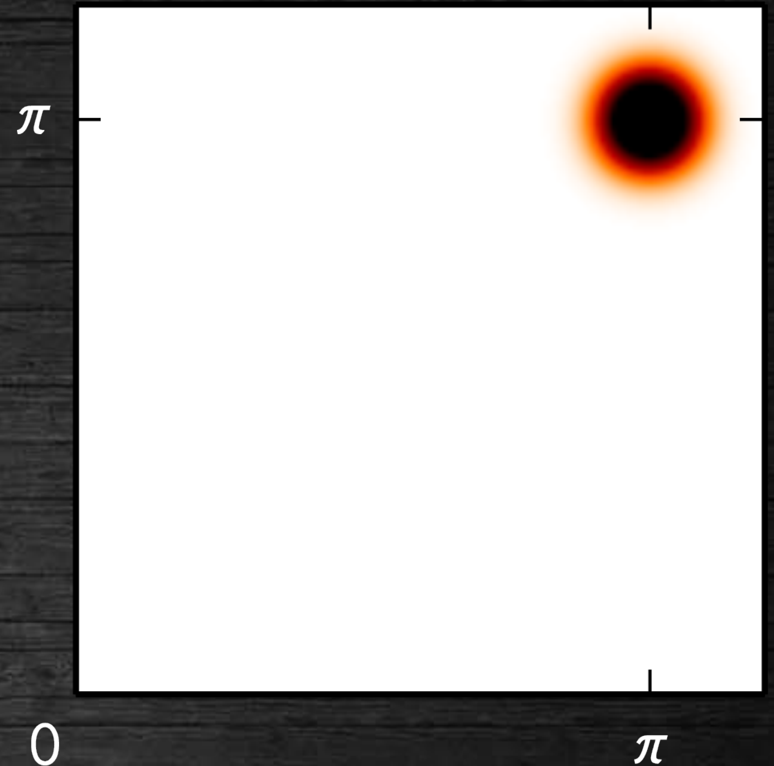
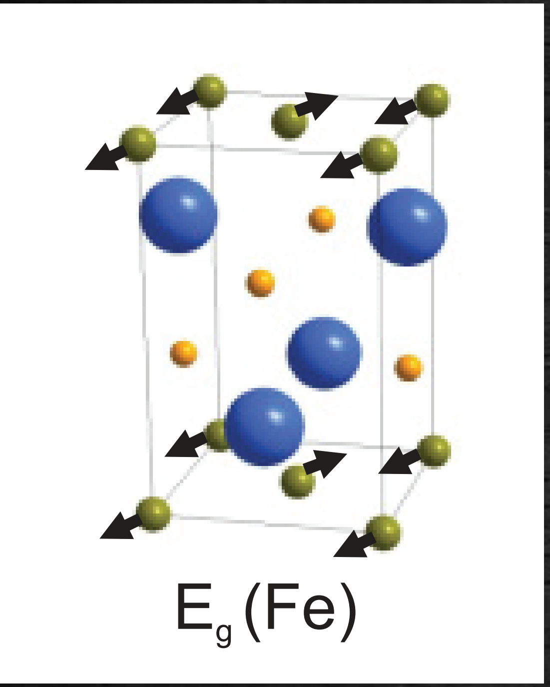


Model Spectral Weight

- Peaked at Q=(π, π) with energy Ω=6meV
- Gaussian with ξ=6a (FWHM: ~12% of π/a)

Eg (Fe) phonon

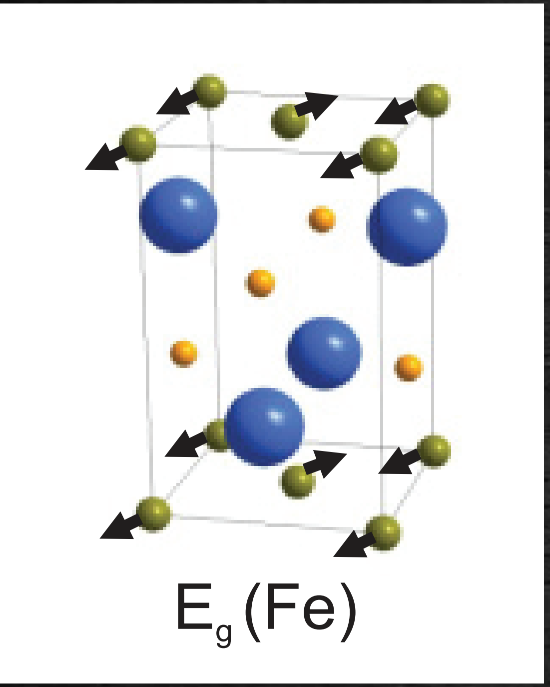
Ω=15meV



- coupling vertex orbital dependent → effective momentum dependence

Eg (Fe) phonon

Ω=15meV



- coupling vertex orbital dependent → effective momentum dependence

- Holstein Eg phonon was shown to induce orbital fluctuations

[Kontani & Onari, PRL 2010]

QPI Calculation with self-energy dressed Greens function

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$$\boxed{\hat{G}^{-1}(\mathbf{k},\omega) = \hat{G}_0^{-1}(\mathbf{k},\omega) - \hat{\Sigma}(\mathbf{k},\omega)}$$

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$$g(\mathbf{q},\omega) \propto \mathrm{Im} \sum_{\mathbf{k}} \left[\hat{G}(\mathbf{k},\omega)\hat{T}\hat{G}(\mathbf{k}+\mathbf{q},\omega)\right]^{11}$$

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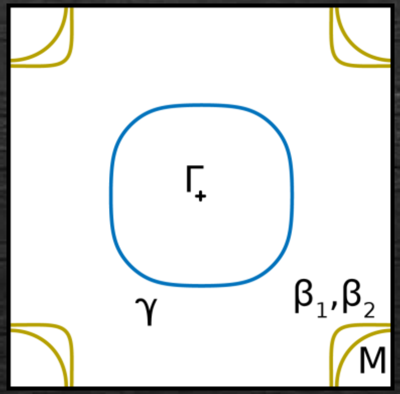

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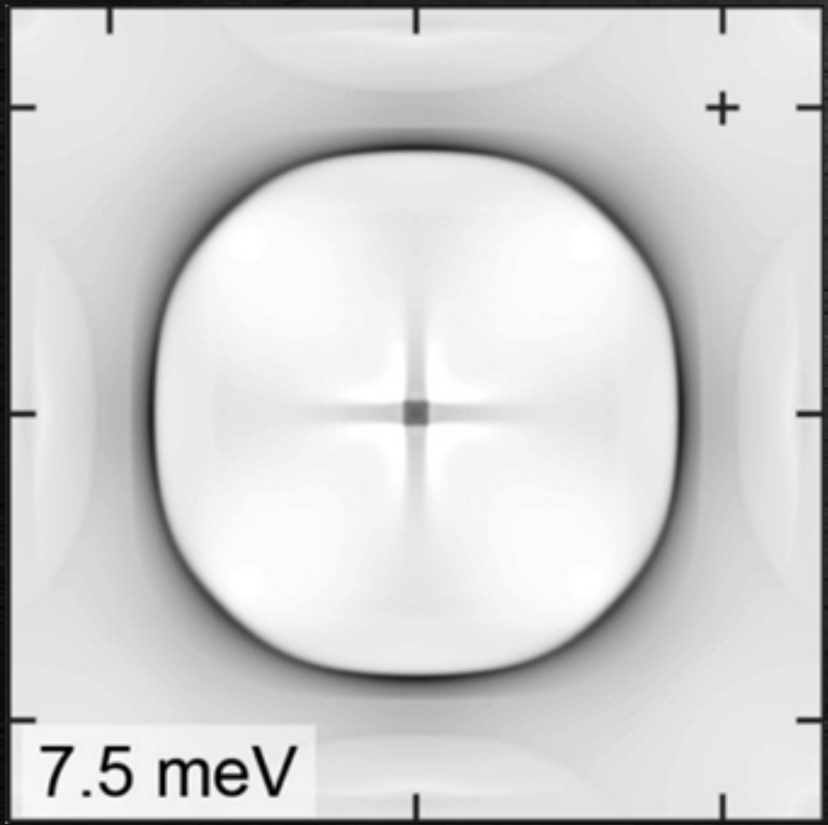
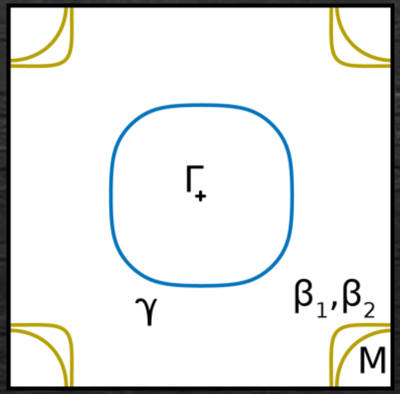


$g(\mathbf{q}, \omega)$ (T-matrix)



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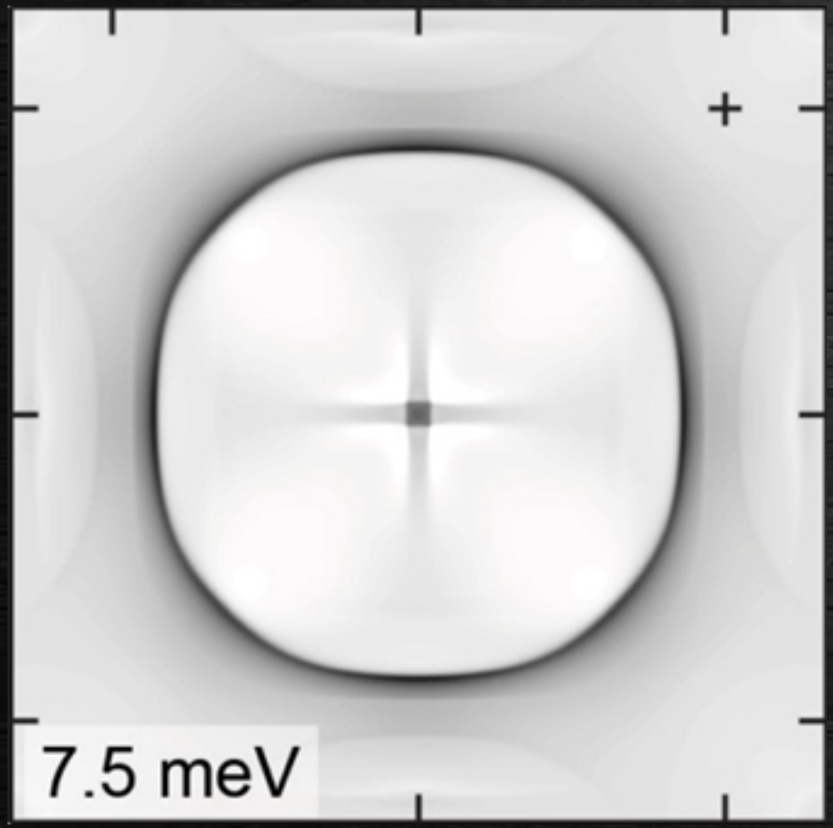

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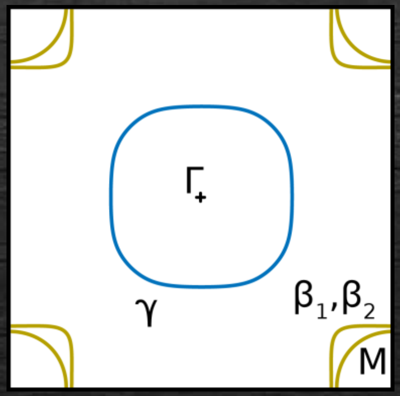
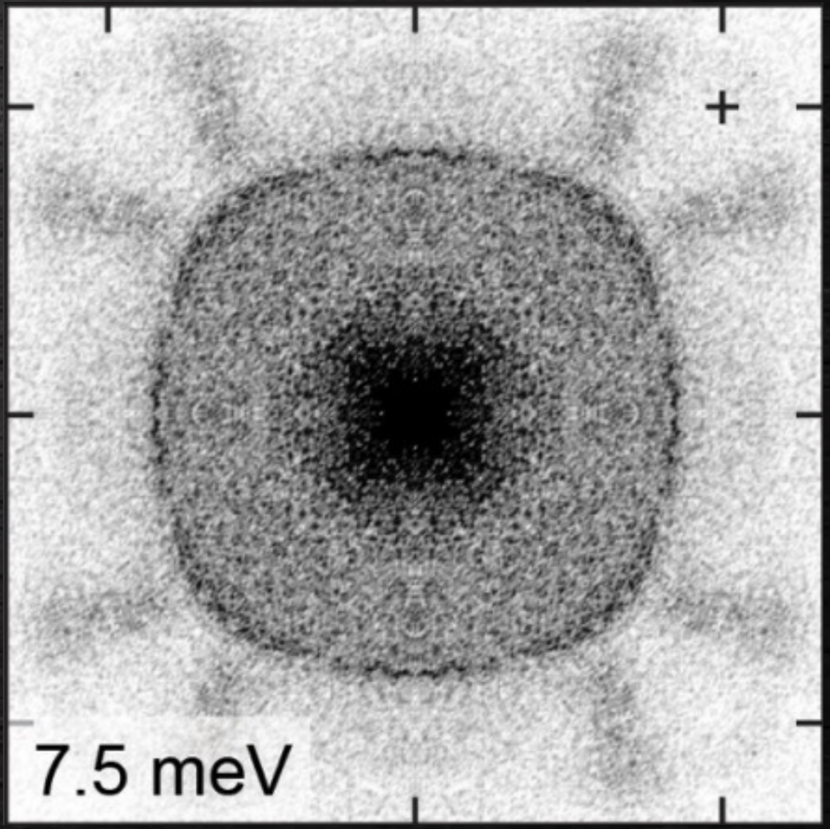


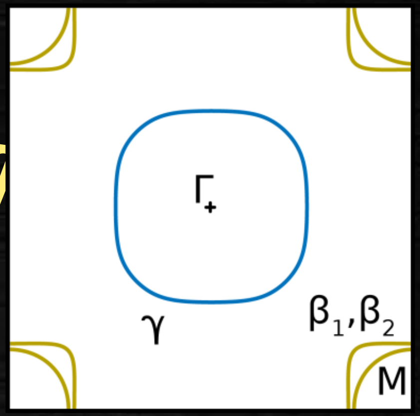


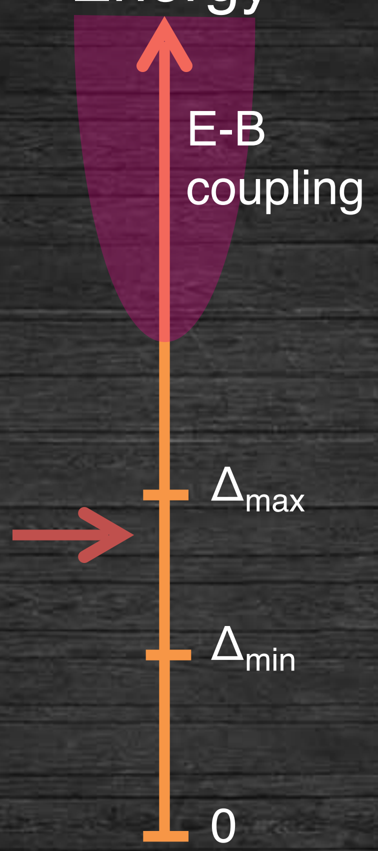
$g(\mathbf{q}, \omega)$ (STS)

Comparison of
Theory and Experiment

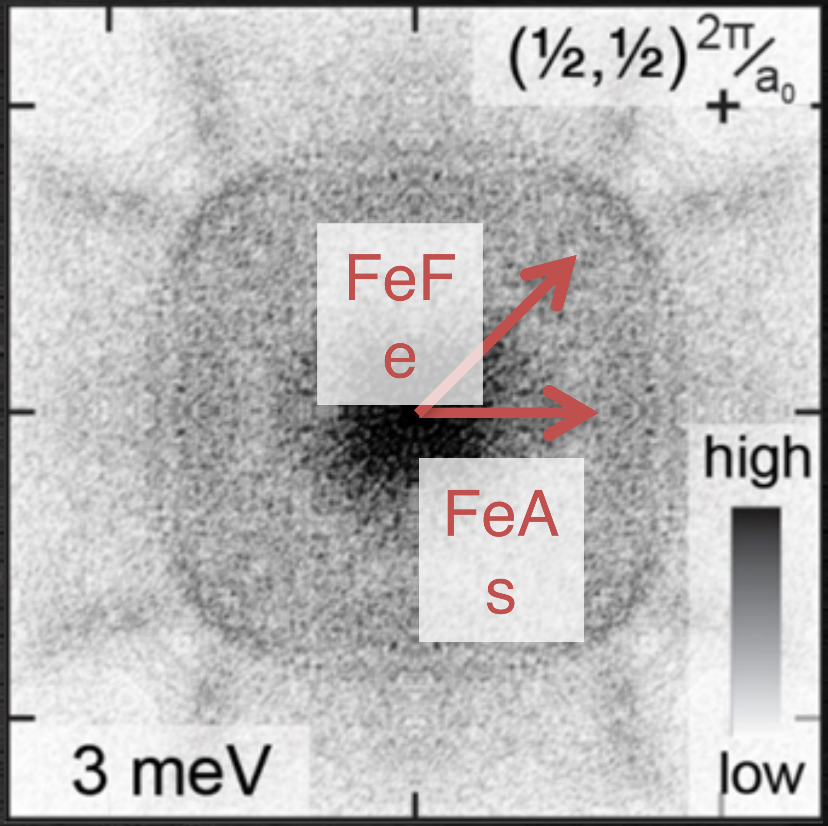
Self-energy due to AFSF

Energy Dependent Anisotropy





STS



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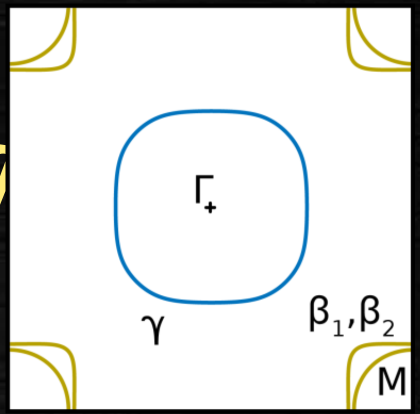

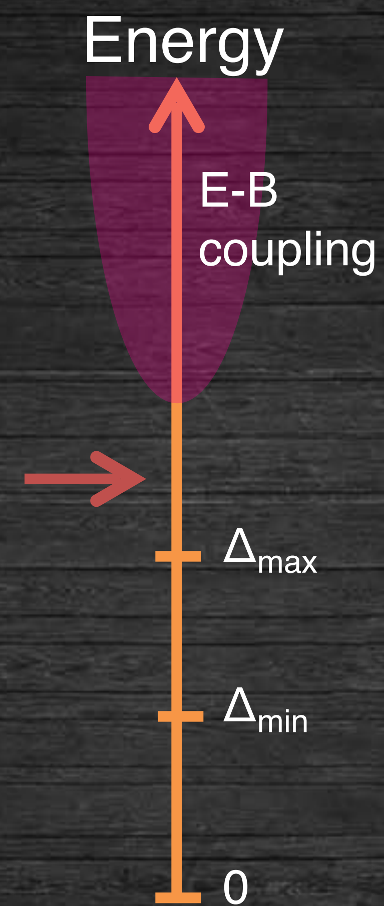

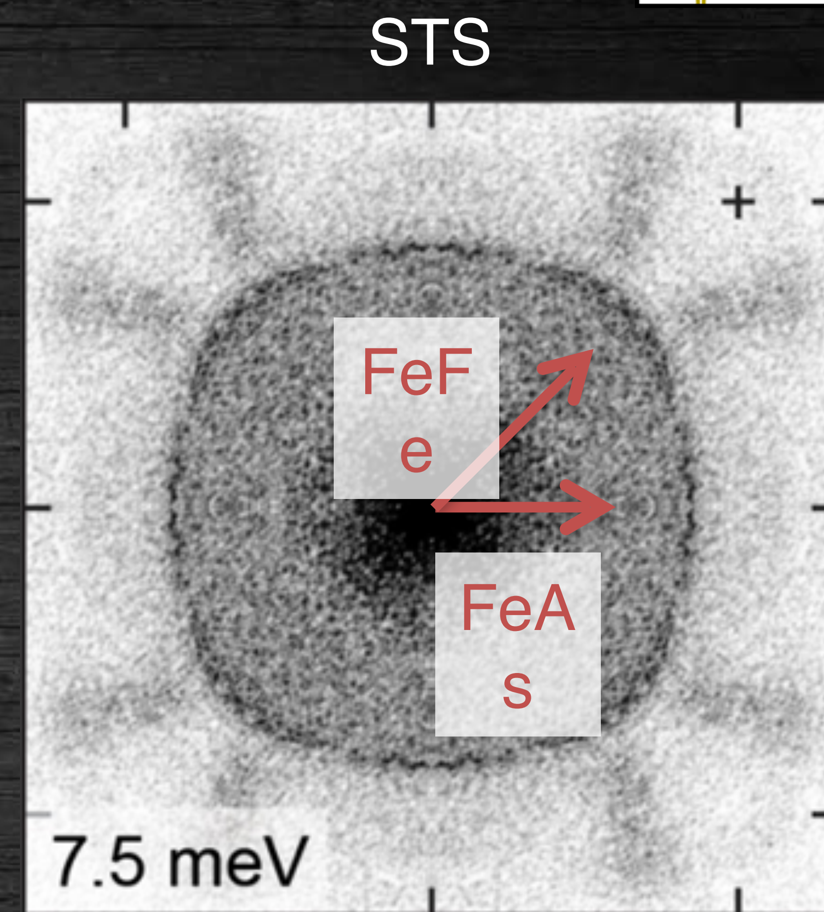

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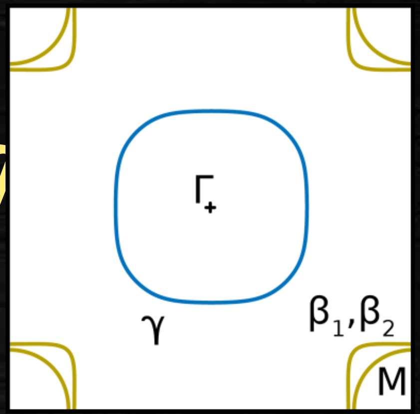

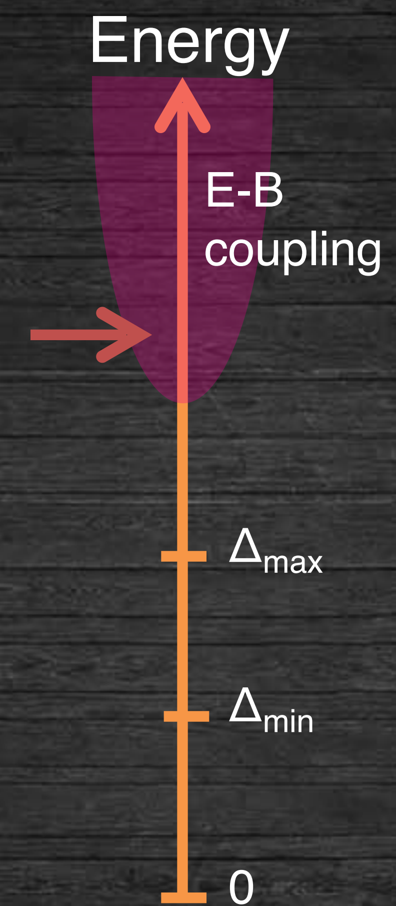

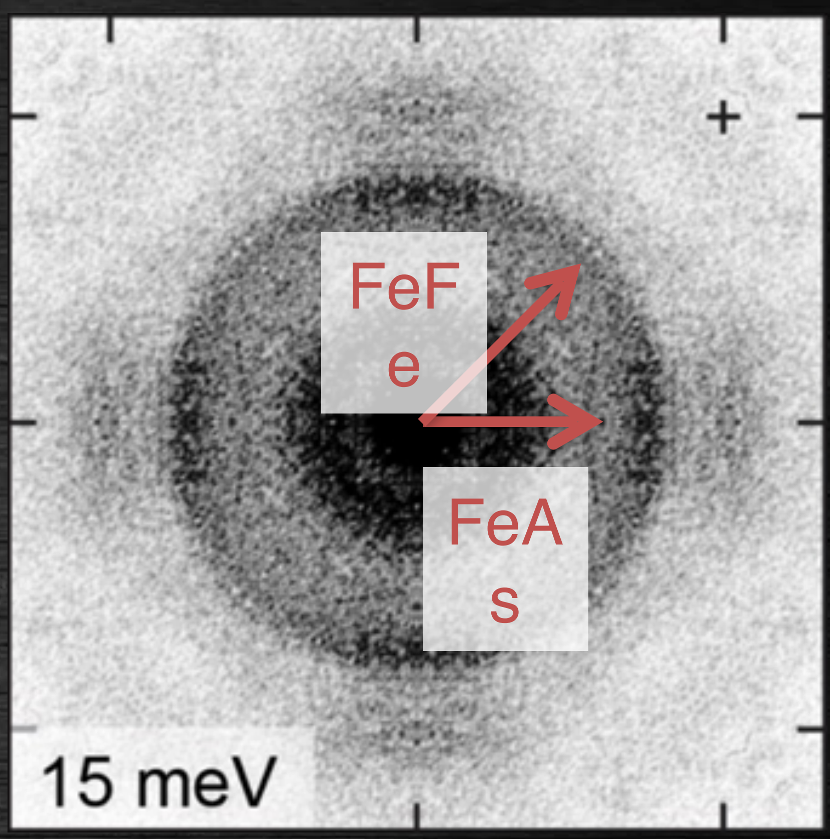

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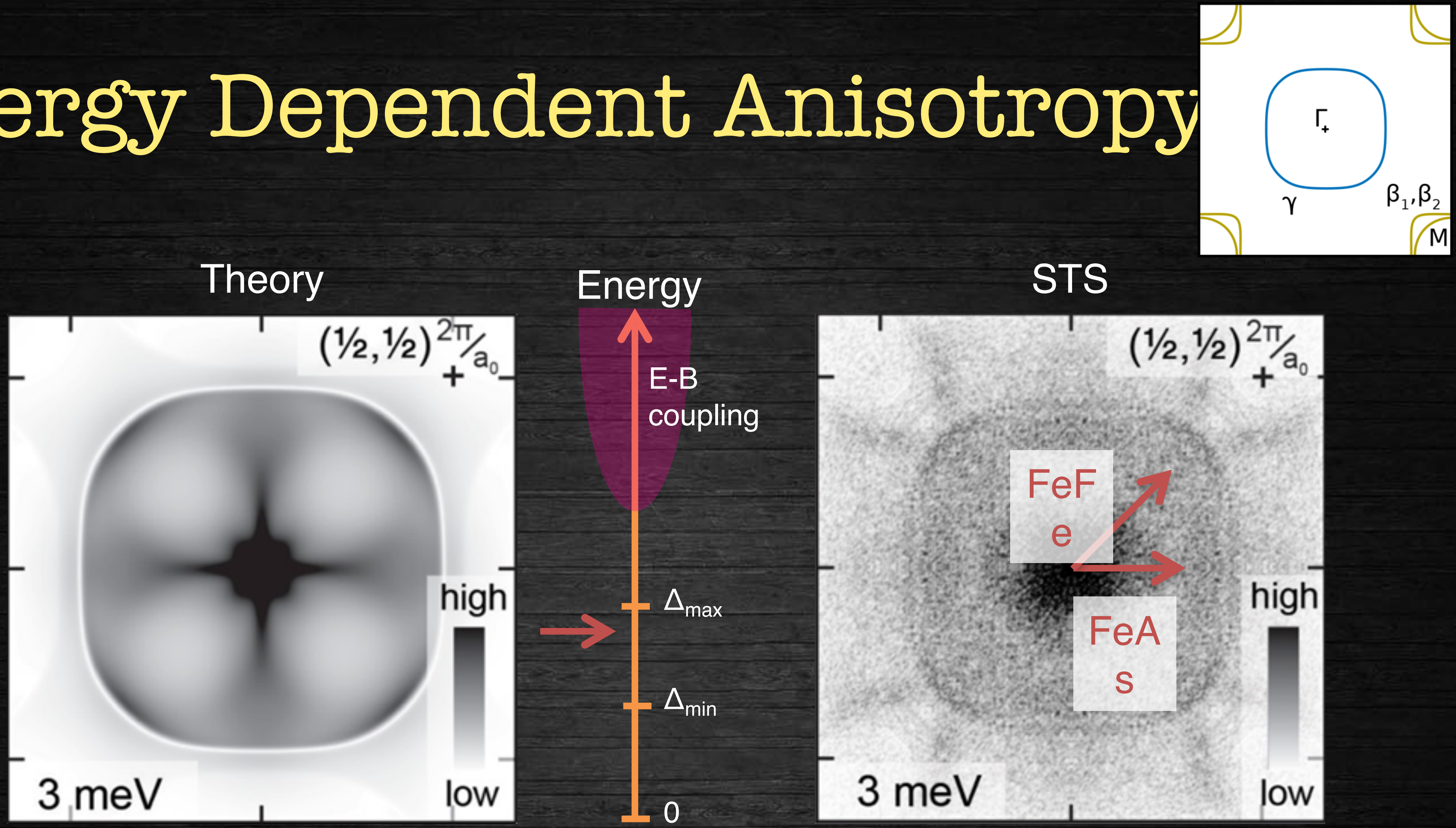

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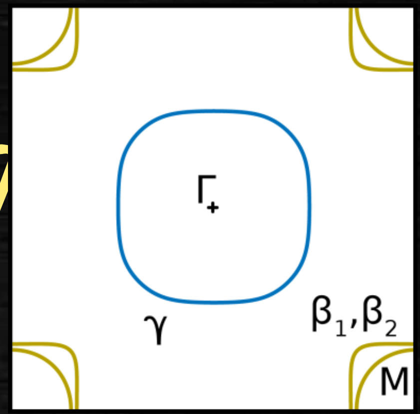
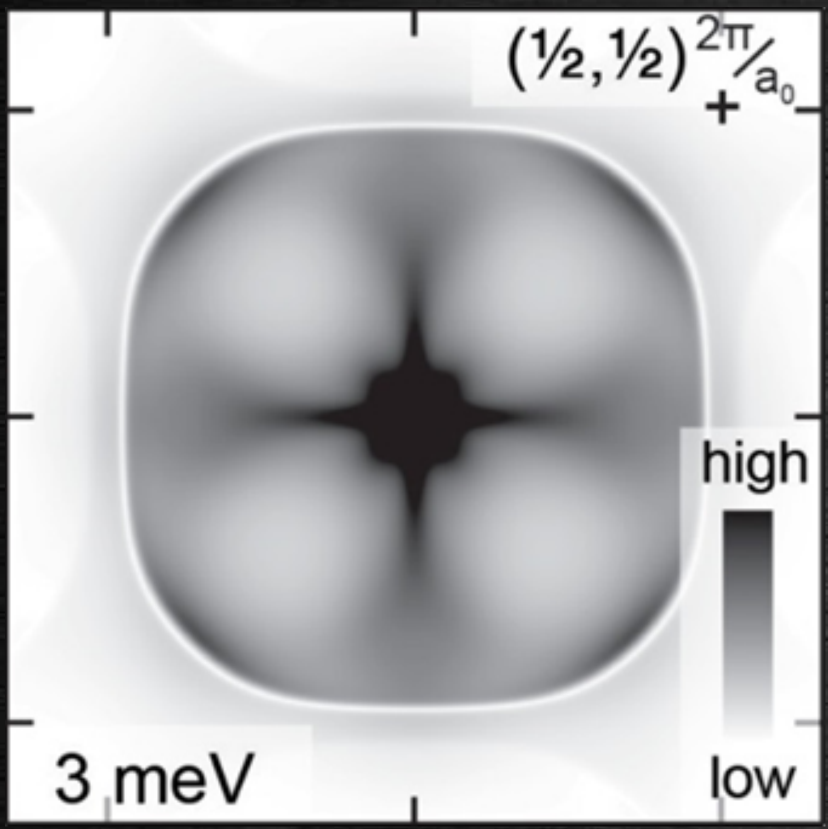
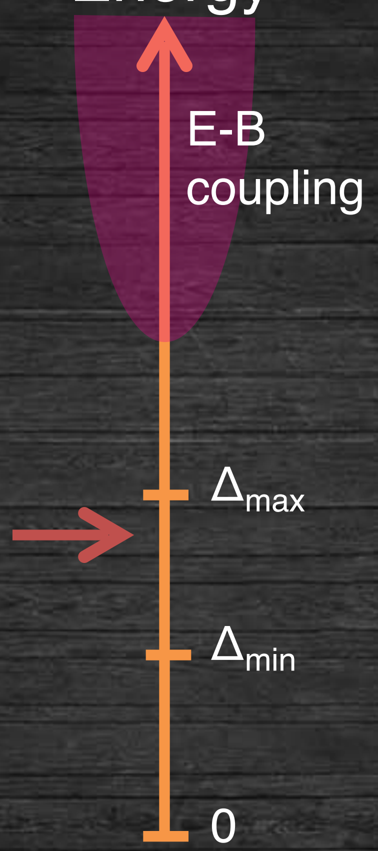


Theory





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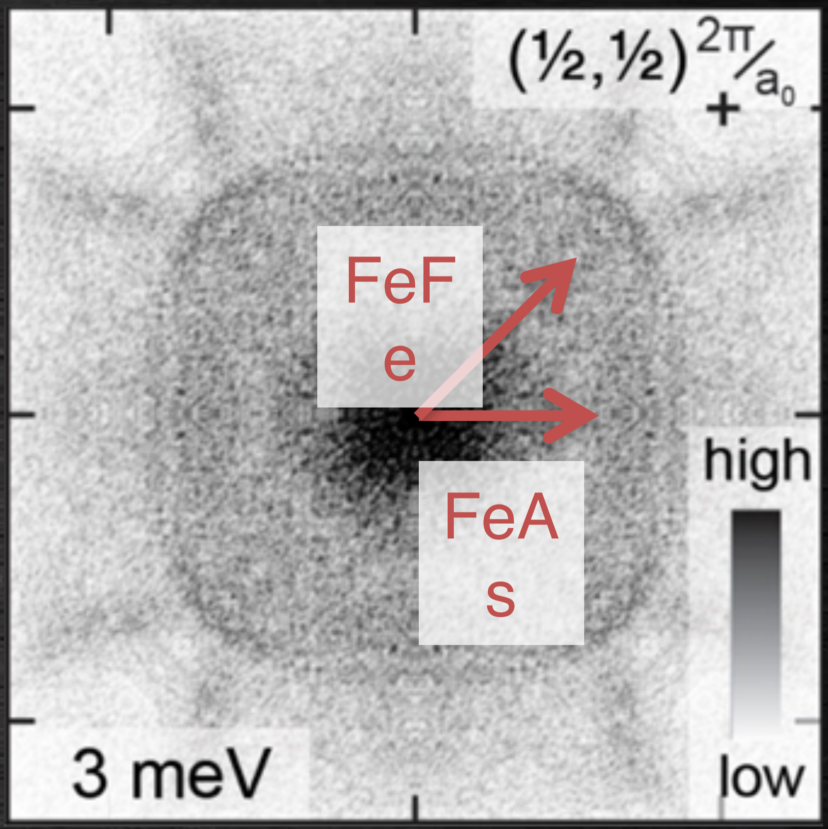
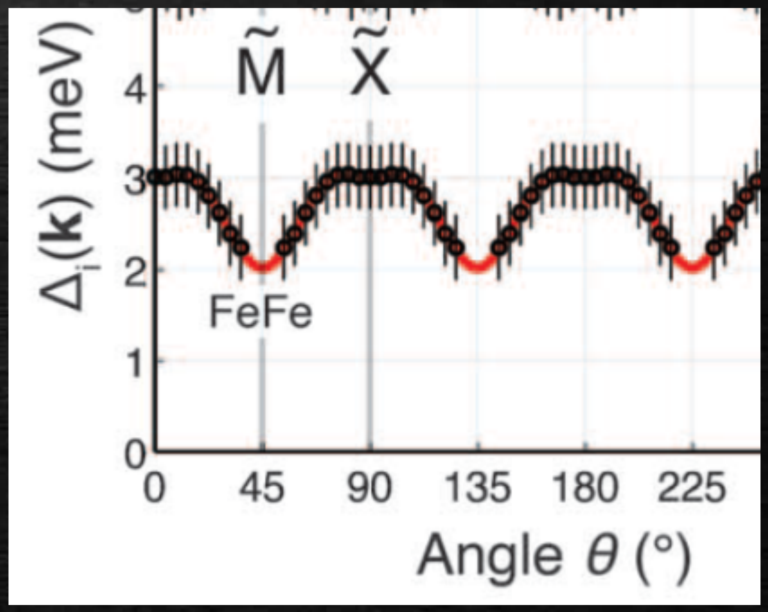
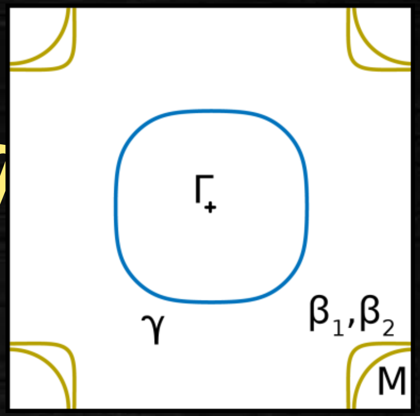
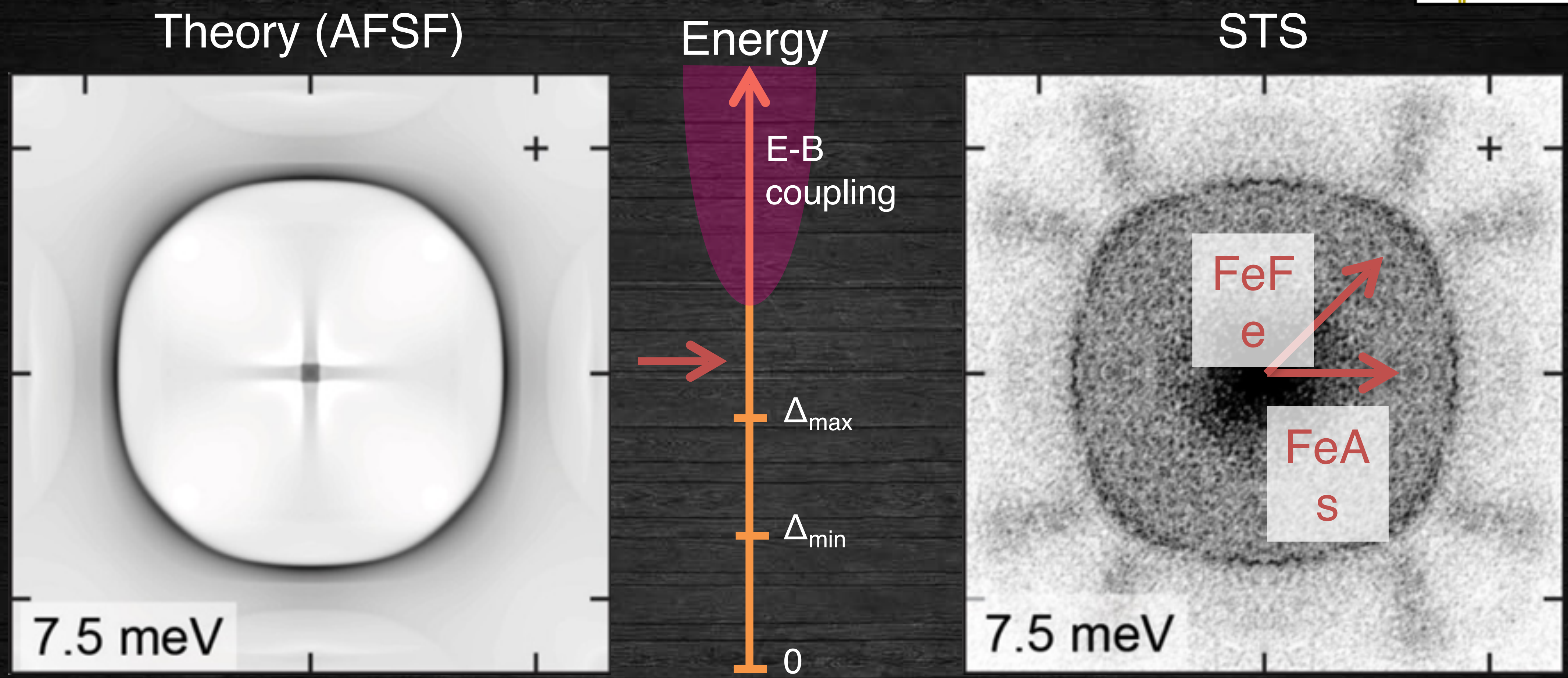




Low energy anisotropy due to gap anisotropy

Energy Dependent Anisotropy





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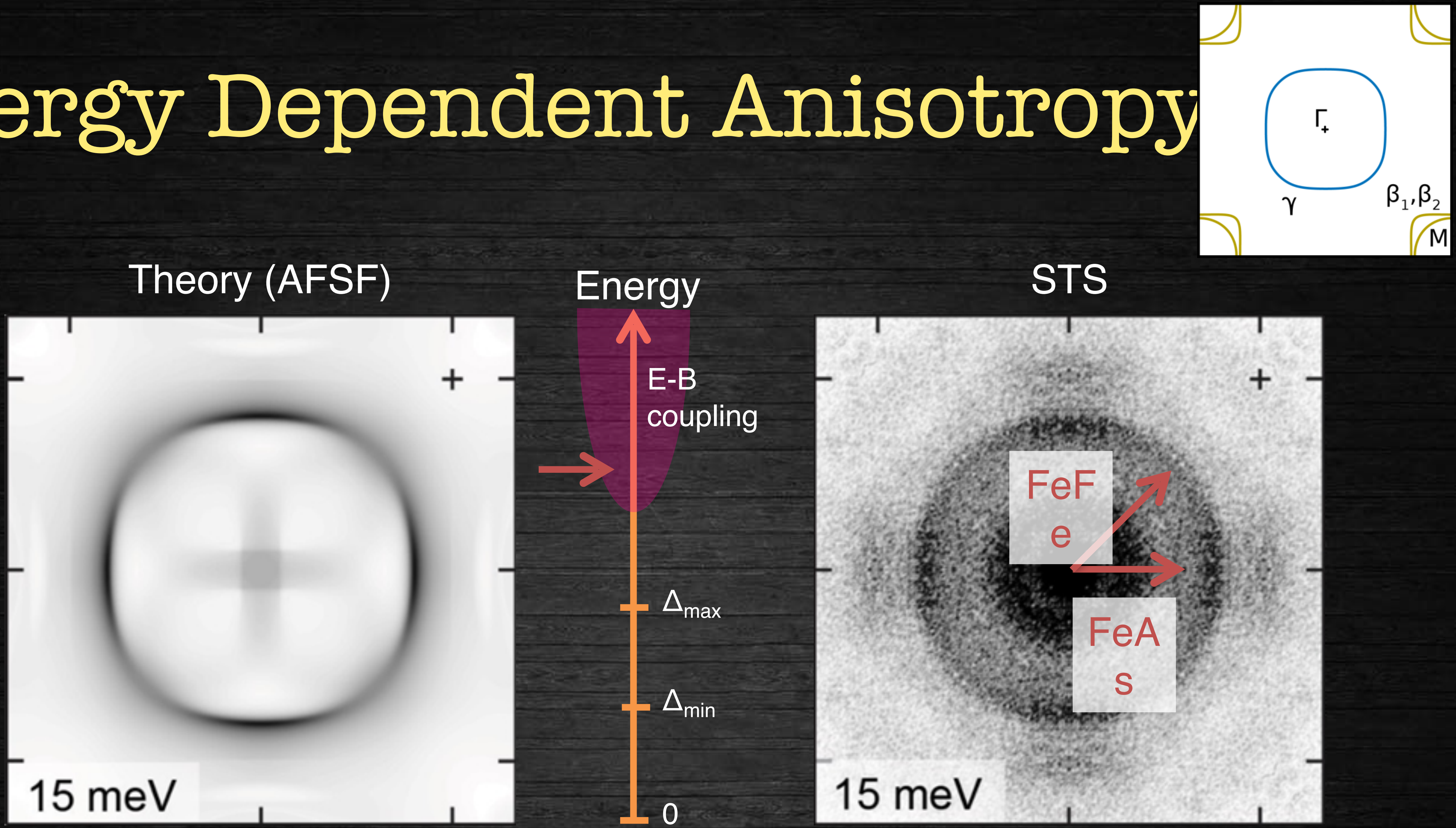

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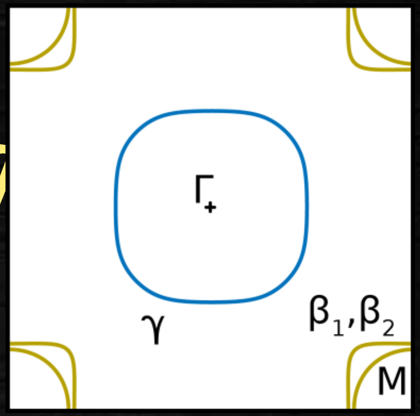
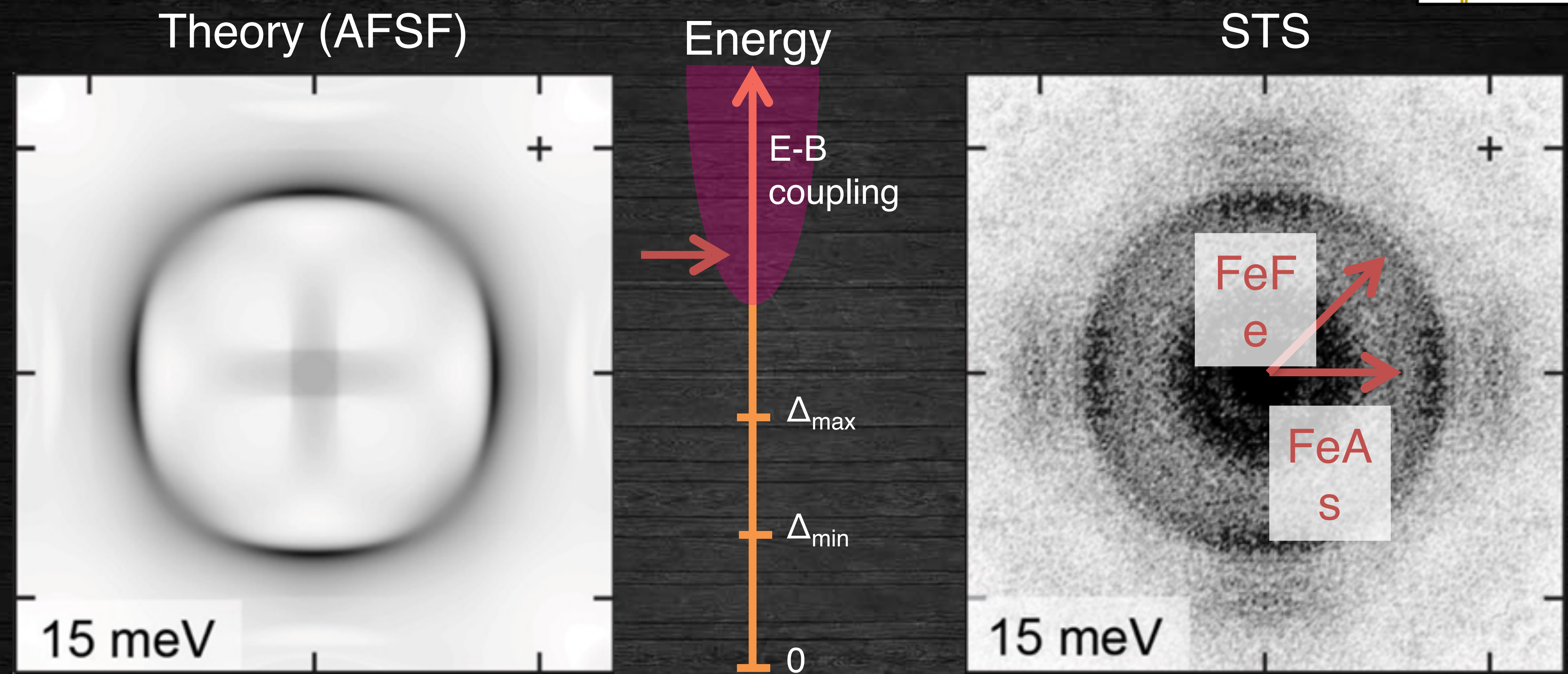




- High energy self-energy effect
  - Intensity suppressed along Fe-Fe

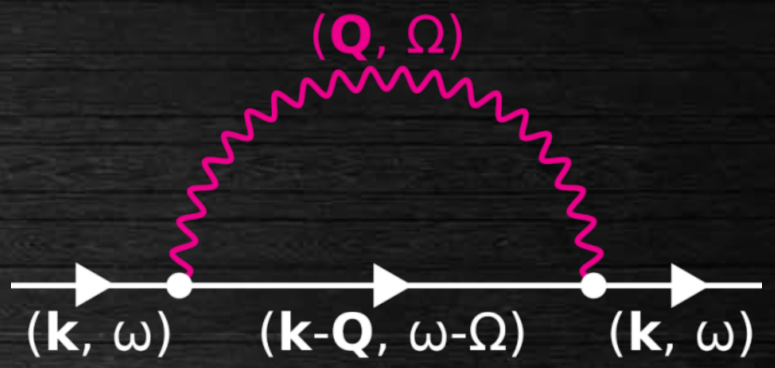
Insight from Kinematics

Insight from Kinematics

- AFSF centered at (Q, Ω)
  - Strong self energy effect when satisfying

$$\omega^{\gamma}_{\mathbf{k}} = \omega^{\beta}_{\mathbf{k}-\mathbf{Q}} + \Omega$$

  - AFSF couples γ pocket to β_1 and β_2
  - *Energy dependent anisotropy*



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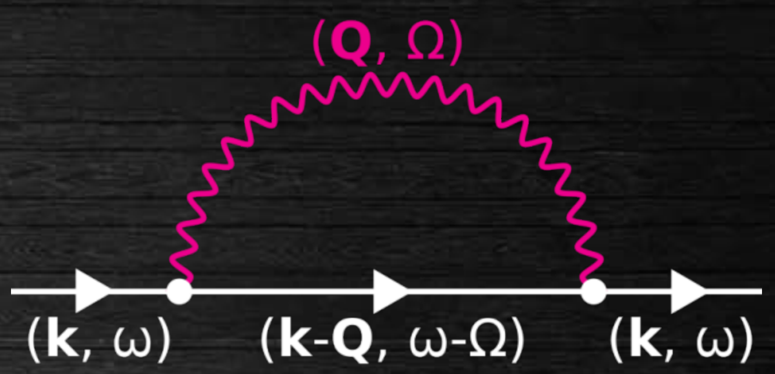
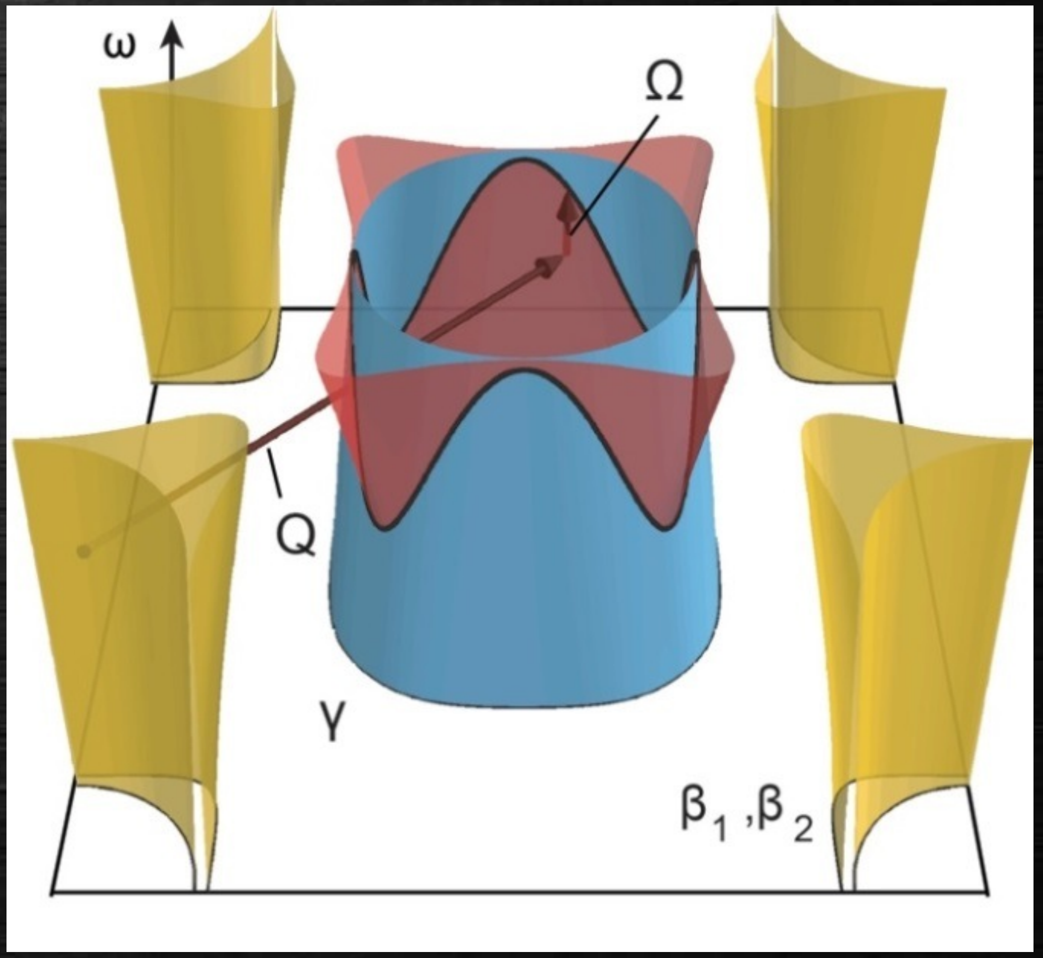
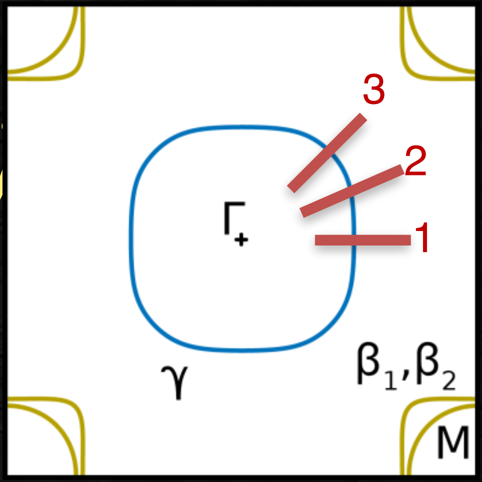
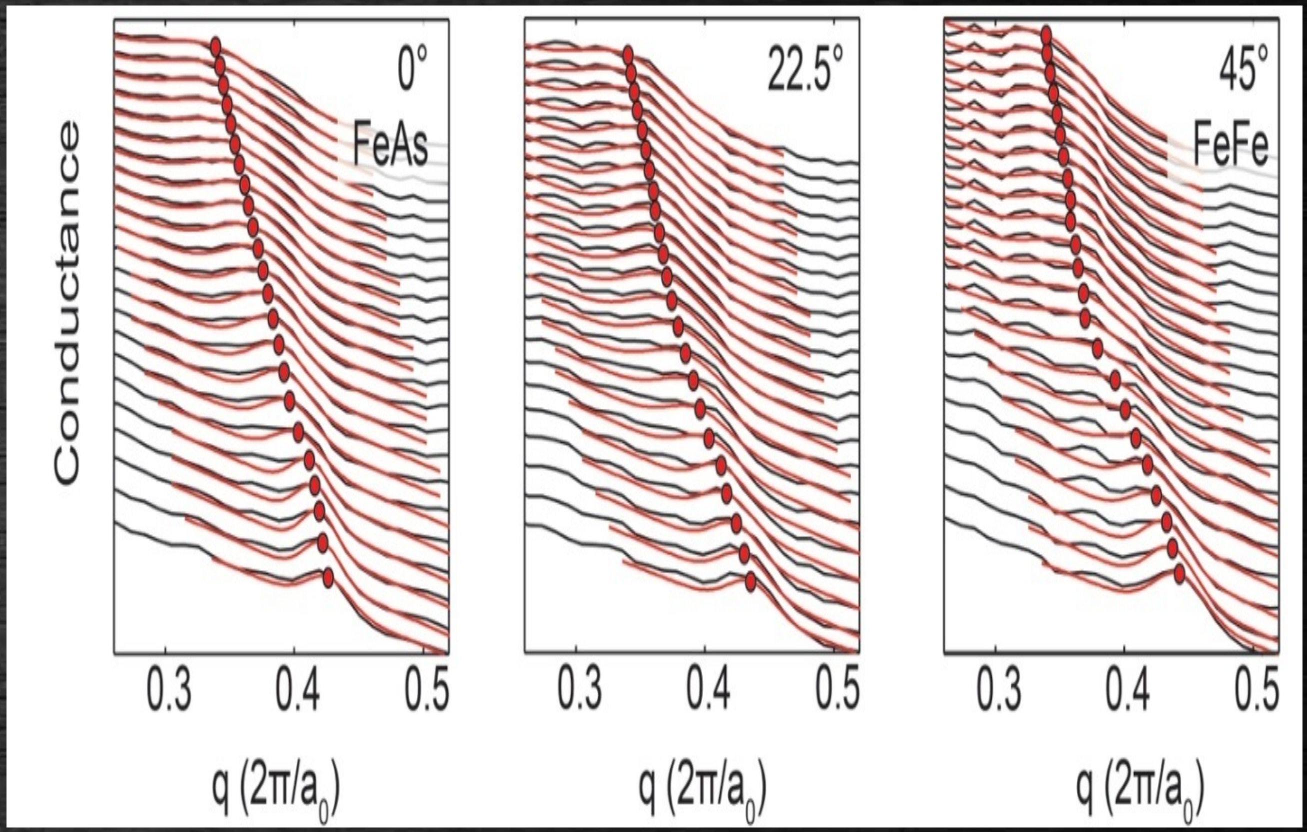




Energy Dependent Anisotropy



- STS



Energy Dependent Anisotropy

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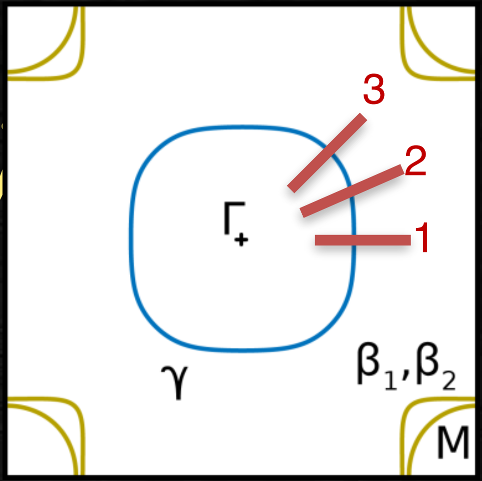
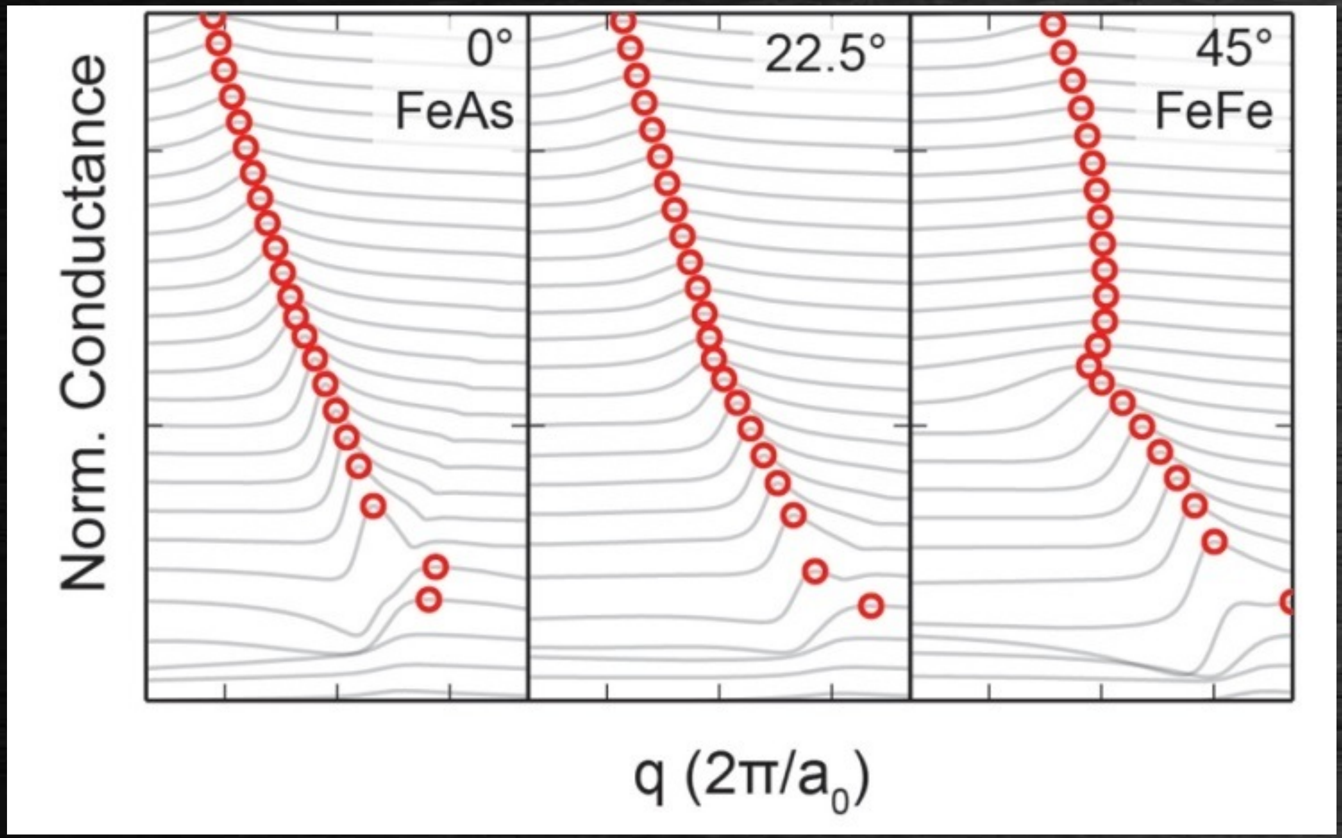
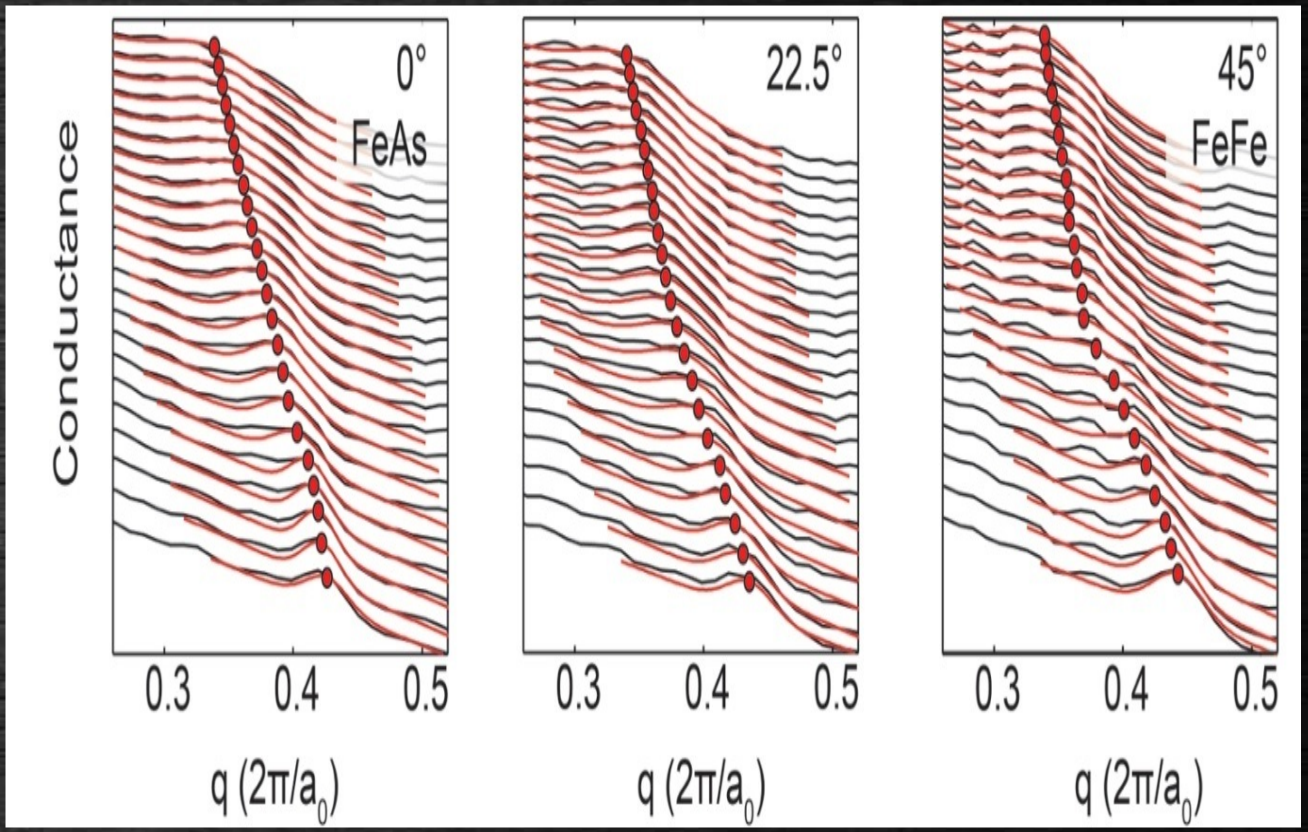
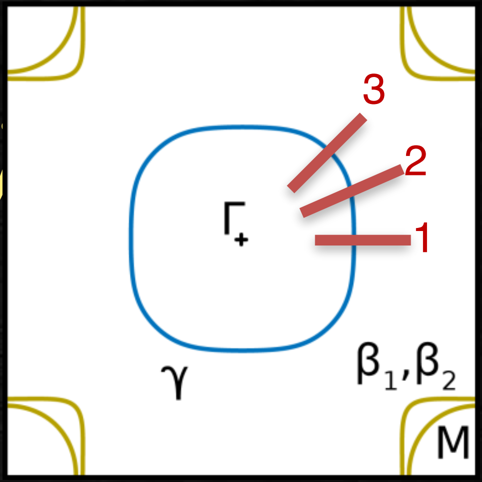


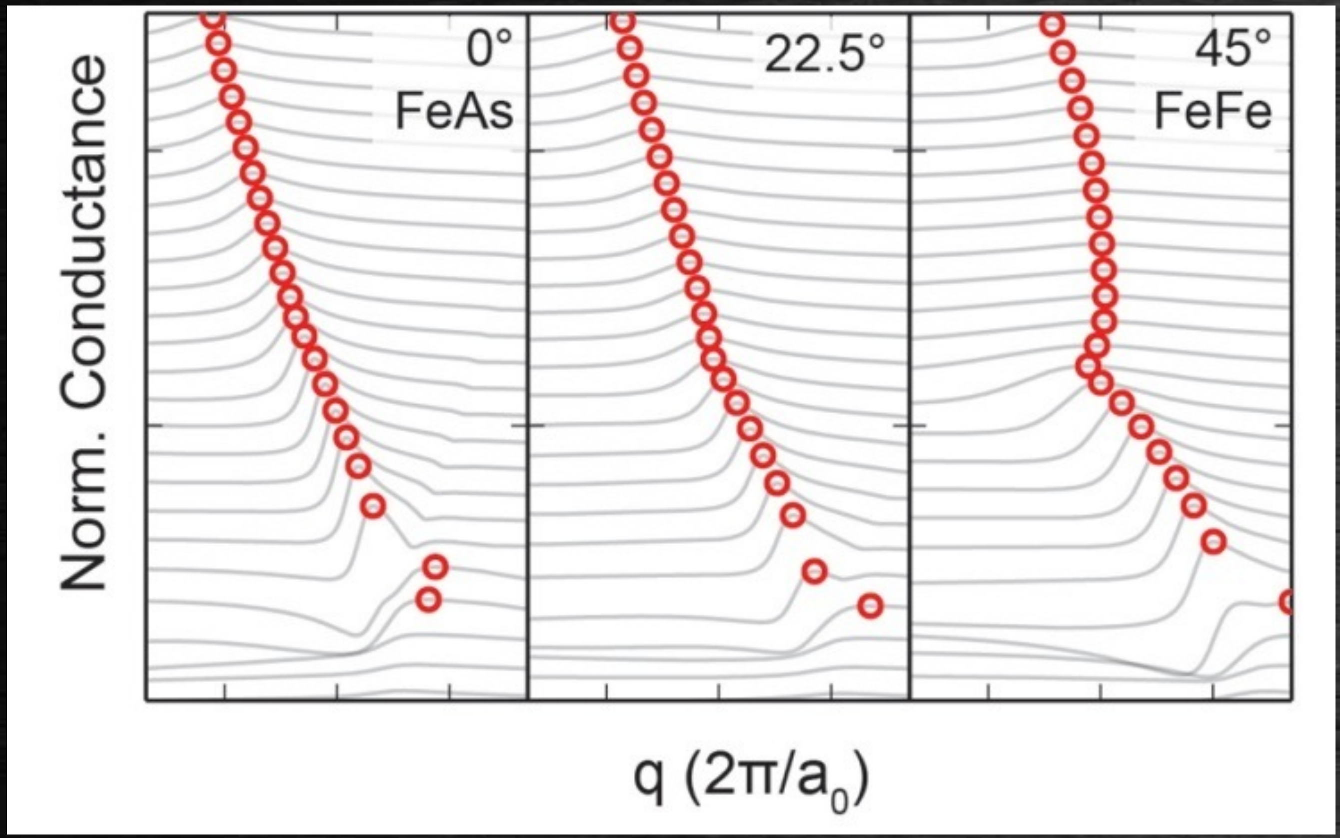


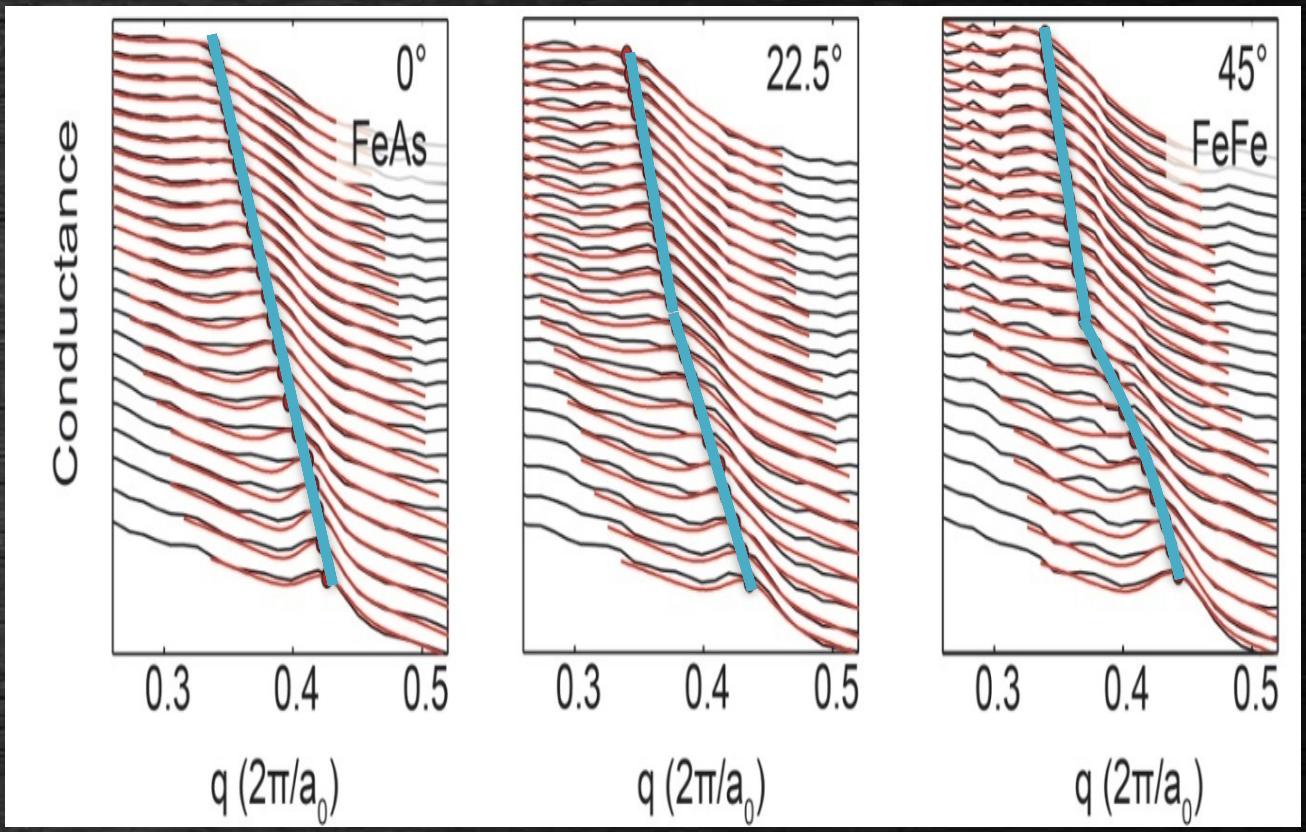


Energy Dependent Anisotropy



- Theory (AFSF)
- STS





Self-energy due to Eg phonon

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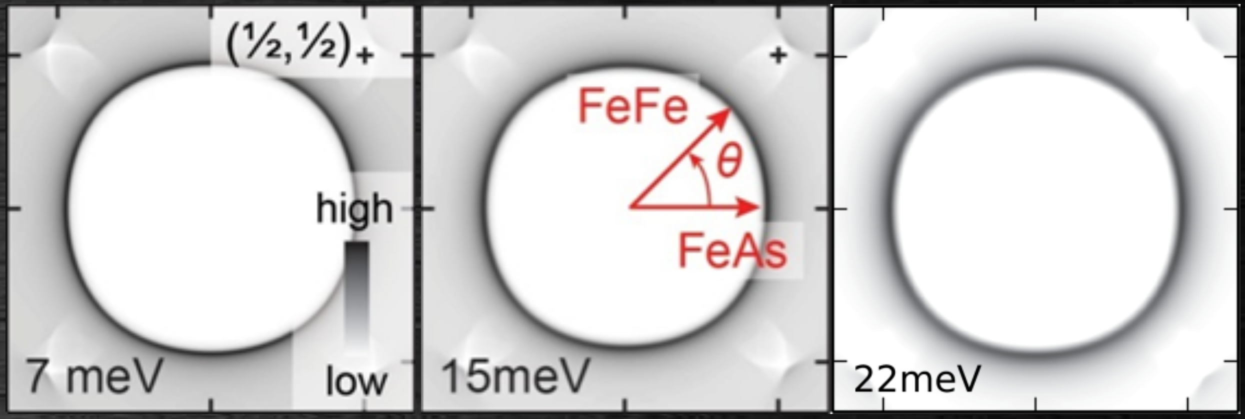

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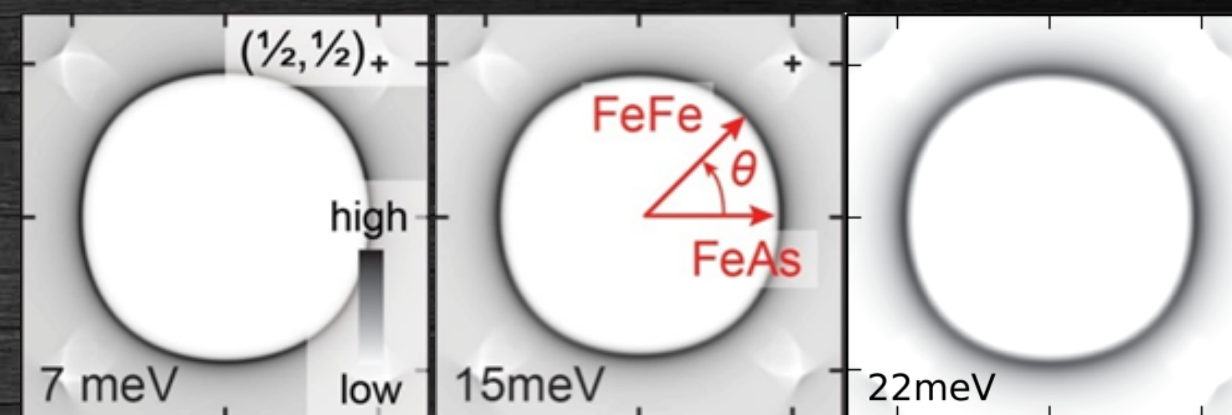

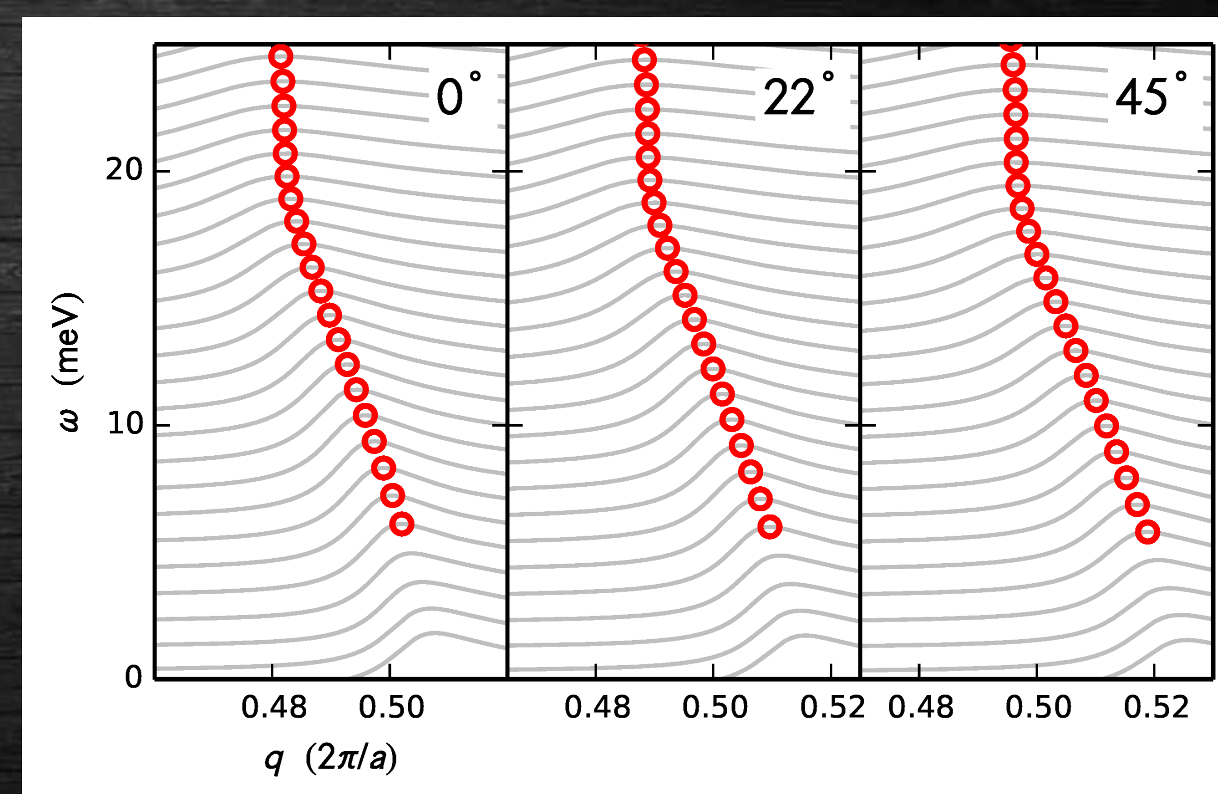

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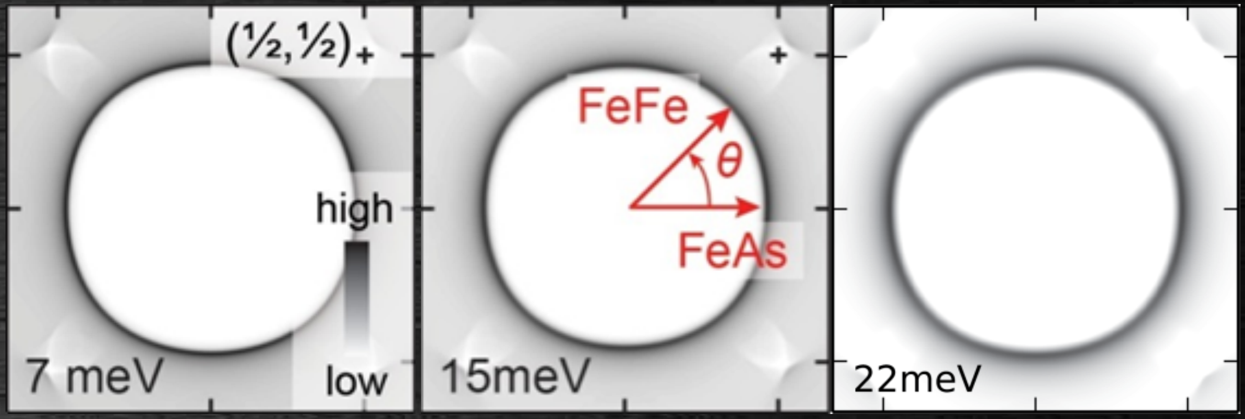

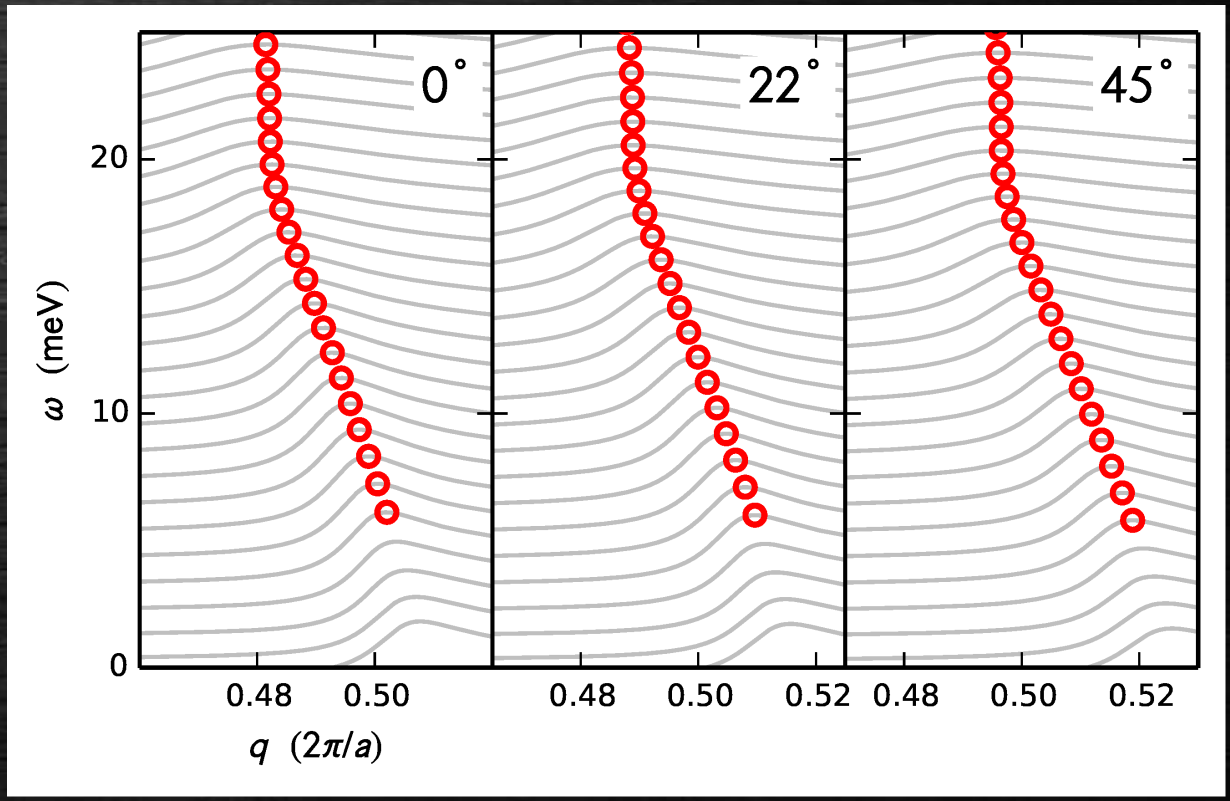

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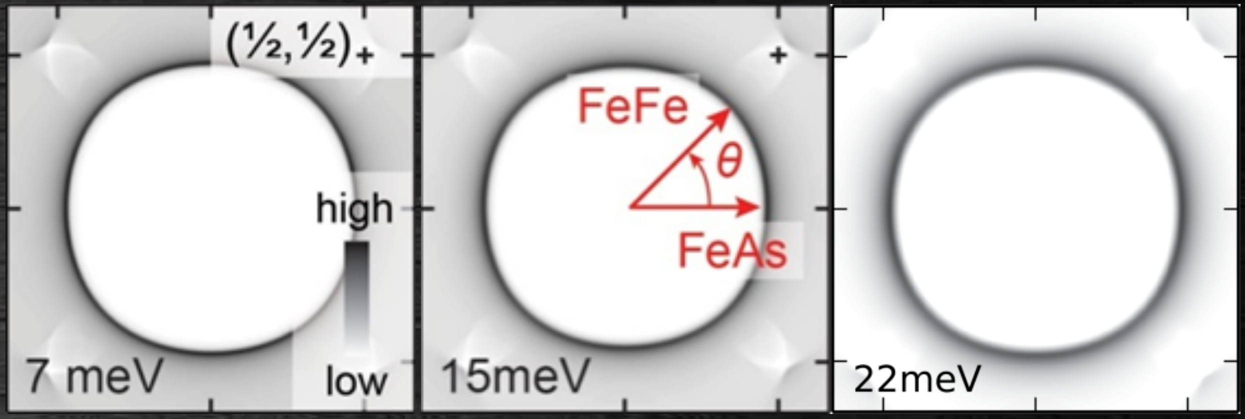
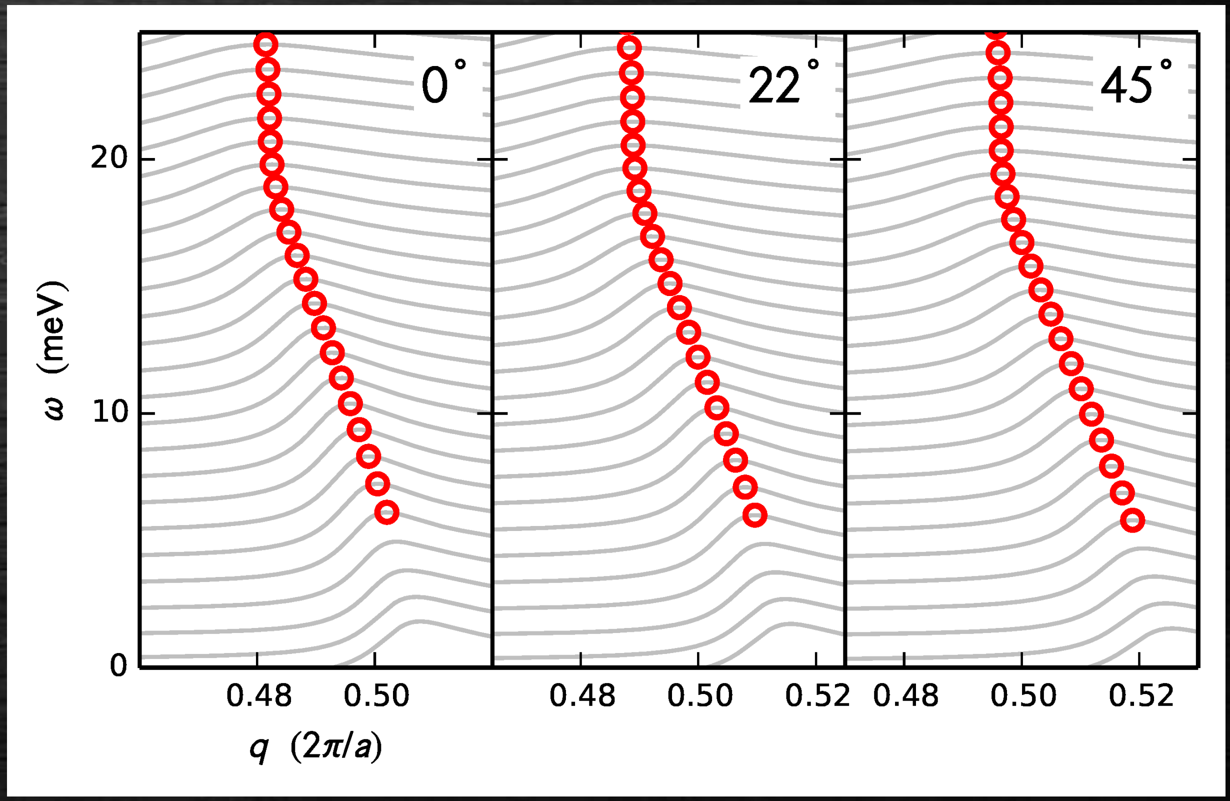


- Isotropic self energy on γ
  - uniform orbital character (d_{xy})
  - kinematics predicts no anisotropy



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- Lowest order self-energy due to electron-boson coupling

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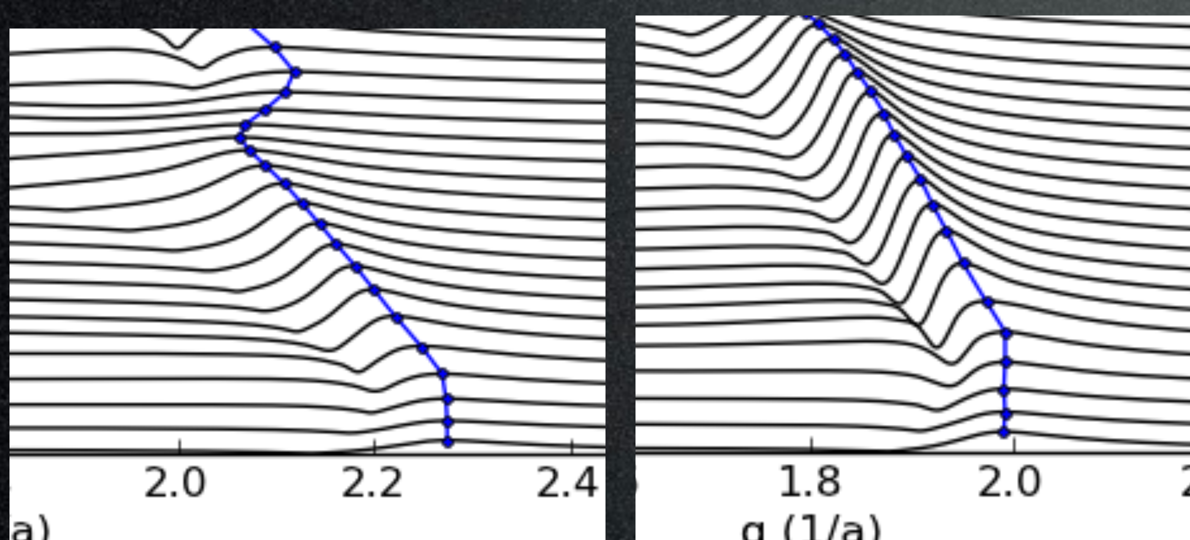
Fe-Fe Fe-As



Mechanism:Summary

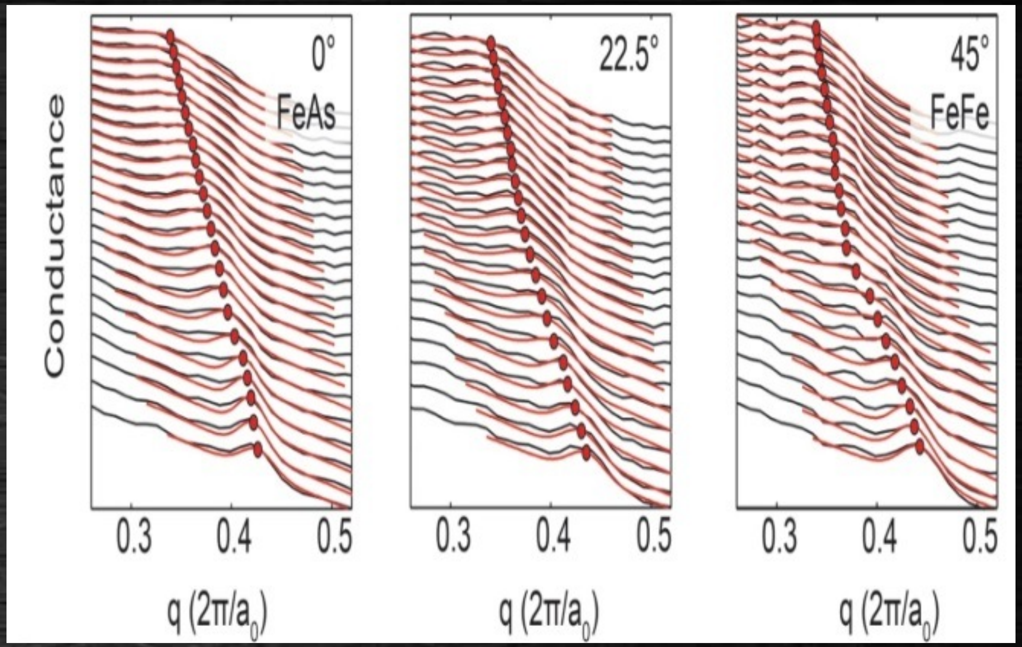
Allan, Lee etal, arXiv:1402.3714, to appear in Nat. Phys.

- Fingerprint of electron-boson coupling in LiFeAs

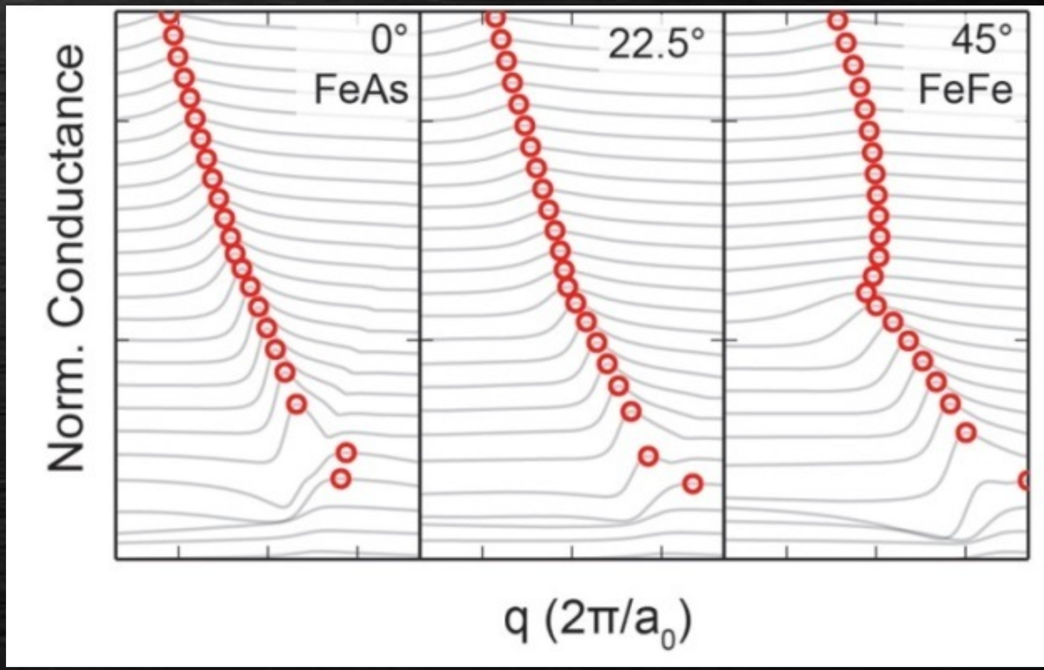
  :energy selective anisotropic self-energy

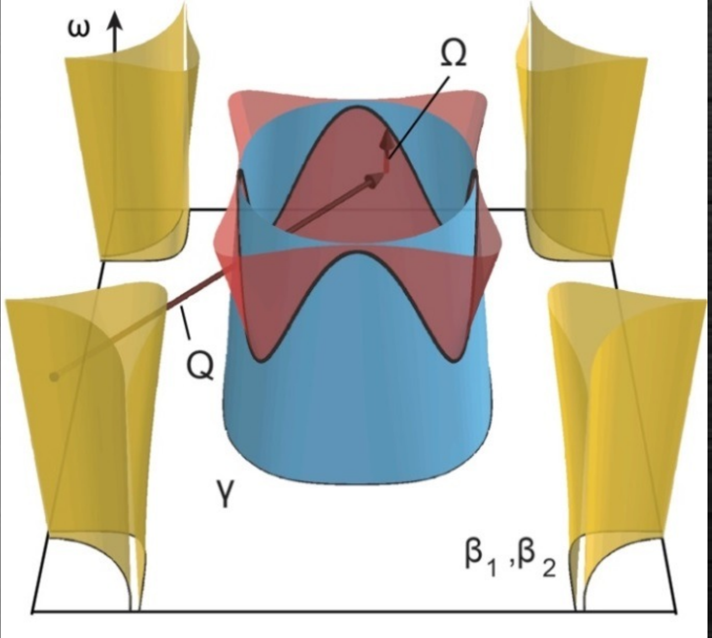
- Mode at finite Q→ anisotropic self energy

STS



AFSF





Collaborators

Experimentalists

J.C. Davis (Cornell, BNL)
H. Eisaki (AIST)
K. Fujita (Cornell)
ChungKoo Kim (Cornell)
Y. Kohsaka (RIKEN)
Jihnhwan Lee (KAIST)
K. Shen (Cornell)
A. Schmit (Berkeley)
S. Uchida (U-Tokyo)

Theorists

M. Lawler (SUNY Binghamton)
A. Mesaros (Cornell, Leiden)
J. Sethna (Cornell)
S. Sachdev (Harvard)
J. Zaanen (Leiden)
Kyungmin Lee (Cornell)
Mark Fischer (Cornell)
Arun Paramekanti (U Toronto)

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Allan, Lee et. al., to appear in Nature Physics (2014)
Fischer, et. al., to appear in NJP (2014)