Microscopic Theory of Coupling of Quantum-critical Fluctuations to Fermions and Superconductivity in Cuprates.

Work done in the last 3 years with

Vivek Aji,
Arcadi Shehter,
Lijun Zhu

following the discovery of Loop-current order in underdoped Cuprates.

Schematic Universal phase diagram of high-T_c superconductors

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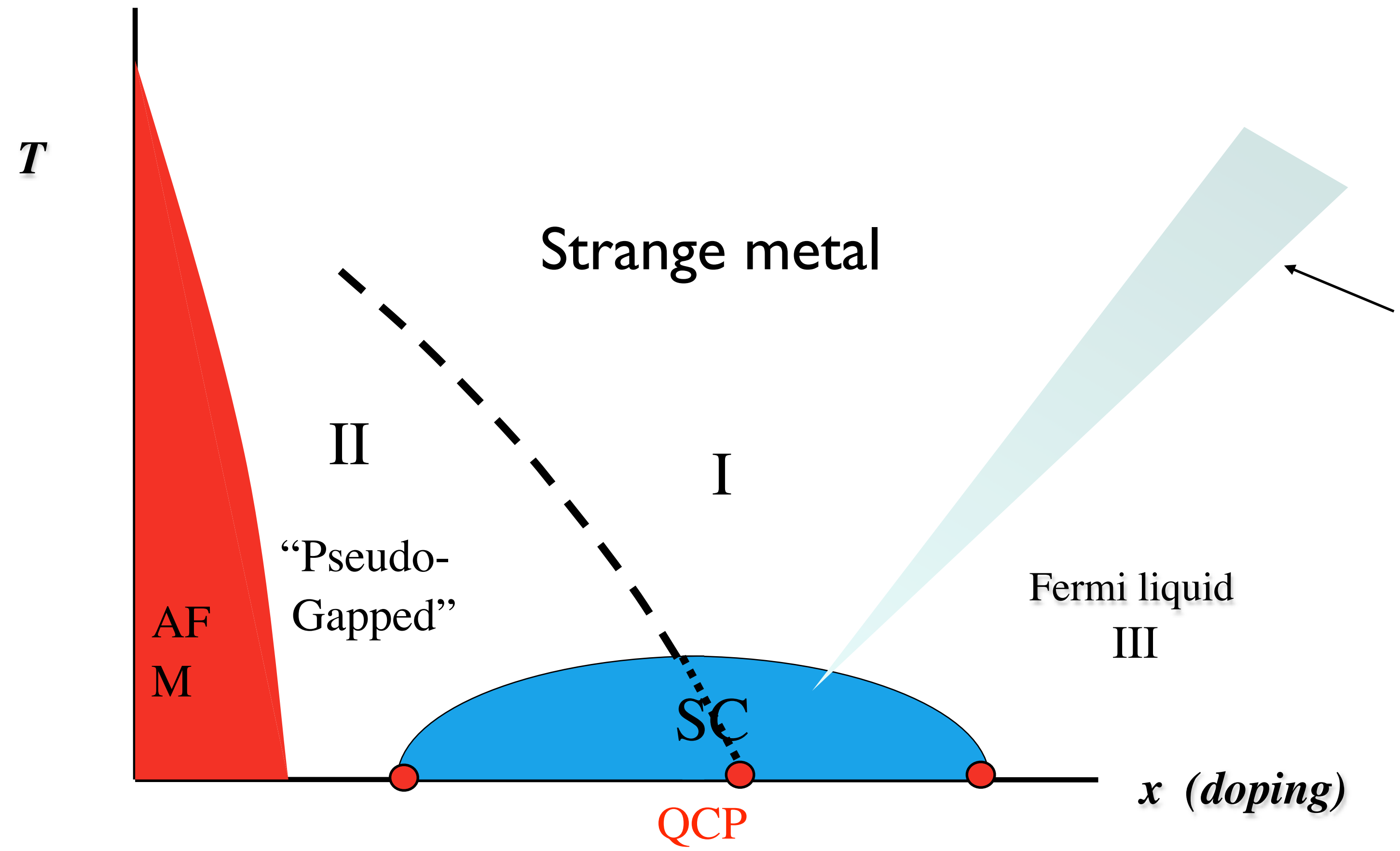

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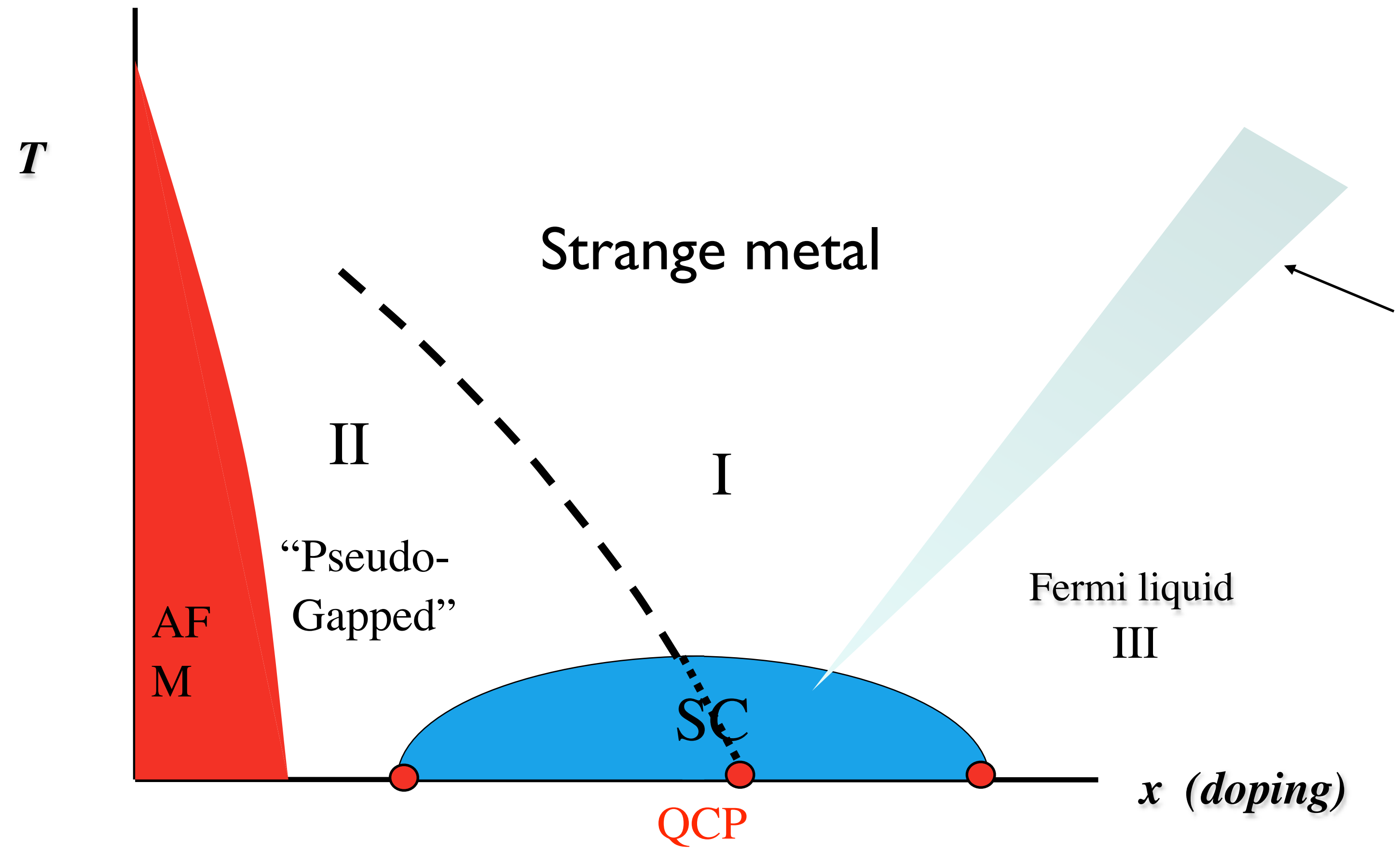
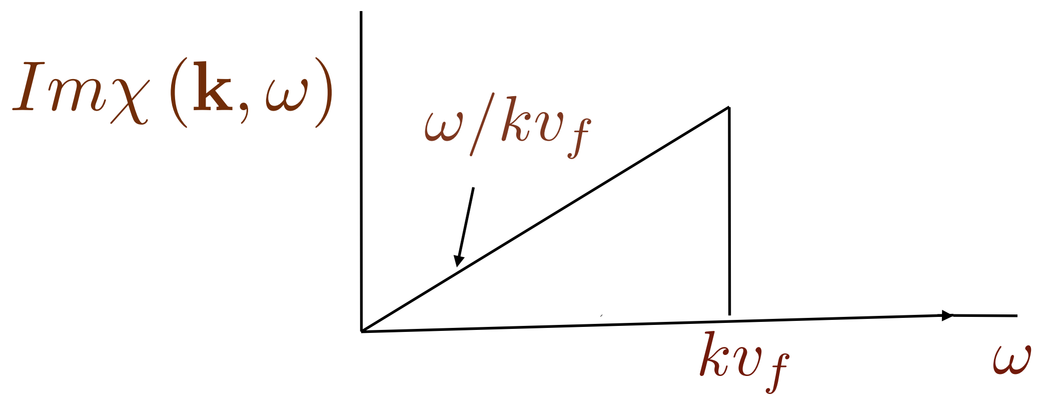


Point of View: These regions are inter-related.

Goal: To explain all universal properties in all three regions from one set of ideas, quantitatively where possible, and make specific verifiable predictions.

Region I: Not a Landau Fermi-liquid.

Landau Fermi Liquid



$\text{Scattering rate} \propto T^2$

Specific Heat ~ T

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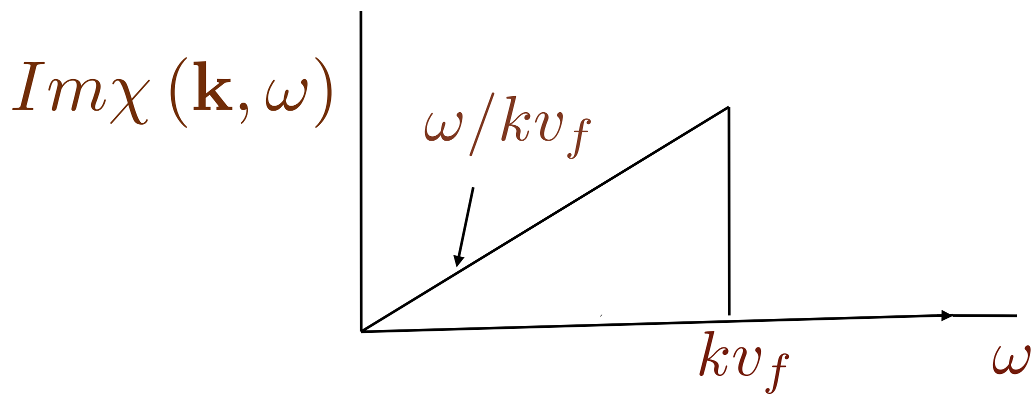

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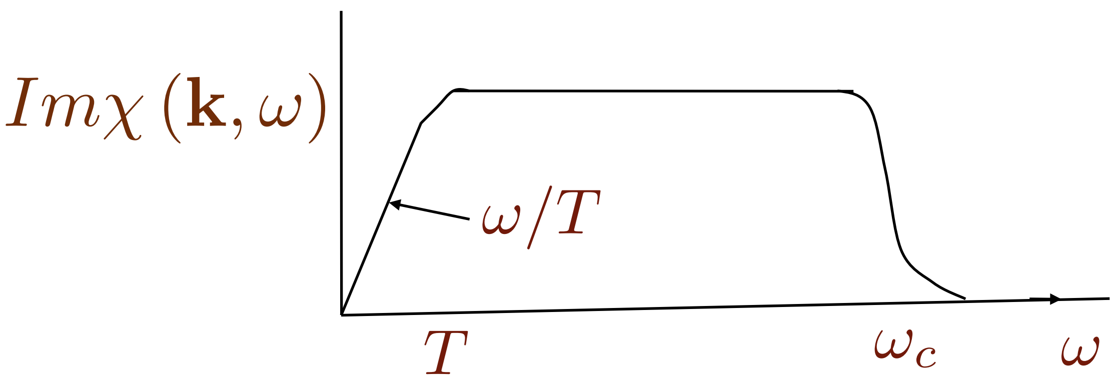

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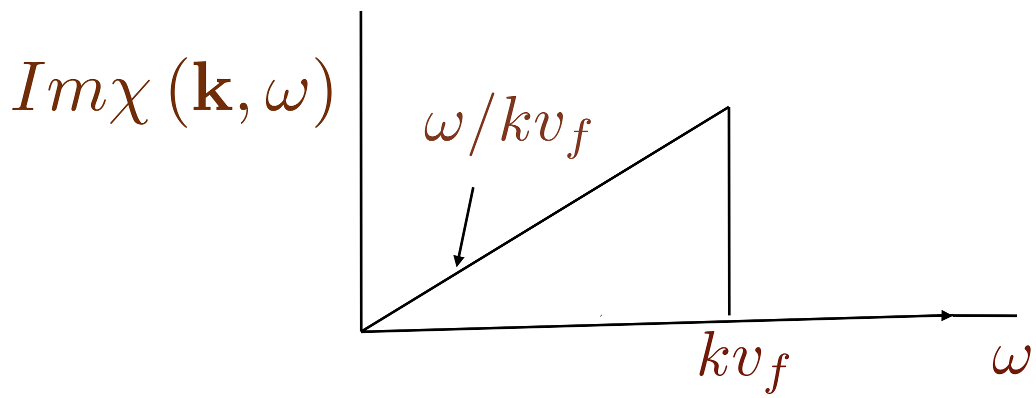

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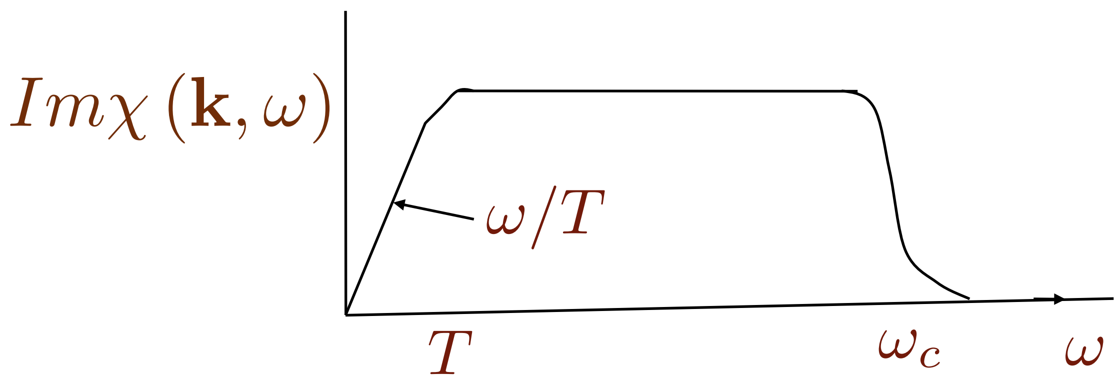

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Local in real space, Singular in time.

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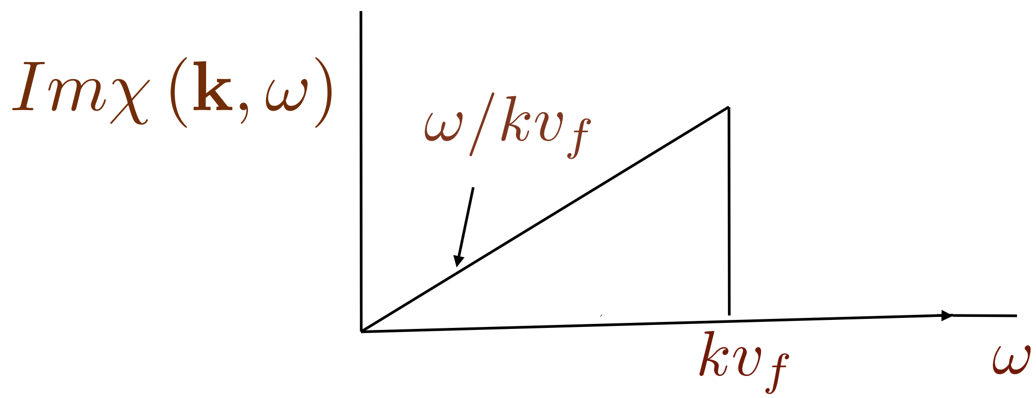

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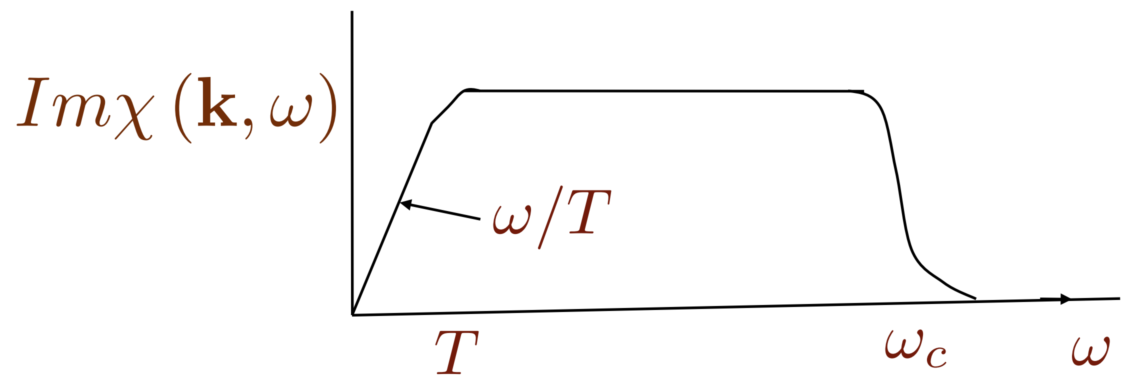

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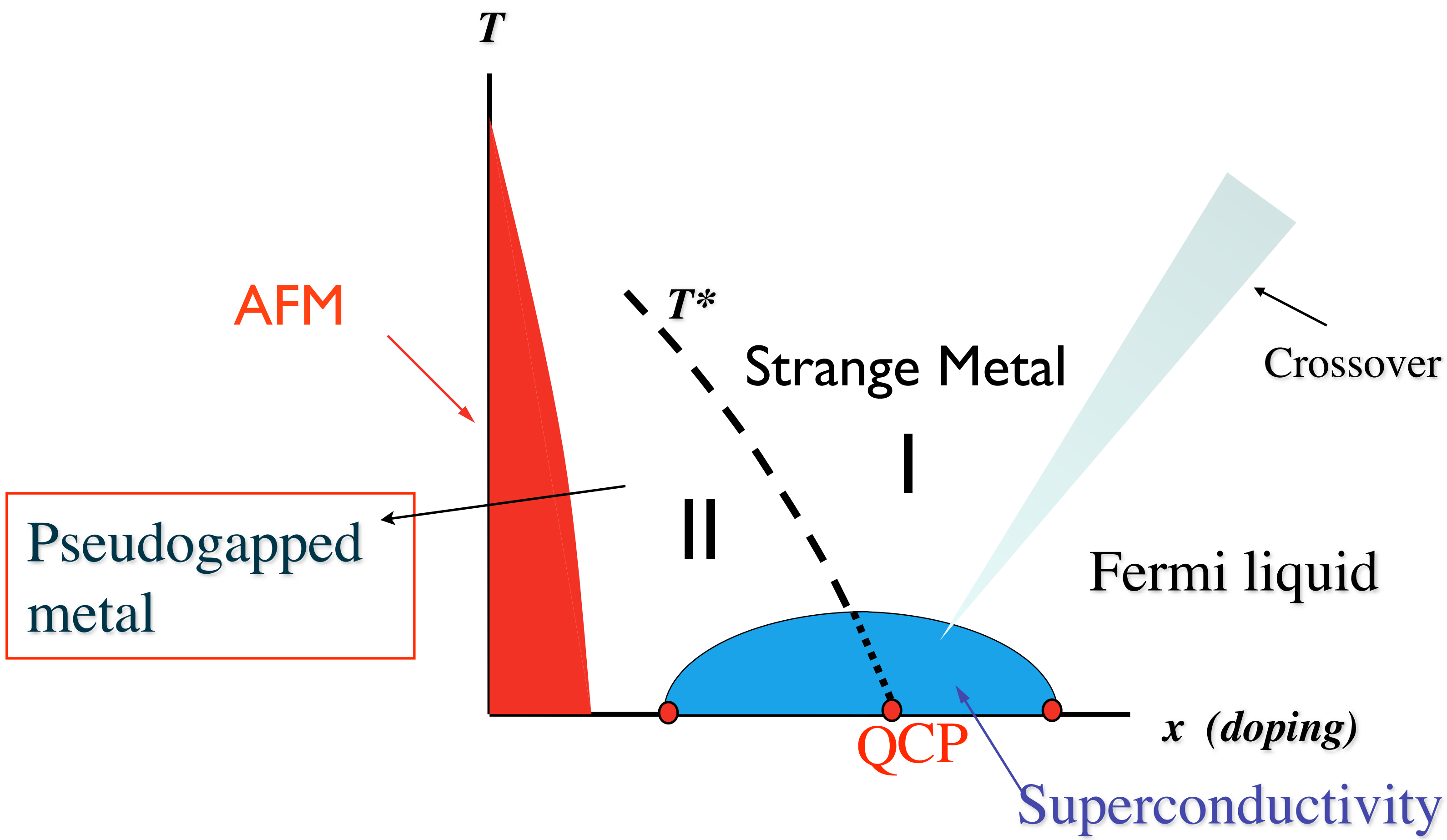
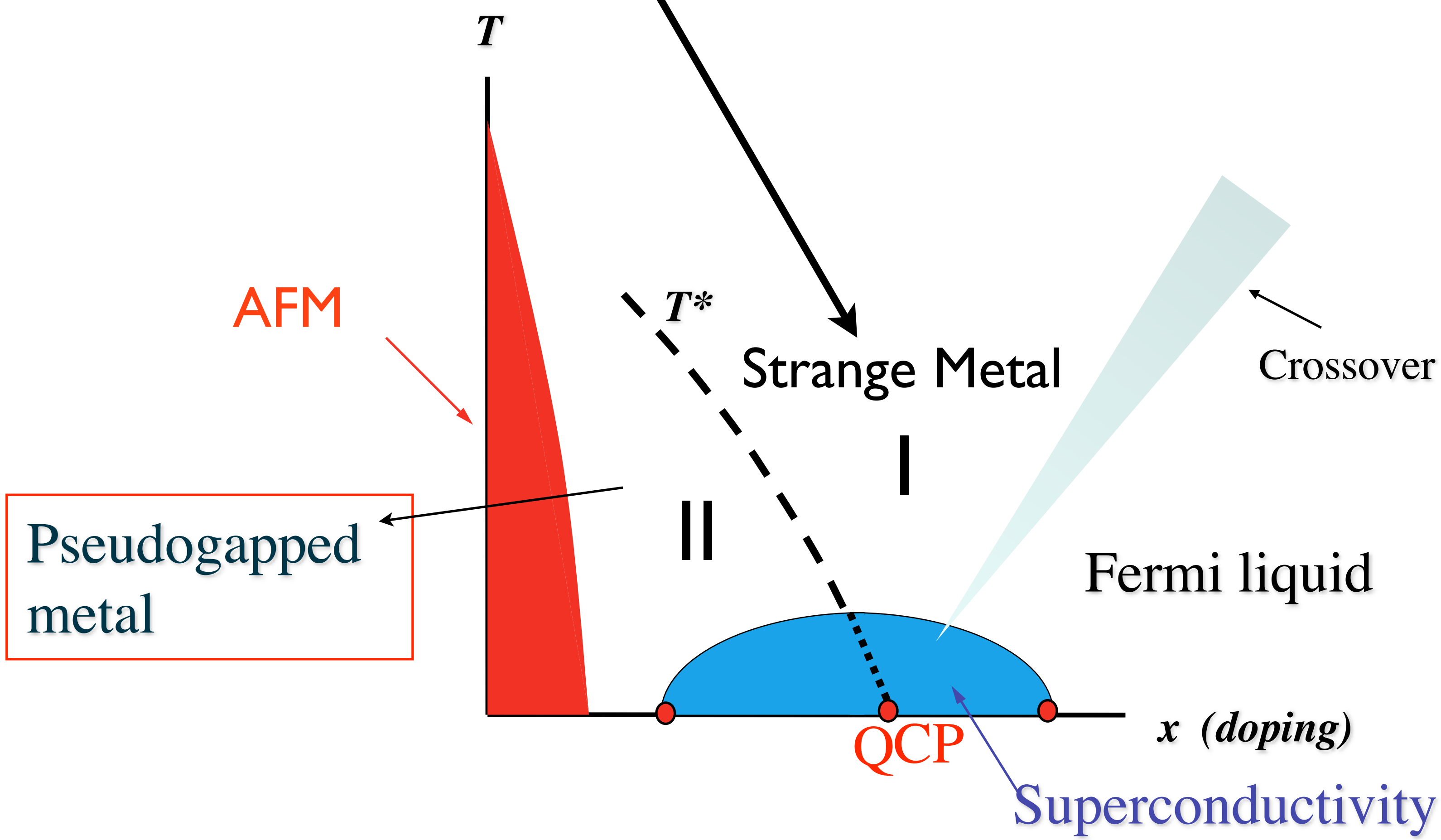
The quantum criticality in heavy-fermions and possibly Pnictides in the same Universality Class.


T
AFM
T*
Strange Metal
Crossover
Pseudogapped
metal
I
II
Fermi liquid
QCP
x (doping)
Superconductivity

Transport properties in Region I can be understood only as due to Quantum-critical Fluctuations leading to a Marginal Fermi-liquid



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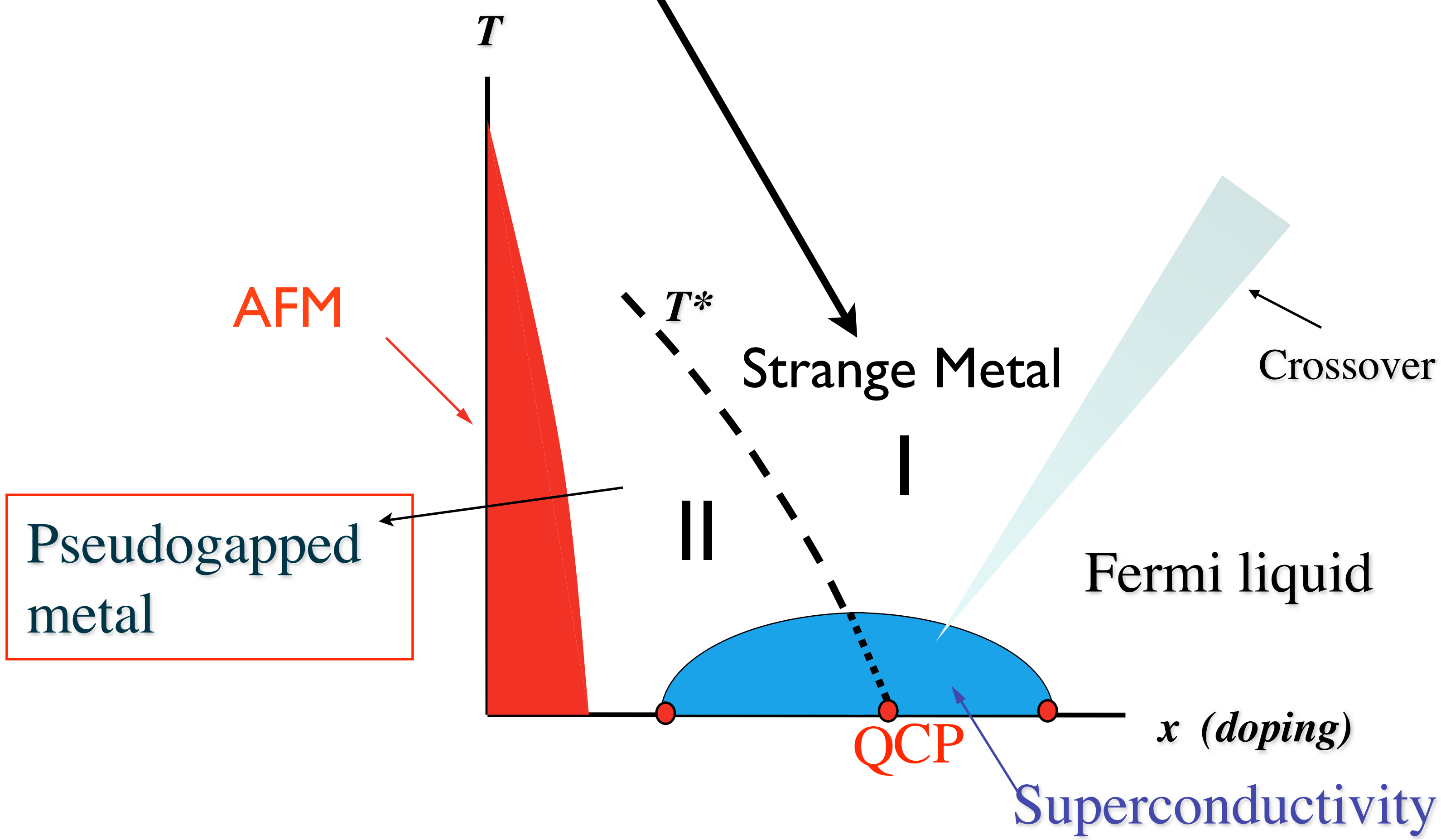

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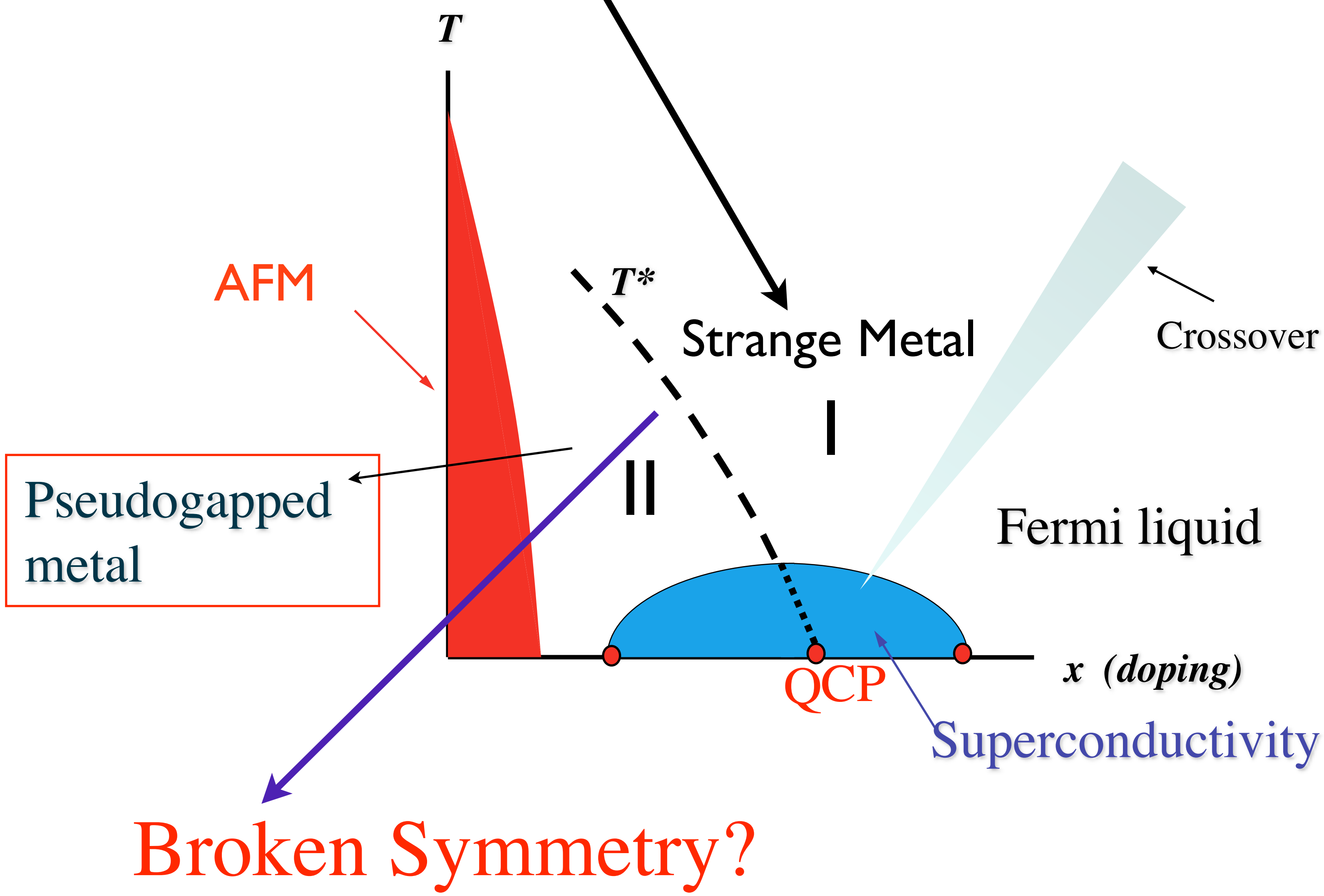

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Model with three orbital per unit-cell, local interactions U and nearest neighbor interactions V:

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Use Operator identity: $V n_i n_j = -V/2\left(|J_{ij}|^2 + n_i + n_j\right).$

$J_{ij} = i c_i^{+} c_j + H.C. \propto current\ operator\ in\ the\ link\ (i-j)$

Mean-Field theory with collective variables on the 8 links per unit-cell constructed from the $|J_{ij}|^2$. Look for phase which does not break Translational symmetry.

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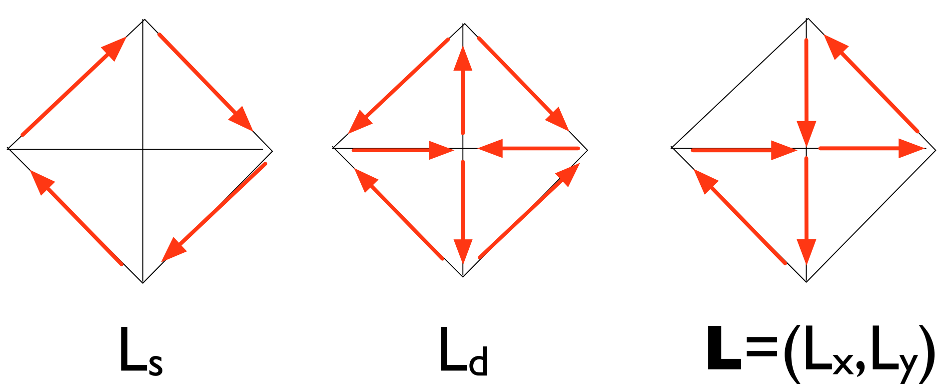
Closed Loop Variables in a unit-cell:



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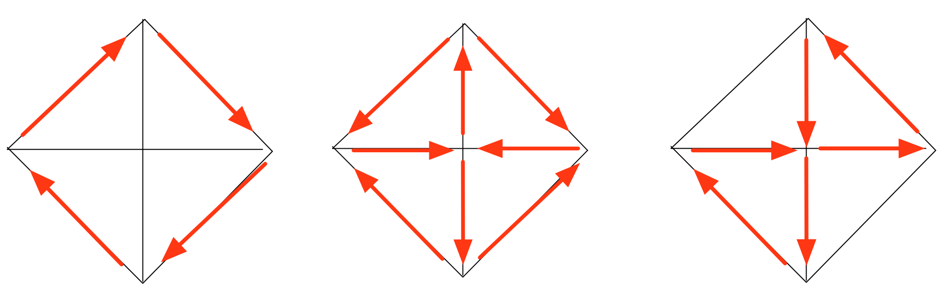

L_s L_d $\mathbf{L}=(L_x,L_y)$

Construct F(L) in mean-field theory and suggest expts.

Broken Symmetry in Underdoped Region.

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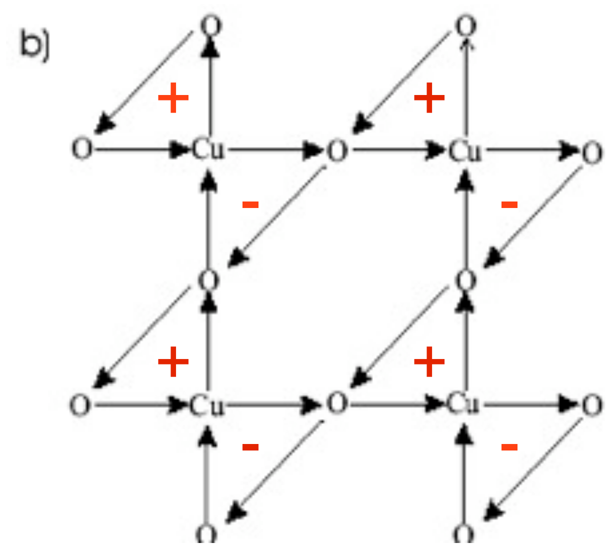

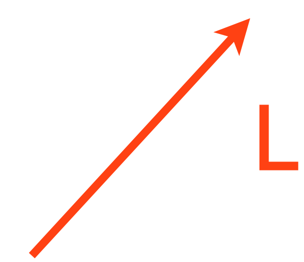

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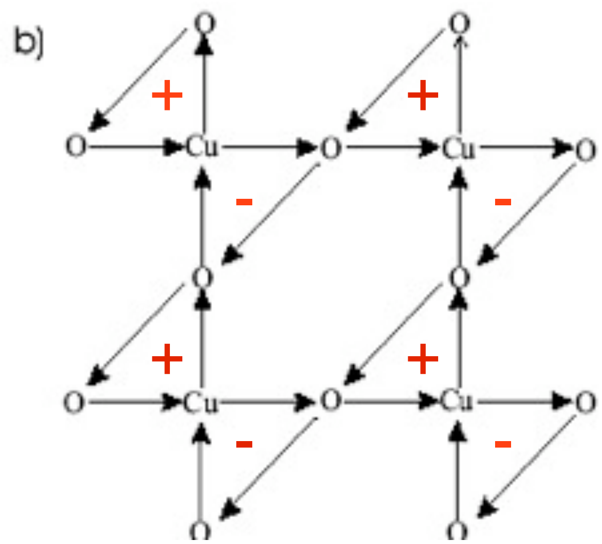

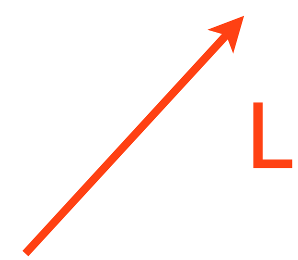

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The direction of moments not consistent with a purely Cu-O planar model. Must take apical oxygen into account (Webber et al.)

Experiments to look for time-reversal breaking in the pseudogap phase

I. Direct Observation by Polarized neutron Diffraction in underdoped YBaCuO of proposed order:(Bourges et al. 2005)

Repeated by Mook et al. (2008)

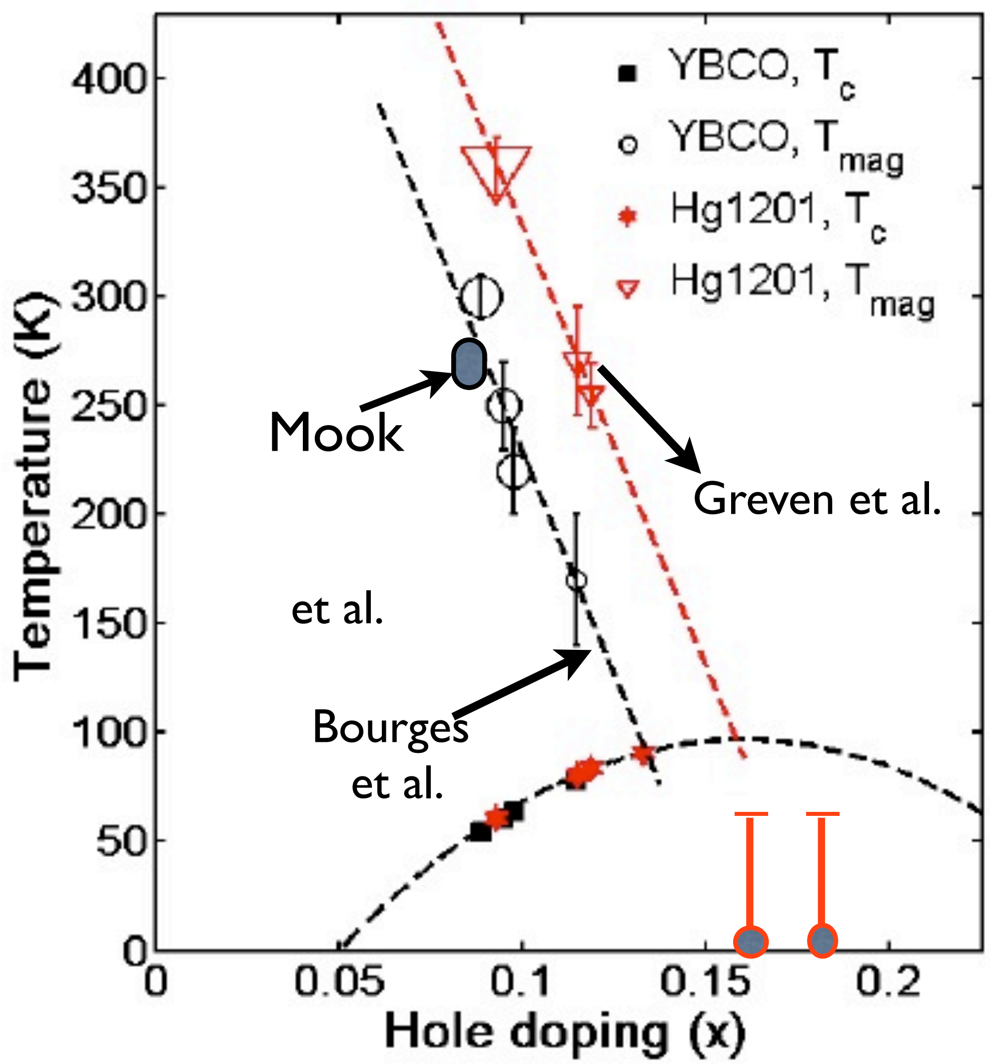
Exactly same order discovered in Underdoped single layer Hg-Cuprates (Greven et al., 2008)

Same Order observed in LSCO (Mesot et al., preprint 2009)

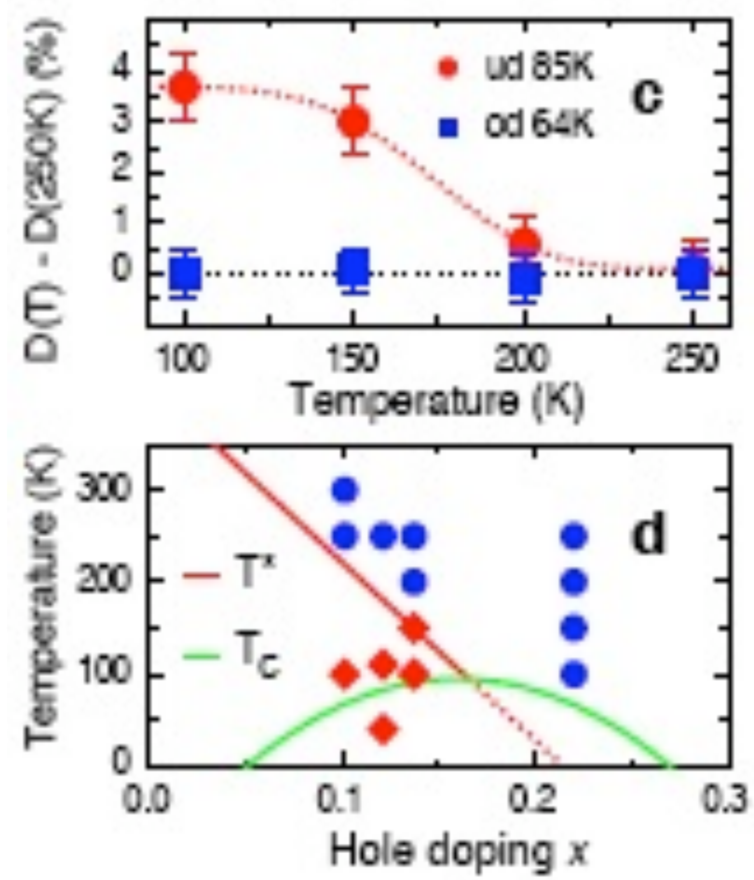
II. Dichroism in Angle-Resolved Photoemission: Experiment by Kaminski et al. (2002) in underdoped BISCCO compounds

III. Observation of Small ferromagnetic moment detected through Kerr effect in underdoped YBa2Cu3Ox :(Kapitulnik)

IV. Thermodynamics Evidence for a Phase Transition at T*(x):
Non-analytic Effect in magnetization even though no singularity in the specific heat. (Leridon, Monod and Colson).



BISCCO: Dichroic ARPES
Kaminksi et al., Nature(2000)

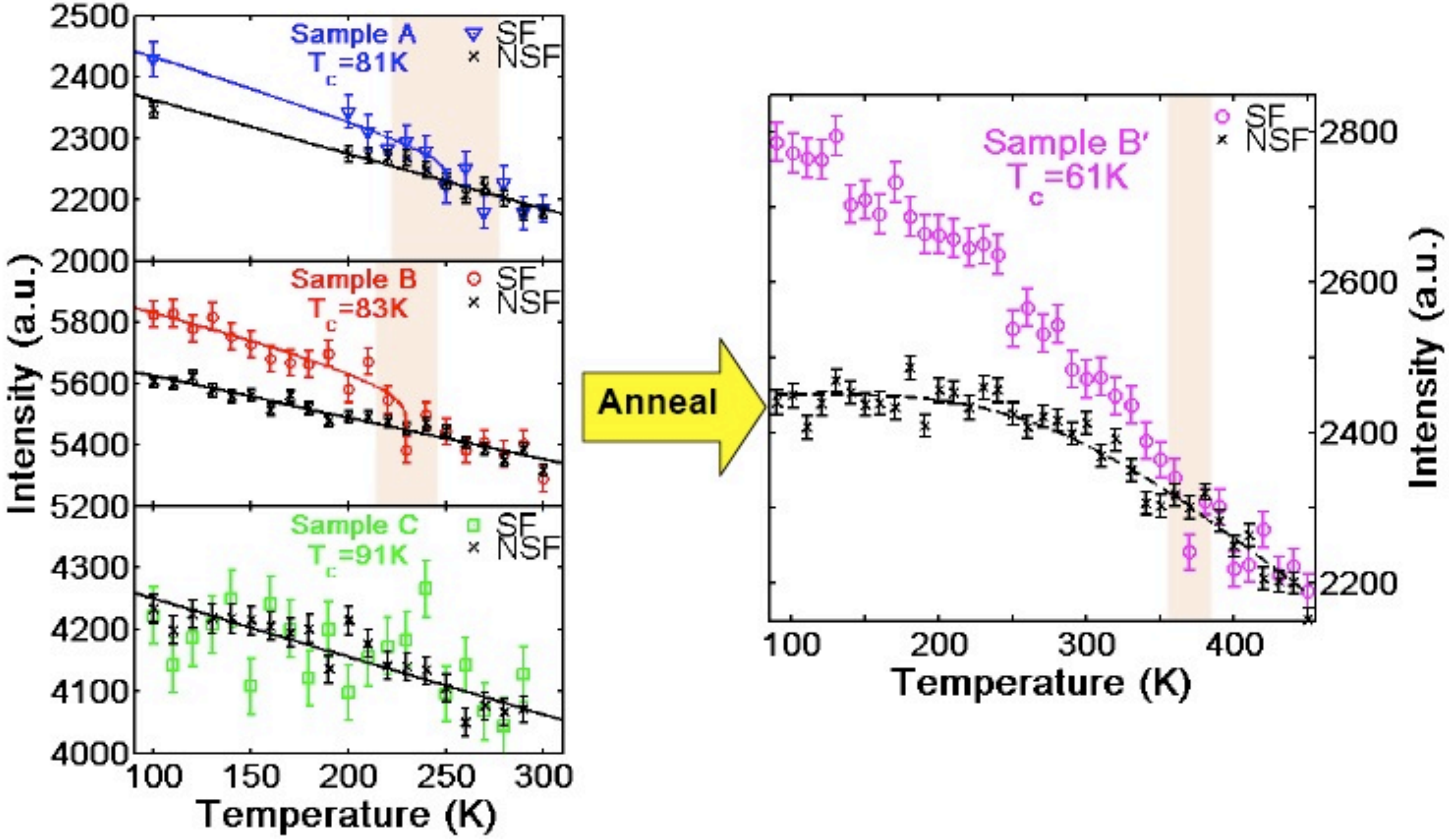


Also new polarized neutron results on LSCO:
Mesot, Bourges et al.

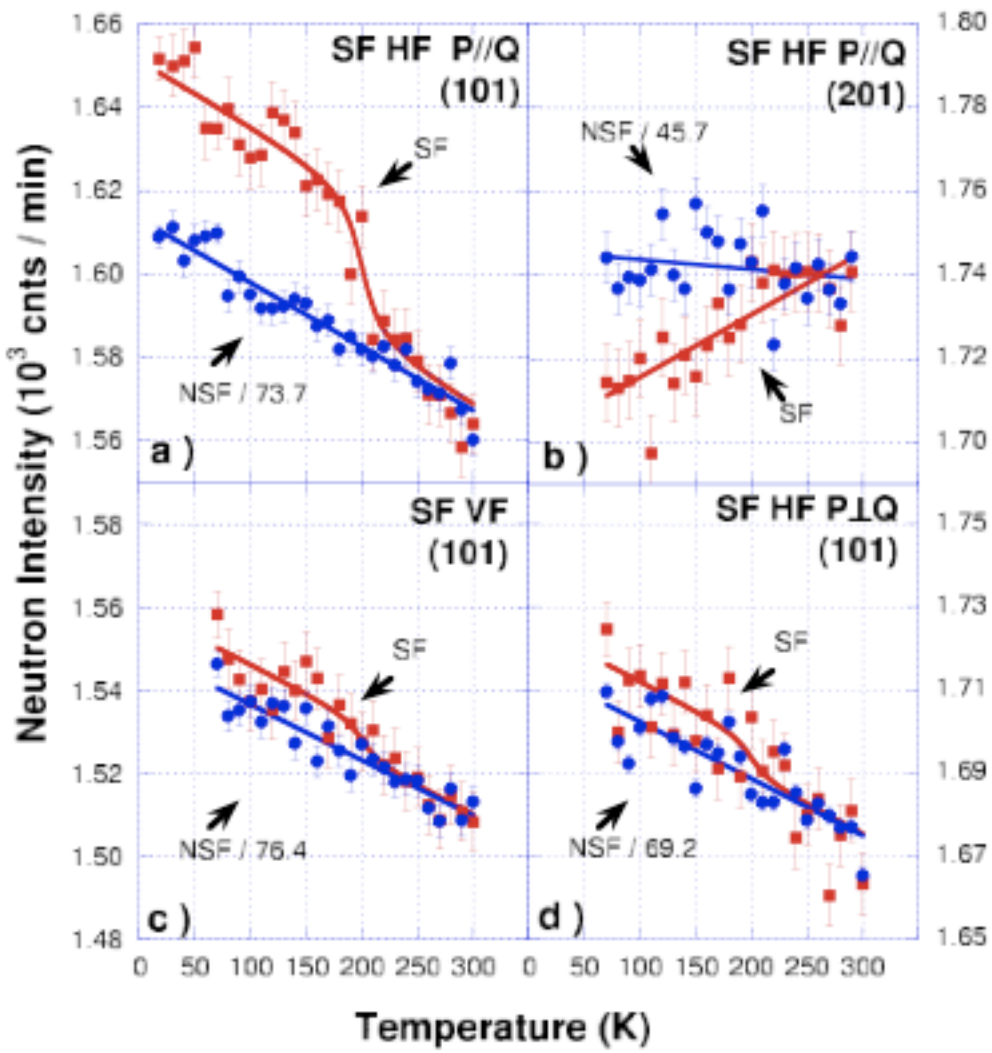
1. Large magnitude Order, $\approx 0.2\mu_B$/unit-cell at the lowest doping.
2. Universality.
3. Direction of Moments not consistent with the simplest 2 d model.

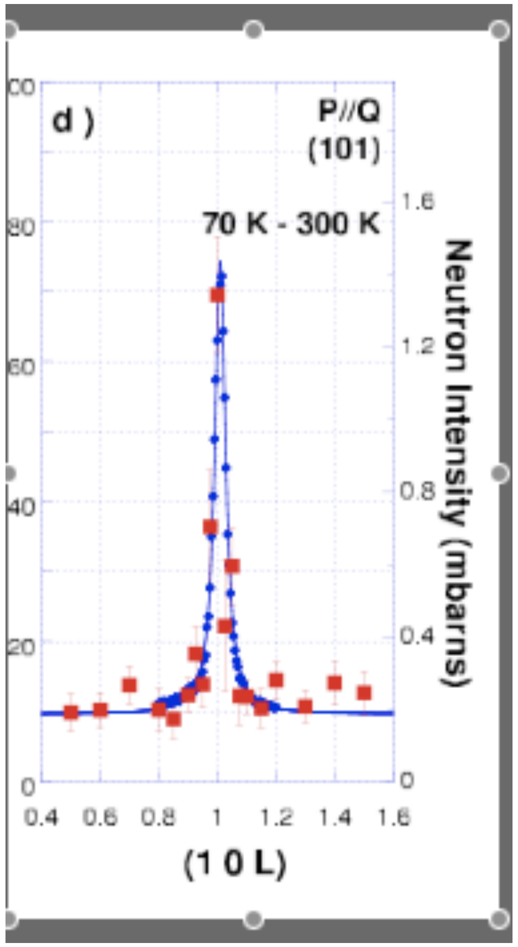
Polarized neutron Scattering in single layer Hg-Cuprates:
Greven et al. (2008).

Bragg Diffraction: (1 0 1), P//Q

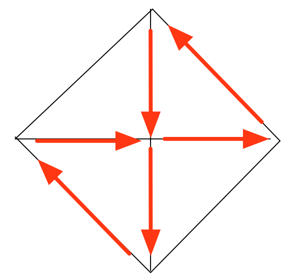


Polarized Neutron scattering: YBCO





H.A. Mook, Y.Sidis, B. Fauque, V. Baledent and P. Bourges, PRB 78, 020506 (R) (2008)



L=(L_x,L_y)

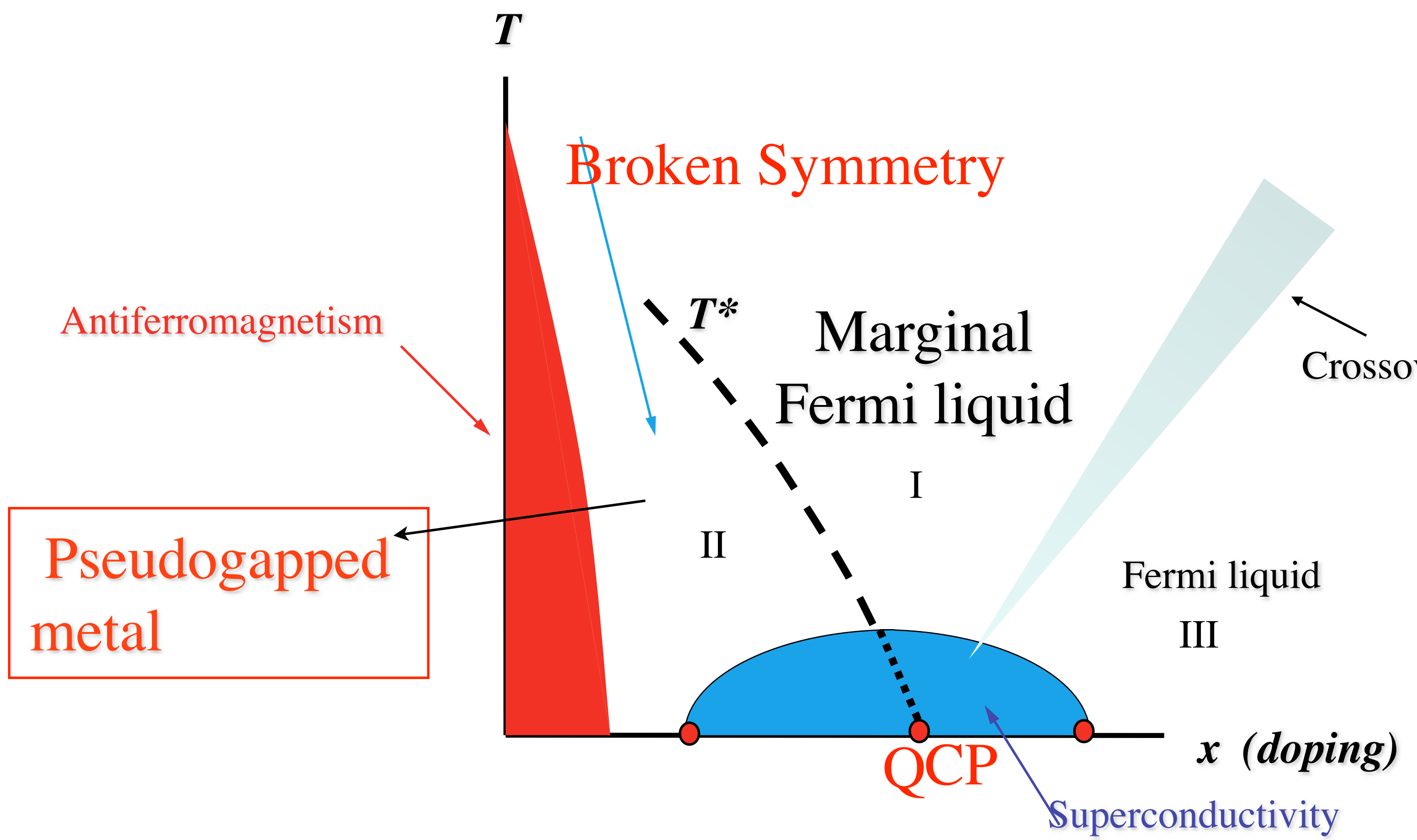
This phase is magneto-electric: $g_{ijk}E_jH_k$ is an allowed term in the Free-energy.

Other symmetry consequences of this form of order:

Magneto-electric tensor: x-ray dichroism (DiMatteo-cmv (2002)
: SHG (Simon-cmv (2002)

Mathematics of the Loop-current Order similar to the Time-reversal breaking in SU(3) models: Cabibo, Kobayashi- Masakawa

Given the experiments, one may assume that this phase exists universally in Region II of the phase diagram setting in at T*(x) where all properties change, and inquire about its consequences.



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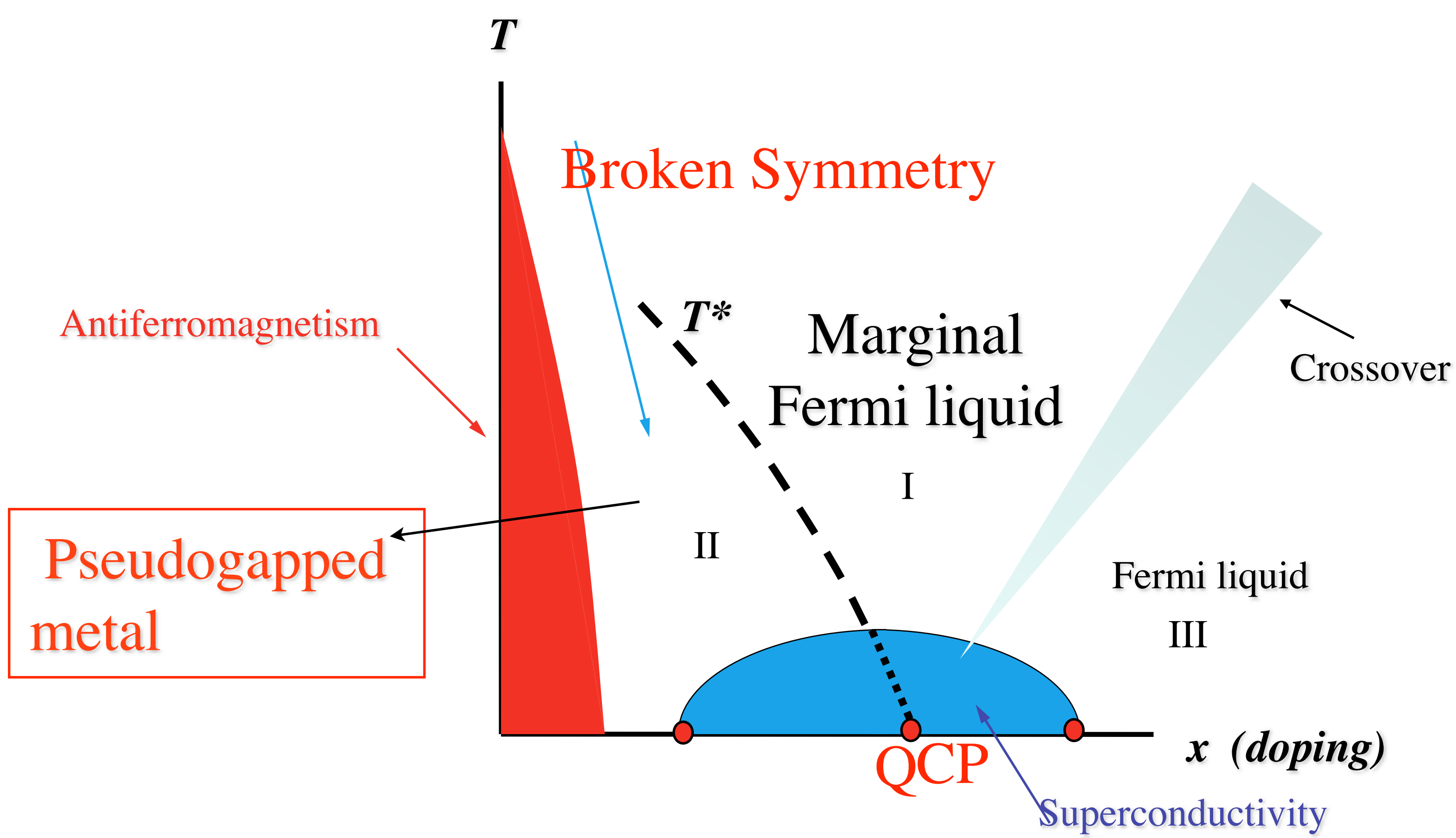

First and most important question:
Can one derive the specific form of Quantum-critical fluctuations necessary for the properties of Region I?

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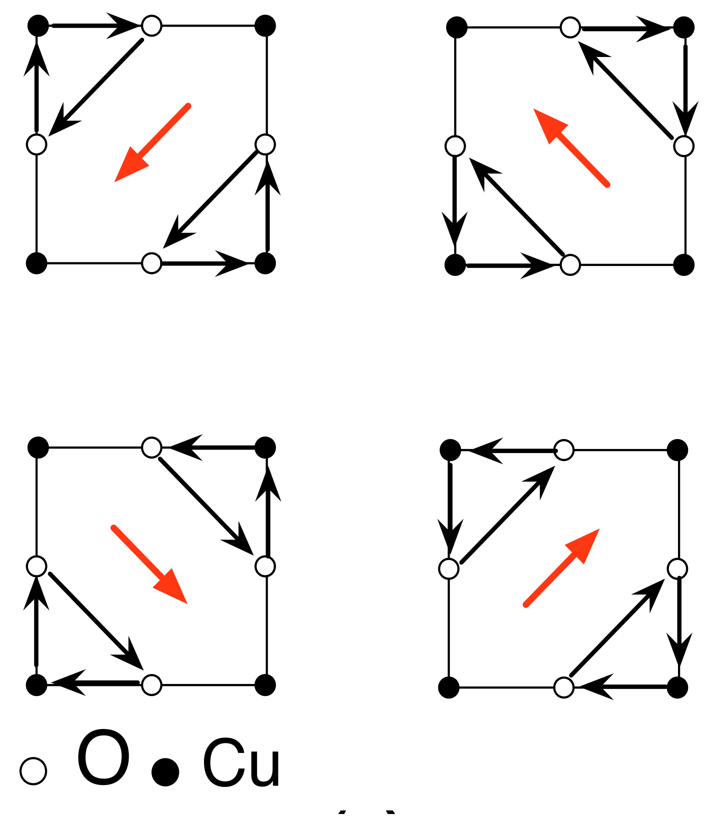

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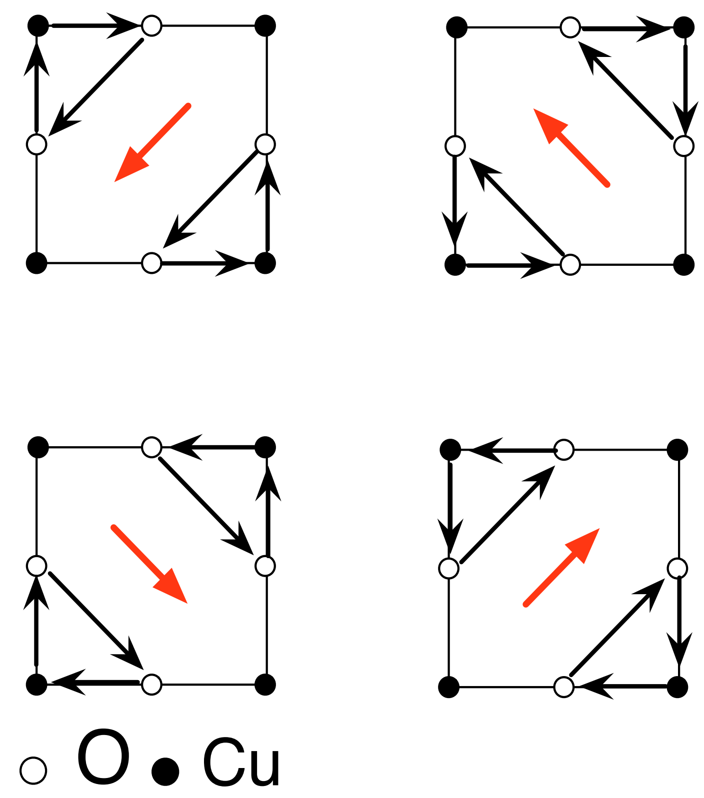

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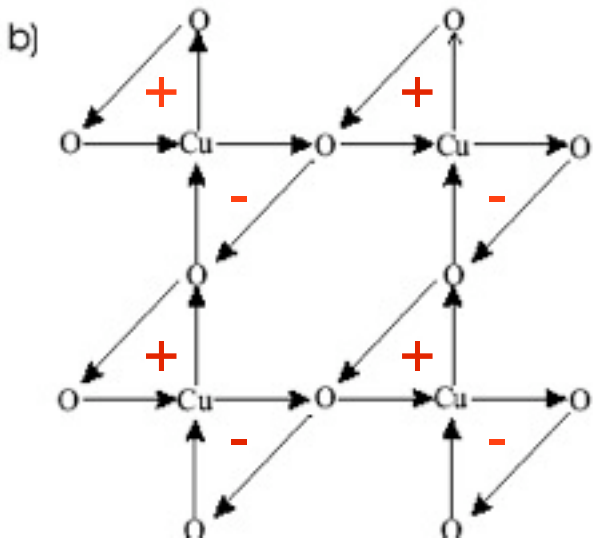
In the fluctuations regime the vector L has the same critical spectra as a model with a continuous rotations of L, i.e. the quantum- XY model.

An effective Hamiltonian for the Loop-Current Order with four states per unit-cell. (ASHKIN-TELLER MODEL)



(σ, τ) : (1,1) (-1,1) (-1,-1) (1,-1)

$$H_{eff} = -\sum_{<i,j>} J_2(\sigma_i\sigma_j + \tau_i\tau_j) + J_4(\sigma_i\tau_i\sigma_j\tau_j)$$

+ Constrained kinetic energy of fermions

+ Interactions of fermion currents linearly with the σ_i and τ_i operators.

For relevant range of parameters, the Ashkin-Teller Model has a smooth specific heat at the Transition even though there is an order parameter singularity (Baxter, Sudbo).

Quantum-Critical Fluctuations

Model is the quantum generalization of the dissipative xy model. It has been analytically solved (Aji-cmv (07).

$$H = \mathcal{L}_i^{z\,2}/2I + J(\mathcal{L}_i^{+}\mathcal{L}_j^{-} + h.c.) + \ Dissipative\ terms\ (\alpha).$$

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We calculate that at the QCP,

$$\chi(r,t;r't') = <\mathcal{L}(r,t)\mathcal{L}(r',t')> = \delta(r-r')\frac{1}{t-t'}$$

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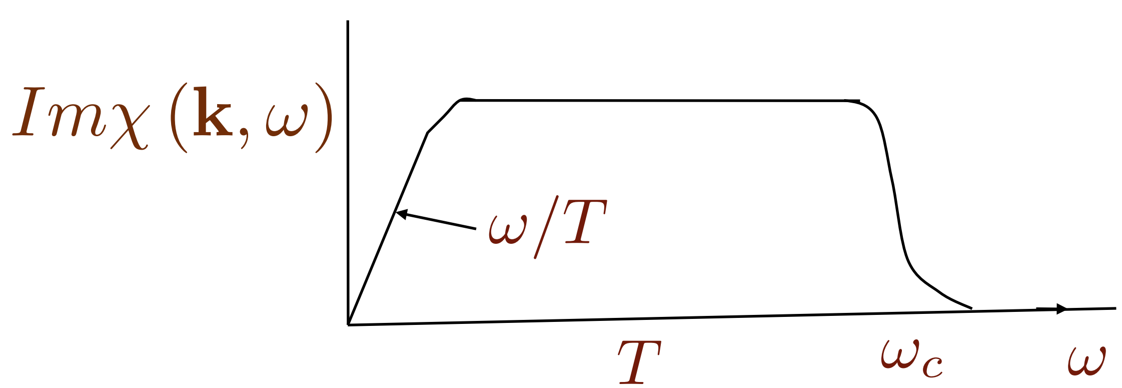


Marginal Fermi-Liquid finally Derived from a Microscopic Model

Theory of Criticality

2D XY model with dissipation

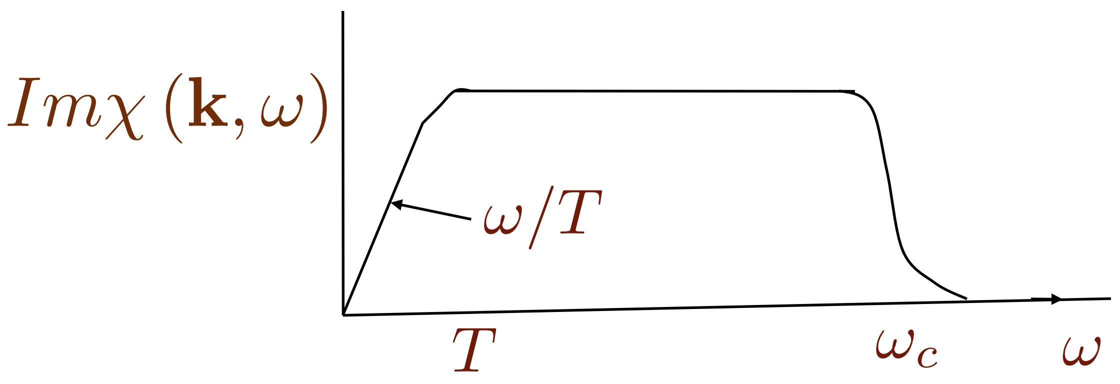
$$S=\int d\tau \sum_{\langle ij\rangle} J\cos\left(\theta_i-\theta_j\right)+\int d\tau \sum_i \frac{\dot{\theta}^2}{C}+\int d\mathbf{k}\mathbf{d}\omega\alpha\left|\omega\right|\mathbf{k^2}\left|\theta_{\mathbf{k},\omega}\right|^{\mathbf{2}}$$

Exact Transformation in terms of two sets of orthogonal variables:

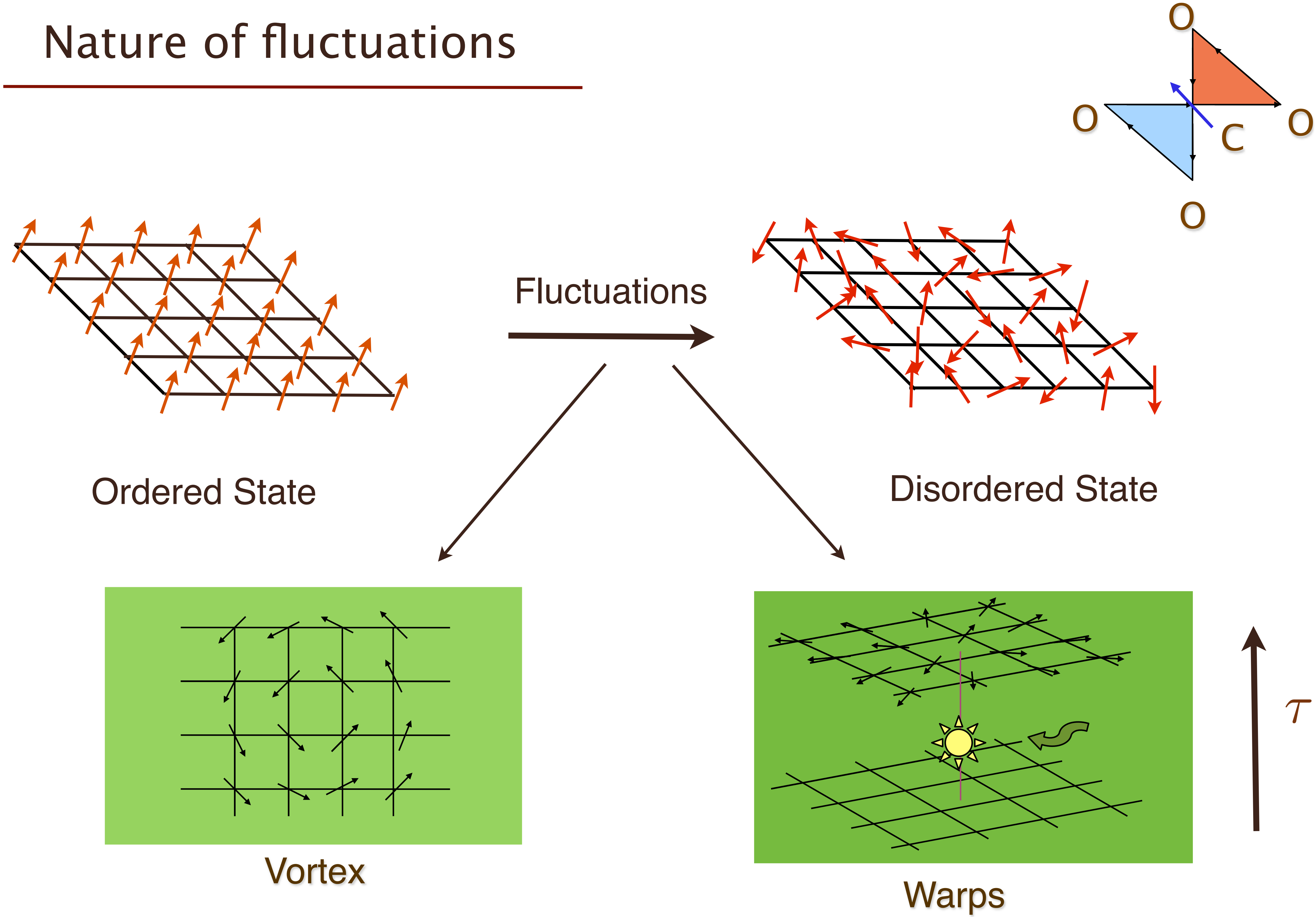
$$\mathrm{S}=\int d\tau d\mathbf{r}\mathbf{d}\mathbf{r}'\mathbf{J}\rho_{\mathbf{v}}(\mathbf{r},\tau)\rho_{\mathbf{v}}(\mathbf{r}',\mathbf{t})\mathbf{ln}\left|\mathbf{r}-\mathbf{r}'\right|+\int \mathbf{d}\mathbf{r}\mathbf{d}\tau\mathbf{d}\tau'\alpha\rho_{\mathbf{w}}(\mathbf{r},\tau)\rho_{\mathbf{w}}(\mathbf{r},\tau')\mathbf{ln}\left|\tau-\tau'\right|$$

Singularities decouple in space and time

Fluctuation spectrum



Nature of fluctuations



Vivek Aji and CMV, PRL 99, 067003 (2007); PRB 2009.

General Remarks:

1. To get quantum-critical fluctuations of this kind, it is necessary to show that at criticality, the partition function can be expressed in terms of variables which are functions only of time and those that are functions of space alone.

2. These variables almost certainly always describe topological excitations.

3. Await Quantum-Monte-Carlo Calculations on this and related models to verify the results.

4. Besides the Cuprates and heavy-fermions (which have also closely related form of criticality) pnictides also seem to be only consistent in their properties with such criticality.

5. "High" Tc from electronic mechanisms is always near quantum-criticality but ordinary criticality is bad for Tc.

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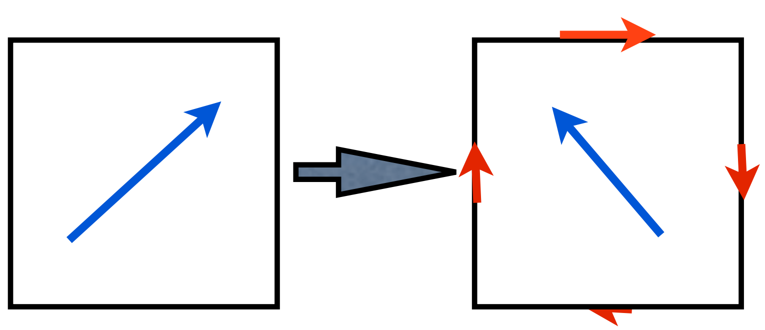

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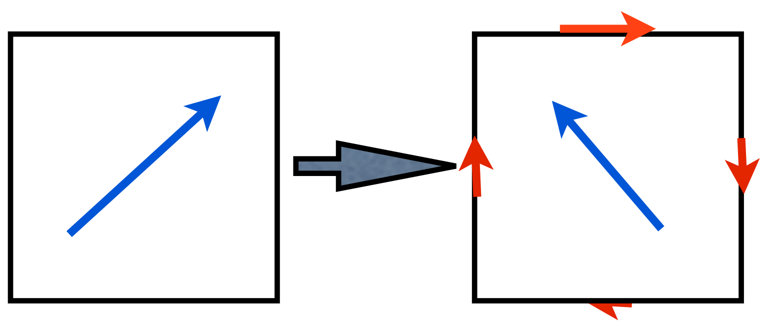


Orbital Moment Analog of the familiar coupling:

$$J\ \psi_k'^{+}\sigma\psi_k \cdot \mathbf{S}$$

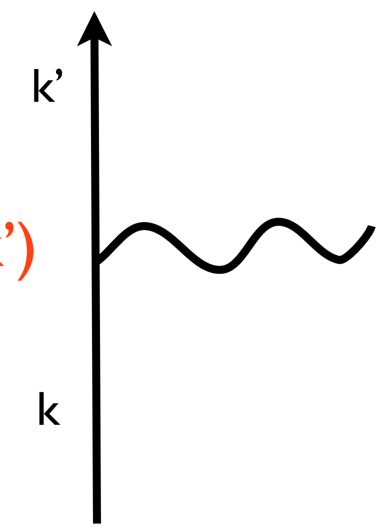
This was used to prove that AFM fl. promote d-wave pairing. Miyake, Schmitt-Rink, cmv (1986).

Fermion-Fluctuation Coupling in Momentum space.

In continuum limit, the coupling Hamiltonian has the form:

$$ig(\mathbf{k}-\mathbf{k}') \times (\mathbf{k}+\mathbf{k}')\psi'^{+}_{\mathbf{k}}\psi_{\mathbf{k}}\mathcal{L}^{\pm}_{(\mathbf{k}-\mathbf{k}')} + h.c.$$

$\gamma(k,k') =$ i g(k X k')



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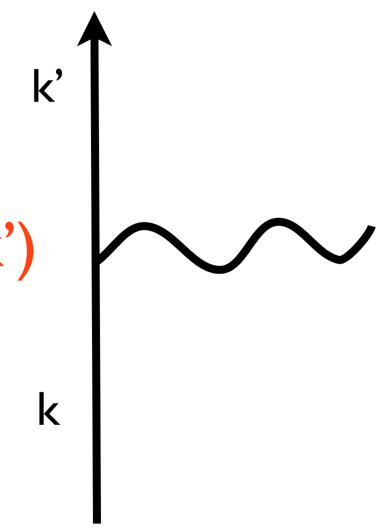

Note the preferential scattering at right angles and the factor i.

Fermion-Fluctuation Coupling in Momentum space.

In continuum limit, the coupling Hamiltonian has the form:

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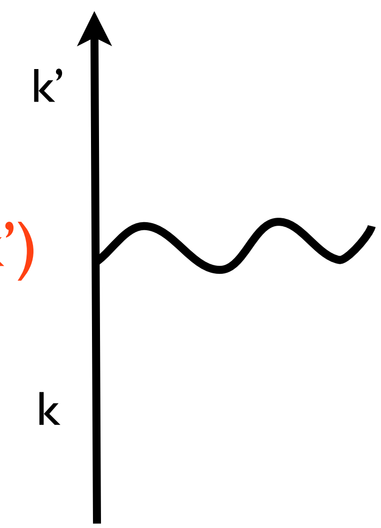
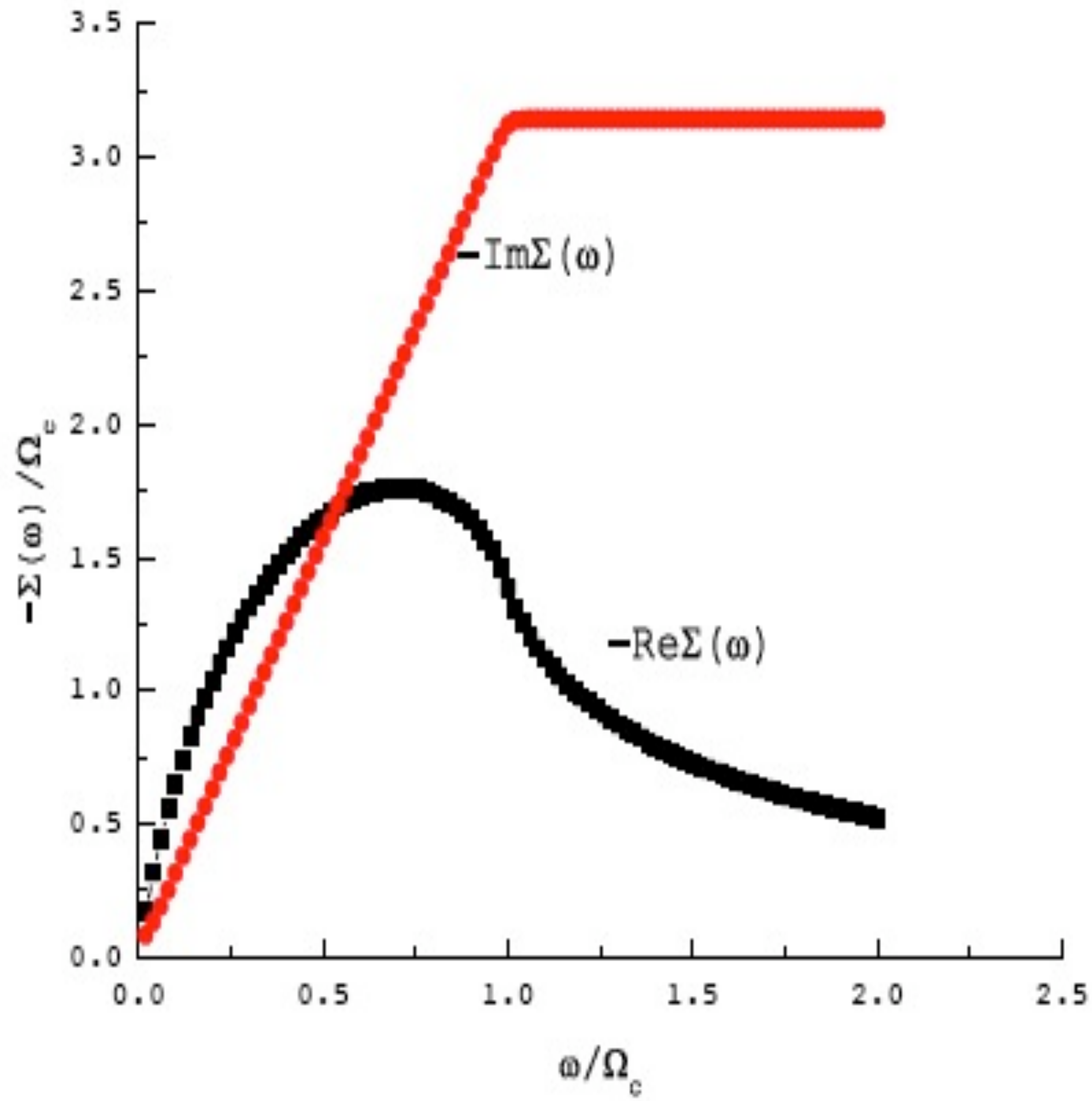


Note the preferential scattering at right angles and the factor i.

Before examining the pairing channel, let us calculate single-particle spectra in the normal state.

Effect of Fluctuations on Single-particle Spectra measured in ARPES

$$Im\Sigma(\omega, k) \propto \lambda(k) \int_0^{\omega} d\omega' Im\chi(\omega') \qquad \lambda(k) = \sum_{k'} |\gamma(k, k')|^2$$



Predicts Linewidth proportional to ω for $\omega \lesssim \omega_c$ and constant beyond. Factor of ~ 2 mom. dependence.

Recent ARPES Experiments to High Energies.

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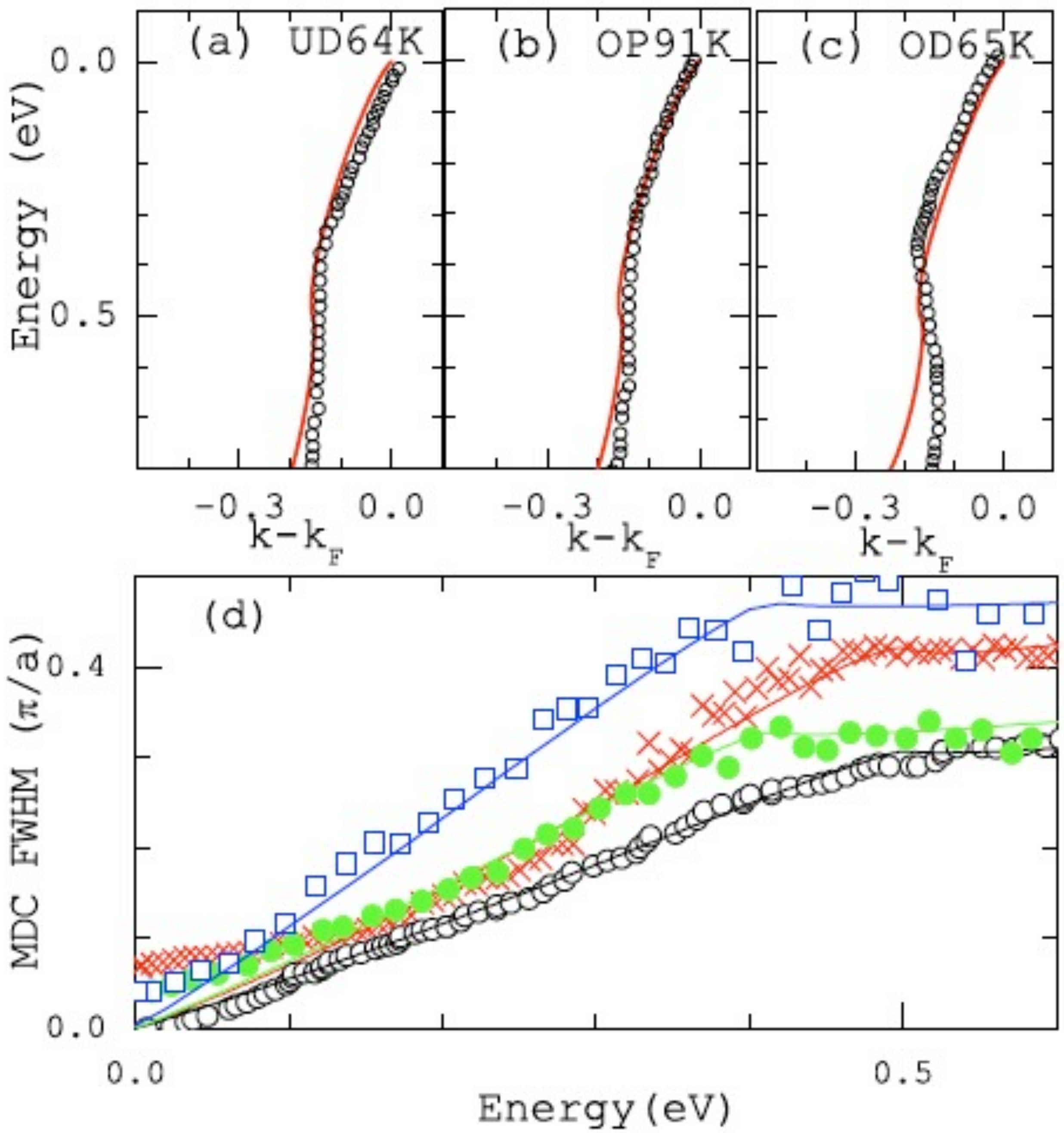
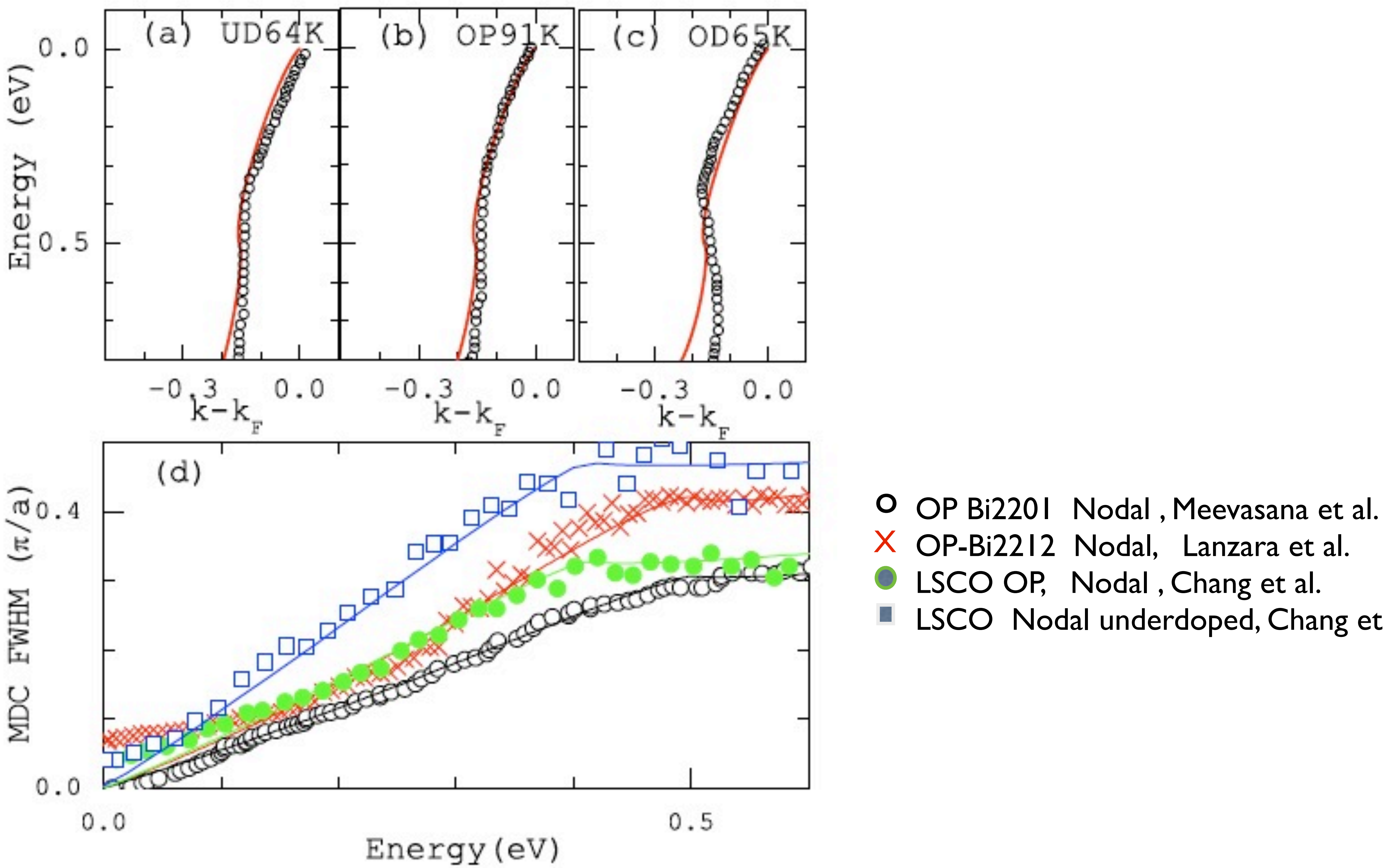


- OP Bi2201 Nodal , Meevasana et al.
- OP-Bi2212 Nodal, Lanzara et al.
- LSCO OP, Nodal , Chang et al.
- LSCO Nodal underdoped, Chang et

Recent ARPES Experiments to High Energies.

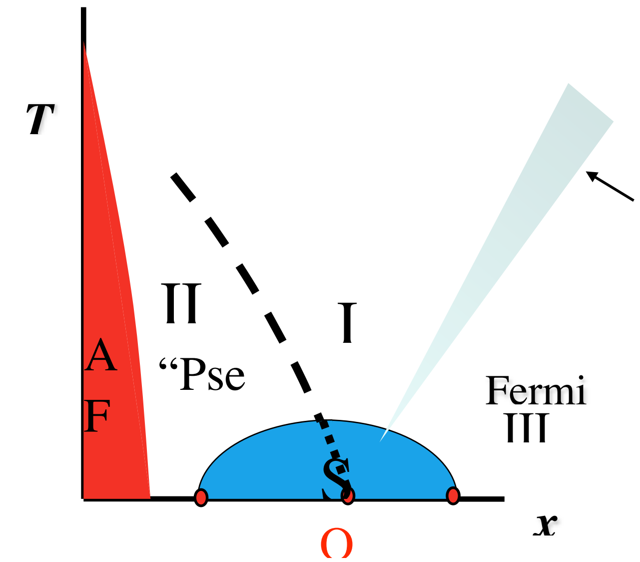


This is an experimental proof of the existence of a distinct spectrum of fluctuations with a well-defined cut-off frequency. This is what couples to fermions at just above Tc.

Single-Particle Spectra in Cuprates measured by ARPES throughout the funnel shaped Quantum-critical region in all Cuprates (underdoped, optimally doped, overdoped) that have been measured have a width

$$= (\pi/2)\lambda\, \omega,\ \ for\ \omega \lesssim \omega_c$$

$$= constant,\ \ for\ \omega \gtrsim \omega_c$$



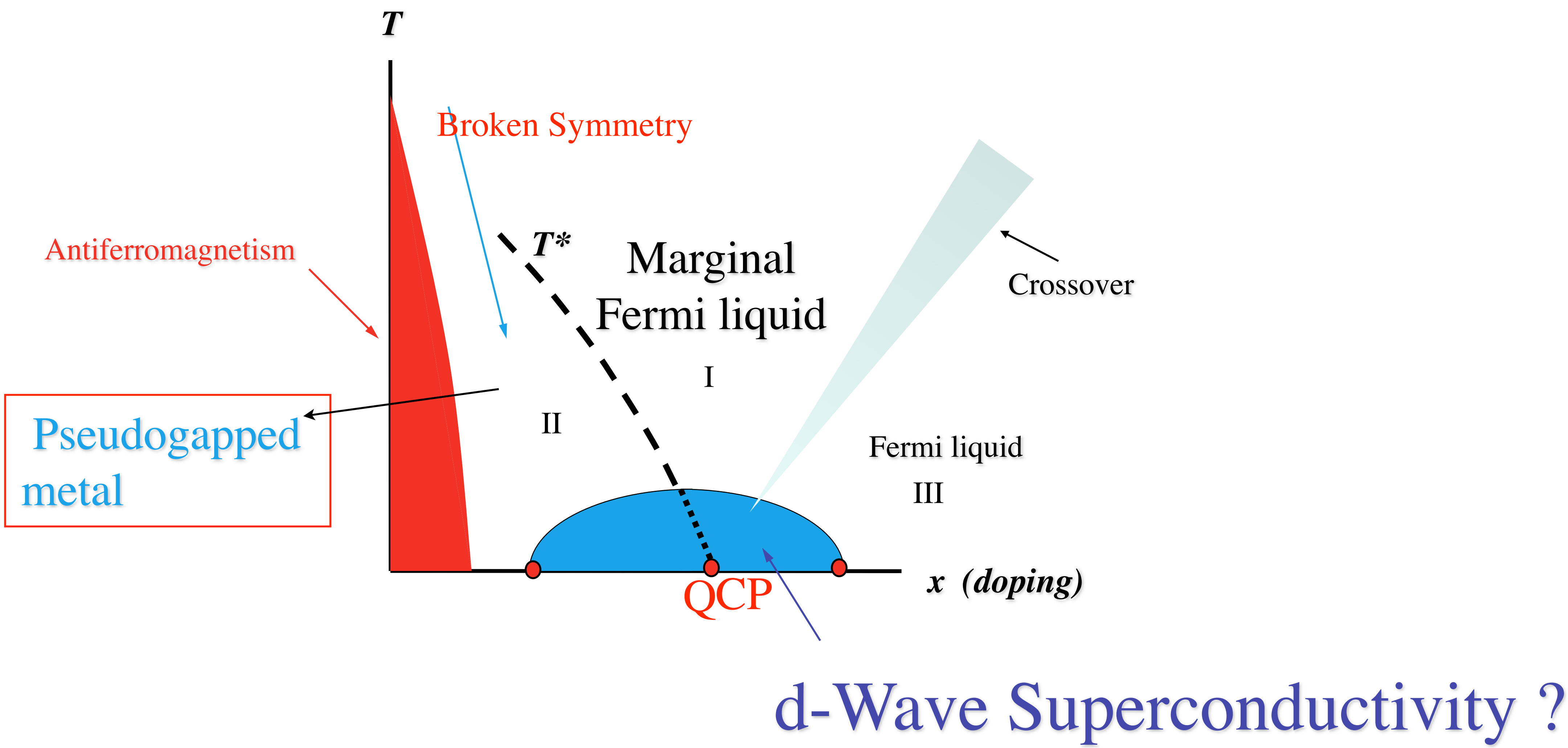
For all data available

$$0.8 < \lambda < 1.1$$

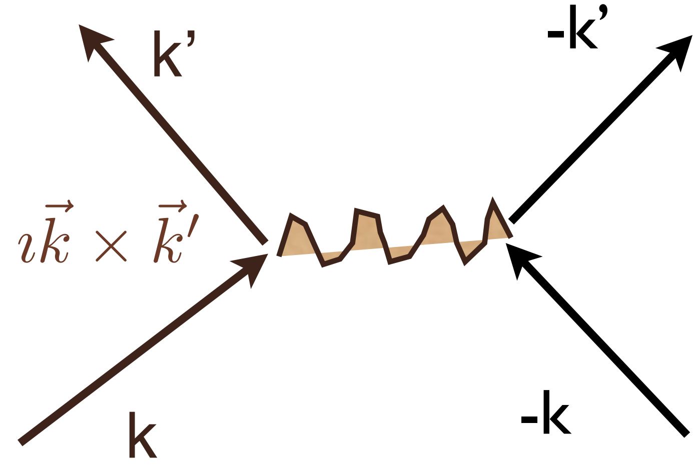
$$0.4 < \omega_c < 0.5\ eV.$$

Linear in T resistivity and optical conductivity in the Strange Metal Region understood by the same parameters to +/-30%.

Next must Prove that the derived QCF spectra couples to Fermions to favor d-wave superconductivity and with right magnitude of parameters.



Pairing



Pairing Vertex: $\left(\imath\vec{k} \times \vec{k}'\right)^2 \Re\chi$

$$\left(\vec{k} \times \vec{k}'\right)^2 = \frac{1}{2}\left[\left(k_x^2 + k_y^2\right)\left(k_x'^2 + k_y'^2\right) - \left(k_x^2 - k_y^2\right)\left(k_x'^2 - k_y'^2\right) - \left(2k_x k_y\right)\left(2k_x' k_y'\right)\right]$$

$$T_c \approx \omega_c \exp(-\frac{1+\lambda_s}{\lambda_d})$$

Arpes data yields $\omega_c \approx 0.4eV, \lambda_s \approx 1$ ⟹ Tc ~ 100 K

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Physics is that for s-wave superconductors low energy scattering does nothing (Anderson's theorem). But not so for d-wave superconductors.

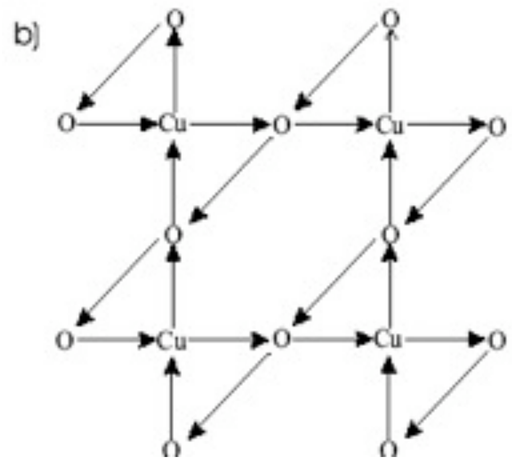
Corollary : When Tc is of order 100K in d-wave, phonon are generally pair-breaking.

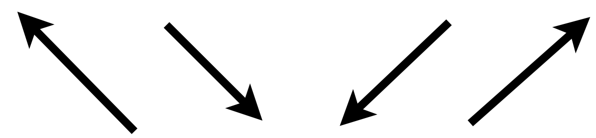
Inversion of ARPES in the normal and superconducting states being carried out to discover the spectrum of the glue for d-wave pairing.

Near Tc, in the quantum-critical regime of x, it is predicted that the spectrum is of the proposed form.

But how will we know that the physics of the spectrum is that of the fluctuations of the discovered loop-current order?

Fluctuations couple the four states which are odd in R and transform as $i(x \pm y)$.





Therefore Fluctuations must transform as

$$i(x\partial/\partial y - y\partial/\partial x)$$

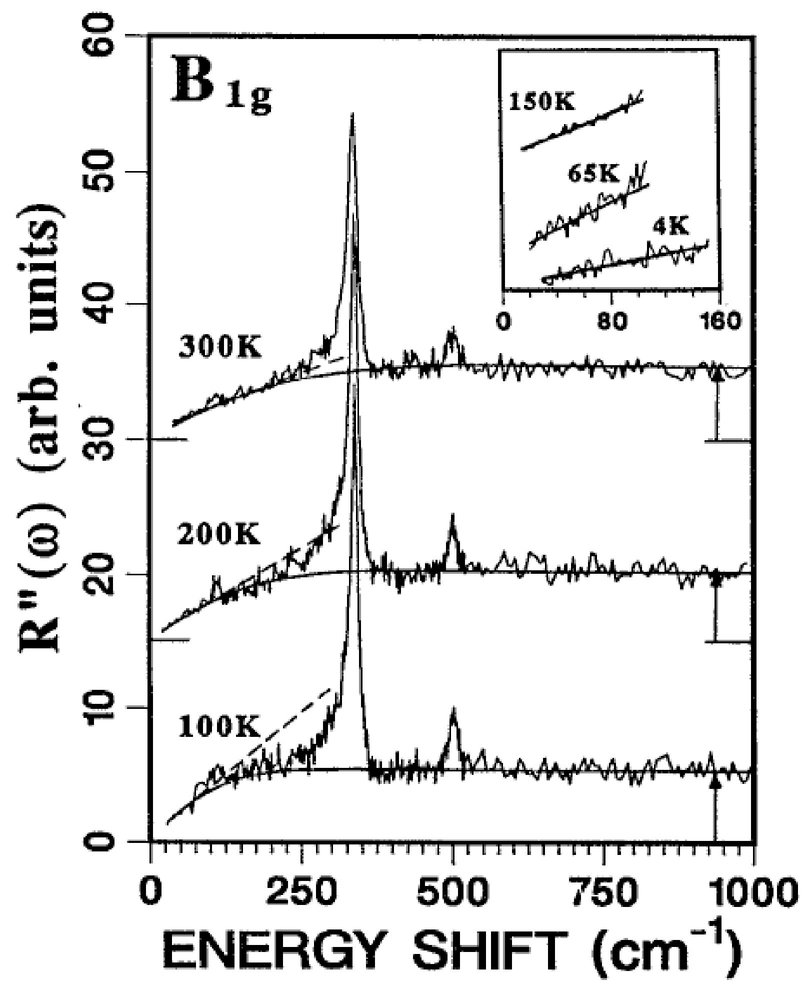
This is A(2g) symmetry in Raman Scattering.

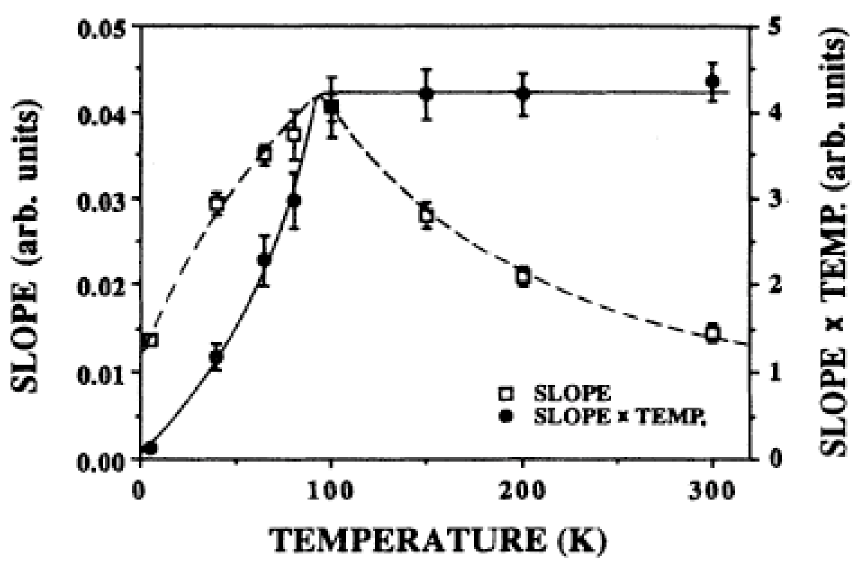
which occurs in experiments in combination with other channels, for example B1g.
I suggest experiments isolating the A(2g) symmetry.

Experimental Evidence of the Derived Spectra

I. Raman Spectra in Optimally doped Cuprates

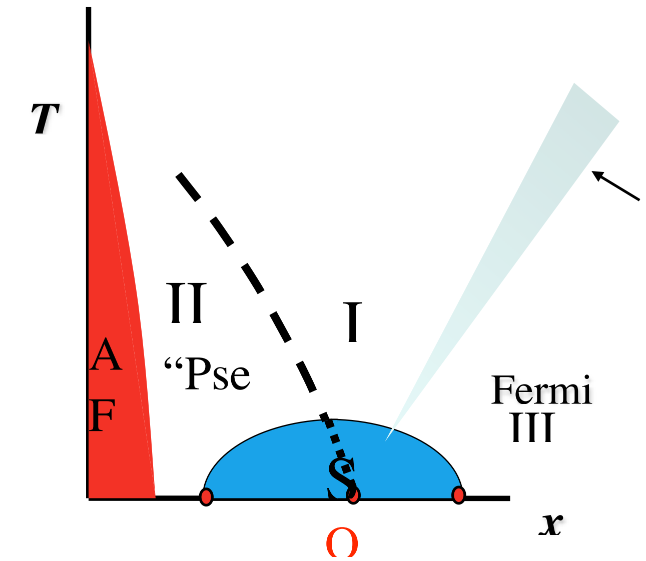
Direct observation of a Quantum critical fluctuations spectra of the derived form:



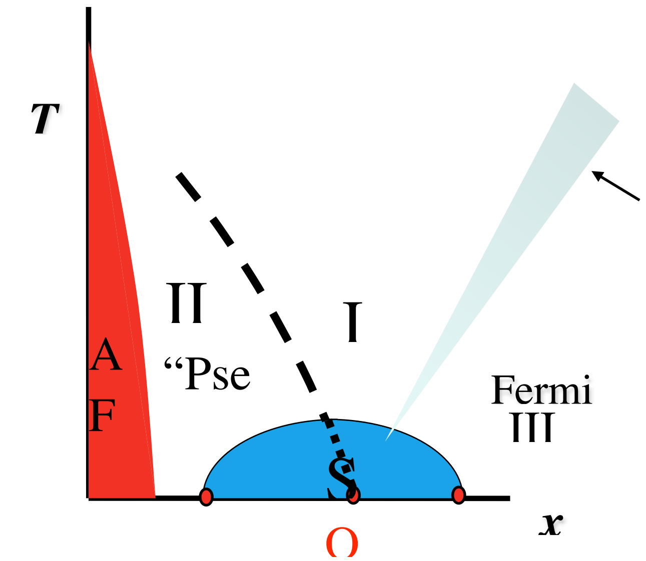


F. Slakey et. al. PRB 43, 3764 (1991)

Conclusions:



Conclusions:



Following the observations of the predicted order in underdoped Cuprates, we have worked to

1. Derive the Quantum-critical Fluctuations to get the Marginal Fermi-liquid State.

2. Calculated the coupling of these fluctuations to fermions to show the coupling is the orbital analog of the coupling to spin-fluctuations with an interesting momentum dependence.

3. Shown unambiguously that pairing in d-wave channel is promoted.

4. Used normal state ARPES to deduce parameters of the QCF's and their coupling to Fermions.

5. Working on inversion of ARPES in the superconducting state with evidence that this method may work if used with care.

6. Working on properties in Region II>

Cu Knight shift in the 123 and 248 layers of Y(2)Ba(4)Cu(7)O(15)

Stern et al. Phys. Rev B 50, (1994).

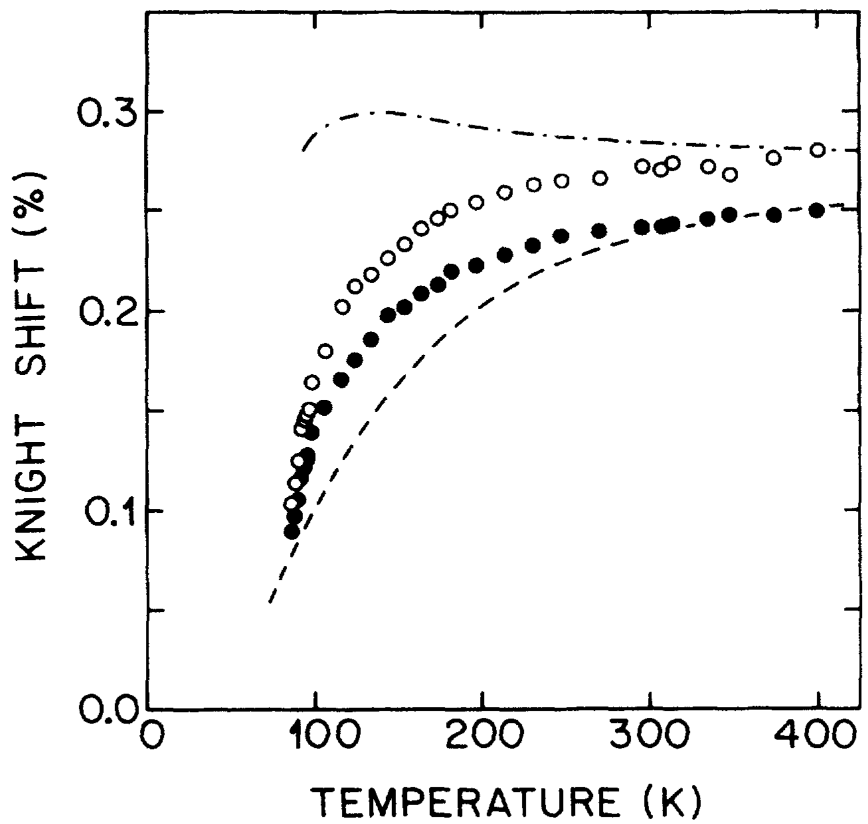


FIG. 7. Temperature dependence of the plane ^{63}Cu Knight shift at Cu(2) (open circles) and Cu(3) sites (filled circles) in $Y_2Ba_4Cu_7O_{15}$ compared to the Knight shift at Cu(2) sites in $YBa_2Cu_3O_7$ (dash-dotted line, Ref. 34) and in $YBa_2Cu_4O_8$ (dashed line, Ref. 6). The external field $\mathbf{B}_0$ lies perpendicular to the crystal **c** axis.

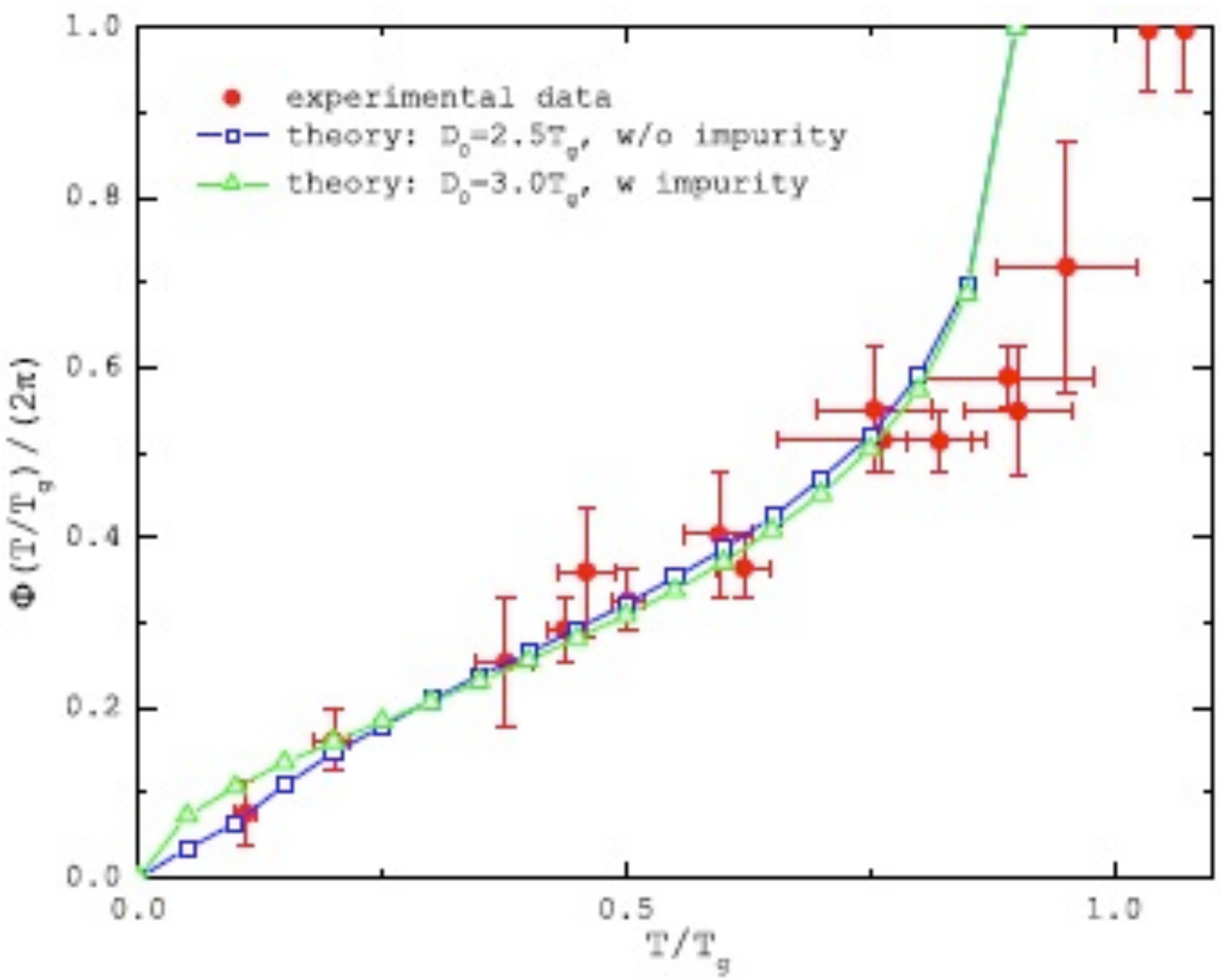
Fermi-Arc Phenomena

with arc length decreasing as Temperature decreases:.

Data consistent with a gap everywhere except at four points in the "normal" Phase in underdoped Cuprates.

Kanigel et al. (2006)

Zhu and cmv (2006) based on cmv (1999).



If Pseudogap state in the Loop-current phase has 4 fermi-points for T=0. It is Consistent with Schubnikov DeHaas with small pockets. But

Separation between Landau levels predicted to be $\propto B^{2/3}$ with absolute magnitude more than an order of magnitude larger than eB/mc.

Significance of Fermi -points

There are strict rules in condensed matter Physics about when a gap in the spectrum can occur.

a. Bloch rules: mix degenerate states at k and k+ G leading to gaps at zone-boundaries.
   i.e. gaps related to translational symmetry.

b. BCS: mix states of (k, σ) and $(-k, -\sigma)$ to produce gaps at chemical potential.

Another Possibility

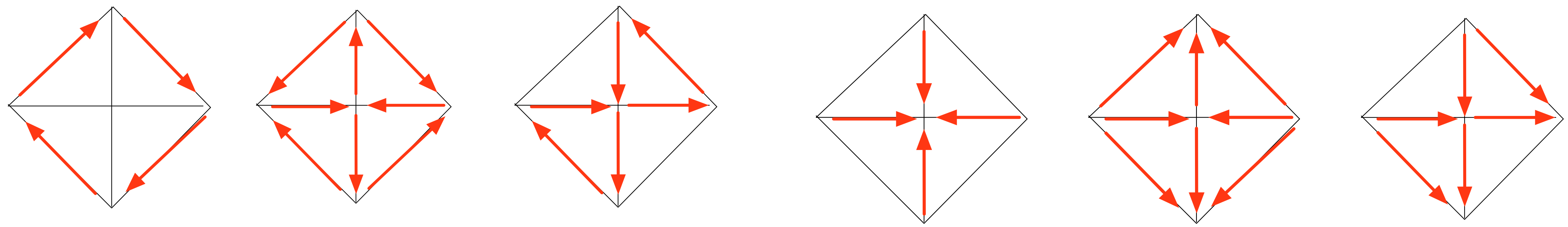
Infinite Range forces: Fermi-surface cannot be stable
For example: Fermi-velocity diverges (i.e. there is a gap)
for unscreened Coulomb interactions.

Also if there is a photon like mode interacting with electrons

with "effective" fine-structure constant of order unity.

At each site in a unit-cell, a gauge transformation is allowed

(8 phase variables)/cell - (3 sites)/cell = (5 physical fields)/cell



L_s L_d $\mathbf{L}=(L_x,L_y)$ a_s a_d $\mathbf{a} = (a_x, a_y)$

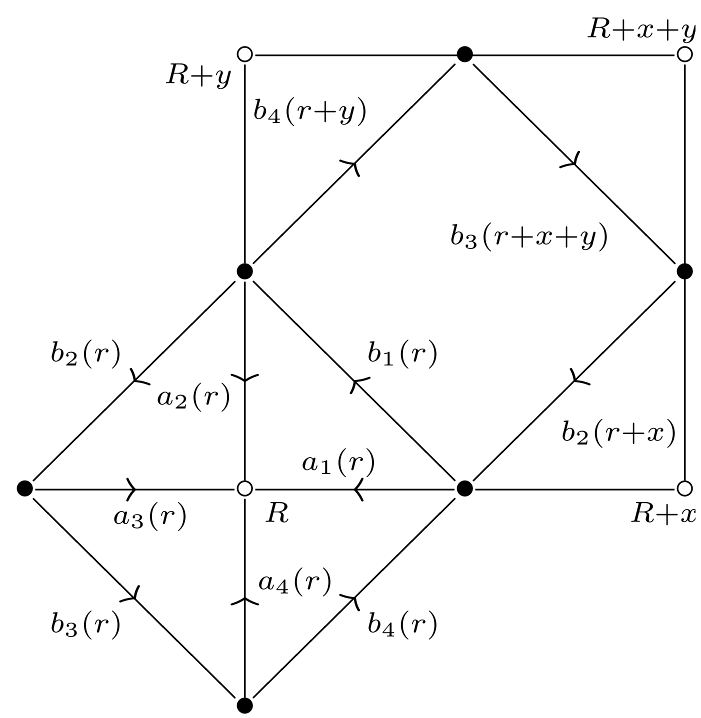
Physical Fields

L_s L_d $\mathbf{L}=(L_x,L_y)$ and transverse part of $\mathbf{a} = (a_x, a_y)$

Only Fields **L** and **a** are relevant for cuprates

$$\mathbf{a} = (a_x, a_y)$$

are necessary to describe the flux in regions of space not covered by the cu-o-o triangles



$\mathbf{L}=(L_x,L_y)$ can order but $\mathbf{a} = (a_x, a_y)$ cannot

$\mathbf{a} = (a_x, a_y)$ is a Gauge field, just like an external electromagnetic potential.

The total free-energy can be derived from microscopic theory starting with

$$\sum_i \sum_{links(i)} |J_{links(i)}|^2 + K.E.$$

$$\text{F} \quad = \quad \text{F(L)+} \; \frac{1}{v^2}|curl\mathbf{a}|^2 + \mathbf{e}^2 + curl(\mathbf{L}) \cdot curl(\mathbf{a}) + ...$$

$$-\mathbf{J} \cdot \mathbf{a} - \mathbf{a} \cdot \mathbf{J} + \mathbf{a}^2 ne^2/2mv + K.E.$$

$$[\mathbf{e}_i, \mathbf{a}_j] = i\delta_{ij}$$

What is v? or what is the fine-structure constant of the theory:

$\alpha \approx V/t$ rather than 1/137.