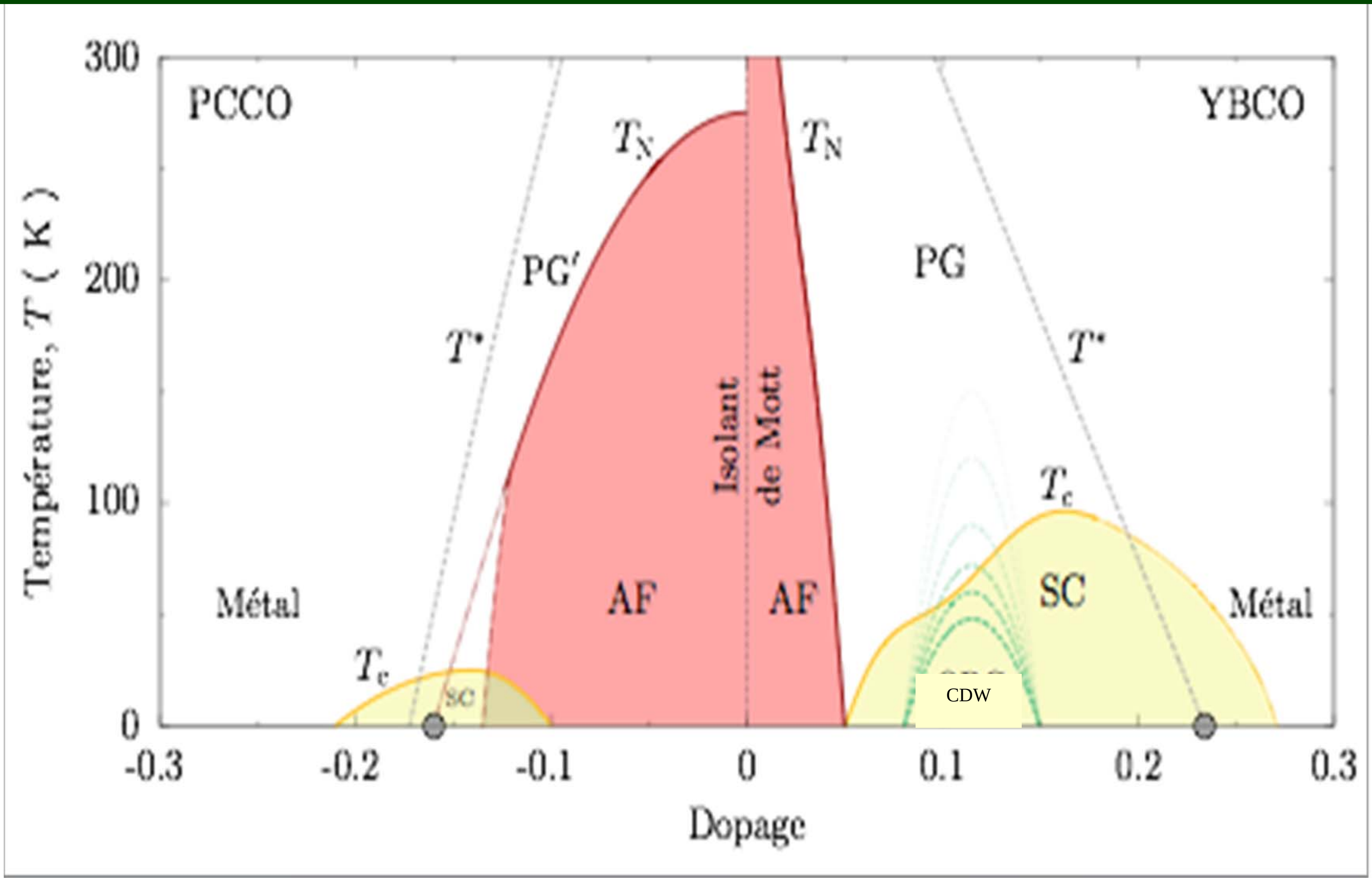
Antiferromagnetic Quantum Critical Behavior and Pseudogap in Electron-Doped Cuprates

A.-M. Tremblay

Quantum Criticality in Correlated Materials and Model Systems”,
Natal, Brazil, July 21 to August 01, 2014

e-doped cuprates, an example of AFM QCP with superconducting dome

Thèse de Francis Laliberté,
Université de Sherbrooke



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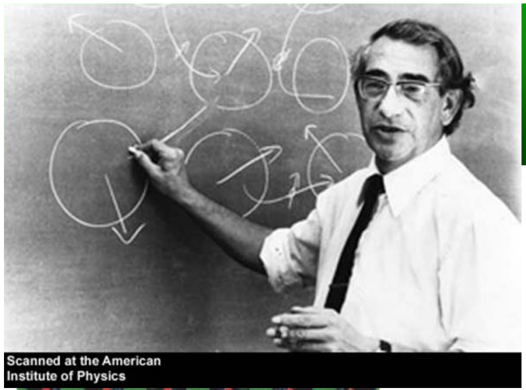
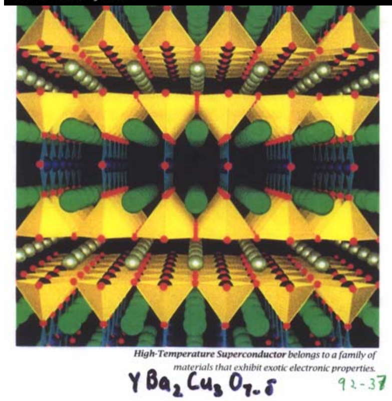
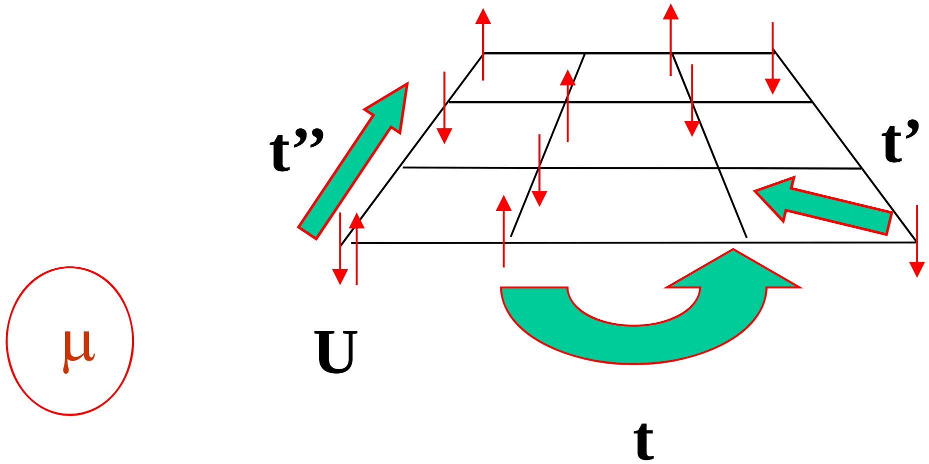
The model

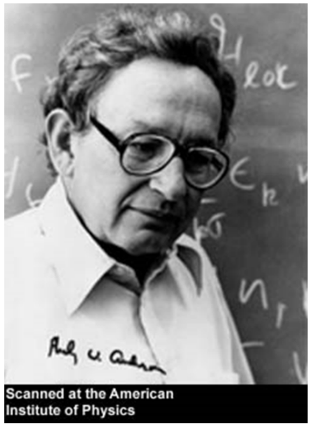
The Hubbard model





Simplest microscopic model for *Cu O* planes.



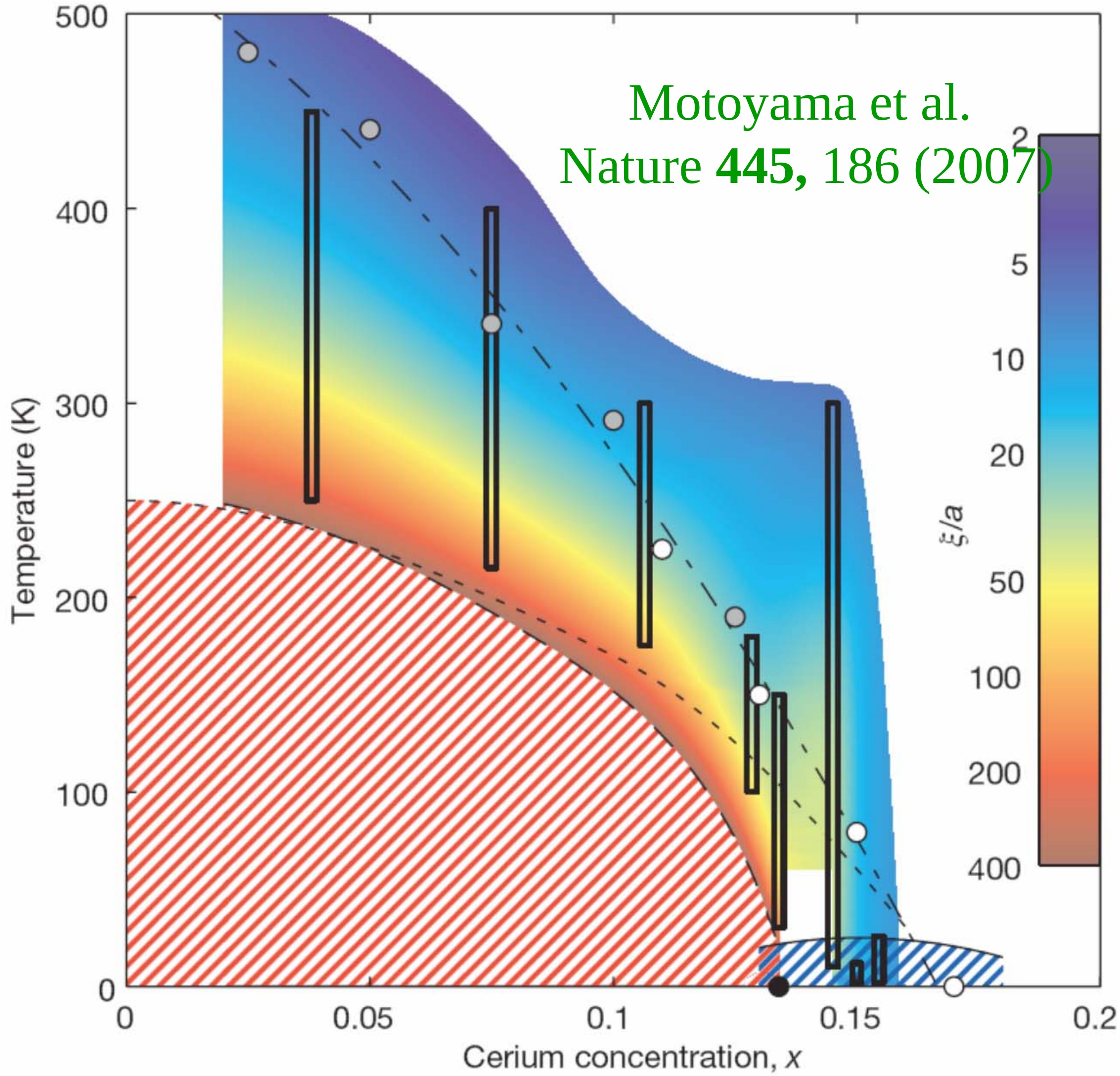


$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

No mean-field factorization for d-wave superconductivity

Some agreement between experiment and theory

Electron doped: Neutron scattering



Motoyama et al.
Nature **445,** 186 (2007)

$$\xi^* = 2.6(2)\xi_{th}.$$

Vilk, A.-M.S.T EPL (1996)
J. Physique (1997)
Kyung, Hankevych,
A.-M.S.T., PRL, sept. 2004

Semi-quantitative agreement for both ARPES and neutron

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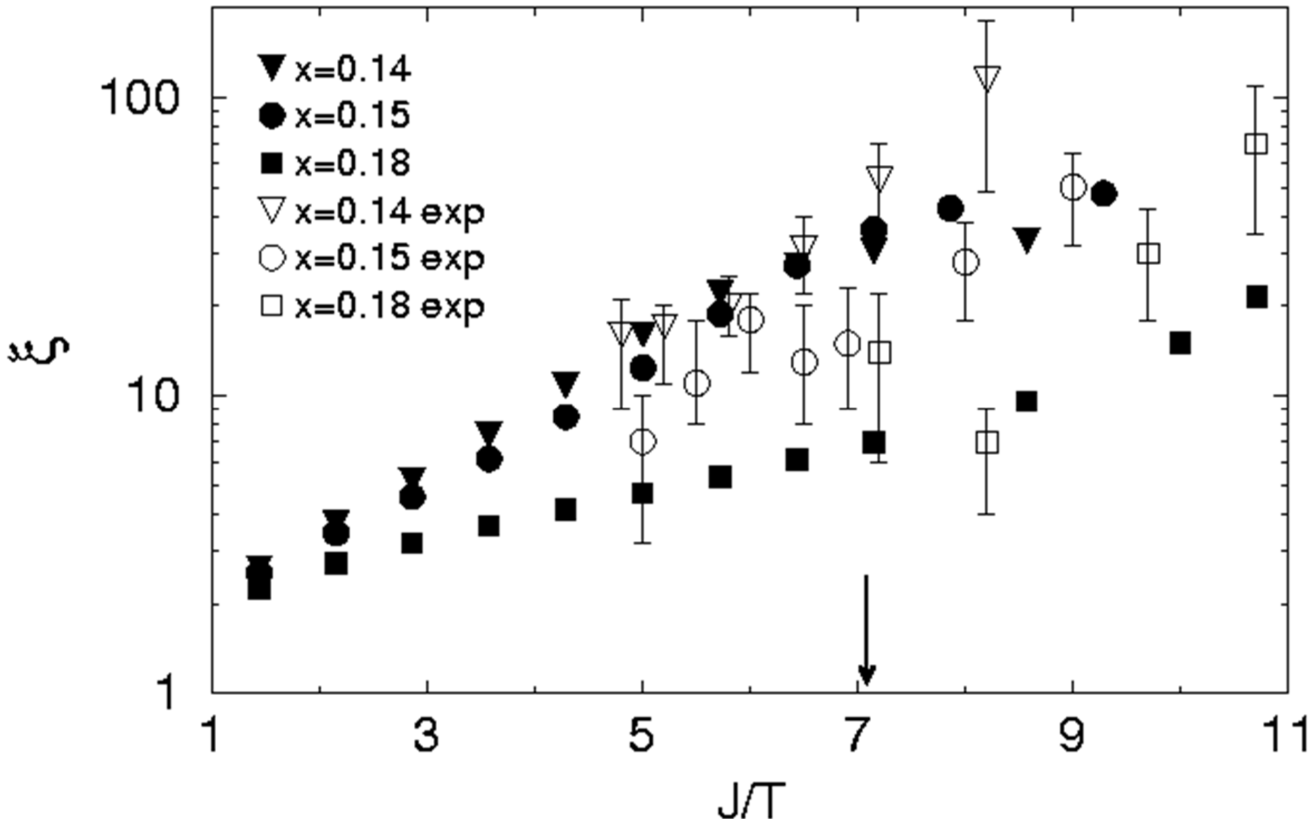
AFM correlation length (neutron)



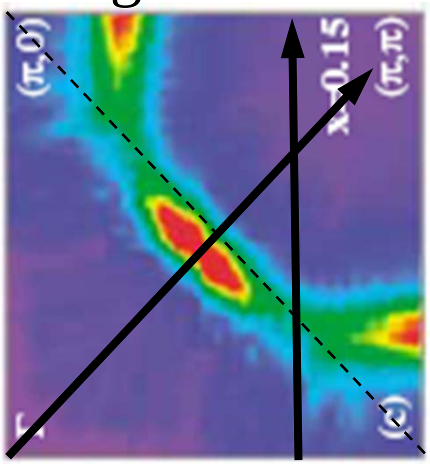
t'= 0.175t ; t'' = 0.05t, U=5.75

Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

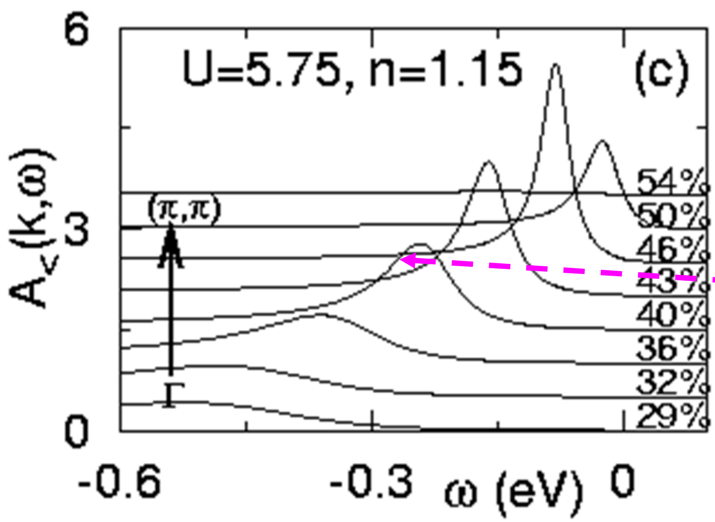
Expt: P. K. Mang et al., PRL **93**, 027002 (2004), Matsuda (1992).

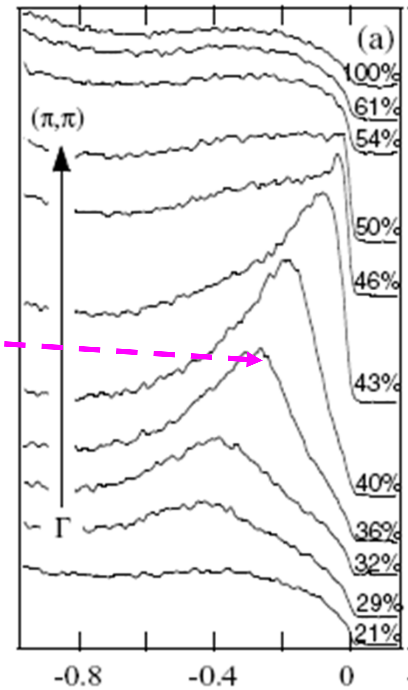
15% doped case: EDCs in two directions

Armitage et al. PRL 2001



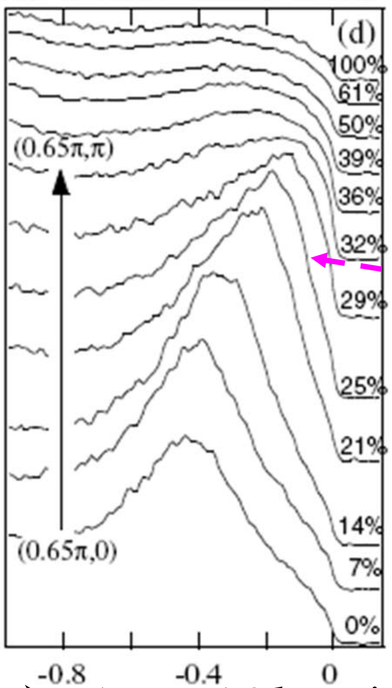
TPSC

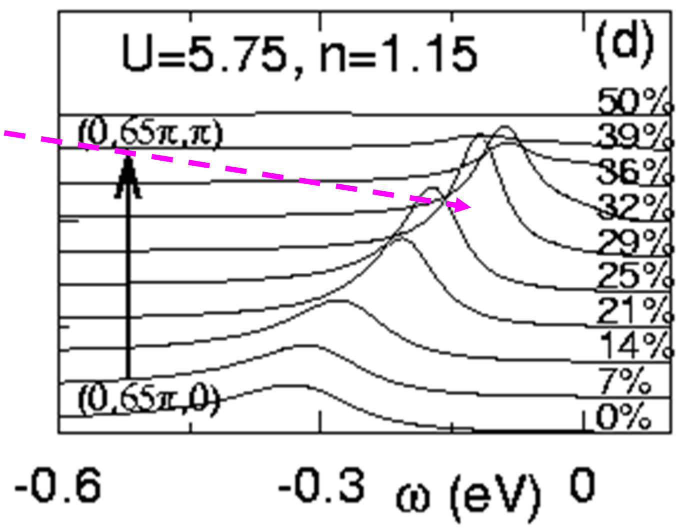




Exp

Exp



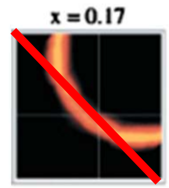


Hankevych, Kyung, A.-M.S.T., PRL (2004).

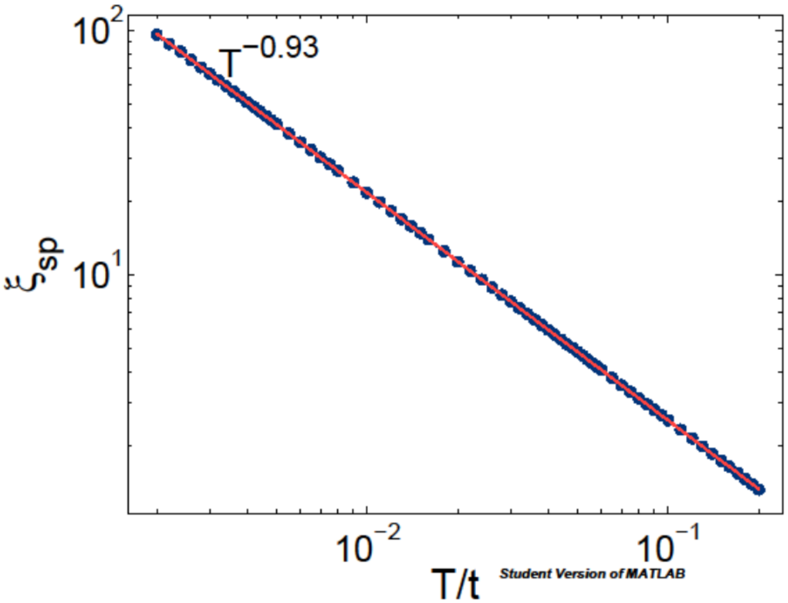
➢ $\Delta_{PG} \approx 10 k_B T^*$ comparable with optical measurements

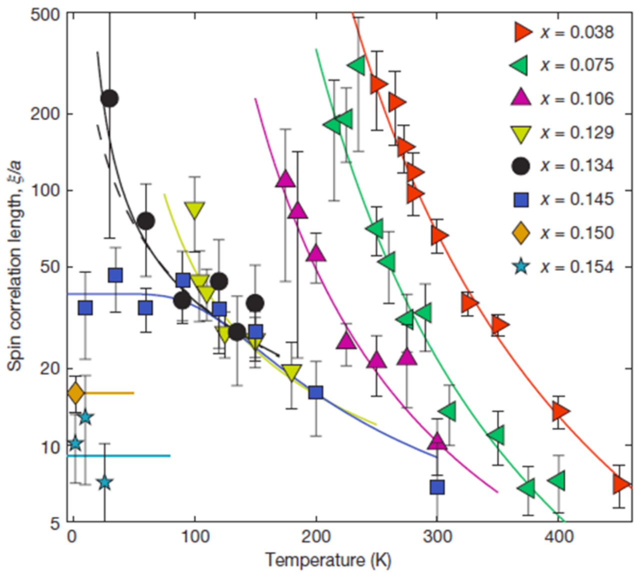
ξ(T) at the QCP

z = 1 Motoyama, Nature 2007



NCCO
Matsui et al. PRB 2007





U=6, t'=-0.175, t''=0.05, n=1.2007

D. Bergeron, D. Chowdhury, M. Punk,
S. Sachdev, and A.-M.S. T
Phys. Rev. B **86**, 155123 (2012)

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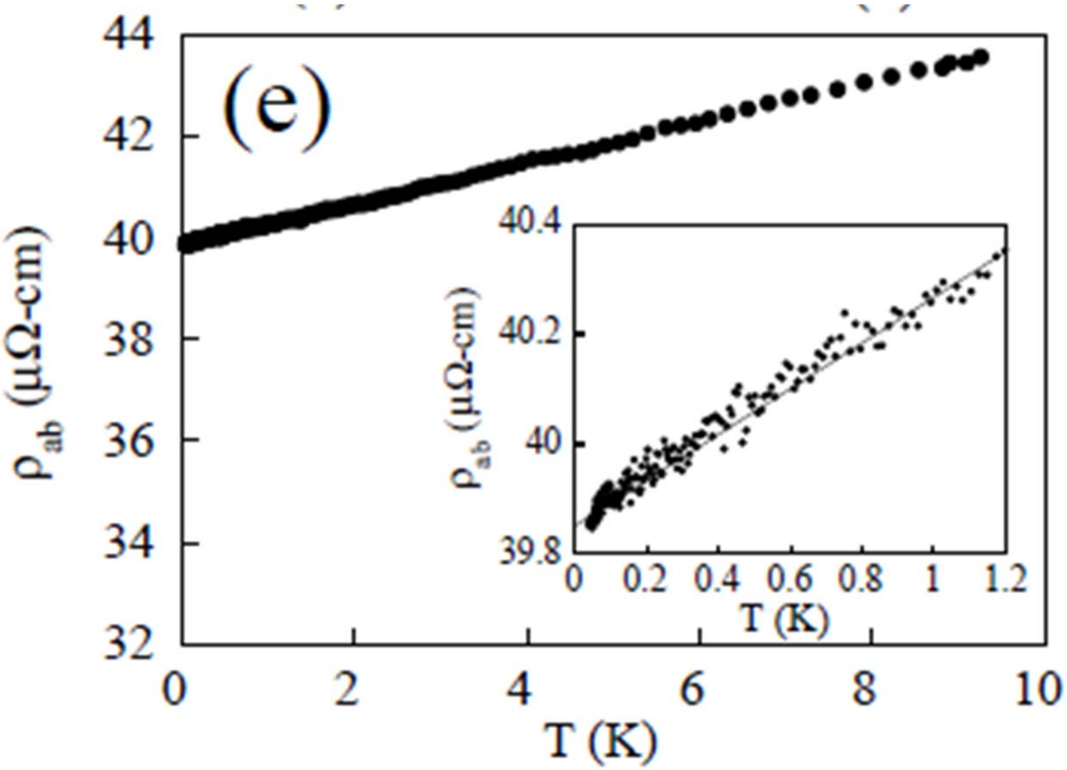
Linear resistivity

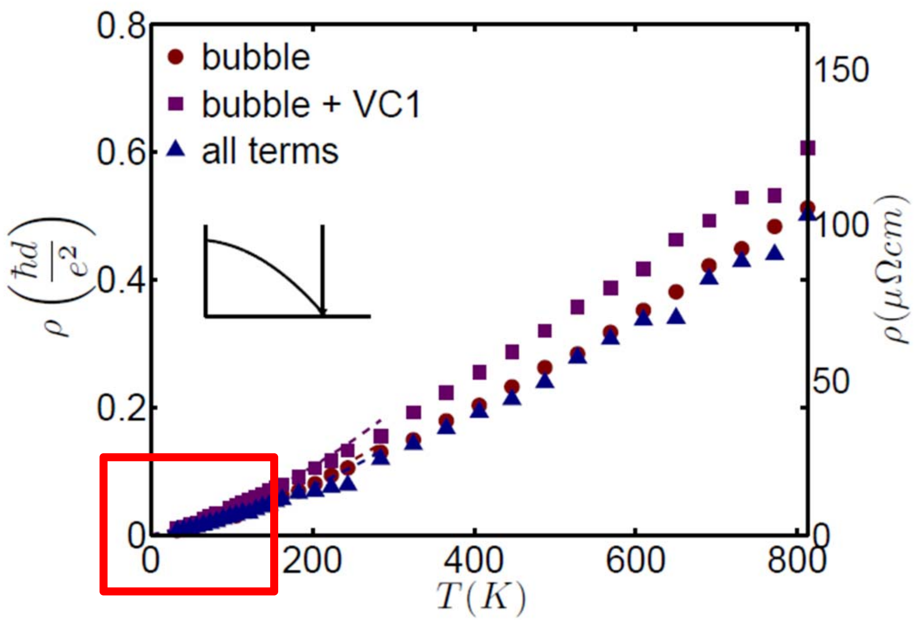


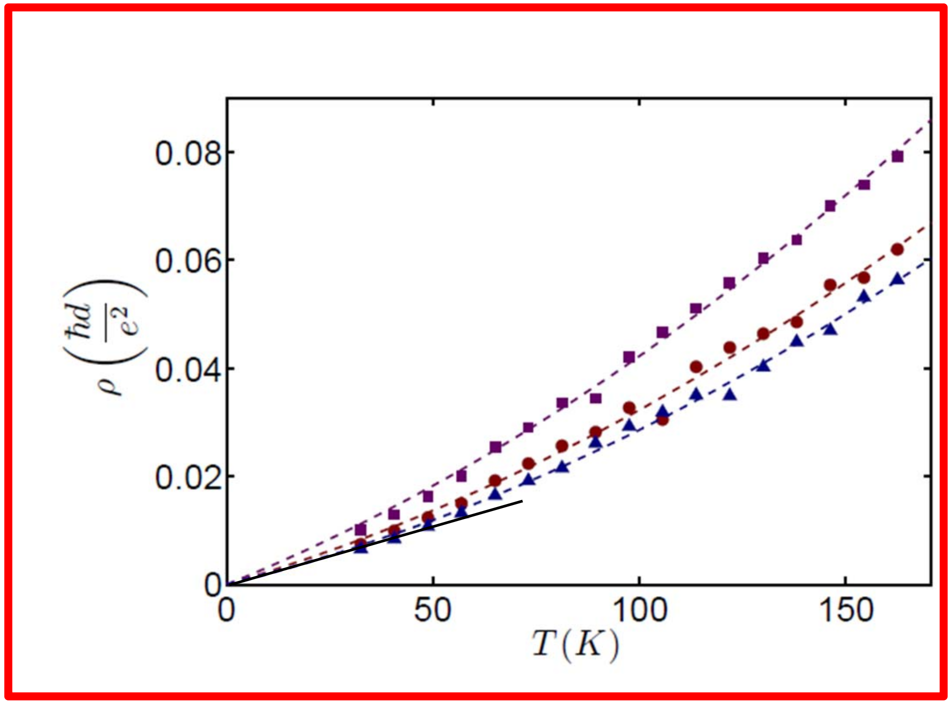
Fournier et al. PRL 1998

At the QCP for finite *t'*

D. Bergeron et al.
Phys. Rev. B **84**, 085128/1-35 (2011)

$U = 6t,\ t' = -0.175t,\ t'' = 0.05t$

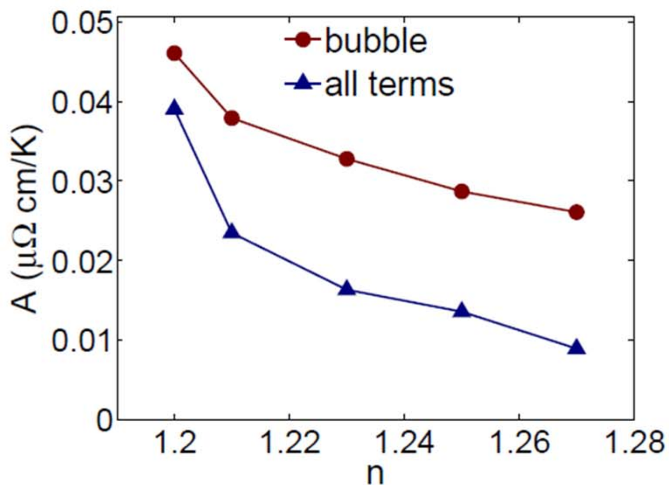


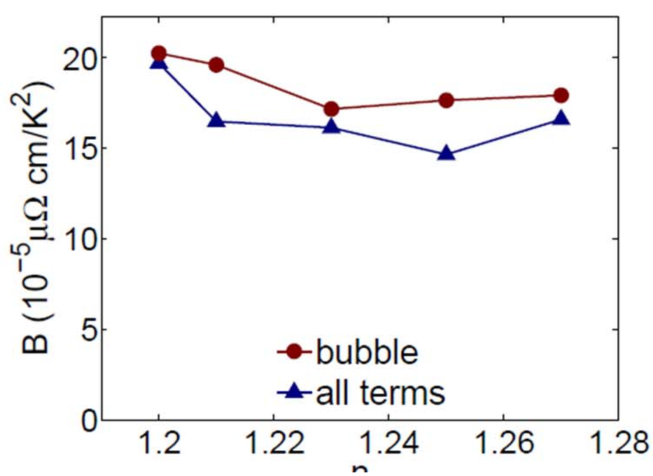


$$\rho(T) = AT + BT^2$$

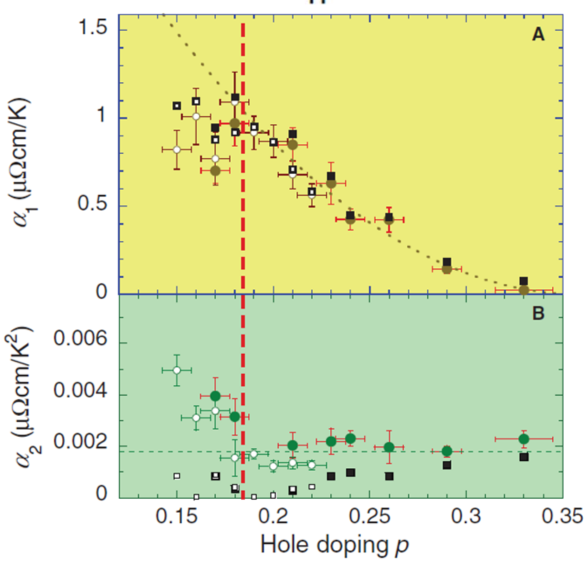
Linearity for $n > n_c$ *and* T_c

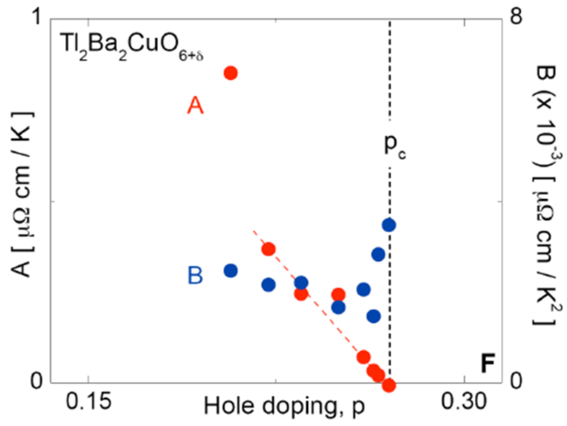
Fitting $\rho(T) = A$ $U = 6t,\ t' = -0.175t,\ t'' = 0.05t$





Cooper et al. Science **323** 30 (2009)





Doiron-Leyraud et al. arXiv:0905.0964

Doiron-Leyraud et al. Phys. Rev. B **80**, 214531 (2009)

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Outline

- e-doped are in weak to intermediate correlation range
- Methodology and benchmarks
- Pseudogap: Vilk criterion $\xi_{AFM} > \xi_{th}$
- Critical point: *z=1*
- Superconductivity

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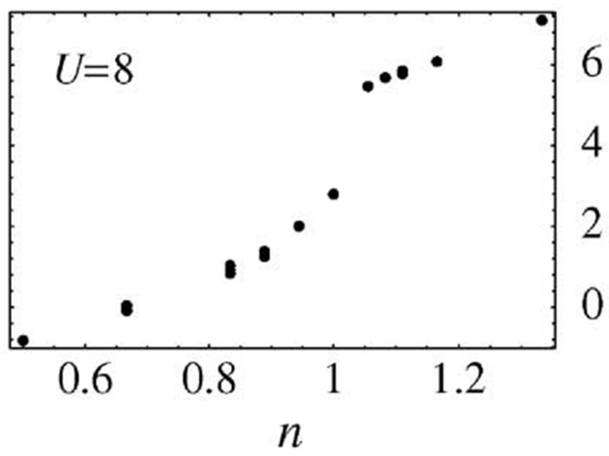
e-doped are in the weak to intermediate range of correlations

e-doped less strongly correlated than h-doped

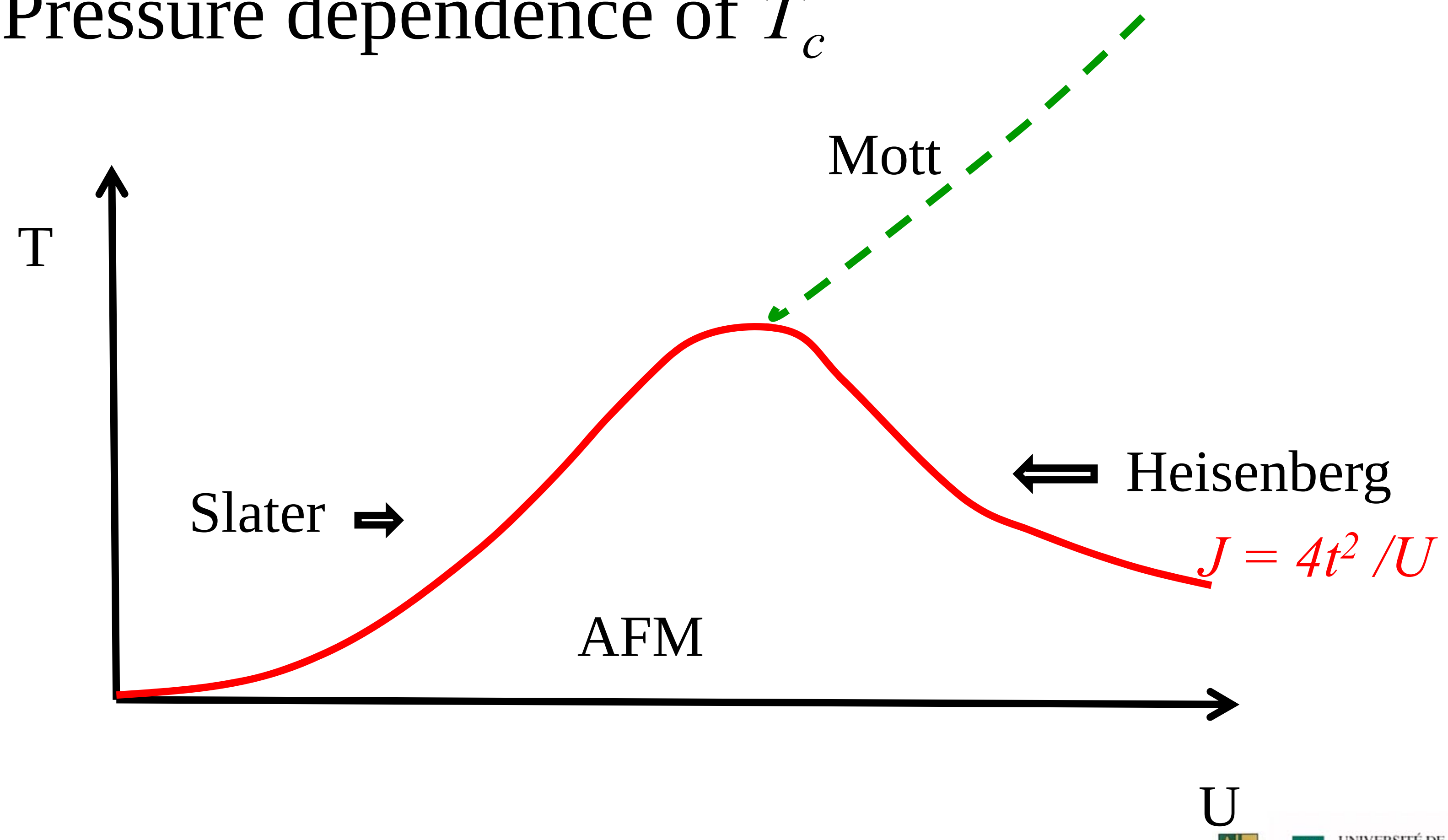
D. Sénéchal, AMST, PRL **92,** 126401 (2004)
C. Weber, K. Haule, G. Kotliar, Nature Physics **6,** 574 (2010)

- Optical gap *1.3* eV vs *2.0* eV
- Compressibility is larger



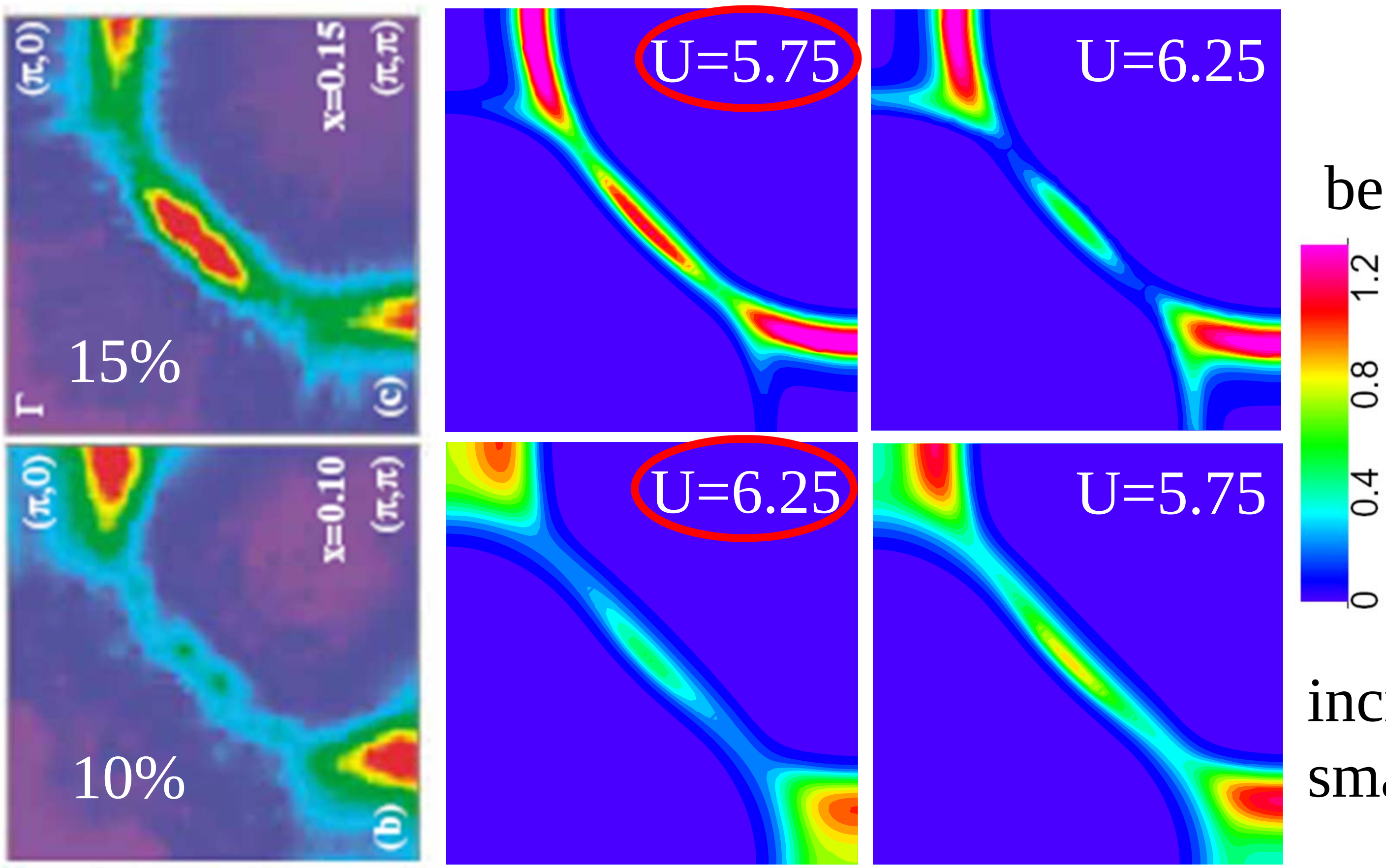
e-doped less strongly correlated than h-doped

- Pressure dependence of T_c



e-doped less strongly correlated than h-doped

Hubbard repulsion *U* has to…



be not too large

increase for smaller doping

B.Kyung *et al.*,PRB **68**, 174502 (2003)

Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

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e-doped less strongly correlated than h-doped

$$\sigma = \frac{ne^2\tau}{m}$$

$$n = \frac{k_F^2}{2\pi d}$$

$$\ell = v_F\tau$$

$$k_F\ell = 1$$

$$\sigma_{MIR} = \frac{1}{d}\frac{e^2}{h}$$

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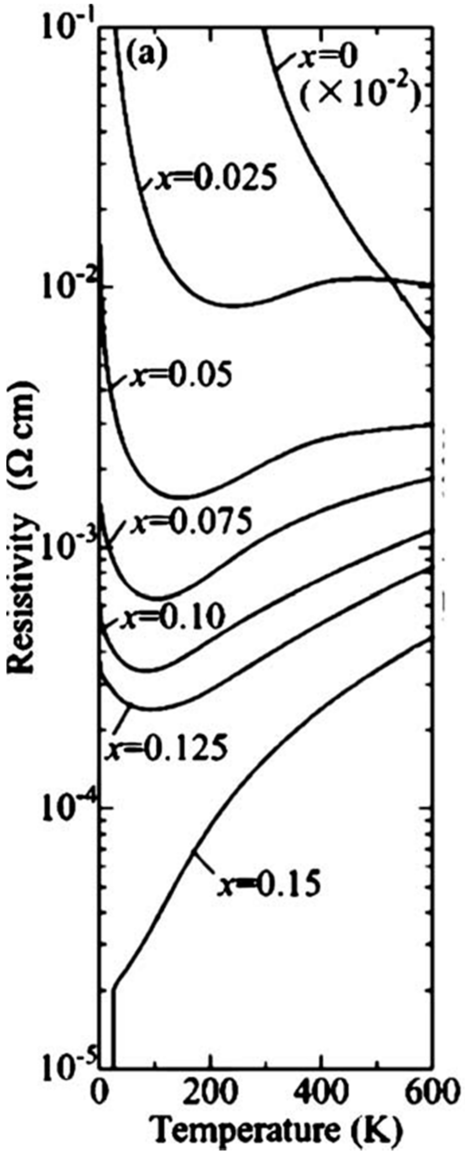
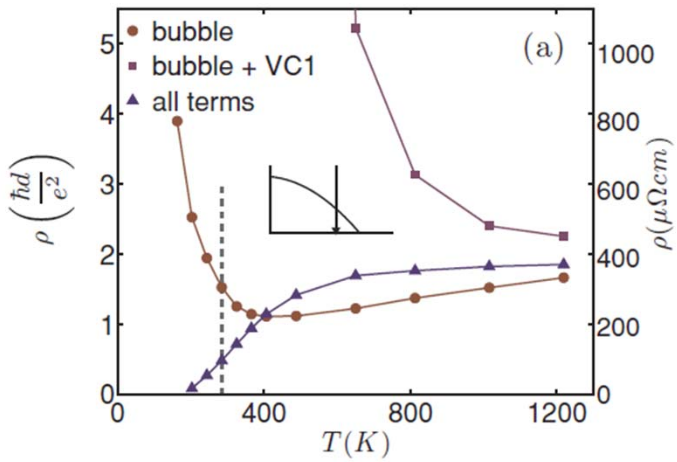
Electron-doped and MIR limit



NCCO



Dominic Bergeron et al. TPSC
PRB **84**, 085128 (2011)

Onose et al. 2004

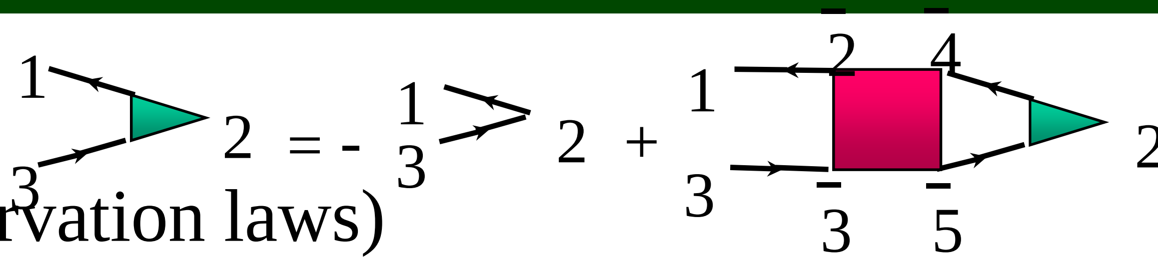
Theoretical difficulties

- Low dimension
  - (quantum and thermal fluctuations)
- Large residual interactions
  - (Potential ~ Kinetic)
  - Expansion parameter?
  - Particle-wave?
- By now we should be as quantitative as possible!

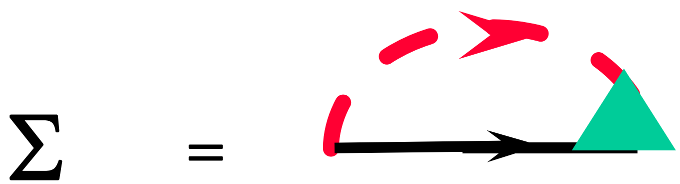
Methodology

Weak to intermediate correlations

Theory difficult even for weak to intermediate correlations!

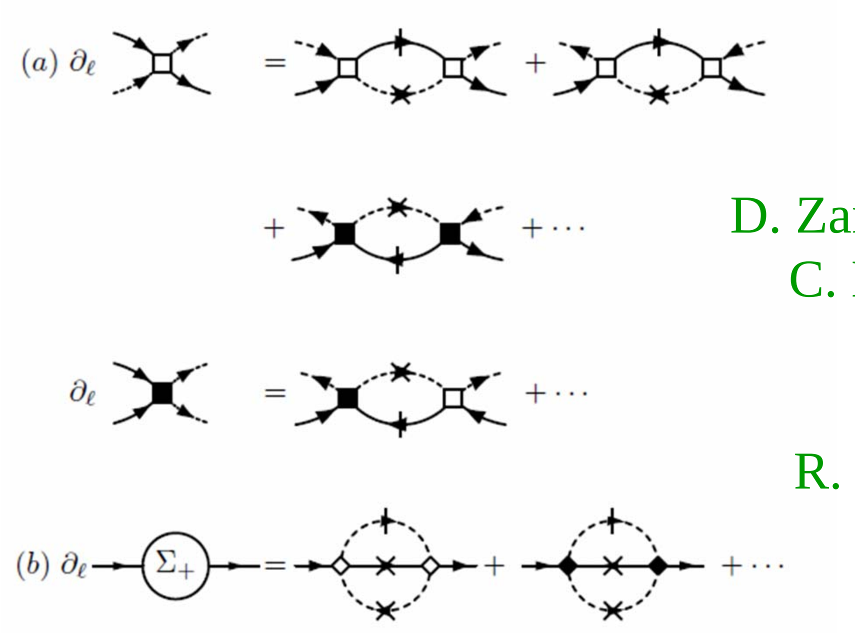


- RPA (OK with conservation laws)
  - Mermin-Wagner
  - Pauli
- Moryia (Conjugate variables HS $\phi^4 = \langle\phi^2\rangle\, \phi^2$)
  - Adjustable parameters: c and U_{eff}
  - Pauli
- FLEX
  - No pseudogap
  - Pauli



Weak correlation methods

- Functional renormalization group



D. Zanchi and H.J. Schulz, PRB 61, 13609 (2000)
C. Honerkamp, et al.PRB 63, 035109 (2001)
Rohe and Metzner (2004)
Katanin and Kampf (2004)
R. Shankar, Rev. Mod. Phys. 66, 129 (1994)
C. Bourbonnais Sedeki PRB 2012

- Other weak coupling methods
  - N.E. Bickers, et al. Phys. Rev. Lett. 62, 961 (1989) FLEX
  - B. Kyung, J.-S. Landry, and A.-M.S.T.,PRB 68, 174502 (2003)

Two-Particle Self-Consistent
TPSC

Theory without small parameter: How should we proceed?

- Identify important physical principles and laws to constrain non-perturbative approximation schemes
  - From weak coupling (kinetic)
  - From strong coupling (potential)
- Benchmark against “exact” (numerical) results.
- Check that weak and strong correlation approaches agree in intermediate range.
- Compare with experiment

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TPSC: general ideas

- General philosophy
  - Drop diagrams
  - Impose constraints and sum rules
    - Conservation laws
    - Pauli principle ($\langle n_\sigma^2 \rangle = \langle n_\sigma \rangle$)
    - Local moment and local density sum-rules
- Get for free:
    - Mermin-Wagner theorem
    - Kanamori-Brückner screening
    - Consistency between one- and two-particle $\Sigma G = U\langle n_\sigma n_{-\sigma} \rangle$

Vilk, AMT J. Phys. I France, **7**, 1309 (1997);
Theoretical methods for strongly correlated electrons also (Mahan, 3rd)

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Benchmark TPSC with Quantum Monte Carlo

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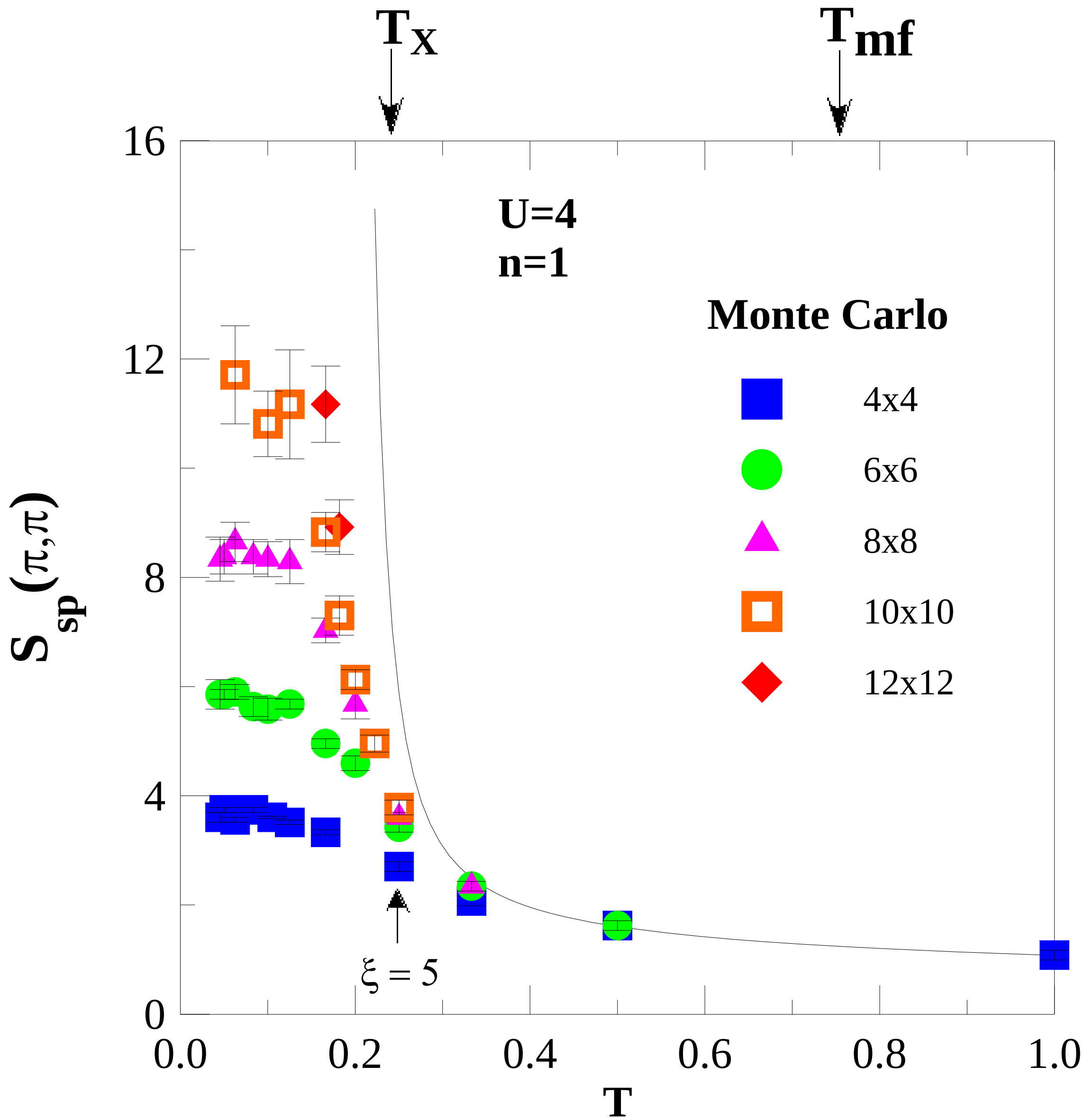
n=1

$\xi \sim \exp\left(C(T)/T\right)$



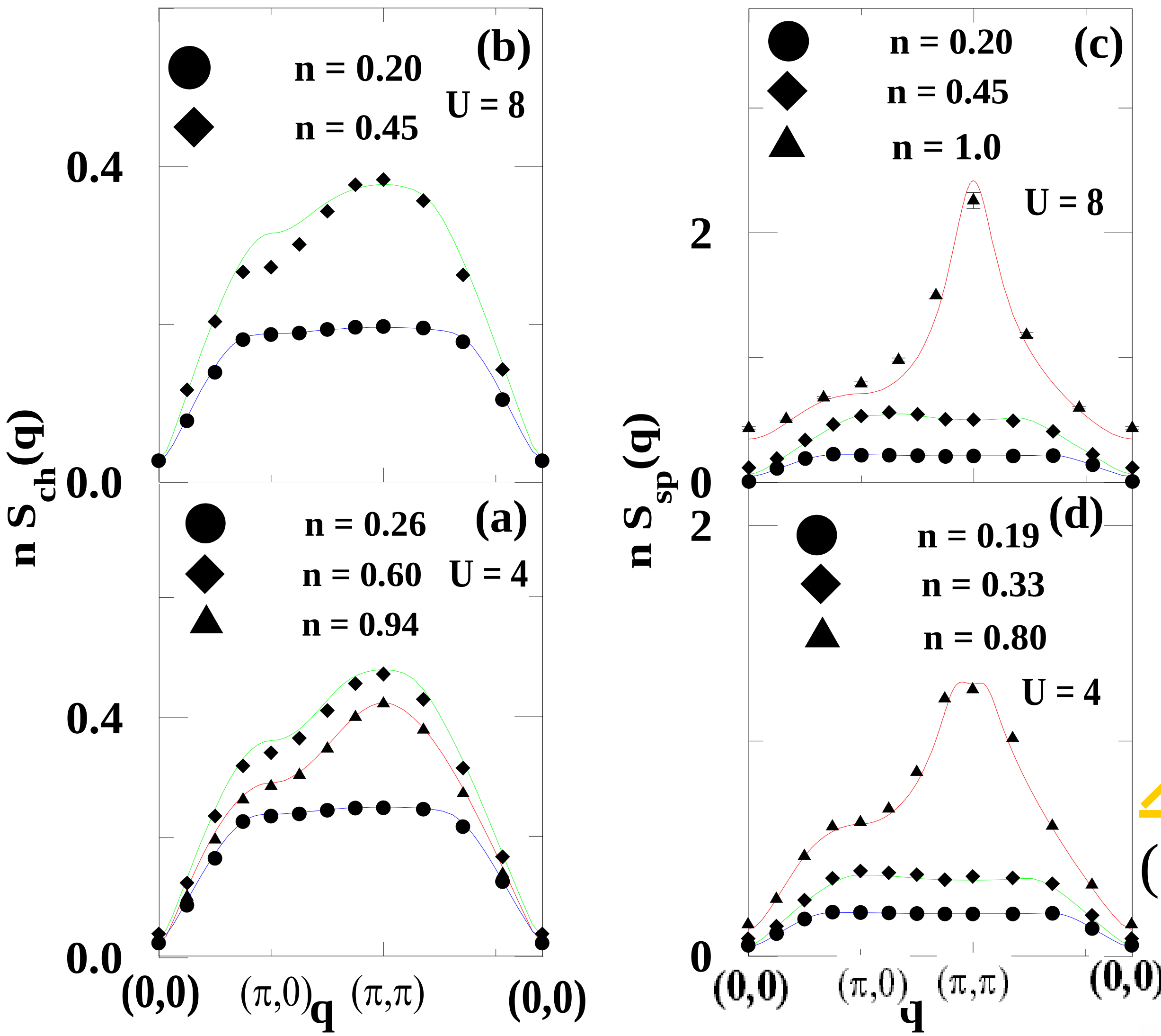
Calc.: Vilk et al. P.R. B **49,** 13267 (1994)

QMC: S. R. White, et al. Phys. Rev. **40**, 506 (1989).

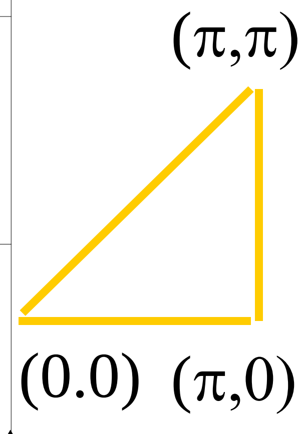
$O(N=\infty)$ A.-M. Daré, Y.M. Vilk and A.-M.S.T Phys. Rev. B **53**, 14236 (1996)

Notes:
-F.L. parameters

-Self also Fermi-liquid



U > 0
β = 5
8 X 8



QMC + cal.: Vilk et al. P.R. B **49,** 13267 (1994)

TPSC for spin fluctuations

$$\chi_{sp}^{(1)}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2}U_{sp}\chi_0(q)}$$

$$\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle - 2\langle n_\uparrow n_\downarrow \rangle$$

$$\frac{T}{N}\sum_q \chi_{sp}^{(1)}(q) = n - 2\langle n_\uparrow n_\downarrow \rangle$$

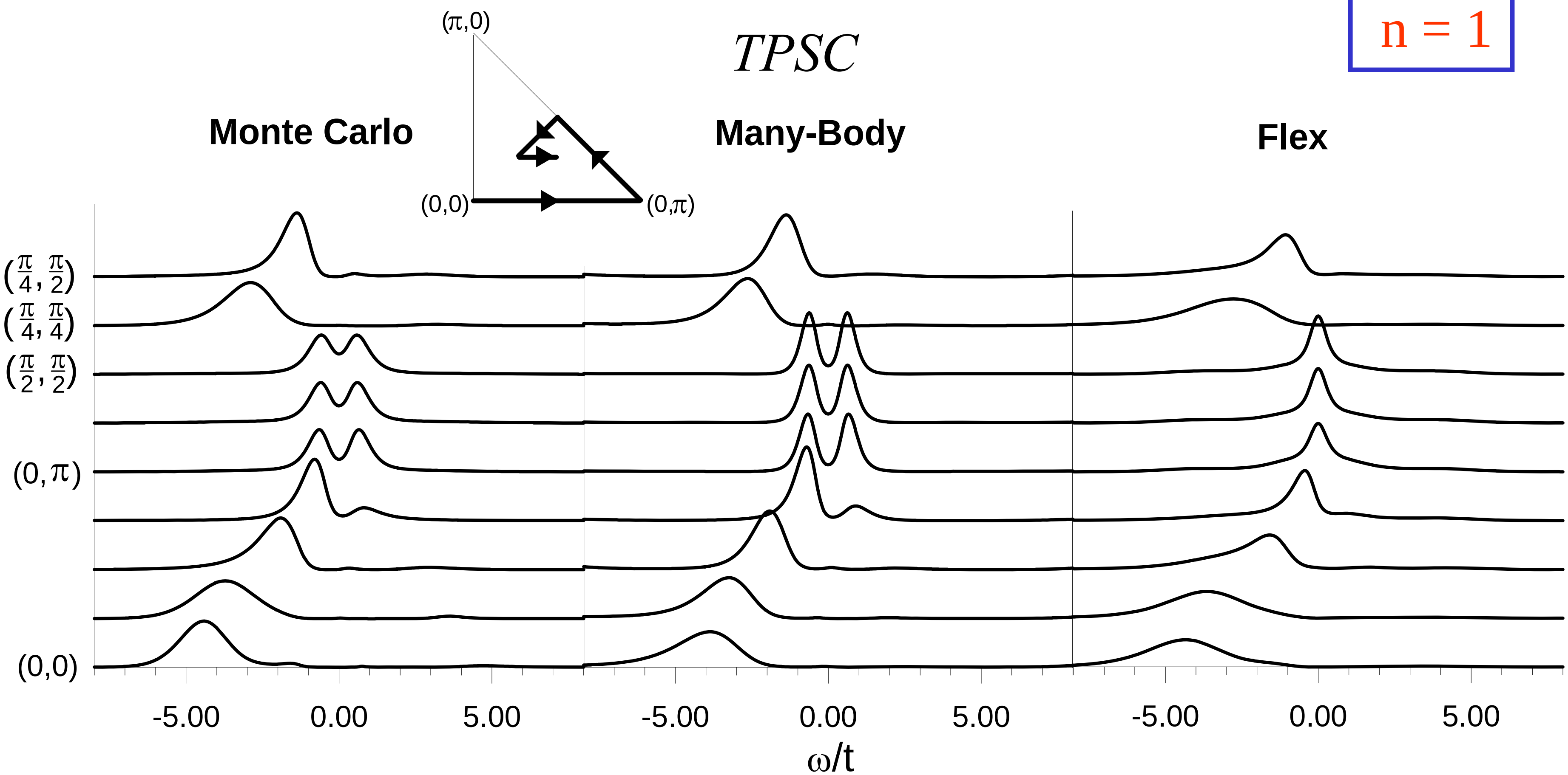
$$U_{sp} = U\frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}$$

Kanamori-Brückner screening

Proofs...

U = 4
β = 5
n = 1

TPSC



Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).

Self-energy in TPSC

$$\chi_{sp}^{(1)}(q) = \frac{\chi_0(q)}{1 - \frac{1}{2}U_{sp}\chi_0(q)}$$

$$\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle - 2\langle n_\uparrow n_\downarrow \rangle \qquad \frac{T}{N}\sum_q \chi_{sp}^{(1)}(q) = n - 2\langle n_\uparrow n_\downarrow \rangle$$

$$U_{sp} = U\frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}$$ Kanamori-Brückner screening

$$\Sigma_\sigma^{(2)}(k) \; = \; U n_{\bar\sigma} + \frac{U}{8}\frac{T}{N}\sum_q \left[3U_{sp}\chi_{sp}^{(1)}(q) + U_{ch}\chi_{ch}^{(1)}(q)\right] G_\sigma^{(1)}(k+q)$$

Does not assume Migdal. Vertex at same level of approximation as G

Internal accuracy check

$$\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}G^{(1)}\right) = U\langle n_\uparrow n_\downarrow \rangle \; = \; \frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}G^{(2)}\right)$$

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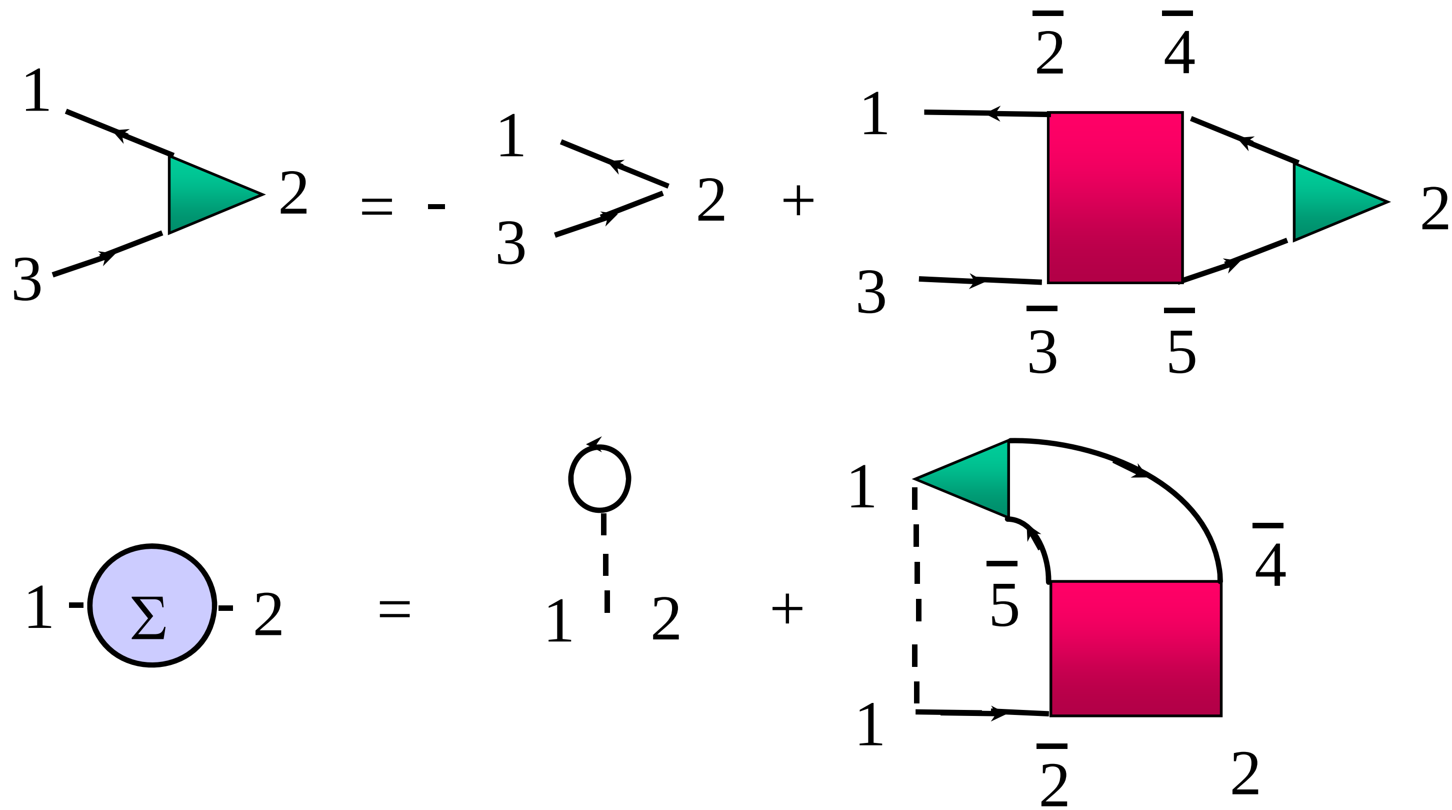
A better approximation for single-particle properties (Ruckenstein)



Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).
Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

N.B.: No Migdal theorem

Pseudogap: $\xi_{AFM} > \xi_{th}$ (Vilk criterion)

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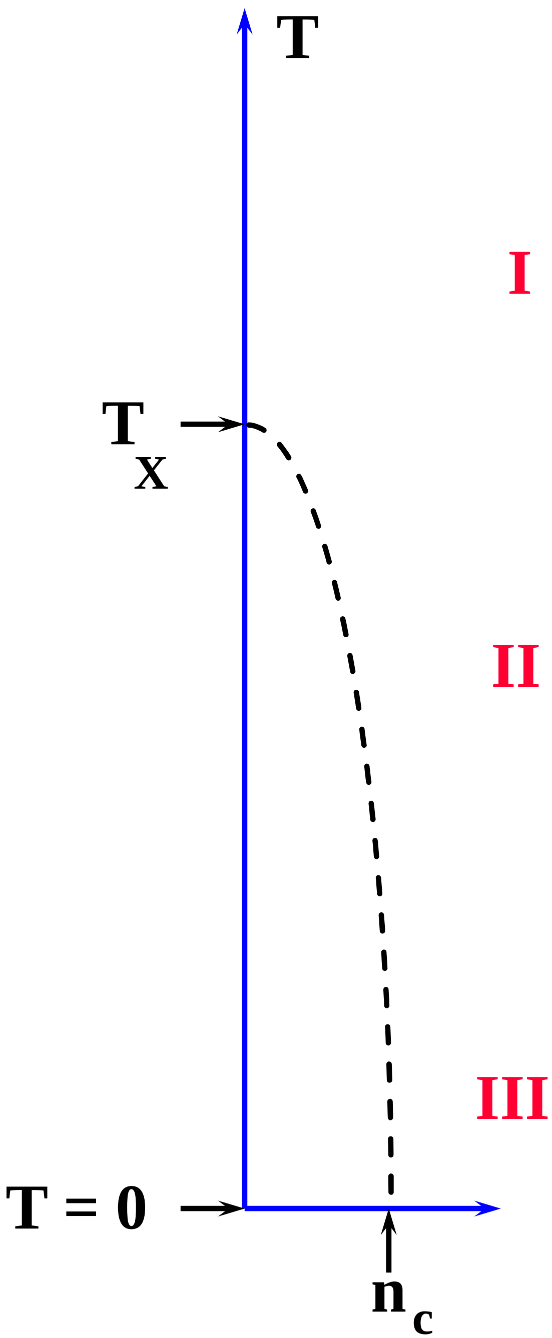
Precursor of SDW state (dynamic symmetry breaking)

- Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769-1771 (1995).
- Y. M. Vilk, Phys. Rev. B 55, 3870 (1997).
- J. Schmalian, *et al.* Phys. Rev. B **60**, 667 (1999).
- B.Kyung *et al.,*PRB **68**, 174502 (2003).
- Hankevych, Kyung, A.-M.S.T., PRL, sept 2004
- R. S. Markiewicz, PRB (2003).


T
I
T_X
II
III
T = 0
n_c

Vilk criterion:

effect of critical fluctuations on particles (RC regime)

$$\hbar\omega_{sf} << k_B T$$

$$\Sigma\left(\mathbf{k}_F, ik_n\right) \propto T\int d^d q \frac{1}{q_\perp^{\,2} + q_\parallel^{\,2} + \xi^{-2}} \frac{1}{ik_n + \varepsilon_{-\mathbf{k}+\mathbf{q}}}$$

$$\operatorname{Im}\Sigma^R\left(\mathbf{k}_F, 0\right) \propto -\frac{T}{v_F}\xi^{3-d}$$

in 2D: $\xi > \xi_{th}$ $\quad (\xi_{th} \equiv \hbar v_F / \pi k_B T)$

$$\Delta\varepsilon \approx \nabla\varepsilon_k \cdot \Delta k \approx v_F \hbar \Delta k = k_B T$$

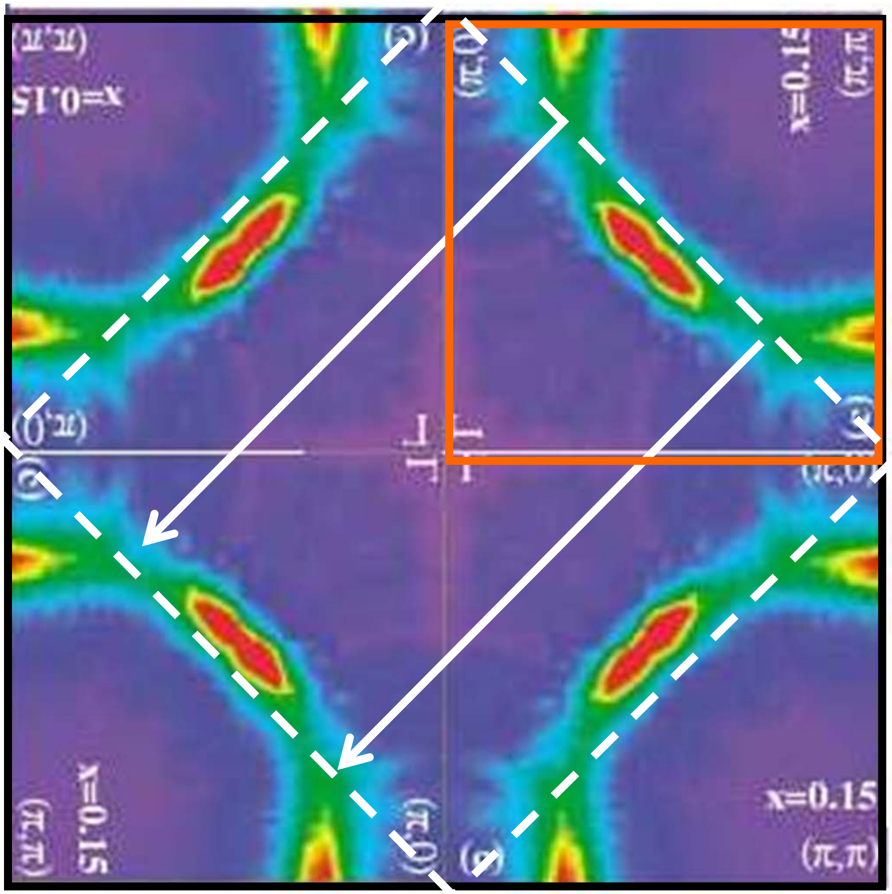
$$\operatorname{Im}\Sigma^R\left(\mathbf{k}_F, 0\right) \propto -U\xi / \left(\xi_{th}\xi_0^2\right) > 1$$

in 3D: Marginal

in 4D: quasiparticle survives up to T_c

Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).
Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

Hot spots from AFM quasi-static scattering

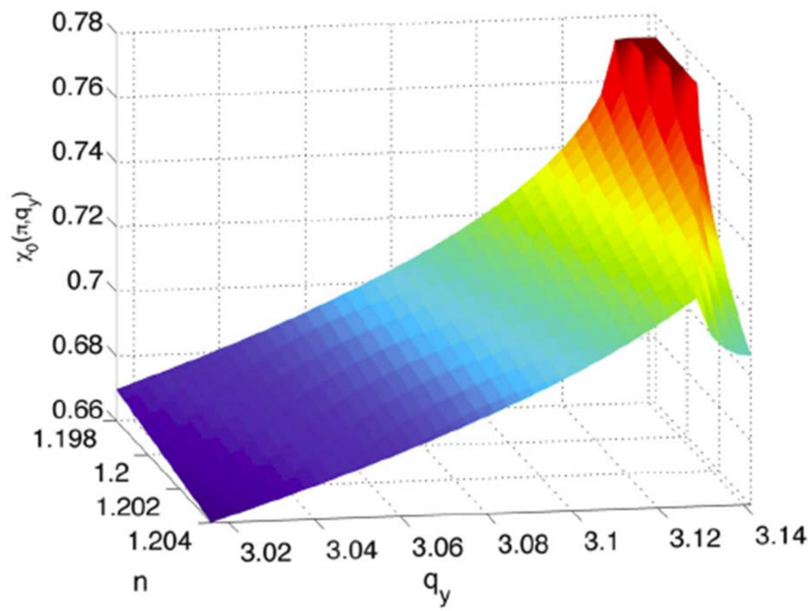


Exponent at the critical point

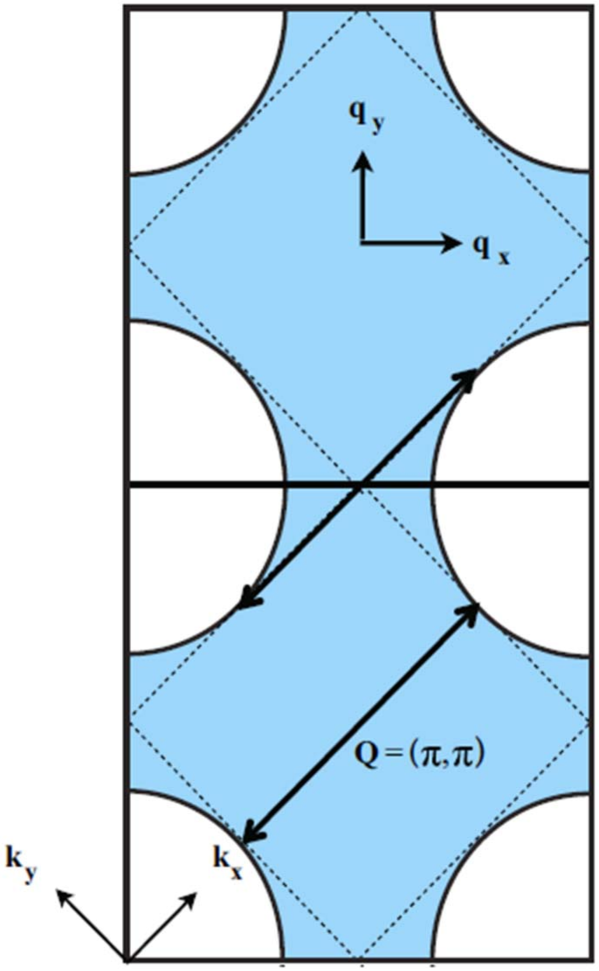
B. L. Altshuler, L. B. Ioffe, and A. J. Millis, PR B **52**, 5563 (1995).
P. Krotkov and A. V. Chubukov, PRL **96**, 107002 (2006).

D. Bergeron, D. Chowdhury, M. Punk, S. Sachdev, and A.-M.S. T
Phys. Rev. B **86**, 155123 (2012) (17 pages)

Touching condition



Lindhard function



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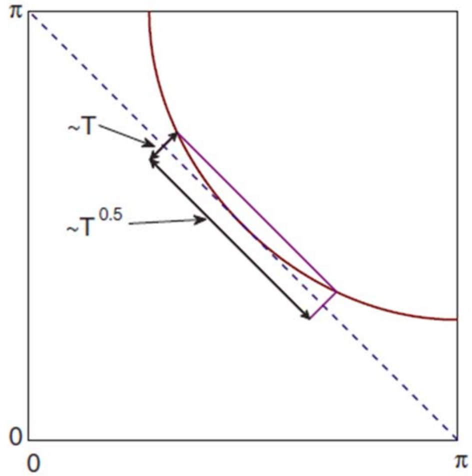
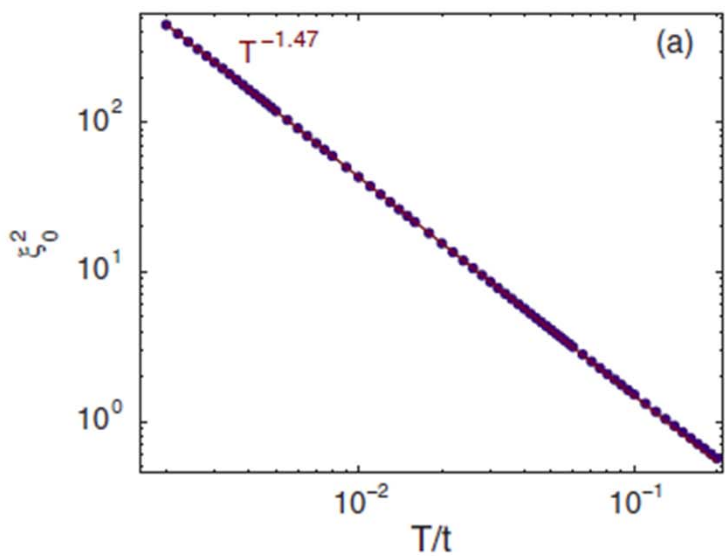
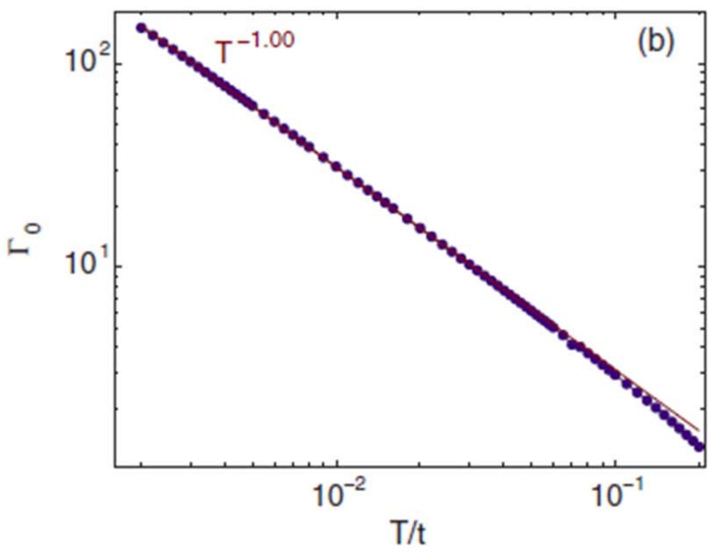
Origin of the change of power law







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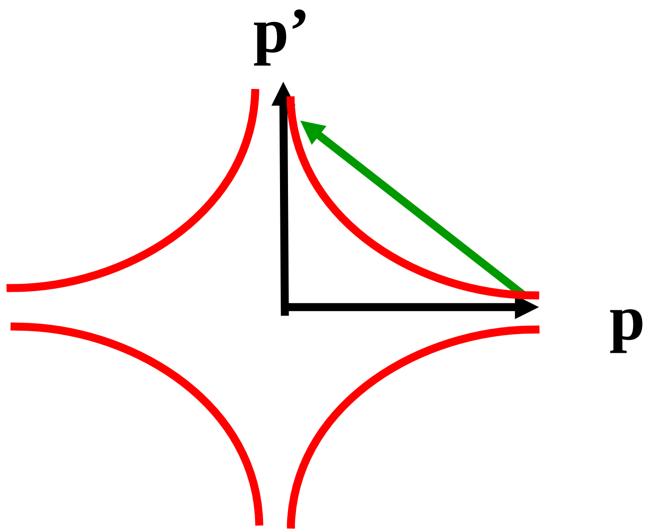
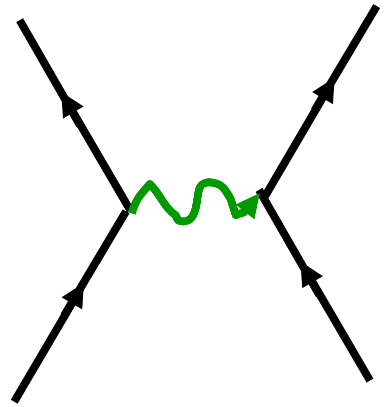
d-wave superconductivity

Cartoon « BCS » weak-coupling picture

$$\Delta_{\mathbf{p}} = -\frac{1}{2V}\sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right)$$





Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

Béal–Monod, Bourbonnais, Emery P.R. B. **34**, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch P.R. B **34**, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. **15**, 524 (1965).

P.W. Anderson Science 317, 1705 (2007)

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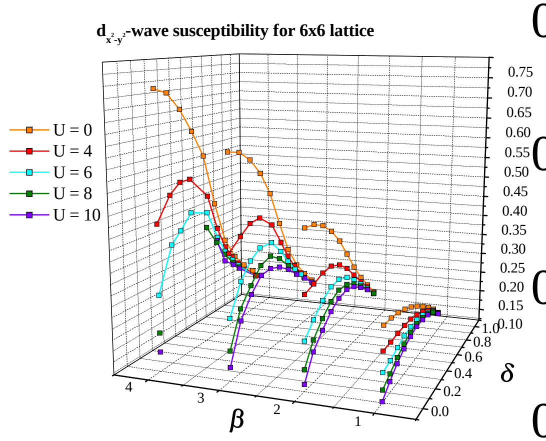

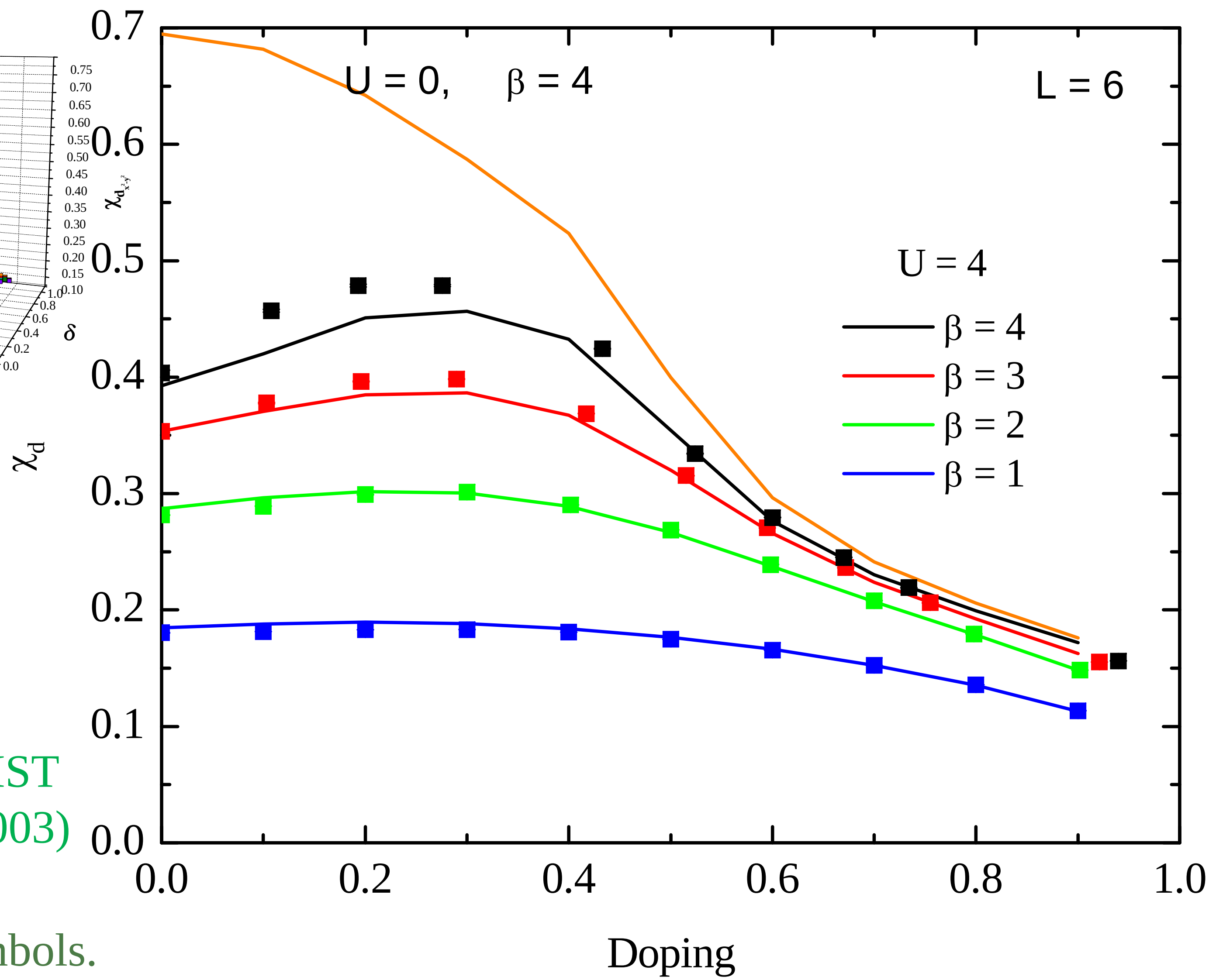

Kyung, Landry AMST
PRB **68**, 174502 (2003)

QMC: symbols.
Solid lines analytical.

Kyung, Landry, A.-M.S.T.

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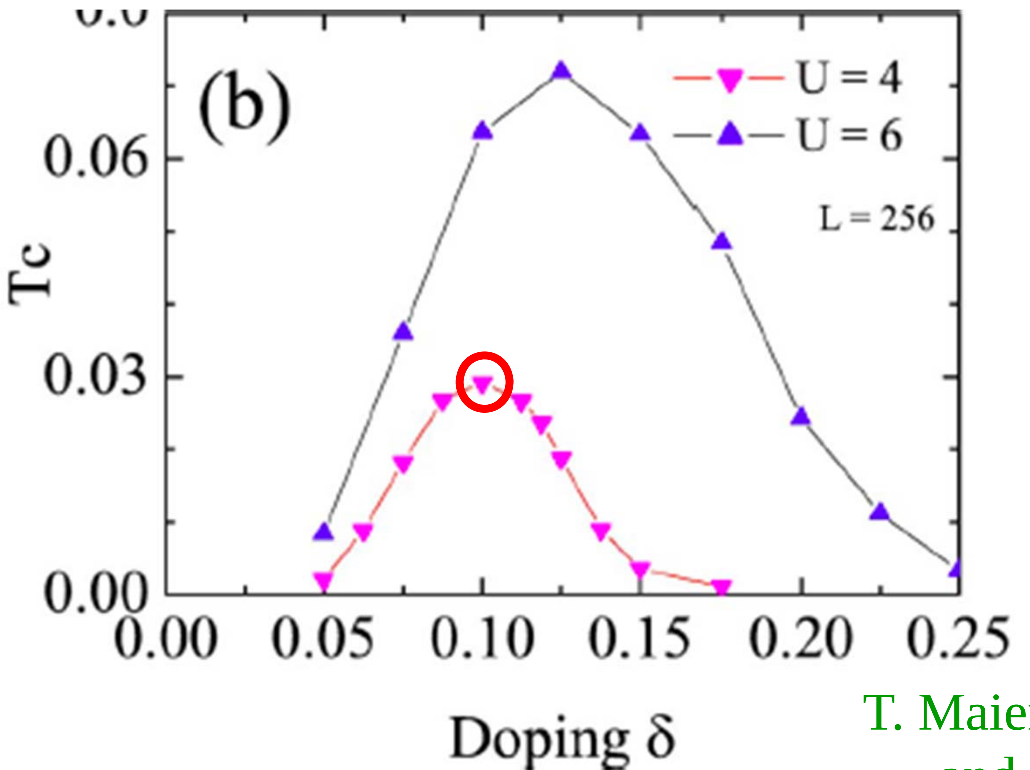
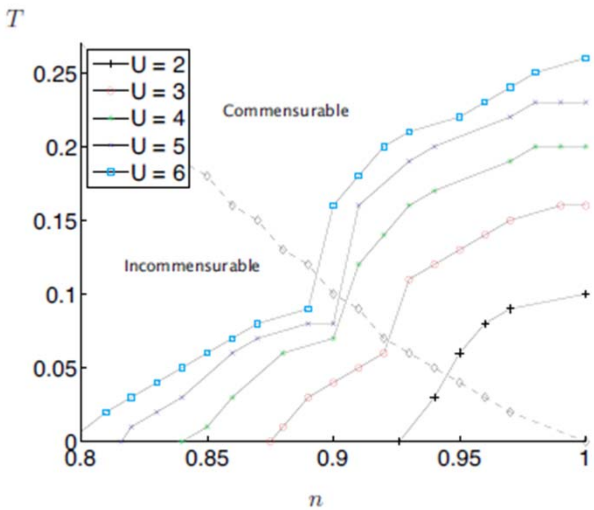
Tc from TPSC

$t' = 0$





S. Roy, PhD thesis 2007
Vilk et al. J. Physique (1997)

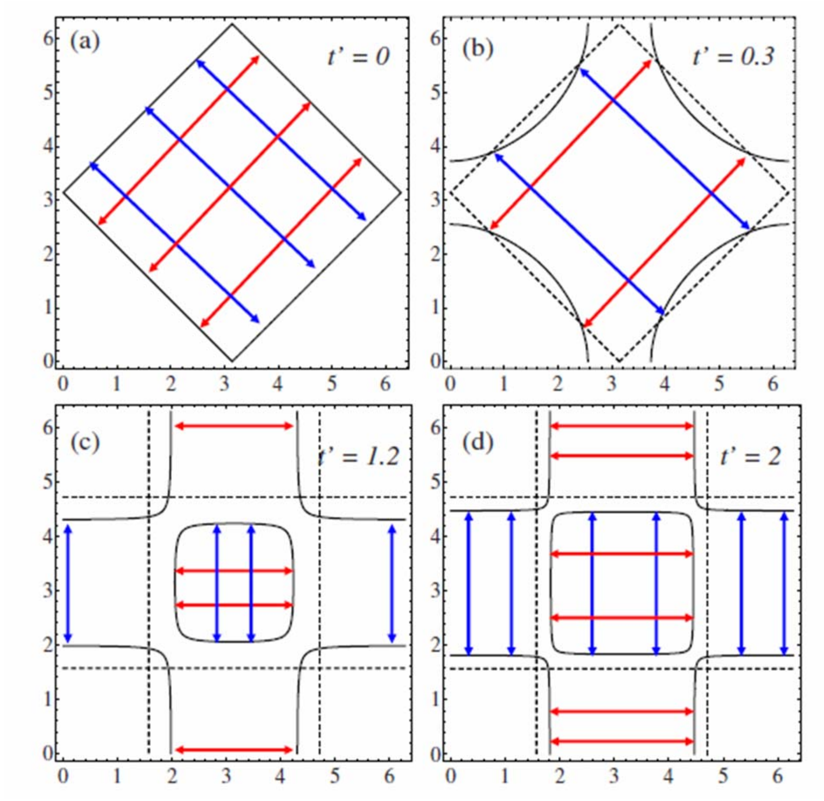
T. Maier, M. Jarrell, T. Schulthess, P. Kent, and J. White, PRL **95**, 237001 2005

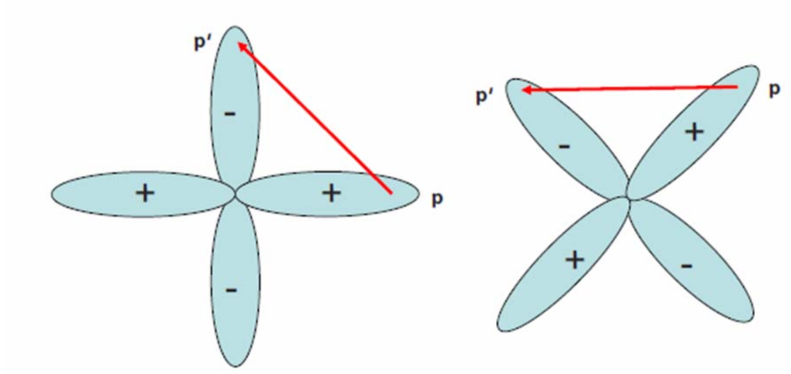
Kyung et al. PRB **68** (2003)

$T_c = 0.023$

More on superconductivity: $n=1$

Relation between symmetry and wave vector of AFM fluctuations





Hassan et al. PRB 2008

T_c depends on t'

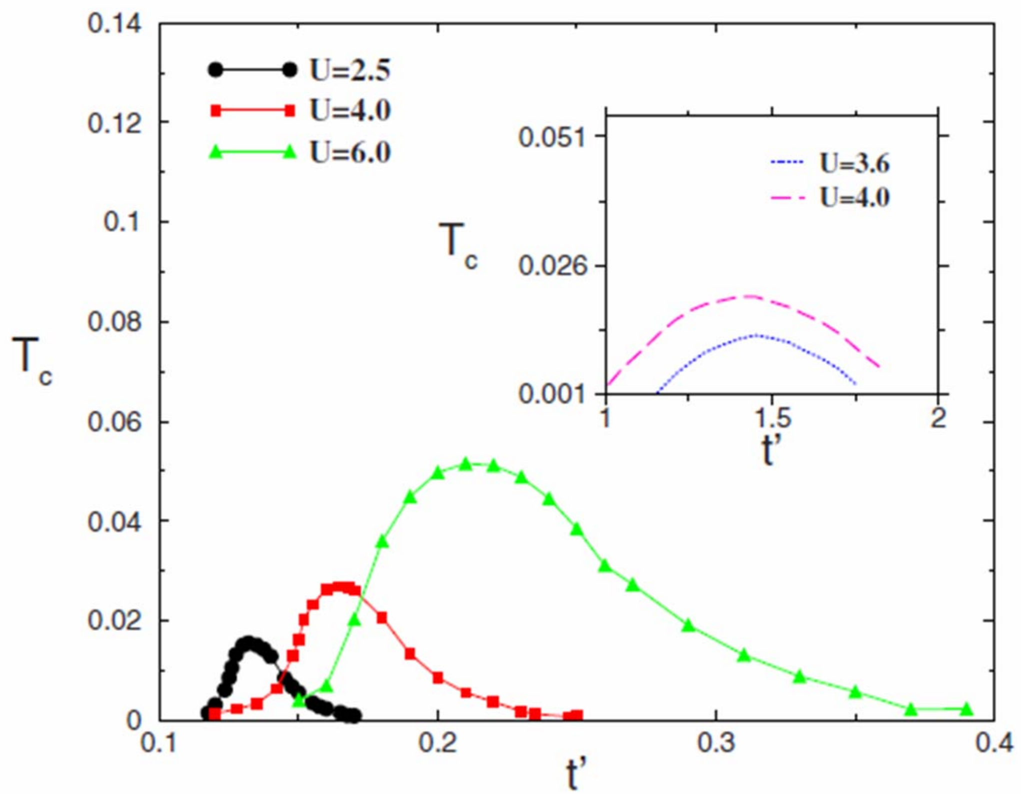


FIG. 5. (Color online) The $d_{x^2-y^2}$ superconducting critical temperature T_c as a function of t' at U=2.5, 3, and 4 for n=1. The inset shows the d_{xy} superconducting critical temperature T_c as a function of t' for U=3.6 and 4.

Hassan et al. PRB 2008

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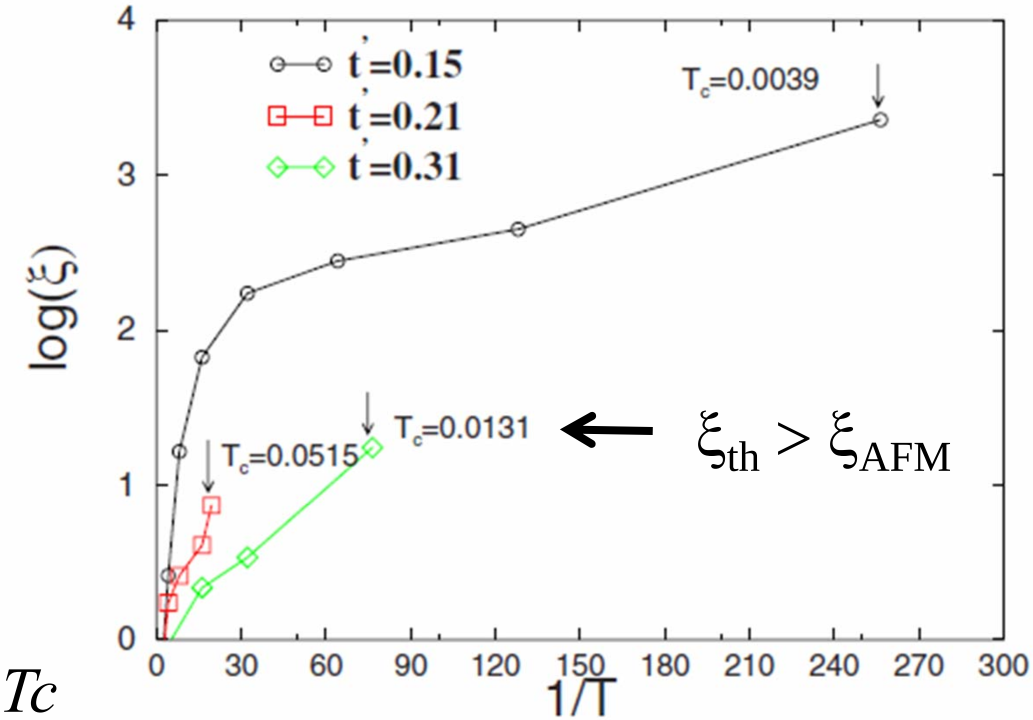
Tc in RC regime or not



$\xi_{th} > \xi_{AFM}$

ξ_{AFM}

~ 10 at optimal *Tc*

FIG. 6. (Color online) Logarithm base ten of the antiferromagnetic correlation length (in units of the lattice spacing) as a function of inverse temperature for three values of $t'=0.15,0.21,0.31$ at $U=4$ for $n=1$. The value of T_c for the corresponding t' is shown on the plot.

Hassan et al. PRB 2008

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Conditions for *d*-wave superconductivity

Hassan, Davoudi, AMST PRB **77**, 094501 2008

- Symmetry related to that of commensurate spin fluctuations
- T_c increases with U
- DOS does not play dominant role
- Optimal frustration
  - In underfrustrated $T_c < T_X$
  - In overfrustrated $T_c > T_X$
  - In all cases $\xi > a$

? Stifening AFM and new mode ?

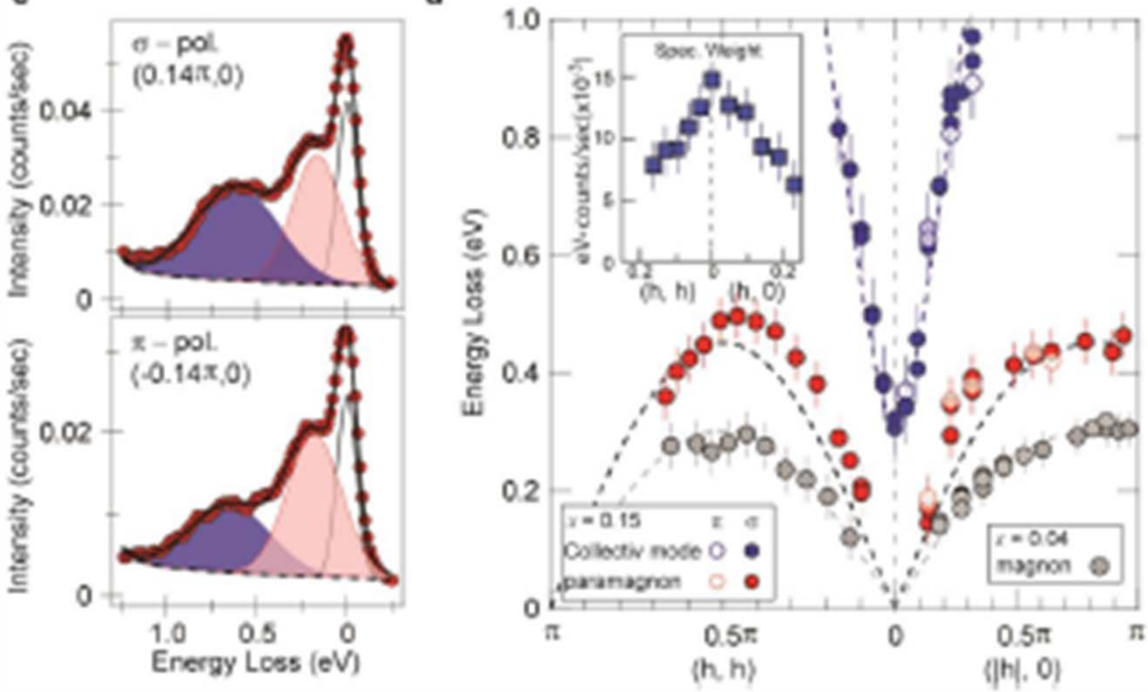

Figure 2

arXiv:1308.4740 [pdf]

W. S. Lee, … M. Greven, T. Schmitt, Z. X. Shen, T. P. Devereaux

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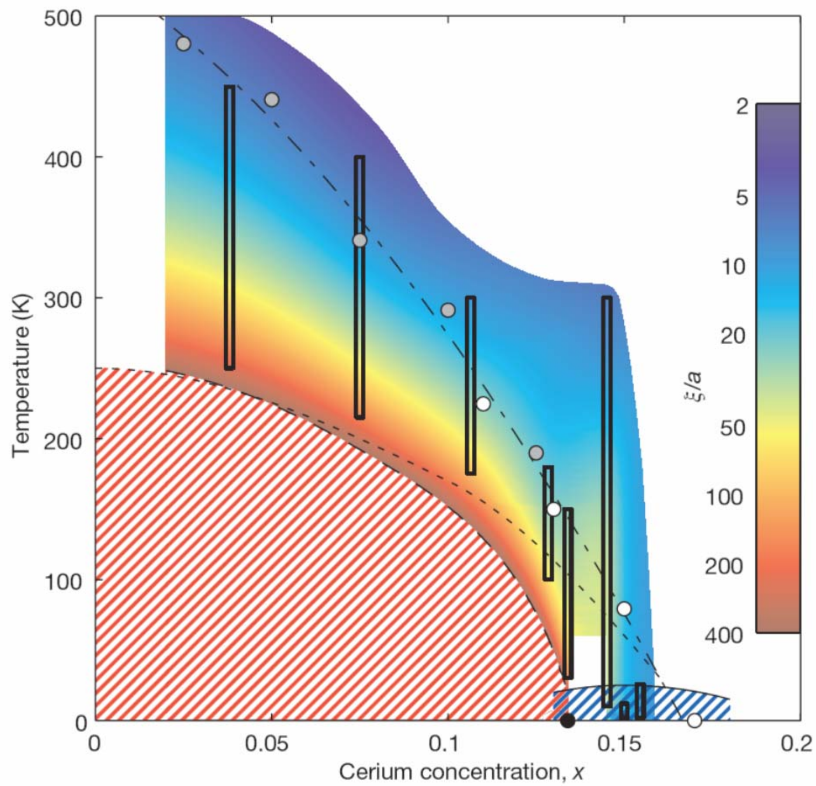
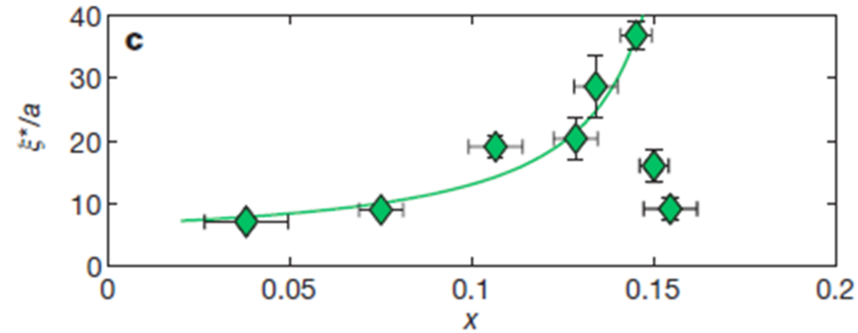
? AFM correlation length at optimal doping ?





Motoyama et al.
Nature **445,** 186 (2007)

Charge ordering in the electron-doped superconductor $Nd_{2-x}Ce_xCuO_4$

Eduardo H. da Silva Neto,[1,2,3,4,*] Riccardo Comin,[1,*] Feizhou He,[5] Ronny Sutarto,[5] Yeping Jiang,[6] Richard L. Greene,[6,4] George A. Sawatzky,[1,2,4] and Andrea Damascelli[1,2,4,†]

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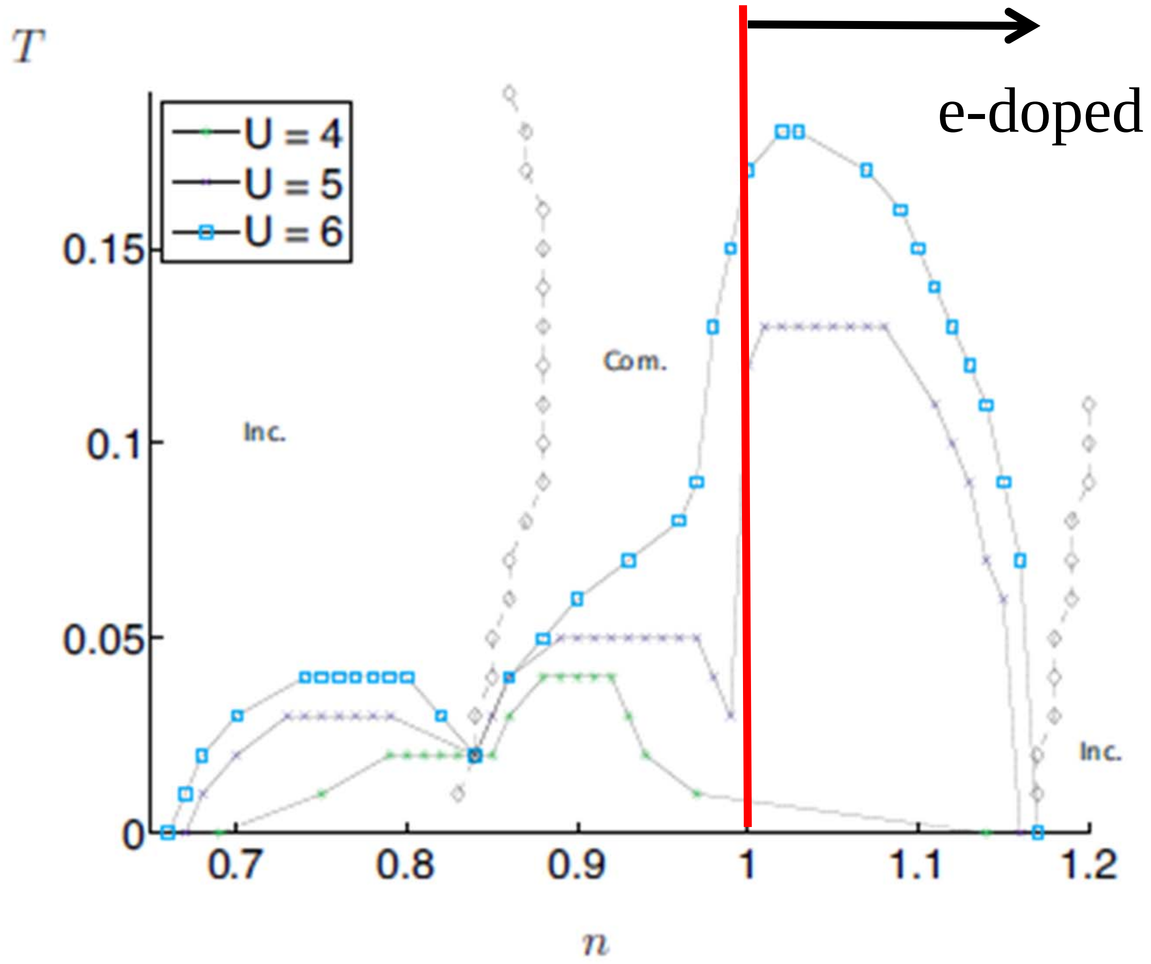
Increased nesting away from *n = 1*



t' = -0.2

S. Roy, PhD thesis, 2007

TPSC: First step

- Consistency between one- and two-particle quantities:

$$\Sigma_\sigma(1,\bar{1})G_\sigma(\bar{1},2) = -U\langle T_\tau n_{-\sigma}(1)c_\sigma(1)c_\sigma^\dagger(2)\rangle\,,$$

$1 = (\mathbf{r}_1, \tau_1)\,.$

- TPSC ansatz:

$$\Sigma_\sigma(1,\bar{1})G_\sigma(\bar{1},2) \approx U_{sp}G_{-\sigma}(1,1^+)G_\sigma(1,2)\,, \quad \text{with} \quad U_{sp} = U\frac{\langle n_\uparrow(1)n_\downarrow(1)\rangle}{\langle n_\uparrow(1)\rangle\langle n_\downarrow(1)\rangle}\,.$$

- $\Rightarrow$ Spin irreducible vertex:

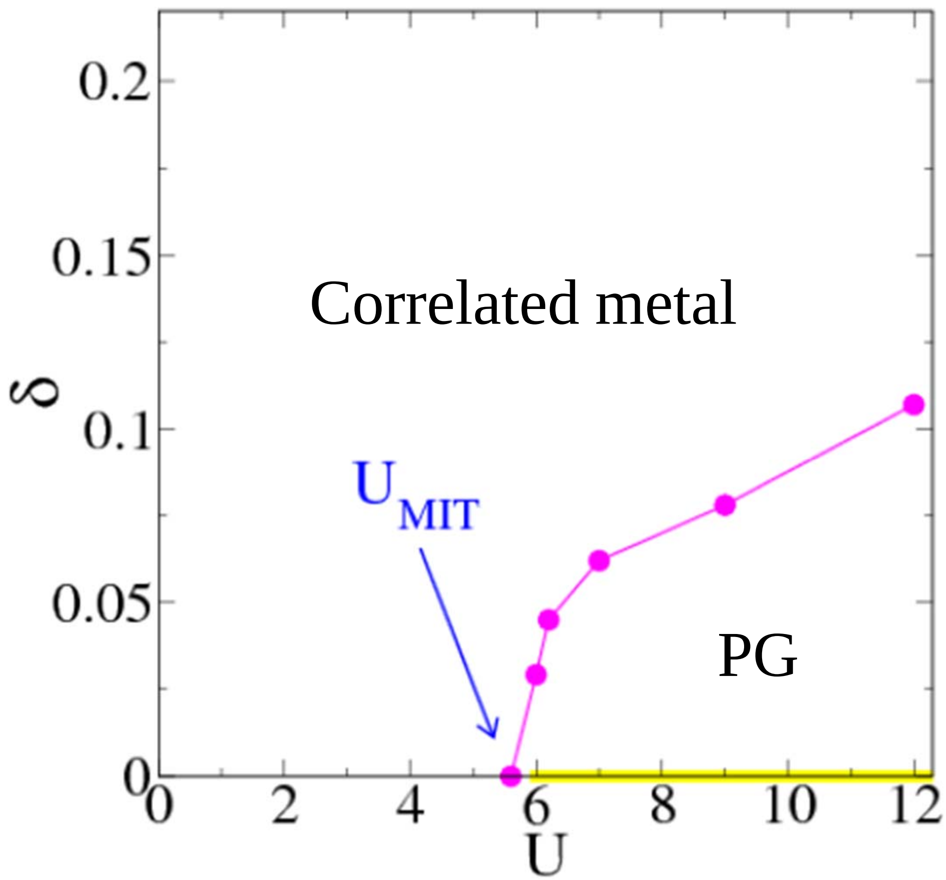
$$\Gamma_{sp}(1,2;3,4) = \frac{\delta\Sigma_\uparrow(1,2)}{\delta G_\uparrow(3,4)} - \frac{\delta\Sigma_\uparrow(1,2)}{\delta G_\downarrow(3,4)} = U_{sp}\delta(1-3)\delta(1^+-4)\delta(1^--2)$$

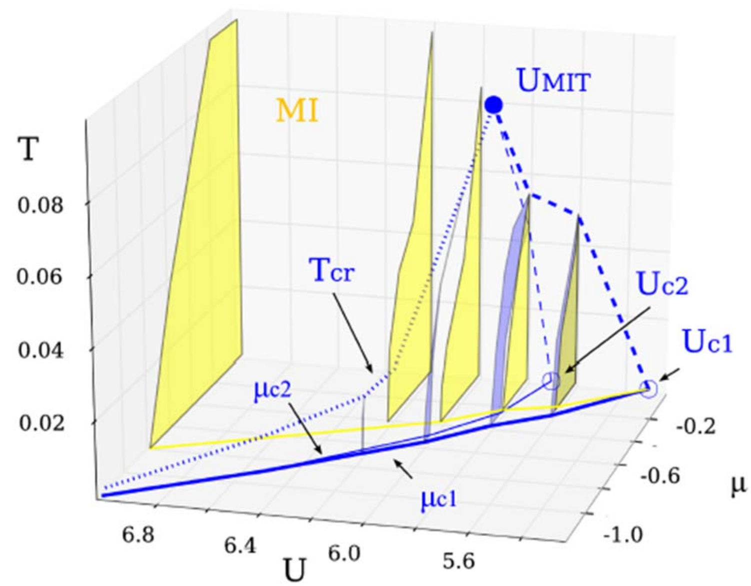
- We also use a local charge irreducible vertex:

$$\Gamma_{ch}(1,2;3,4) = \frac{\delta\Sigma_\uparrow(1,2)}{\delta G_\uparrow(3,4)} + \frac{\delta\Sigma_\uparrow(1,2)}{\delta G_\downarrow(3,4)} \approx U_{ch}\delta(1-3)\delta(1^+-4)\delta(1^--2)$$

Hole-doped : Link to Mott transition up to optimal doping

Doping dependence of critical point as a function of U





Sordi et al. PRL 2010, PRB 2011

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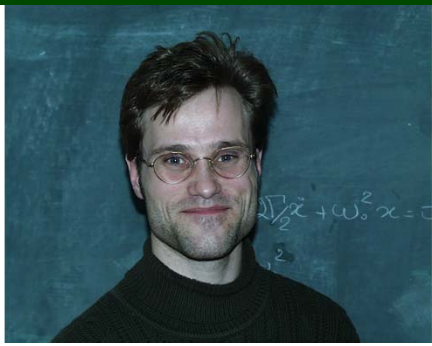
Conclusion

- e-doped better understood with one-band Hubbard than h-doped (less strongly correlated)
- Mechanism for pseudogap is different on h-doped side (Related to Mott physics) (Vilk criterion not satisfied)
- Certain anomalies explainable by charge order? Or interference between channels?

Collaborators



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Hugo Touchette

J.-S. Landry

Collaborators

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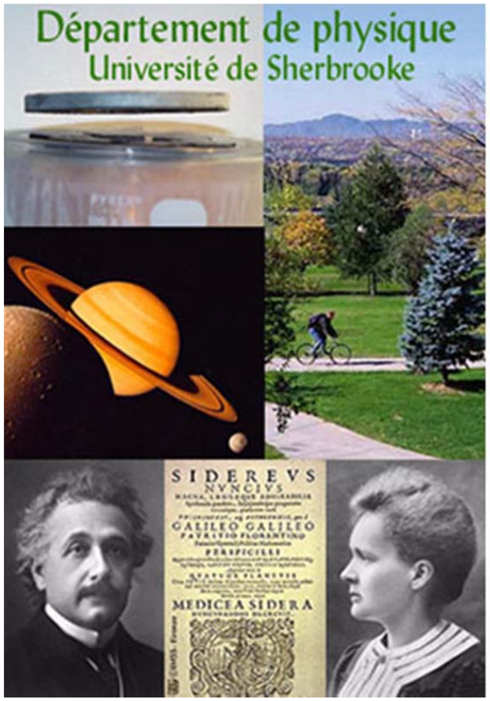

André-Marie Tremblay

CANADA RESEARCH CHAIRS
CHAIRES DE RECHERCHE DU CANADA

RQMP

Le regroupement québécois sur les matériaux de pointe

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Reviews: A.-M.S.T. arXiv: 1107.1534
and arXiv: 1310.1481

Merci

Thank you

A.-M.S. Tremblay
"Strongly correlated superconductivity"
Chapt. 10 : *Emergent Phenomena in Correlated Matter Modeling and Simulation, Vol. 3,* E. Pavarini, E. Koch, and U. Schollwöck (eds.)
Verlag des Forschungszentrum Jülich, 2013