Lecture 3:
Spin-fluctuation induced superconductivity: Electron-Doped High T_c Superconductors and Two-Particle Self-Consistent Approach

André-Marie Tremblay

Université de Sherbrooke

Collège de France, 23 mars 2015

17h00 à 18h30

Main collaborators on TPSC


Liang Chen


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Dominic Bergeron


Bahman Davoudi


Syed Hassan


Steve Allen

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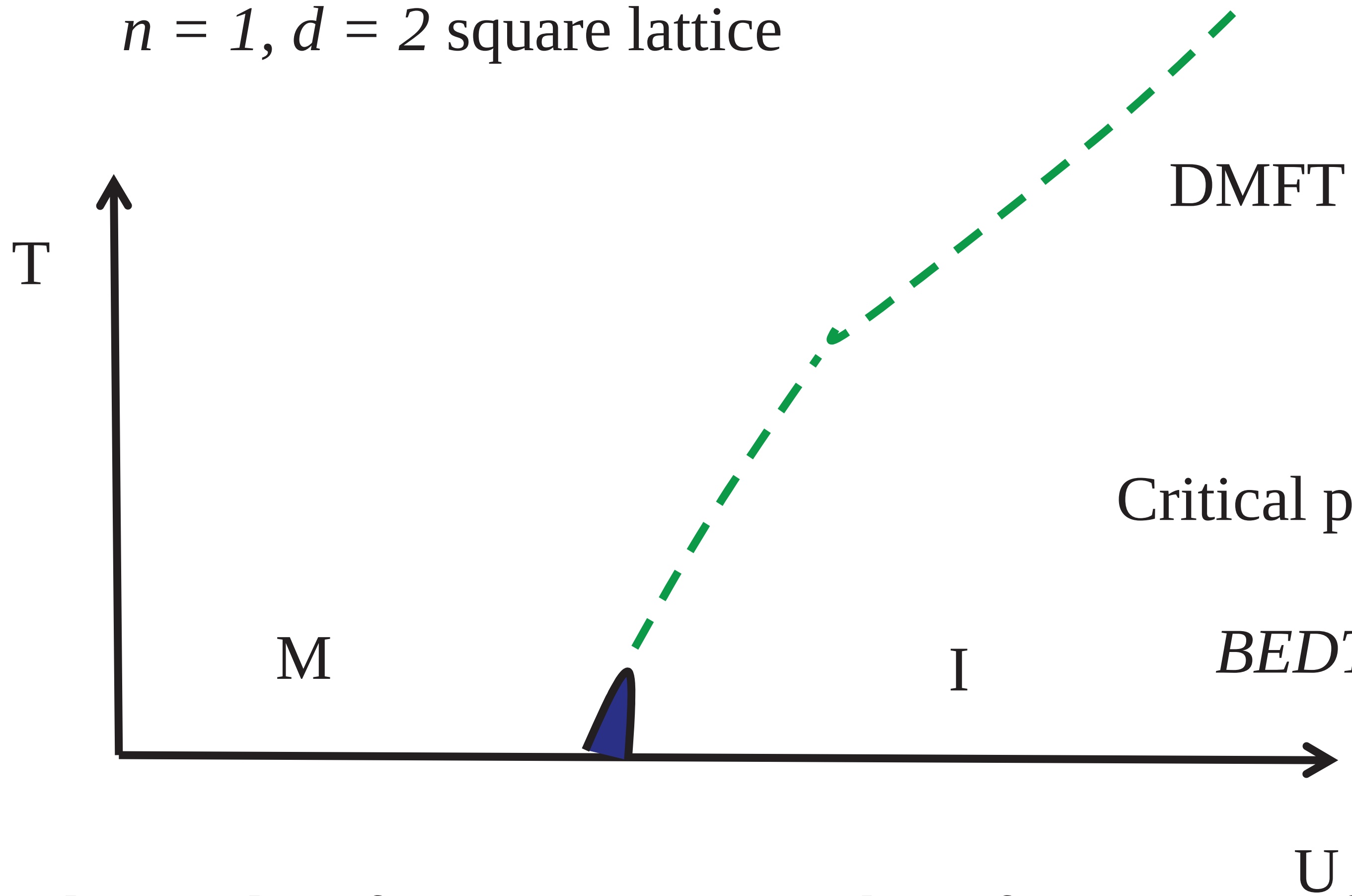
Three broad classes of mechanisms for pseudogap

- Phase with a broken symmetry (discrete)
- Mott Physics
- Precursor of LRO ($d = 2$)
  - Mermin-Wagner allows a large fluctuation regime
  - Even with weak correlations

Local moment and Mott transition

n = 1, d = 2 square lattice



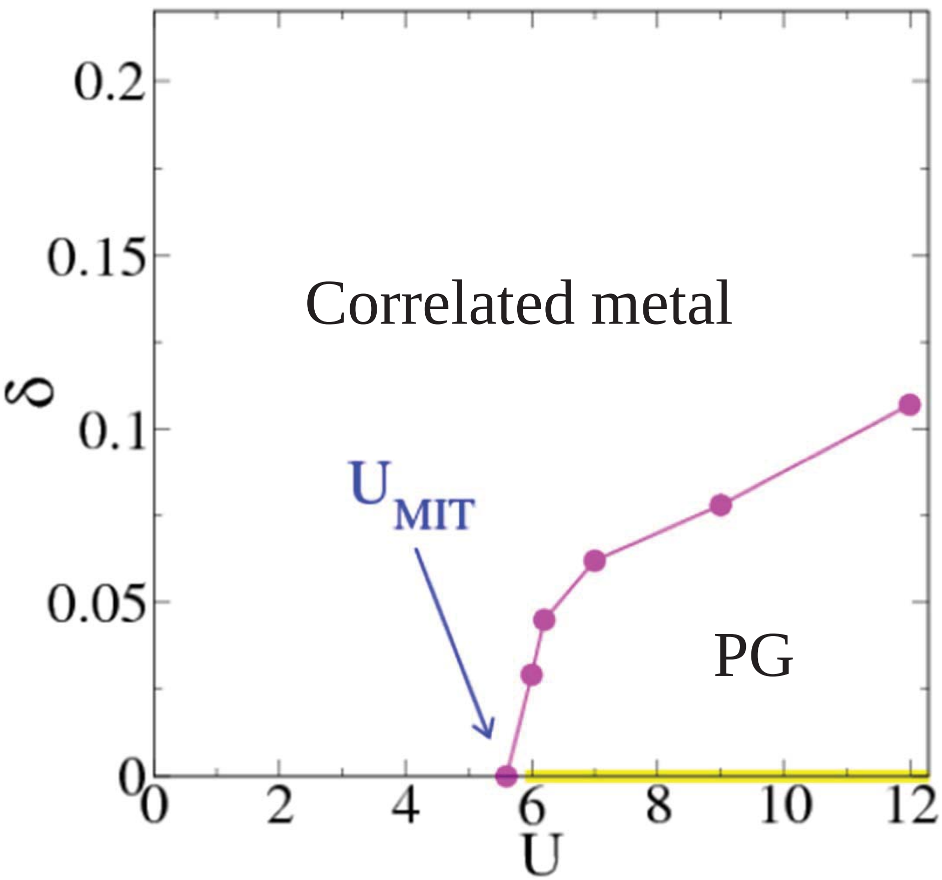
Critical point visible in

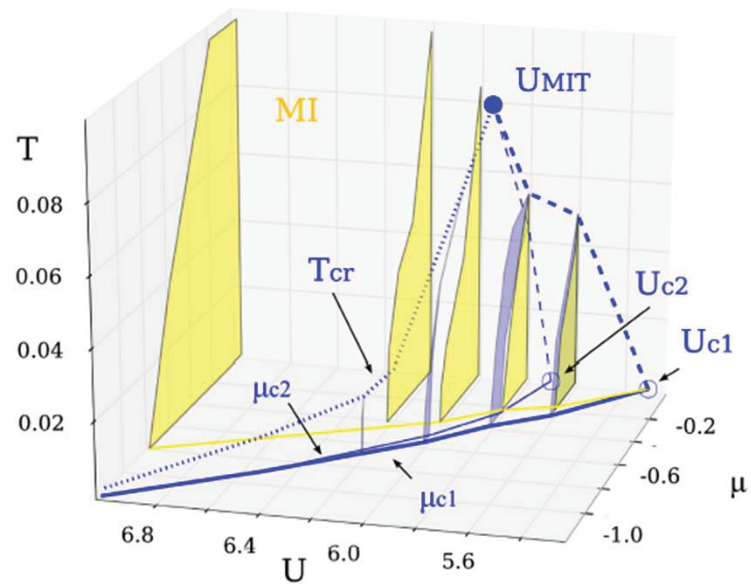
BEDT organics

Understanding finite temperature phase from a *mean-field theory* down to $T = 0$

A finite-doping first order transition, linked to Mott transition up to optimal doping

Doping dependence of critical point as a function of *U*





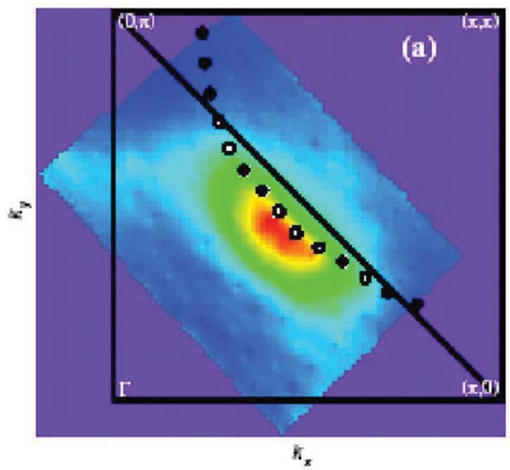
Sordi et al. PRL 2010, PRB 2011

Strong correlation pseudogap (U > 8t)

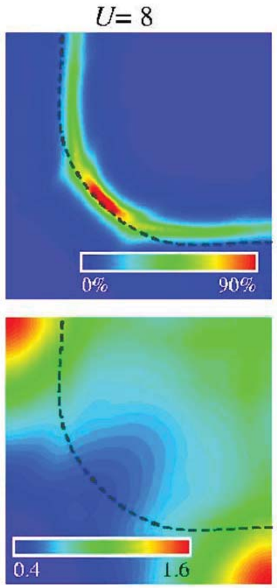
- Different from Mott gap that is local (all k) not tied to $\omega=0$.
- Pseudogap tied to $\omega=0$ and only in regions nearly connected by (π,π). (e and h),
- Pseudogap is independent of cluster shape (and size) in CPT.
- Not caused by AFM LRO
  - No LRO, few lattice spacings.
  - Not very sensitive to *t'*
  - Scales like *t*.

Sénéchal, AMT, PRL **92**, 126401 (2004).

Hole-doped, 10%



F. Ronning et al. Jan. 2002, $Ca_{2-x}Na_xCuO_2Cl_2$



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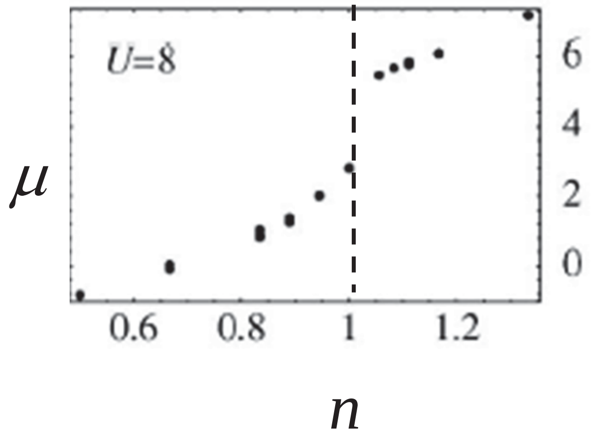
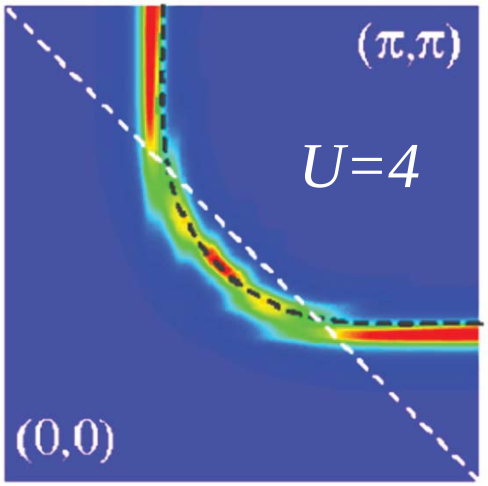
Weak-correlation pseudogap (e-doped cuprates)

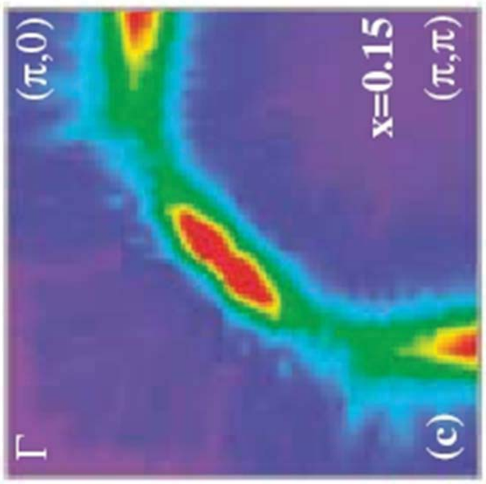
- In CPT
  - is mostly a depression in weight
  - depends on system size and shape.
  - located precisely at intersection with AFM Brillouin zone
- Coupling weaker, better screened *U(n)* ~ dμ/dn



Armitage et al. PRL 88 257001 (2002)

Sénéchal, AMT, PRL **92**, 126401 (2004).

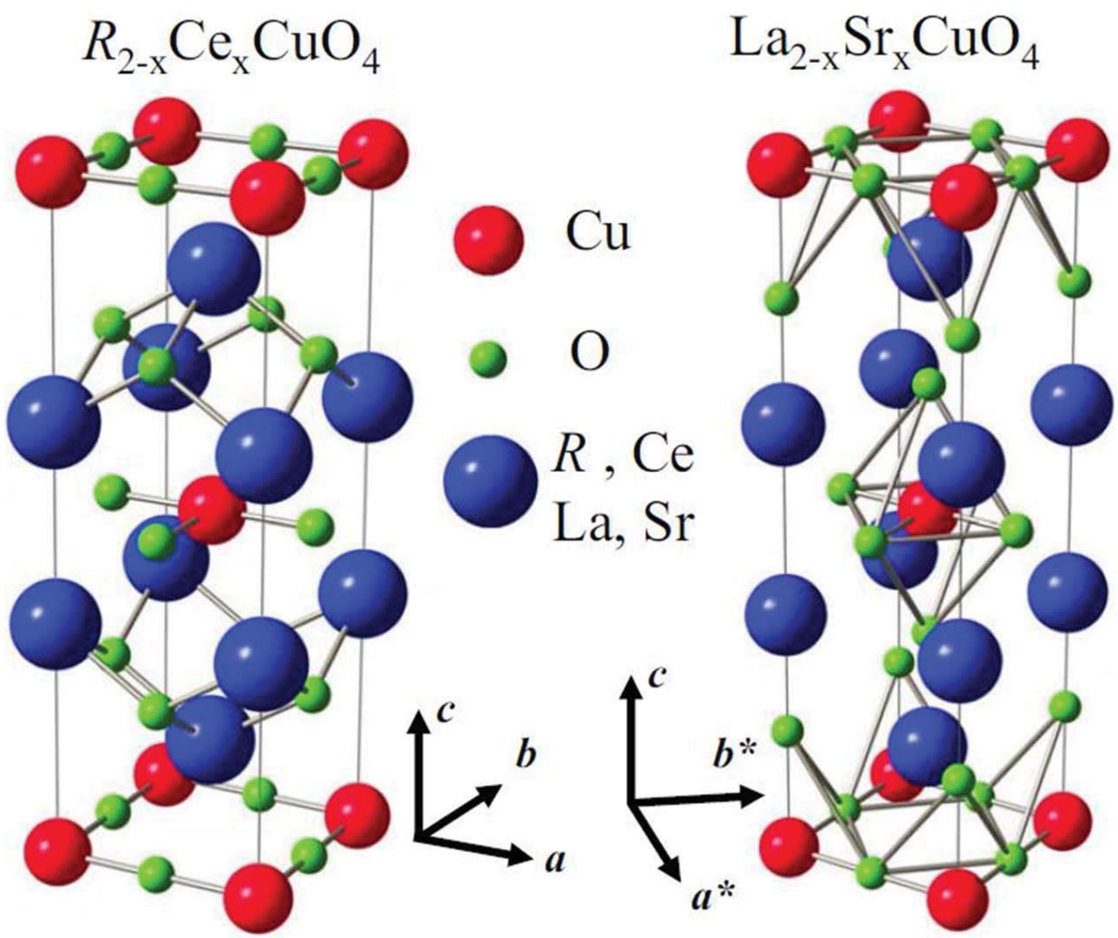




Middle segment disappears for *U*~ 6, (also slave bosons)

Q. Yuan, F. Yuan, and C. S. Ting, PRB **72**, 054504 (2005).

Different cristal structures

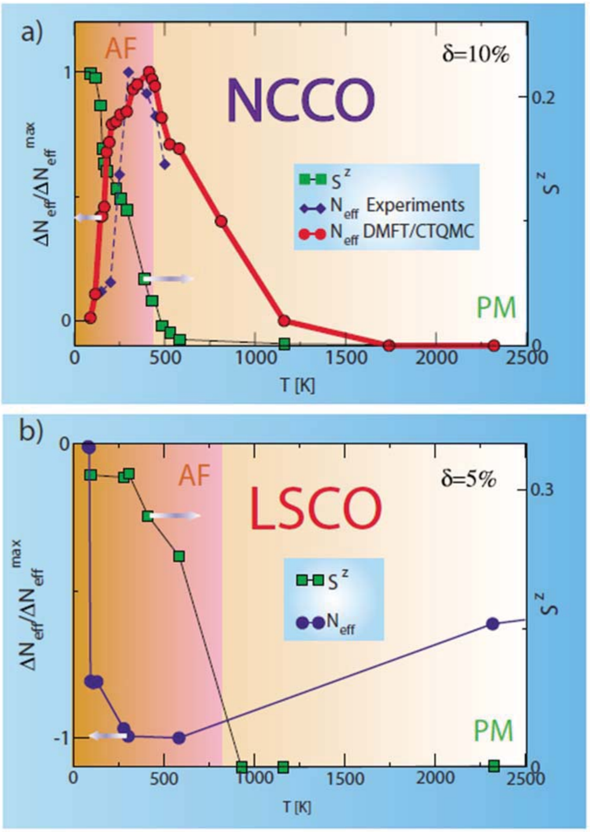


N. P. Armitage, P. Fournier, and R. L. Greene RMP **82**, 2421 (2010)

LDA + DMFT

C. Weber, K. Haule, G. Kotliar, PRB **82**, 125107 2010
C. Weber, K. Haule, G. Kotliar, Nature Physics, **6,** 574 (2010)

N_{eff} - $N_{eff}(89\ K)$



$$N_{\rm eff} = (2\, m_{\rm e} V / \hbar \pi e^2) \int_0^{\Lambda} \sigma'(\omega)\, d\omega$$

$\Lambda \sim 1.4\ eV$

Experiments, dashed line

Y. Onose, Y. et al. PRB **69**, 024504 (2004).

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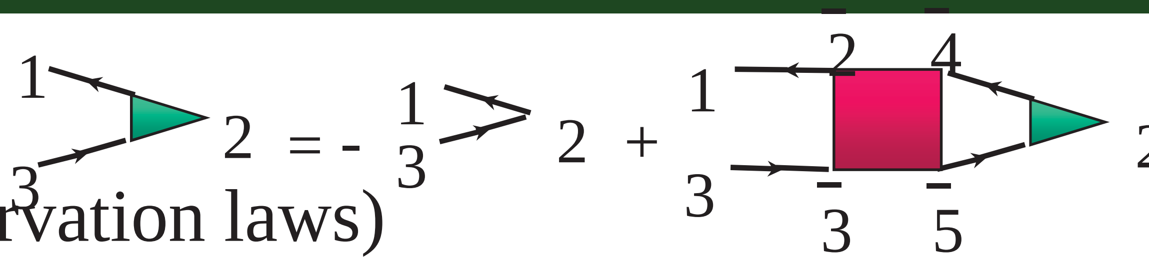
Theoretical difficulties

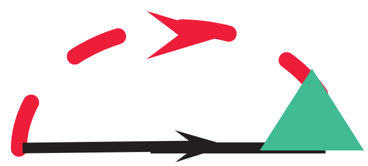
- Low dimension
  - (quantum and thermal fluctuations)
- Large residual interactions
  - (Potential ~ Kinetic)
  - Expansion parameter?
  - Particle-wave?
- By now we should be as quantitative as possible!

Theory difficult even at weak to intermediate correlation!



- 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
- Renormalization Group
  - 2 loops

Σ =



Zanchi Schultz, (2000)
Rohe and Metzner (2004)
Katanin and Kampf (2004)

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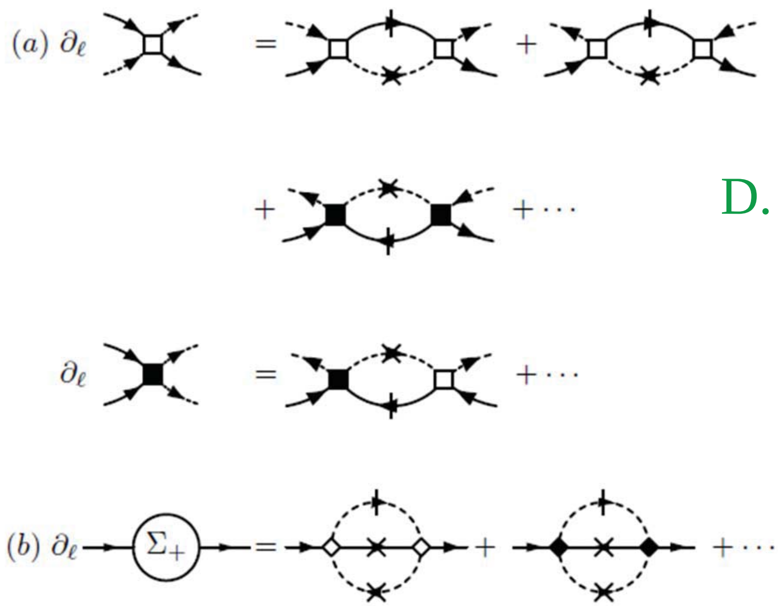
Weak correlation methods

- 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

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

Outline for today

- Comparisons with experiment
  - Agreement does not mean accurate solution of Hubbard
- Benchmarks
  - Quantum Monte Carlo for large systems
- How it works
  - Physical principles
- ___________________________
- Derivation and analytic: Mermin-Wagner + pseudogap

A.-M.S.T, *Theoretical Methods for Strongly Correlated Systems*, edited by A. Avella and F. Mancini (Springer, New York, 2011), Chap. 13, p. 409; e-print arXiv:1107.1534.

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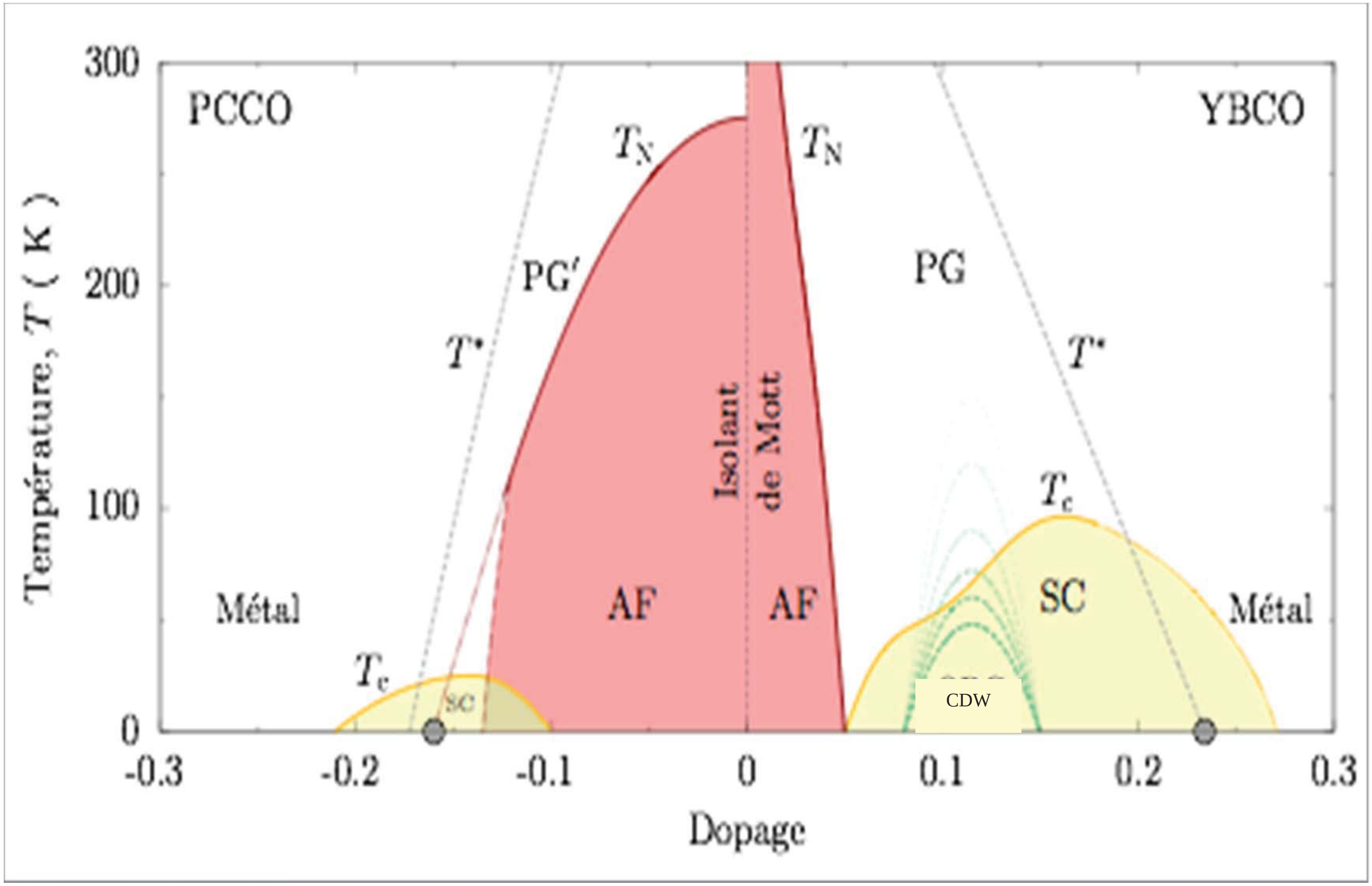
TPSC: Theory vs experiment

The pseudogap in electron-doped cuprates

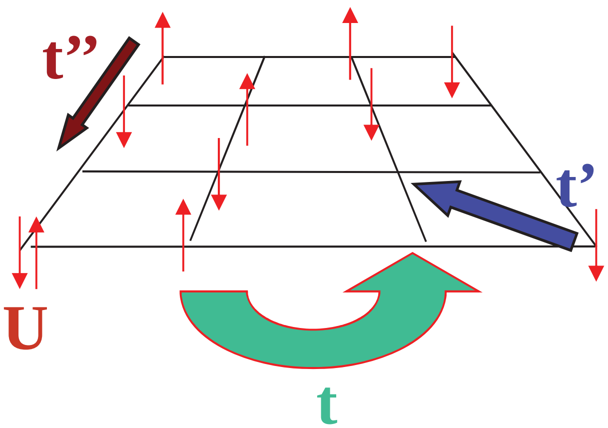
Our road map

Thèse de Francis Laliberté, Université de Sherbrooke



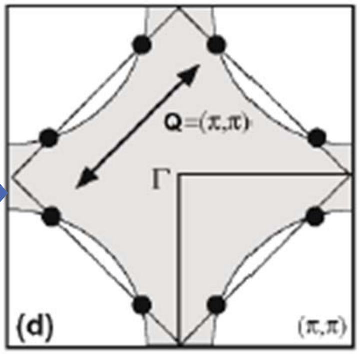
Model parameters

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



fixed

$t' = -0.175t$, $t'' = 0.05t$
$t = 350$ meV, $T = 200$ K



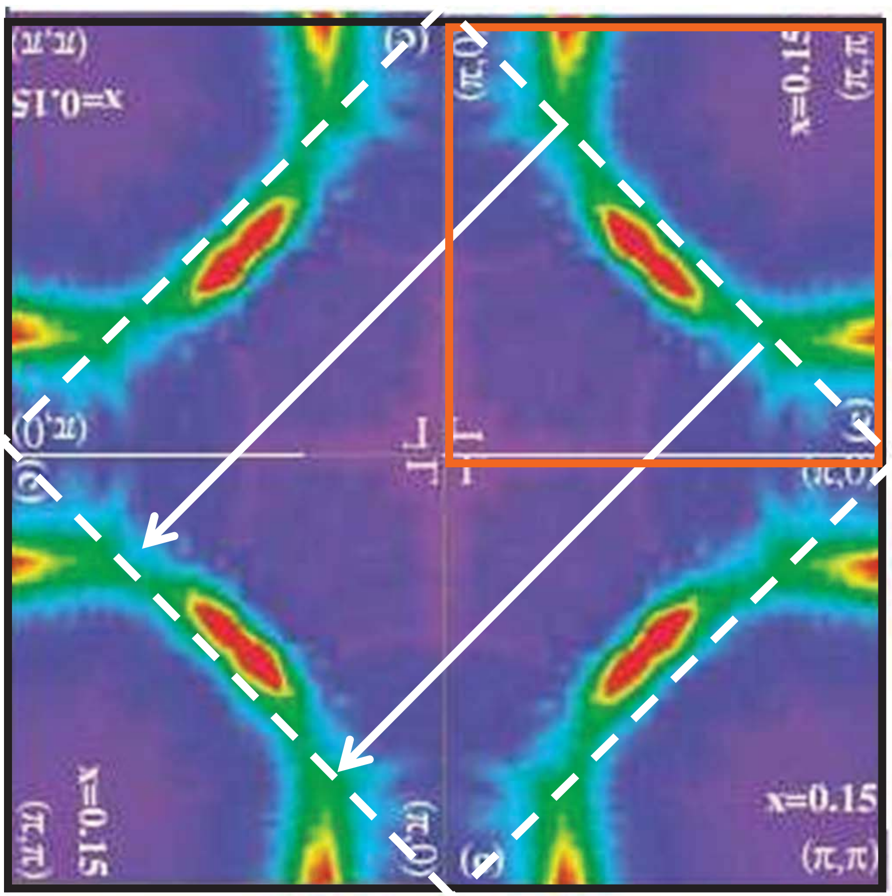
Weak coupling $U<8t$

$n=1+x$ – electron filling

Hot spots from AFM quasi-static scattering

Mermin-Wagner

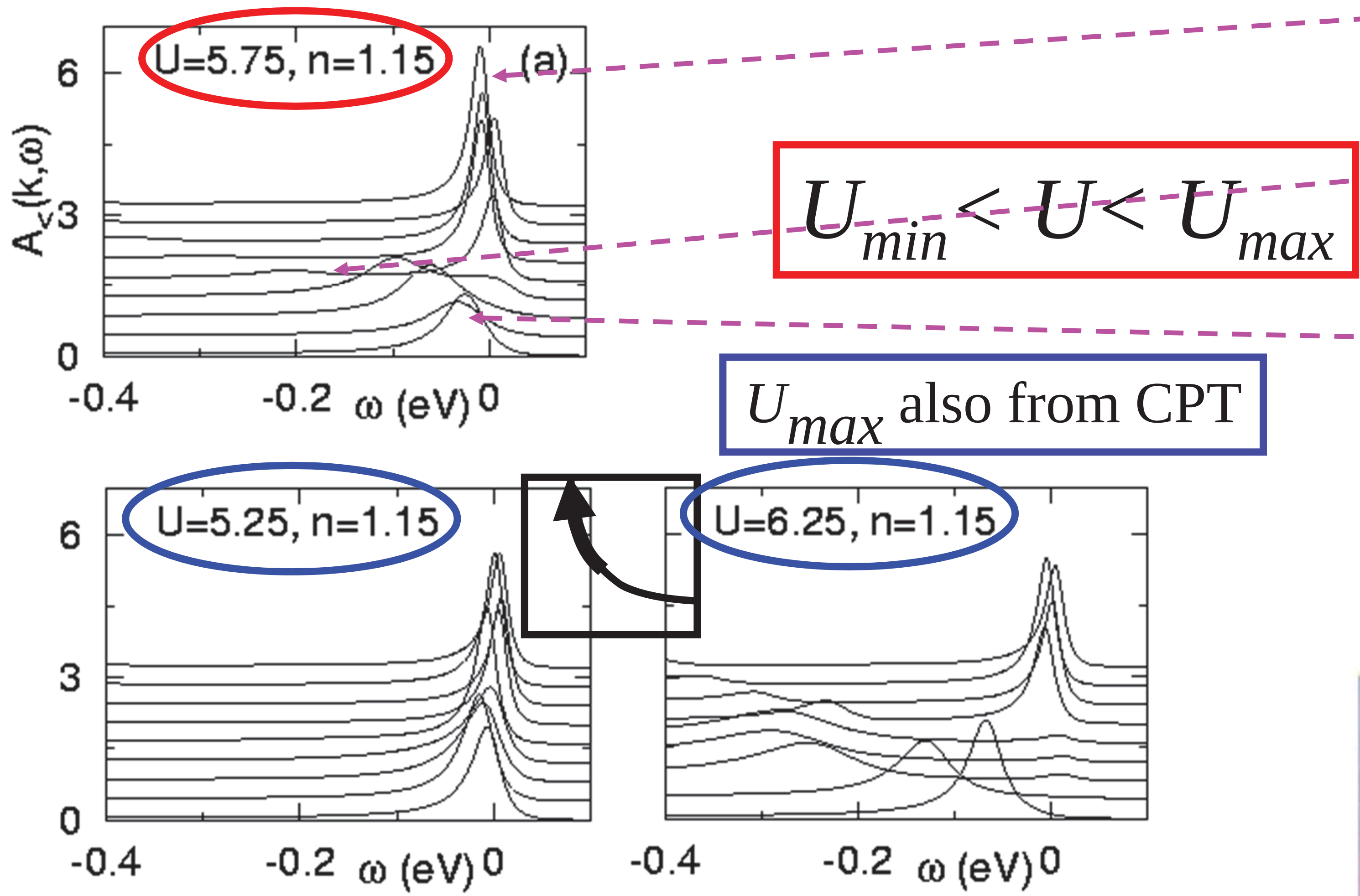
$d = 2$

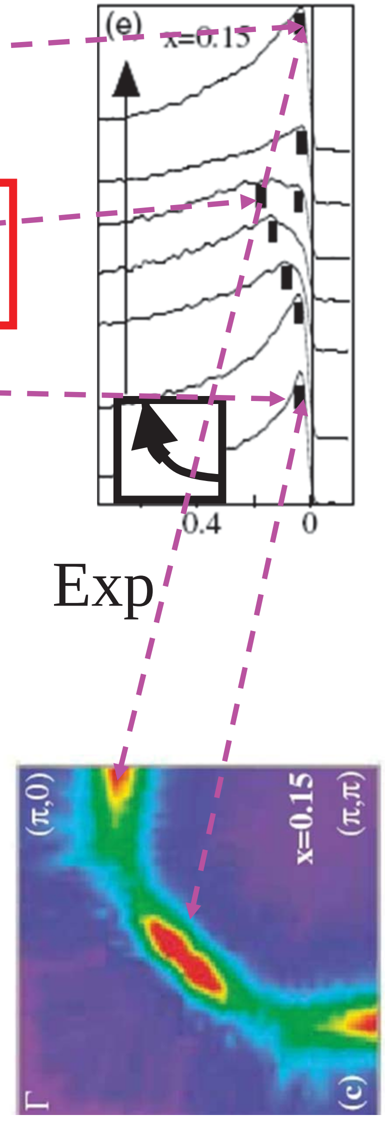


Vilk, A.-M.S.T (1997)
Kyung, Hankevych,
A.-M.S.T., PRL, 2004

Armitage et al. PRL 2001

15% doping: EDCs along the Fermi surface TPSC

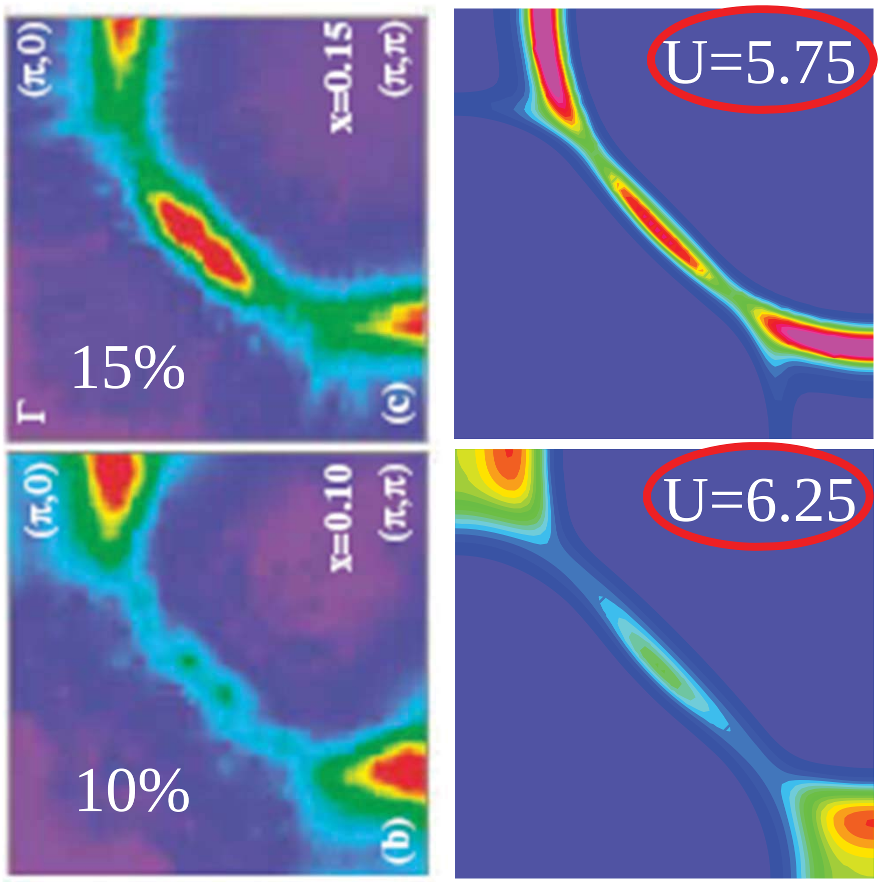




Hankevych, Kyung, A.-M.S.T., PRL, sept. 2004

Fermi surface plots

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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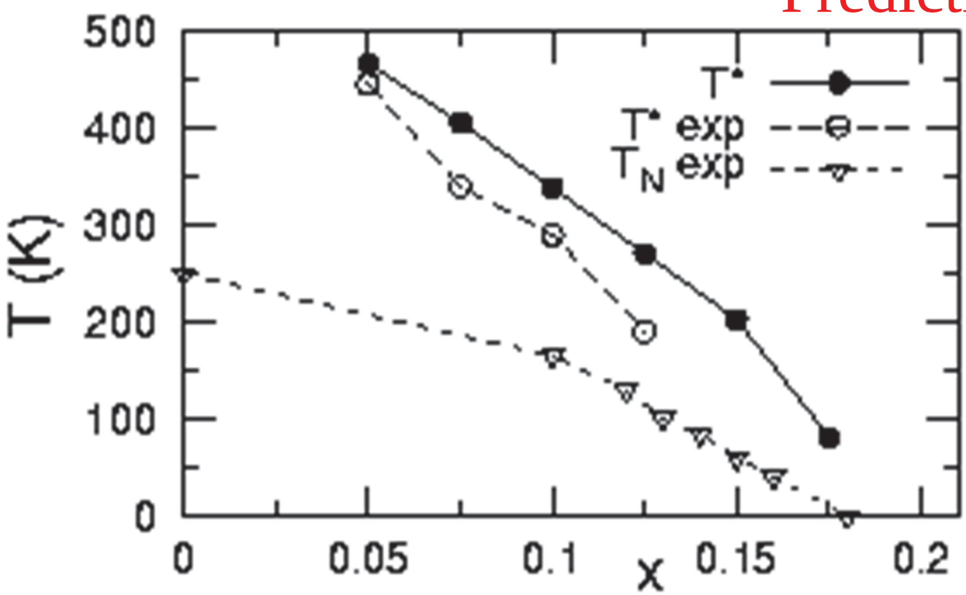
Pseudogap temperature and QCP



Prediction ➢ $\xi \approx \xi_{th}$ at PG temperature T^*, and $\xi > \xi_{th}$ for $T < T^*$

supports further AFM fluctuations origin of PG

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

Hankevych, Kyung, A.-M.S.T., PRL 2004 : Expt: Y. Onose et al., PRL (2001).

Thermal de Broglie wavelength

$$\Delta\varepsilon \sim k_B T$$

$$\nabla_{\mathbf{k}}\varepsilon \; \Delta k \sim k_B T$$

$$\xi_{th} \sim \frac{v_F}{T}$$

$$\Delta k \sim \frac{k_B T}{\hbar v_F}$$

$$\frac{2\pi}{\xi_{th}} \sim \frac{k_B T}{\hbar v_F}$$

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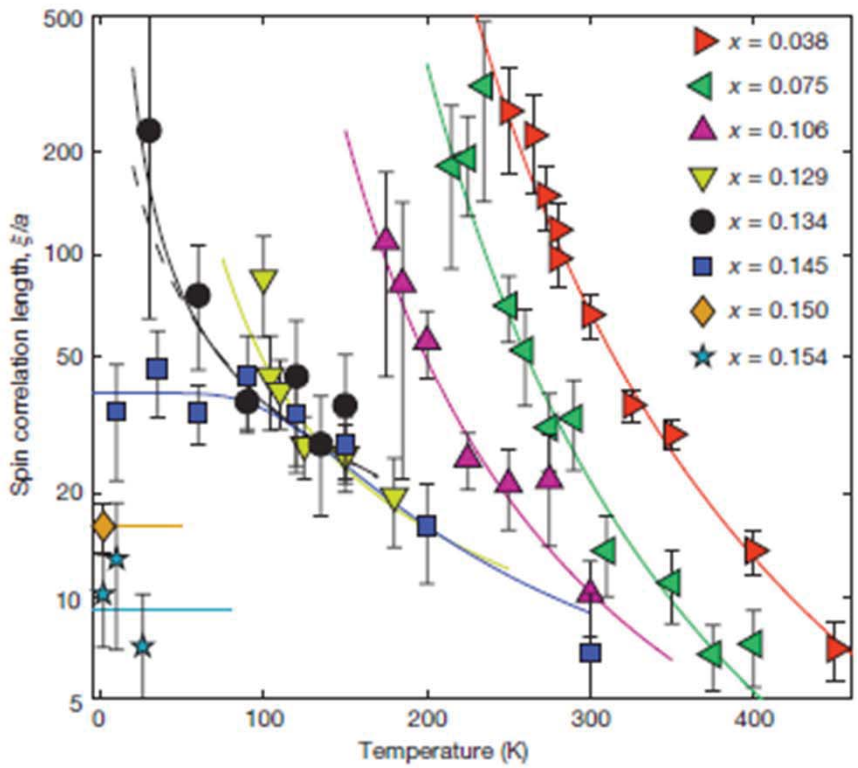
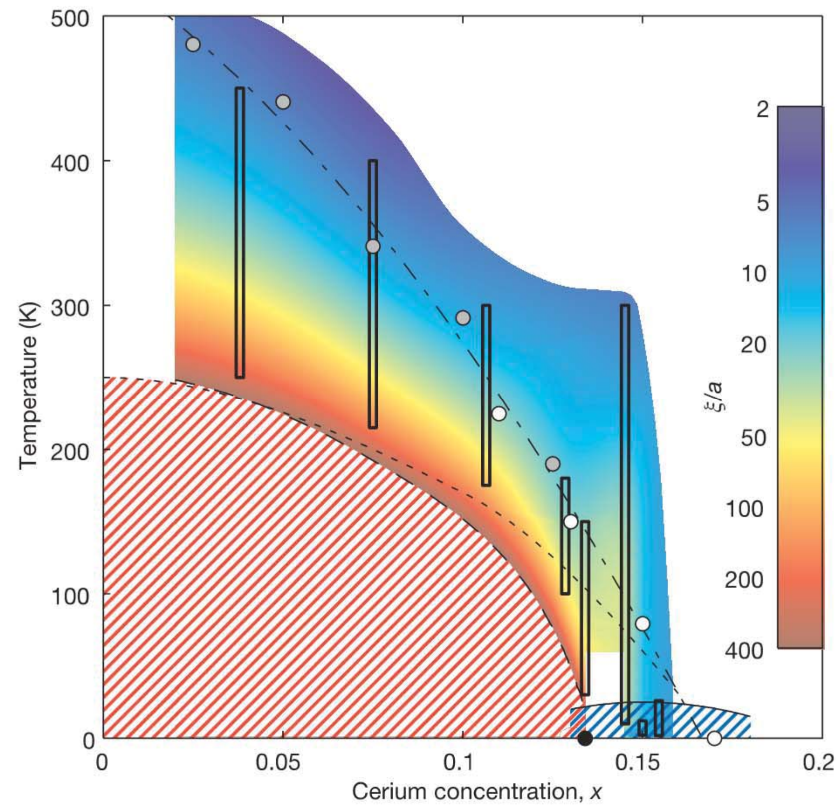
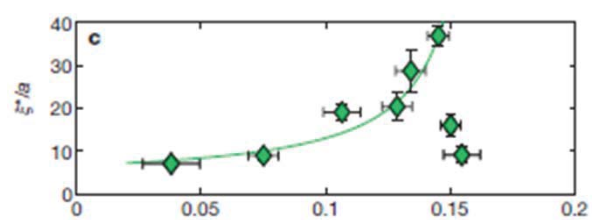
e-doped pseudogap

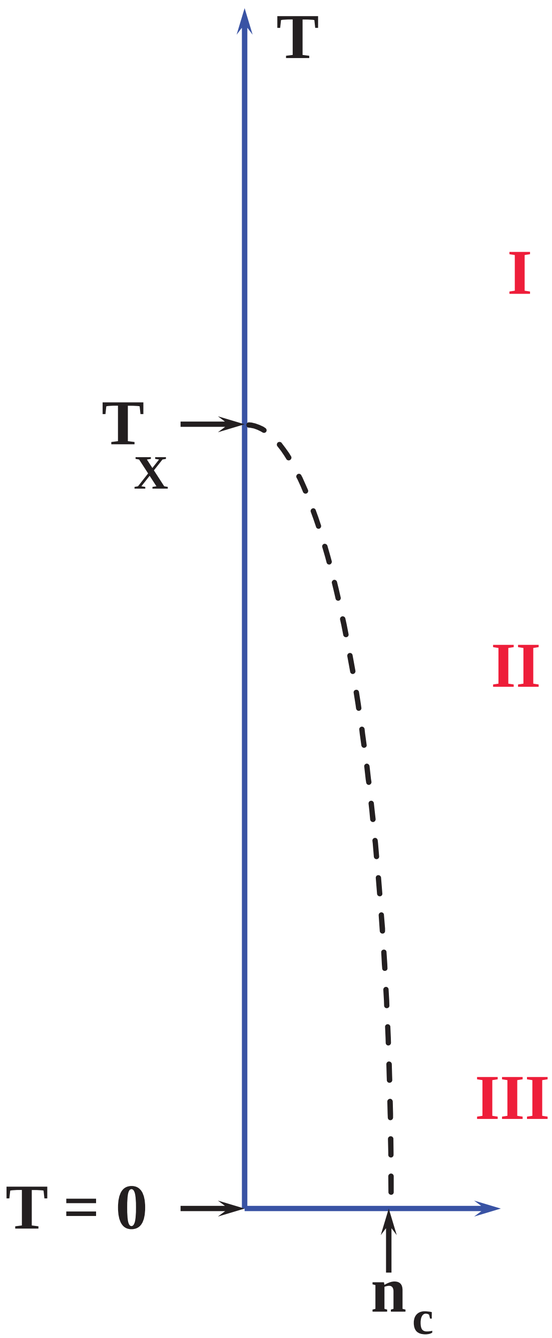
E. M. Motoyama et al.. Nature 445, 186–189 (2007).





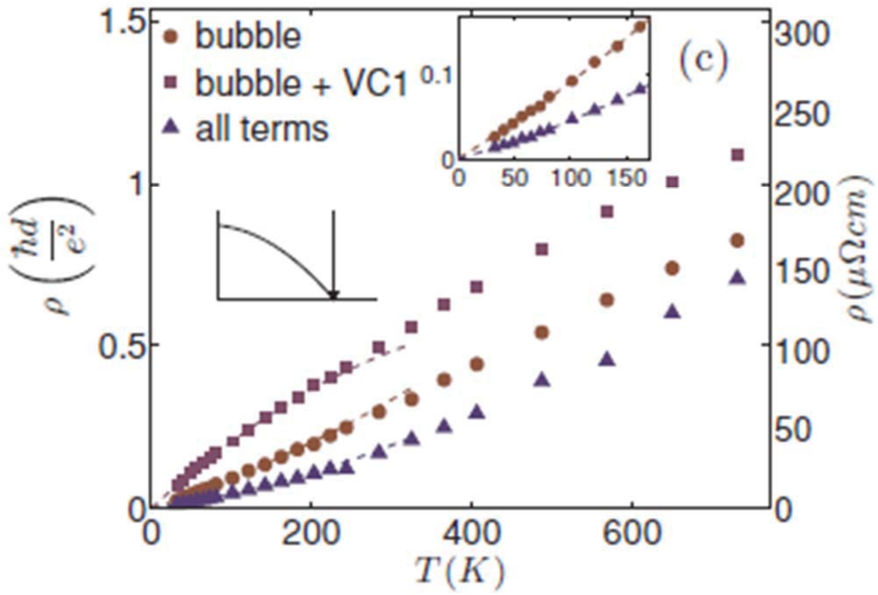


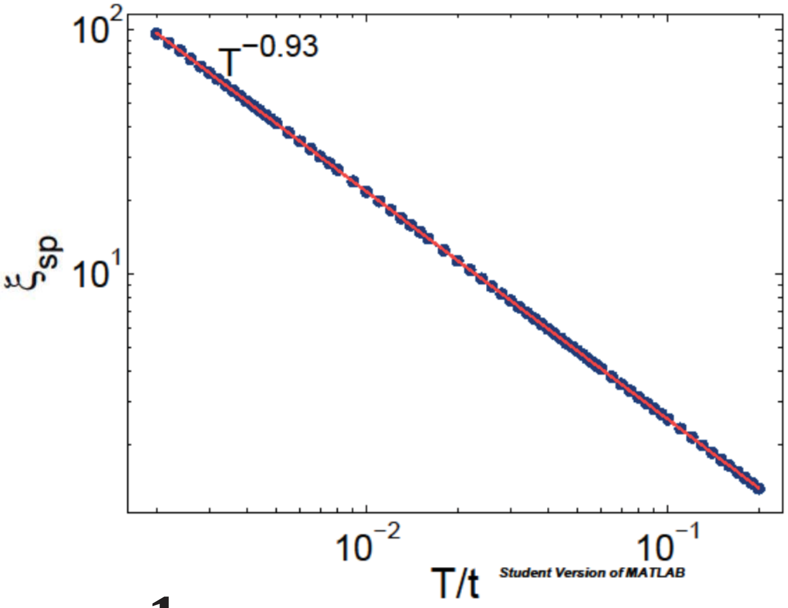
Vilk criterion $\xi^{*} = 2.6(2)\xi_{\rm th}.$


T
I
T_X
II
III
T = 0
n_c

ξ(T) at the QCP

NCCO
Matsui et al. PRB 2007





z = 1

Motoyama, Nature 2007

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

Bergeron, Hankevych, Kyung, A-M.S.T. PRB **84**, 085128 (2011)
Bergeron, Chowdhury, Punk, Sachdev PRB **86**, 155123 (2012)TPSC

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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
- Kusko *et al*. PRB **66**, 140513 (2002).

Benchmarks for TPSC

Normal state

Spin and charge fluctuations: the equations

$$\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \sum_{\mathbf{q}} \sum_{i\omega_n} \frac{\chi^{(1)}(q)}{1 - \frac{1}{2} U_{sp} \chi^{(1)}(q)} = n - 2 \langle n_\uparrow n_\downarrow \rangle$$

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

Kanamori-Brückner

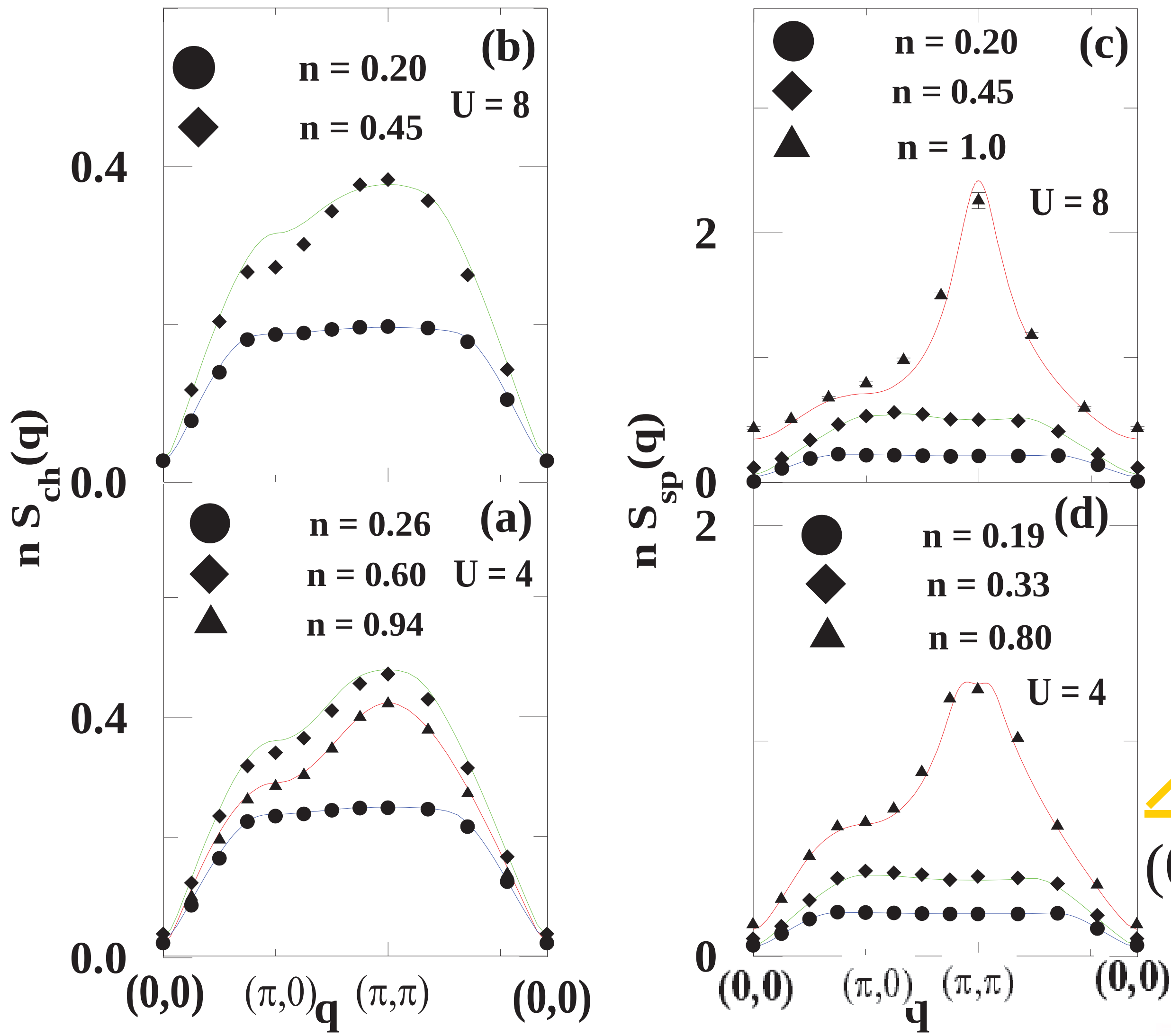
$$\frac{T}{N} \sum_{\mathbf{q}} \sum_{i\omega_n} \frac{\chi^{(1)}(q)}{1 + \frac{1}{2} U_{ch} \chi^{(1)}(q)} = n + 2 \langle n_\uparrow n_\downarrow \rangle - n^2$$

Benchmark comparison with QMC

<u>Notes:</u>

-F.L. parameters

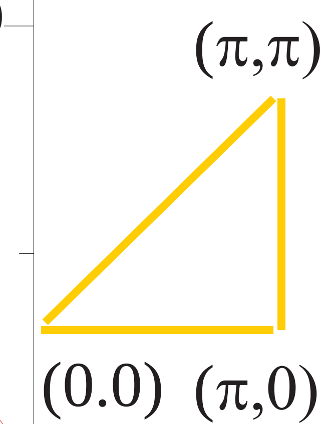
-Self also Fermi-liquid



$U > 0$

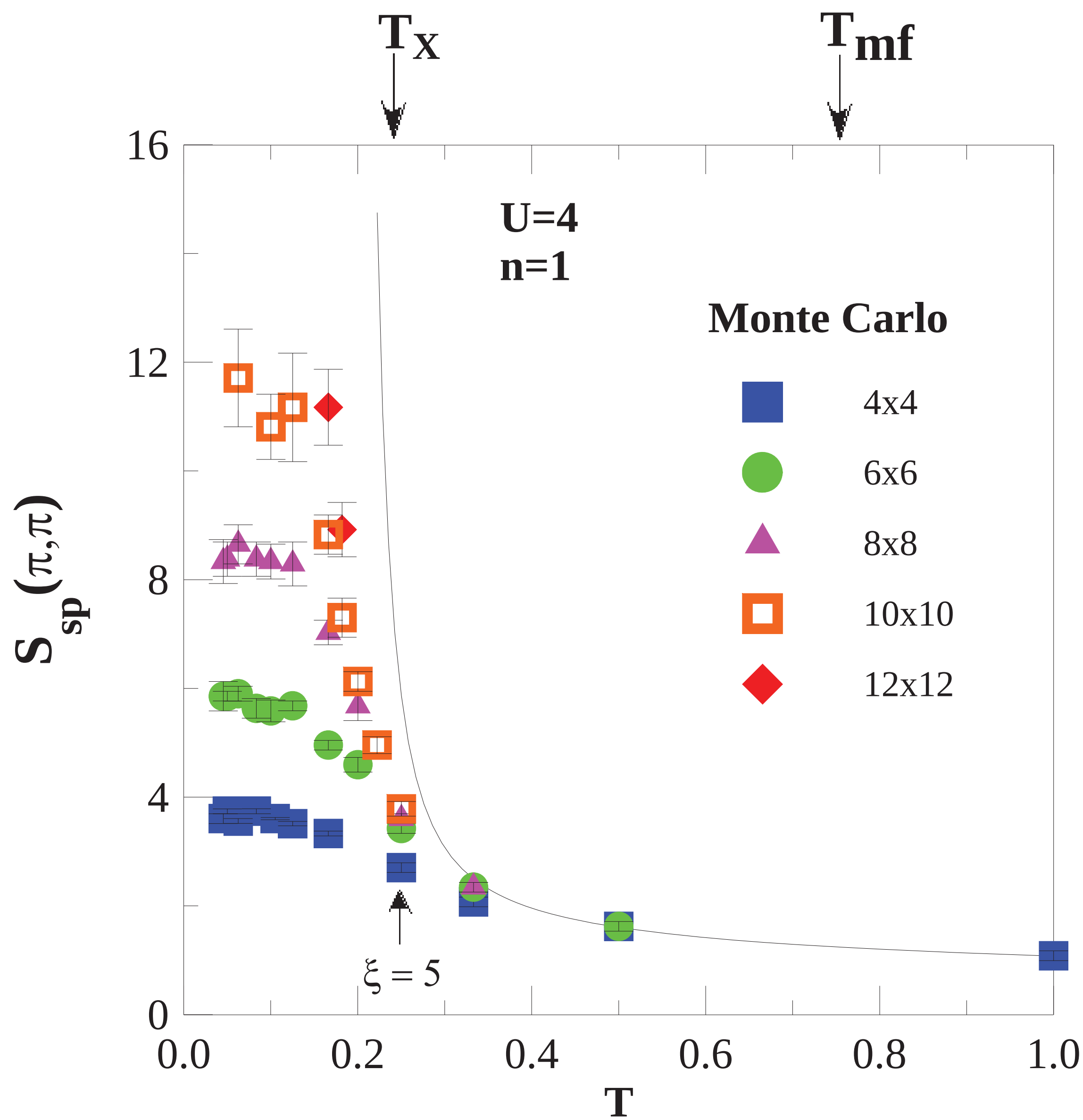
$\beta = 5$

8 X 8



QMC + cal.: Vilk et al. P.R. B **49,** 13267 (1994) *n=1*

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



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

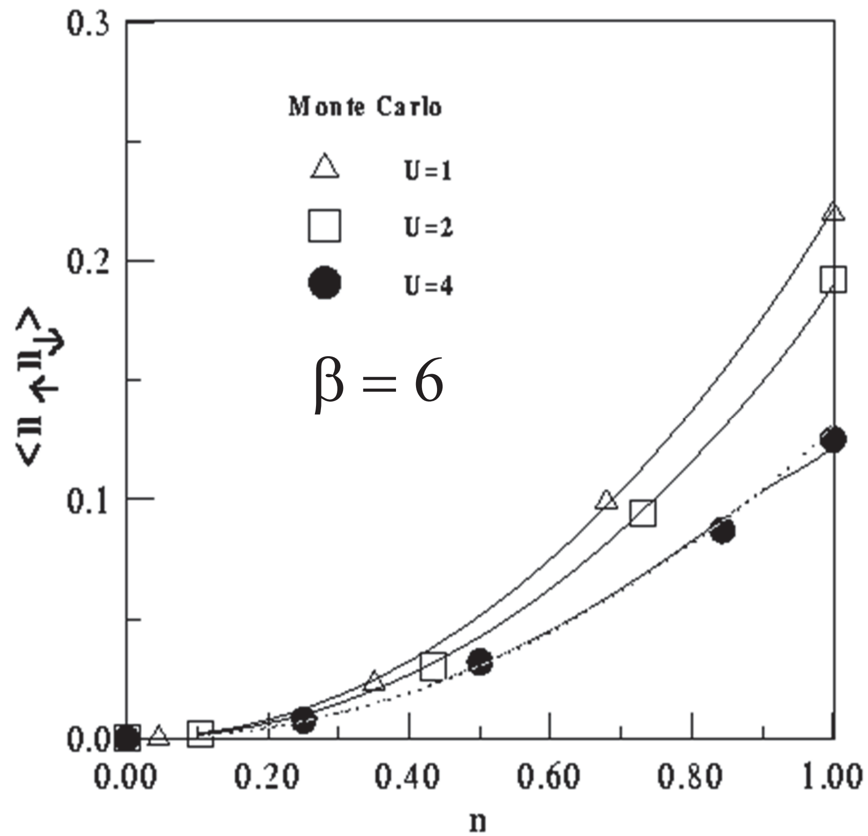
QMC: S. R. White, et al. Phys. Rev. **40**, 506 (1989).

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

Benchmark comparison with QMC

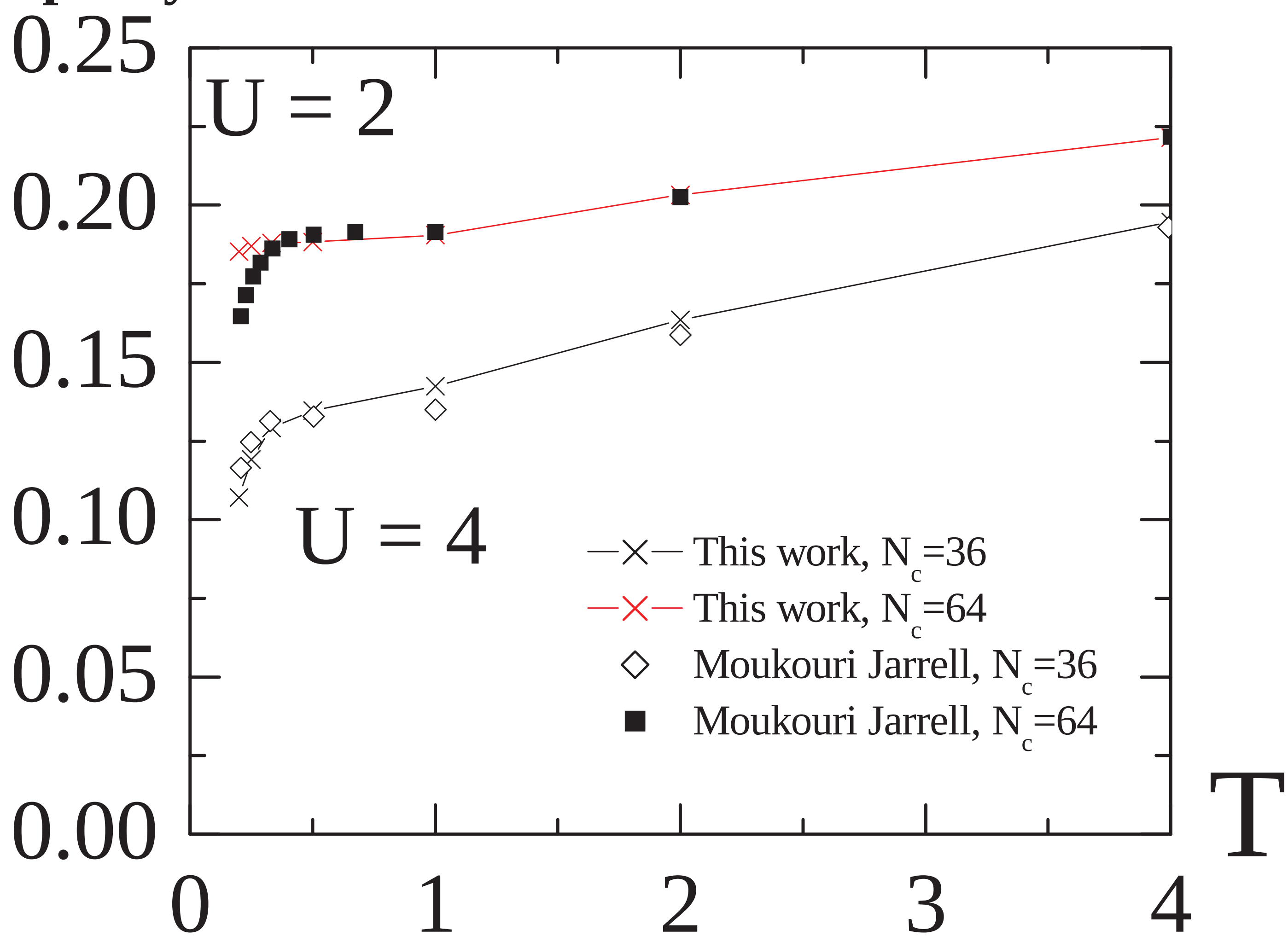
$$\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle - 2\langle n_\uparrow n_\downarrow \rangle$$

- Double occupancy and filling serve as initial conditions for spin and charge structure factor.



Vilk, et al. J. Phys. I France, **7**, 1309 (1997).
QMC : Moreo et al. P.R.B. **41**, 2313 (1990)

Double occupancy :



Dip at low *T* is absent in *d = 3*

Daré, Albinet, P.R. B 61, 4567 (2000).

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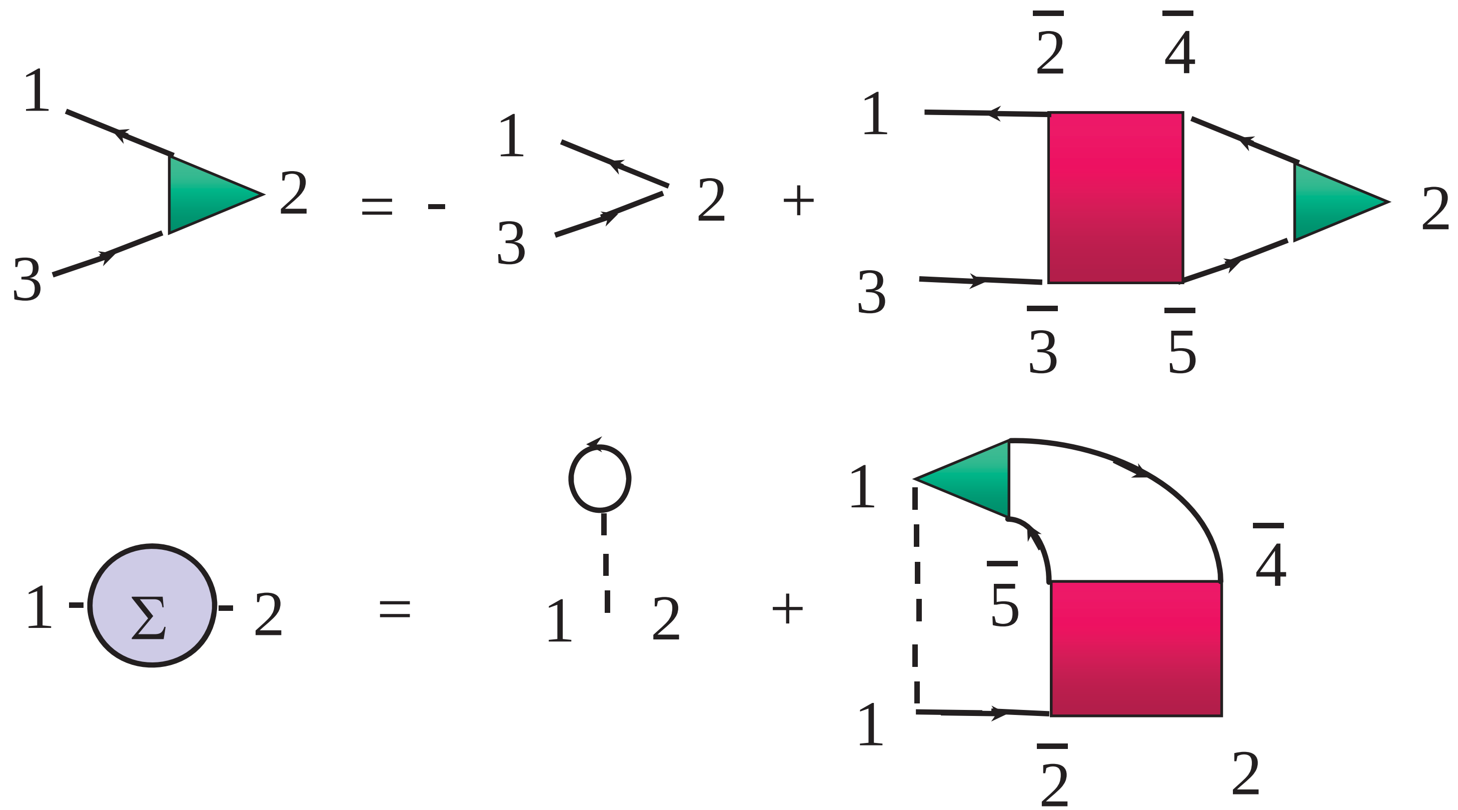
TPSC: Single-particle properties

A better approximation for single-particle properties (Ruckenstein)

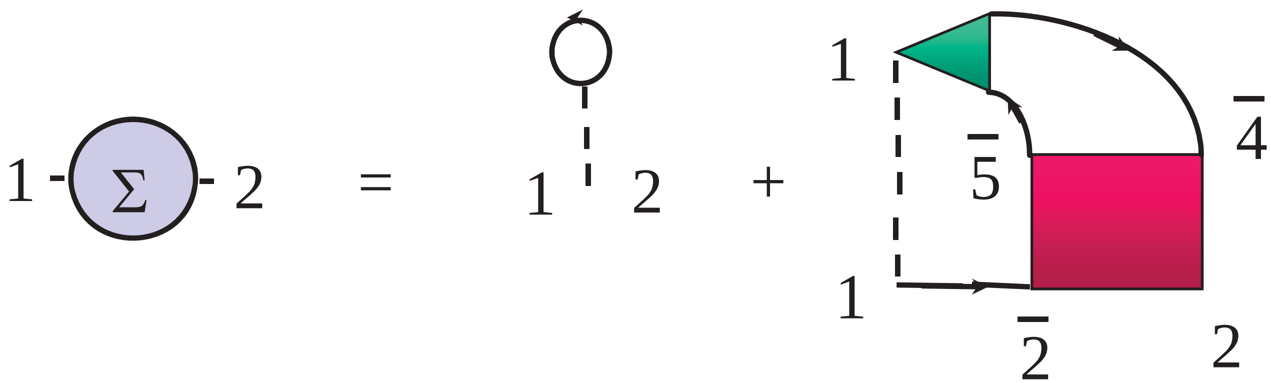


Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).
Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

N.B.: No Migdal theorem

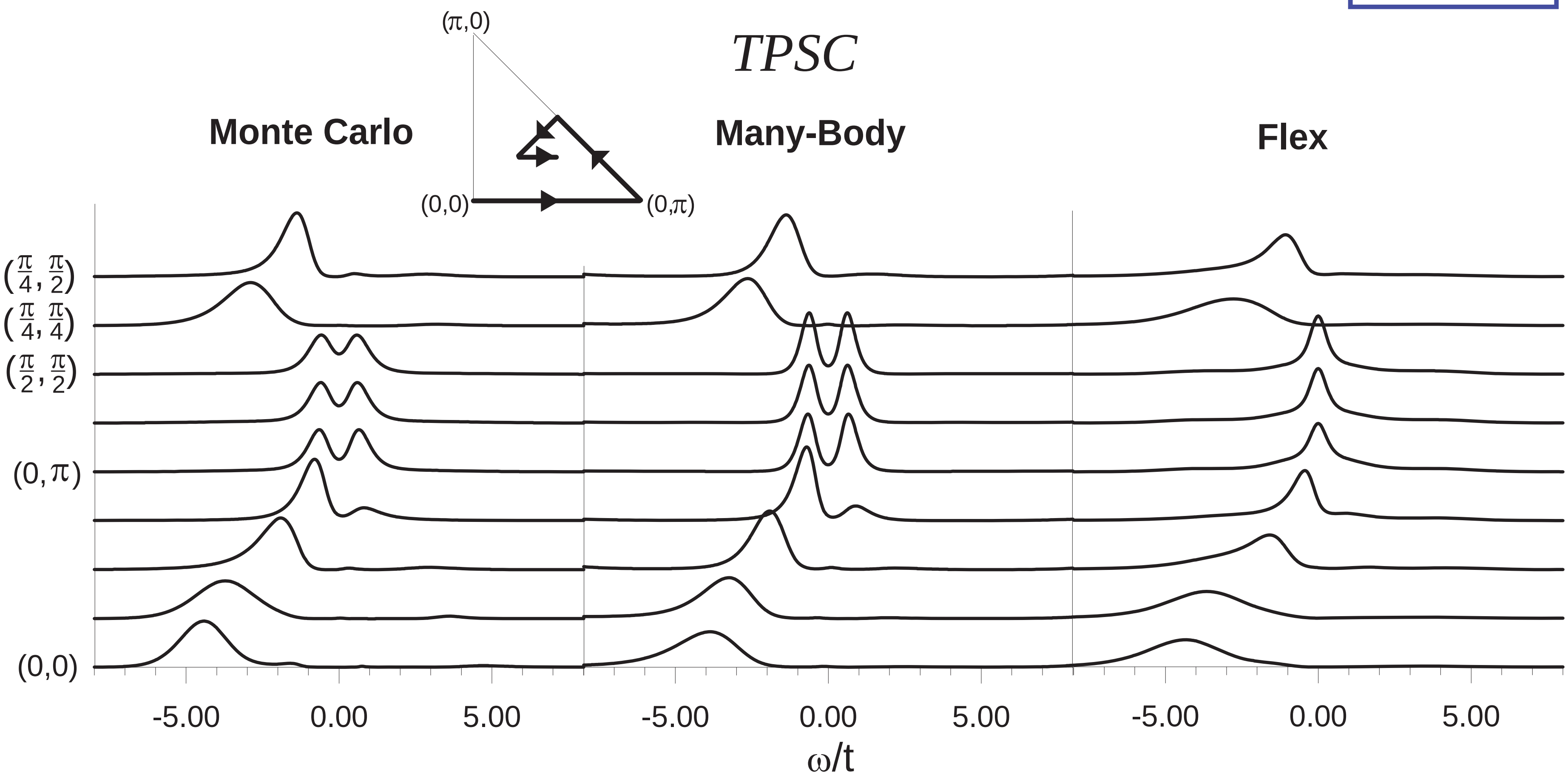
One-particle spectral weight: the equation

$$\Sigma_{\sigma}^{(2)}(k) = Un_{-\sigma} + \frac{U}{8}\frac{T}{N}\sum_{q}\left[3U_{sp}\chi_{sp}(q) + U_{ch}\chi_{ch}(q)\right]G_{\sigma}^{(1)}(k+q).$$



Proofs...

$U = +4$
$\beta = 5$



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

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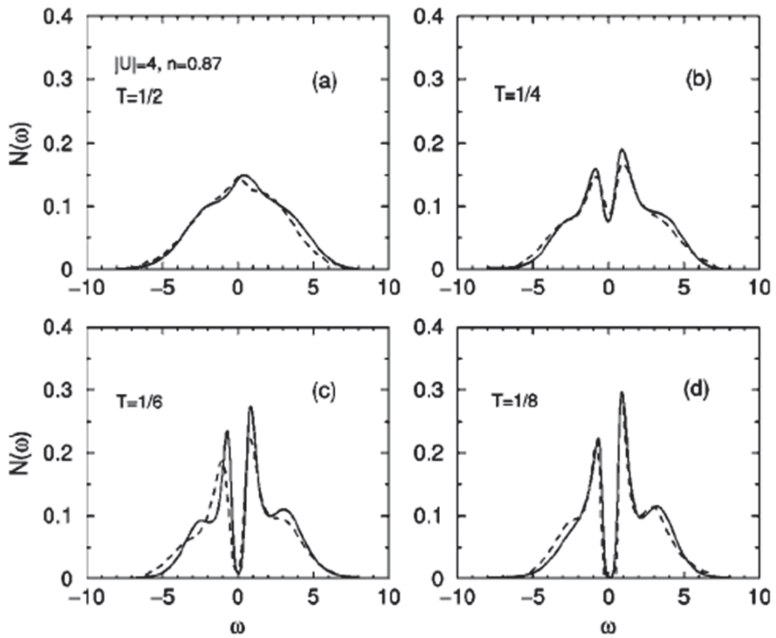
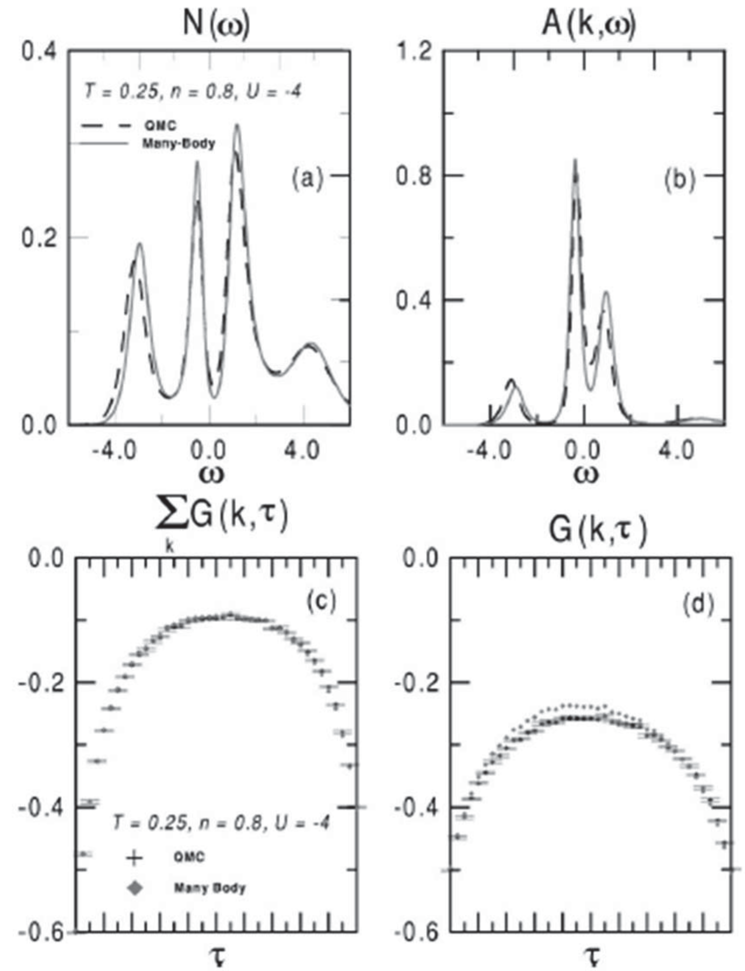
Additional results obtained with TPSC Attractive Hubbard model





•Kyung, Allen, A.-M.S.T. PRB **64**, 075116 (2001)

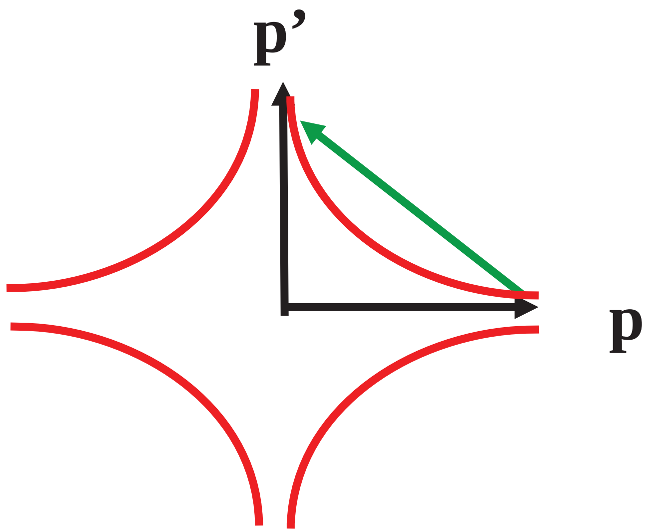
Superconductivity

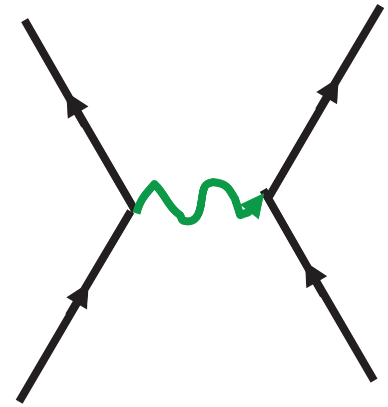
Weakly correlated case

(e-doped ?)

Cartoon « BCS » weak-coupling picture

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





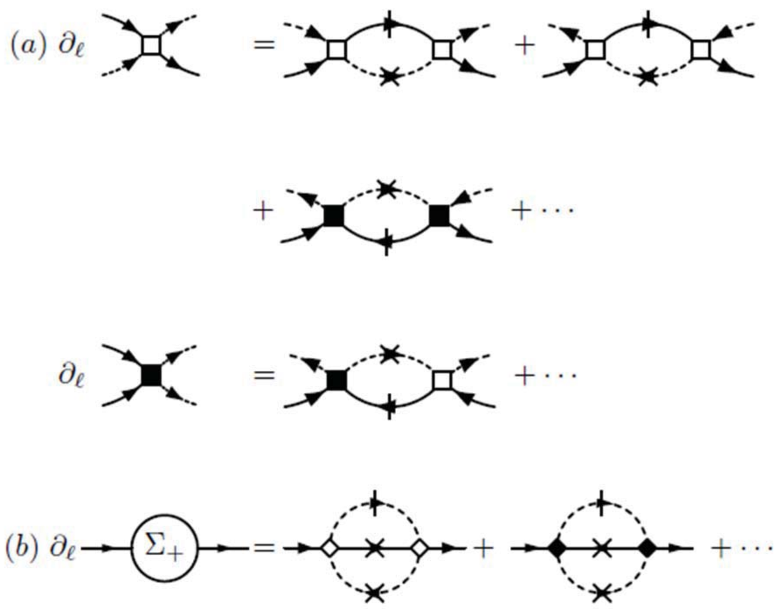
Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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)

Weak coupling methods

- Functional renormalization group



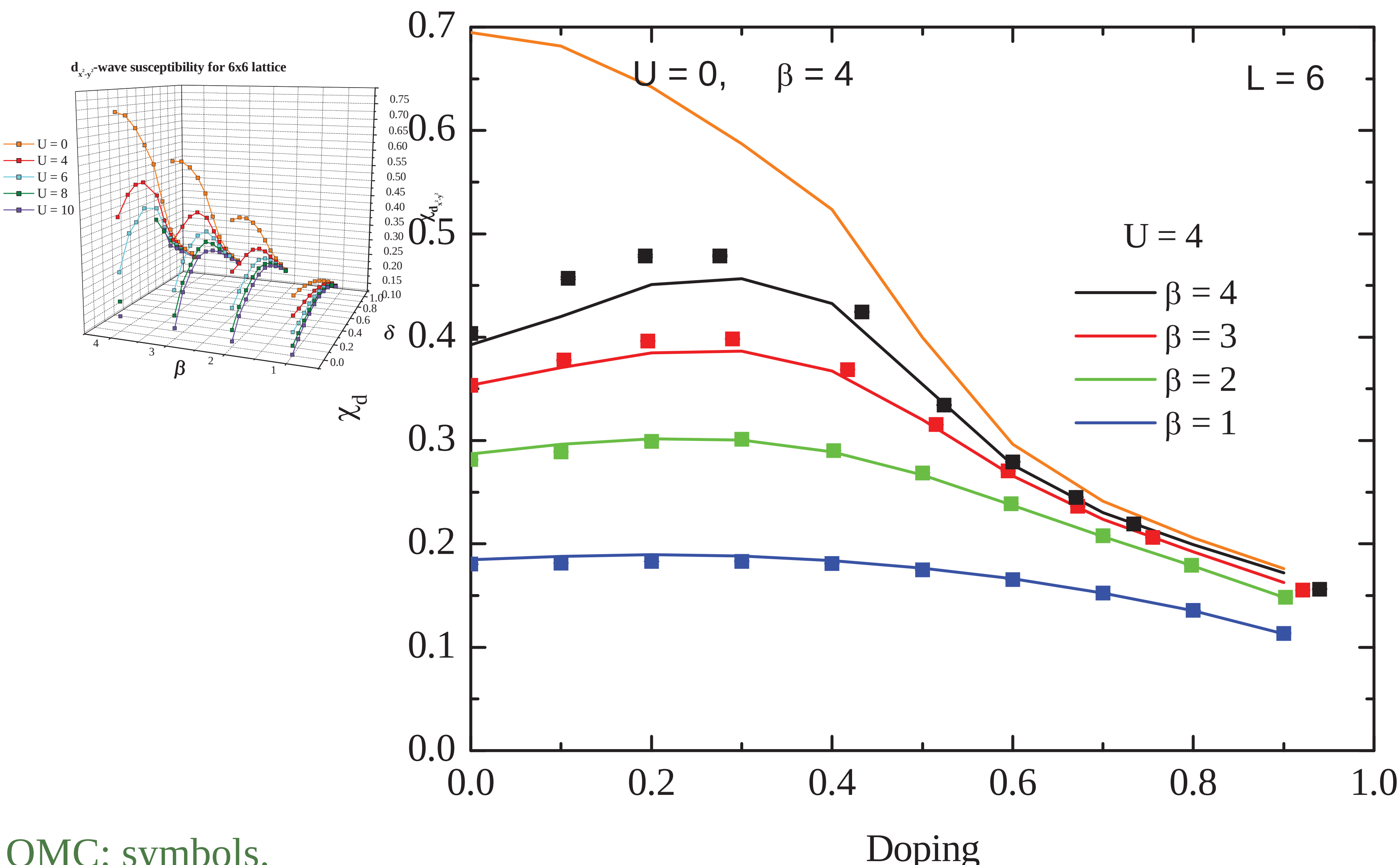
Zanchi, Schultz 2000
Honerkamp, Salmhofer 2000 +
Bourbonnais Sedeki PRB 2012

- Weak coupling perturbation theory

S. Maiti and A.V. Chubukov: arXiv:1305.4609

Results from TPSC

Benchmark, SC state



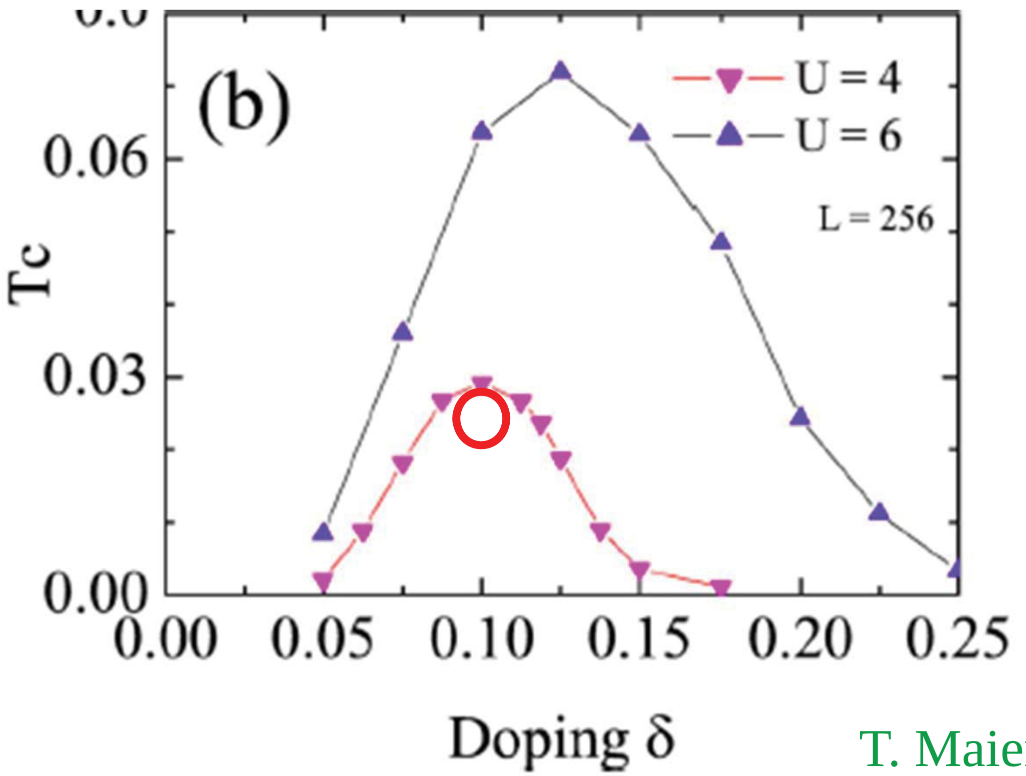
QMC: symbols.

Solid lines analytical.

Kyung, Landry, A.-M.S.T. PRB (2003)

Tc from TPSC

t' = 0

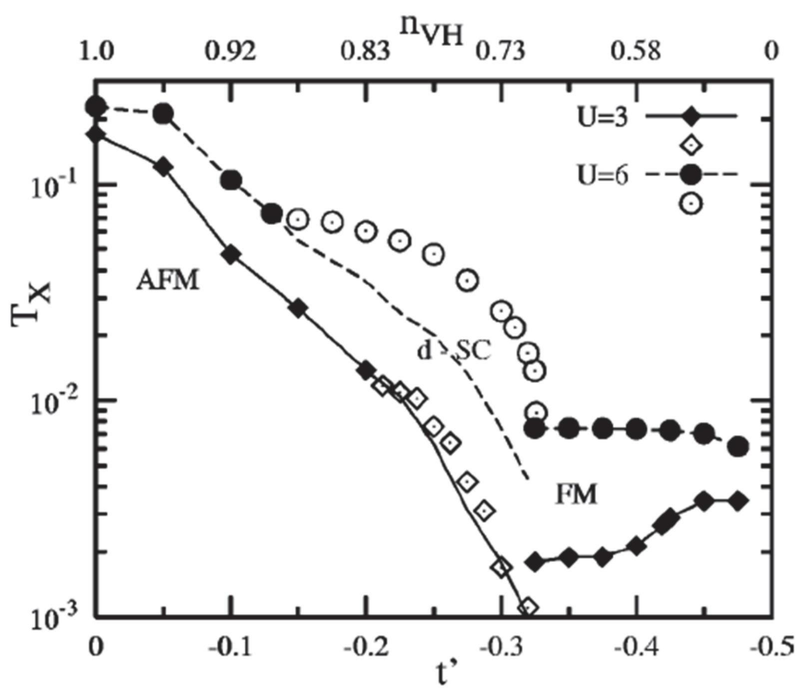


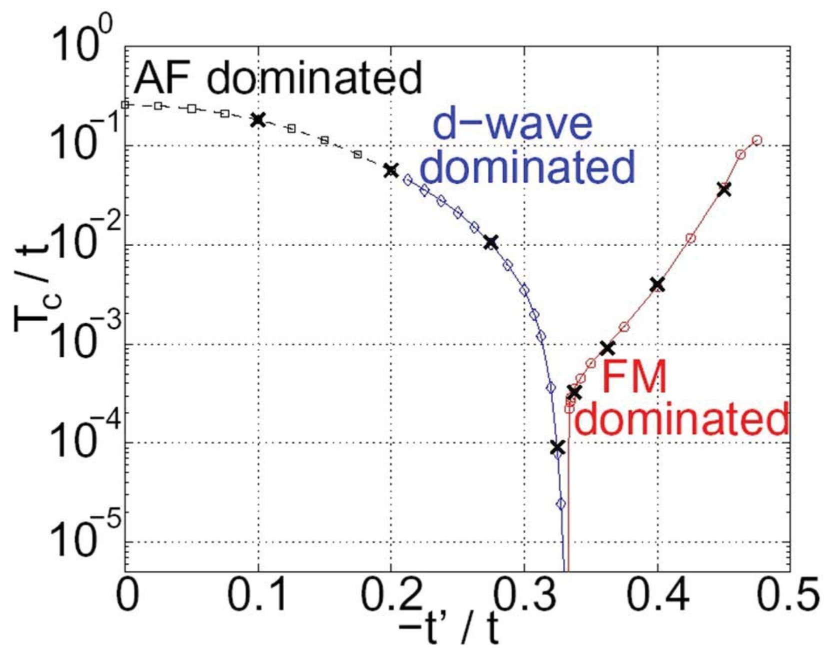
Kyung et al. PRB **68** (2003)

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

DCA: $T_c = 0.023$

Additional results obtained with TPSC
Instabilities at the van Hove point





U = 3

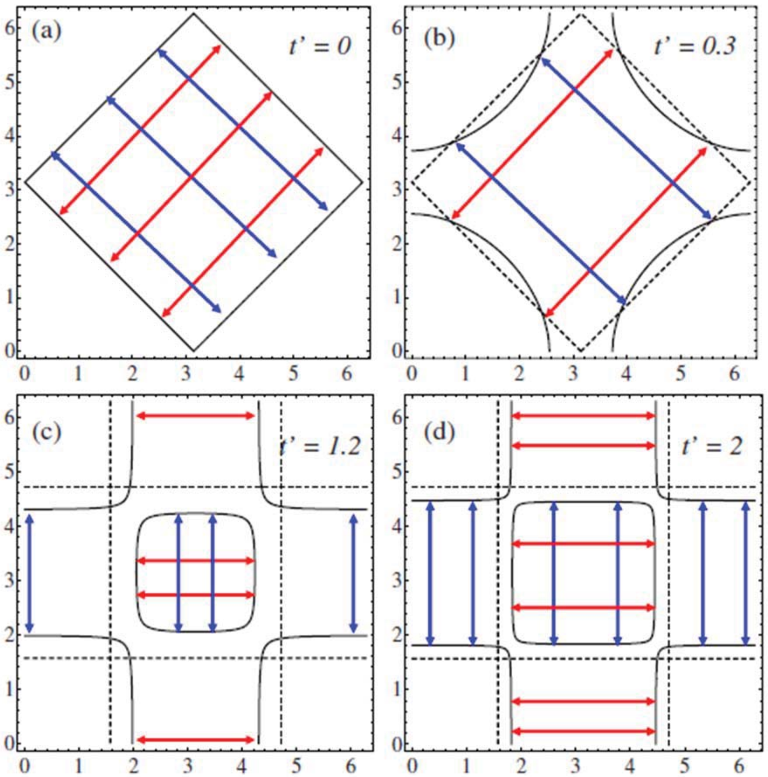
•Hankevych, Kyung, A.-M.S.T. PRB **68**, 214405 (2003)

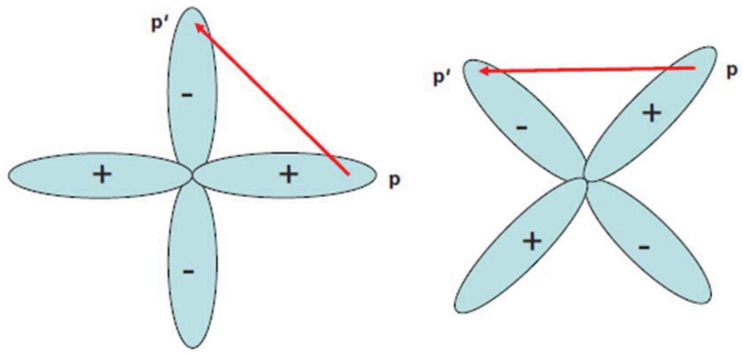
•Honerkamp and Salmhofer, PRL **87**, 187004 (2001)

Physics of superconductivity: TPSC

Predictions, SC state

Relation between symmetry and wave vector of AFM fluctuations





Hassan et al. PRB 2008

T_c depends on t'

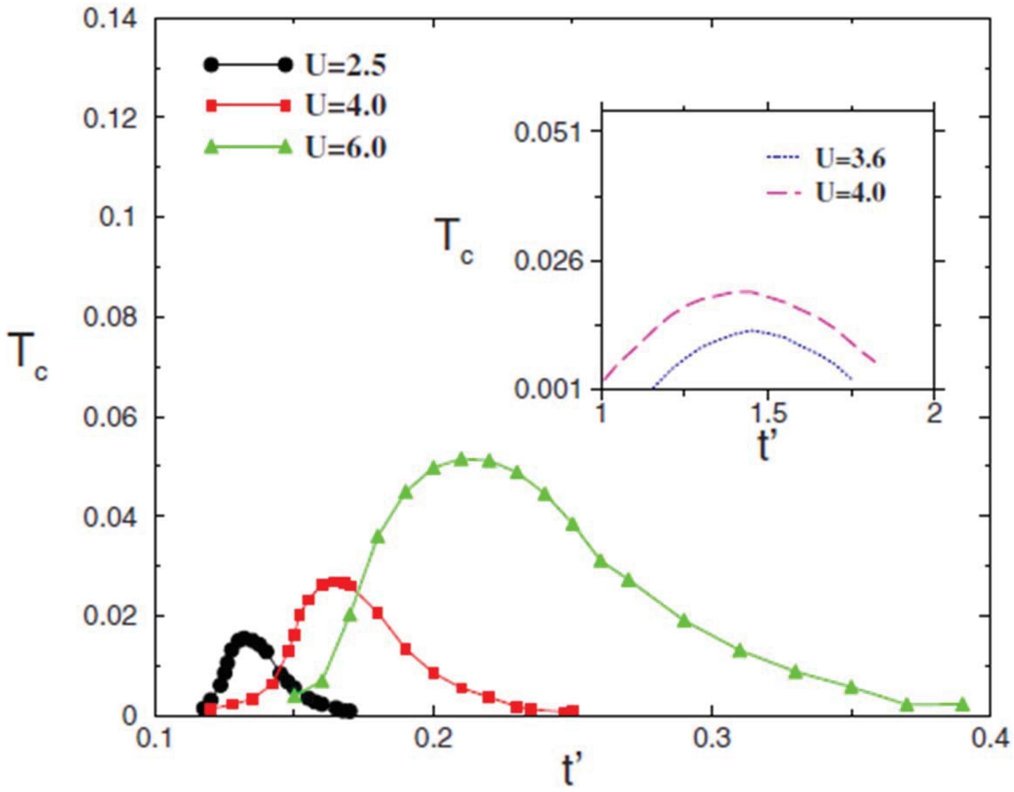


FIG. 5. (Color online) The $d_{x^2-y^2}$ superconducting critical temperature T_c as a function of t' at U=2.5, 3, and 4 for n=1. The inset shows the d_{xy} superconducting critical temperature T_c as a function of t' for U=3.6 and 4.

Hassan et al. PRB 2008

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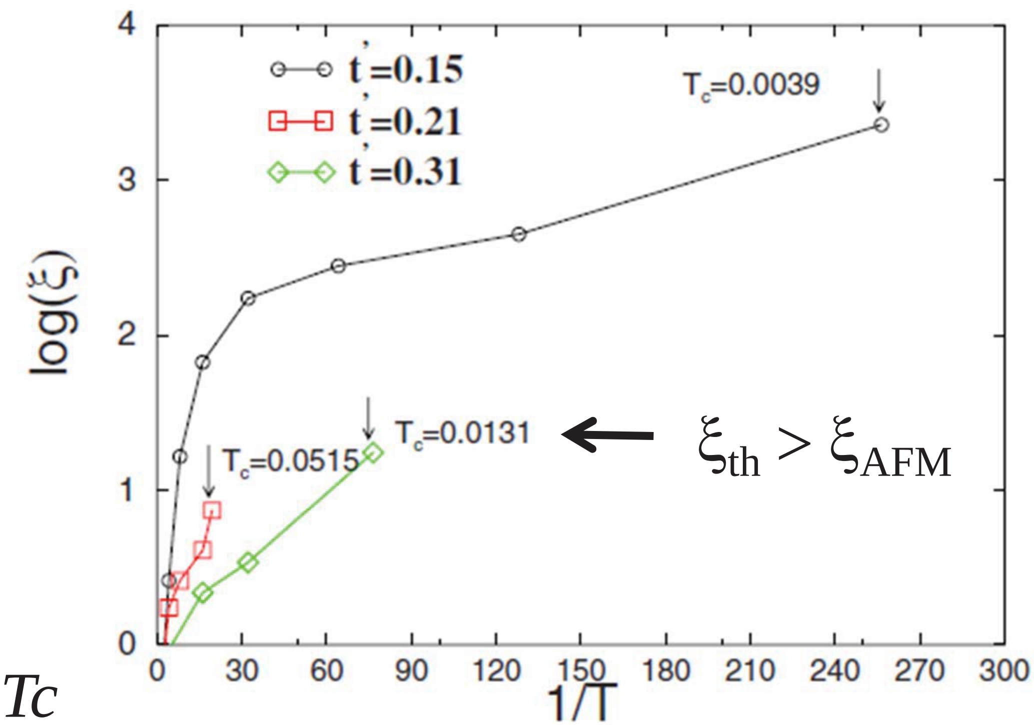
Tc in RC regime or not



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

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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Bio break

A.-M.S.T, *Theoretical Methods for Strongly Correlated Systems*, edited by A. Avella and F. Mancini (Springer, New York, 2011), Chap. 13, p. 409; e-print arXiv:1107.1534.

TPSC: How it works

e-doped

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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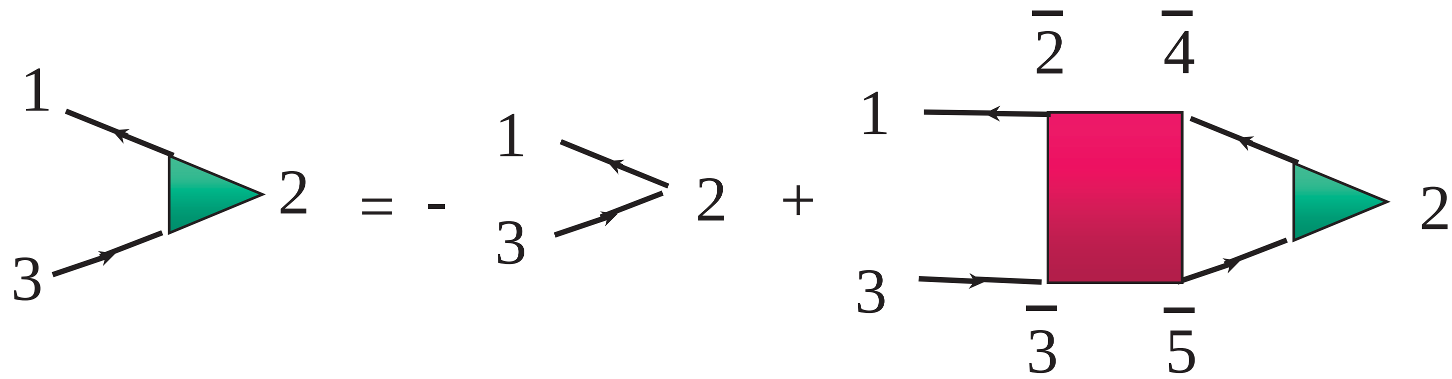
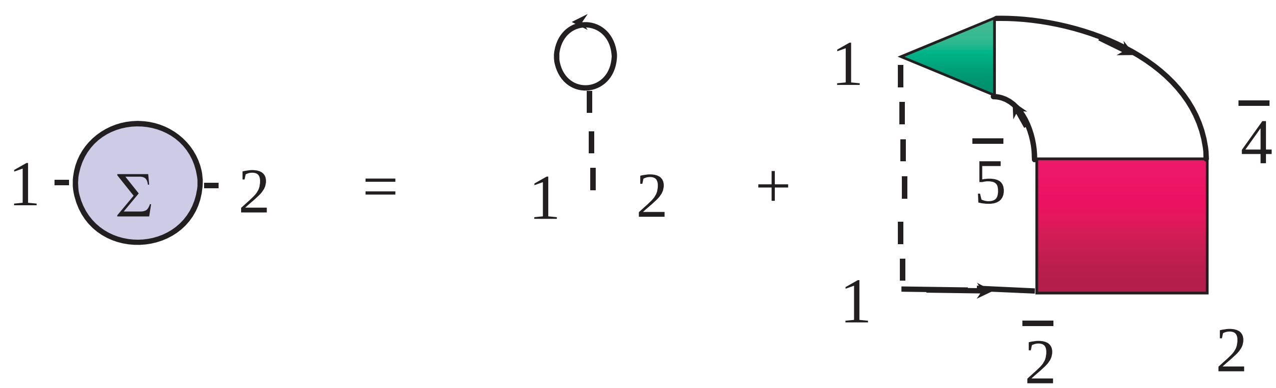
TPSC: Single-particle properties

A better approximation for single-particle properties (Ruckenstein)

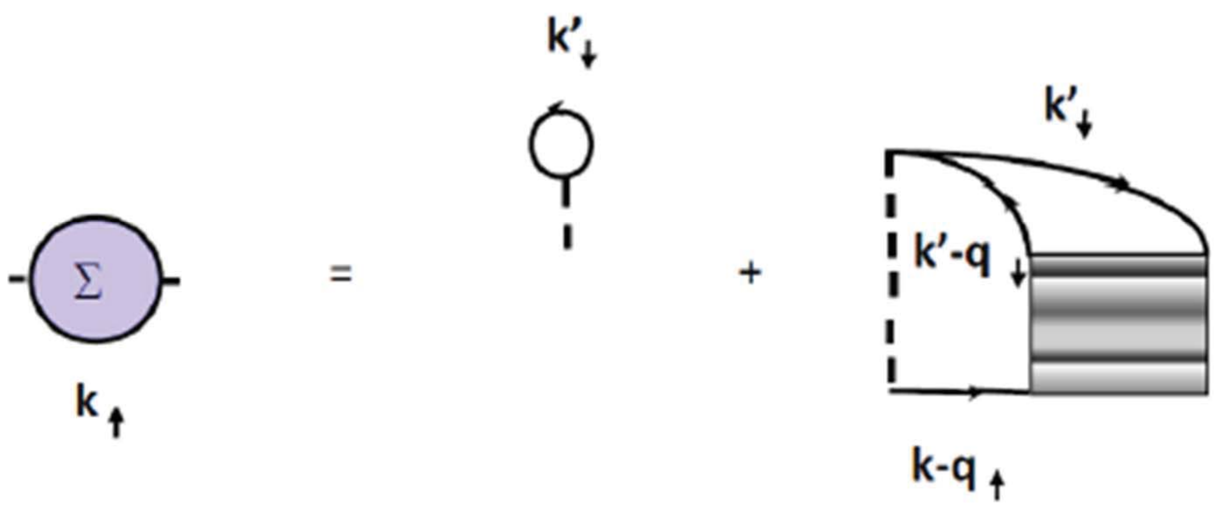




Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).
Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

N.B.: No Migdal theorem

Crossing symmetry



Self-energy in TPSC

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

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

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

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

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

Kanamori-Brückner screening

=

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Internal accuracy check

Internal accuracy check

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

f- sum rule (conservation law)

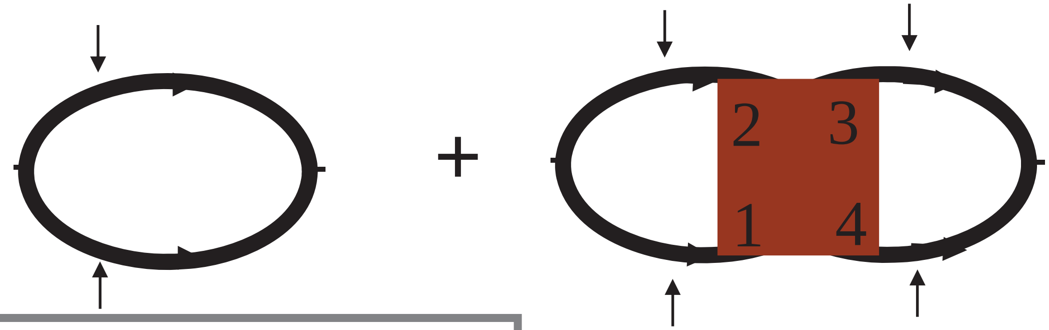
$$\int \frac{d\omega}{\pi}\omega\chi''_{ch,sp}(\mathbf{q},\omega) = \lim_{\eta\to 0} T\sum_{i\omega_n}\left(e^{-i\omega_n\eta} - e^{i\omega_n\eta}\right) i\omega_n\chi_{ch,sp}(\mathbf{q}, i\omega_n)$$

$$= \frac{1}{N}\sum_{\mathbf{k}\sigma}\left(\epsilon_{\mathbf{k+q}} + \epsilon_{\mathbf{k-q}} - 2\epsilon_{\mathbf{k}}\right) n_{\mathbf{k}\sigma}$$

TPSC superconductivity

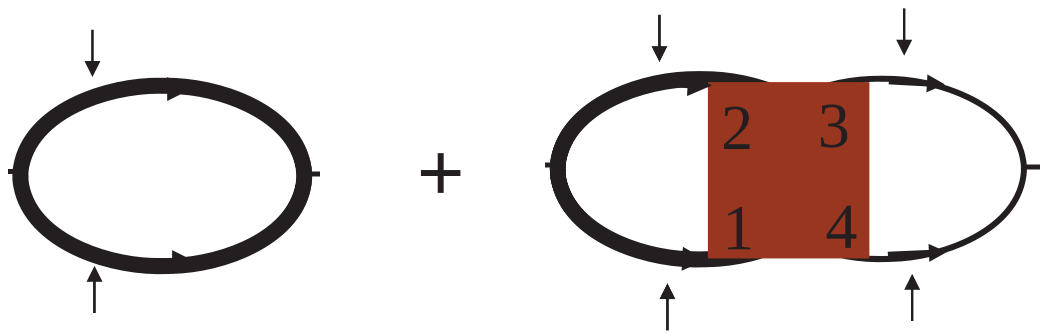
Method

$$\chi_d = \frac{\delta G}{\delta \eta} =$$

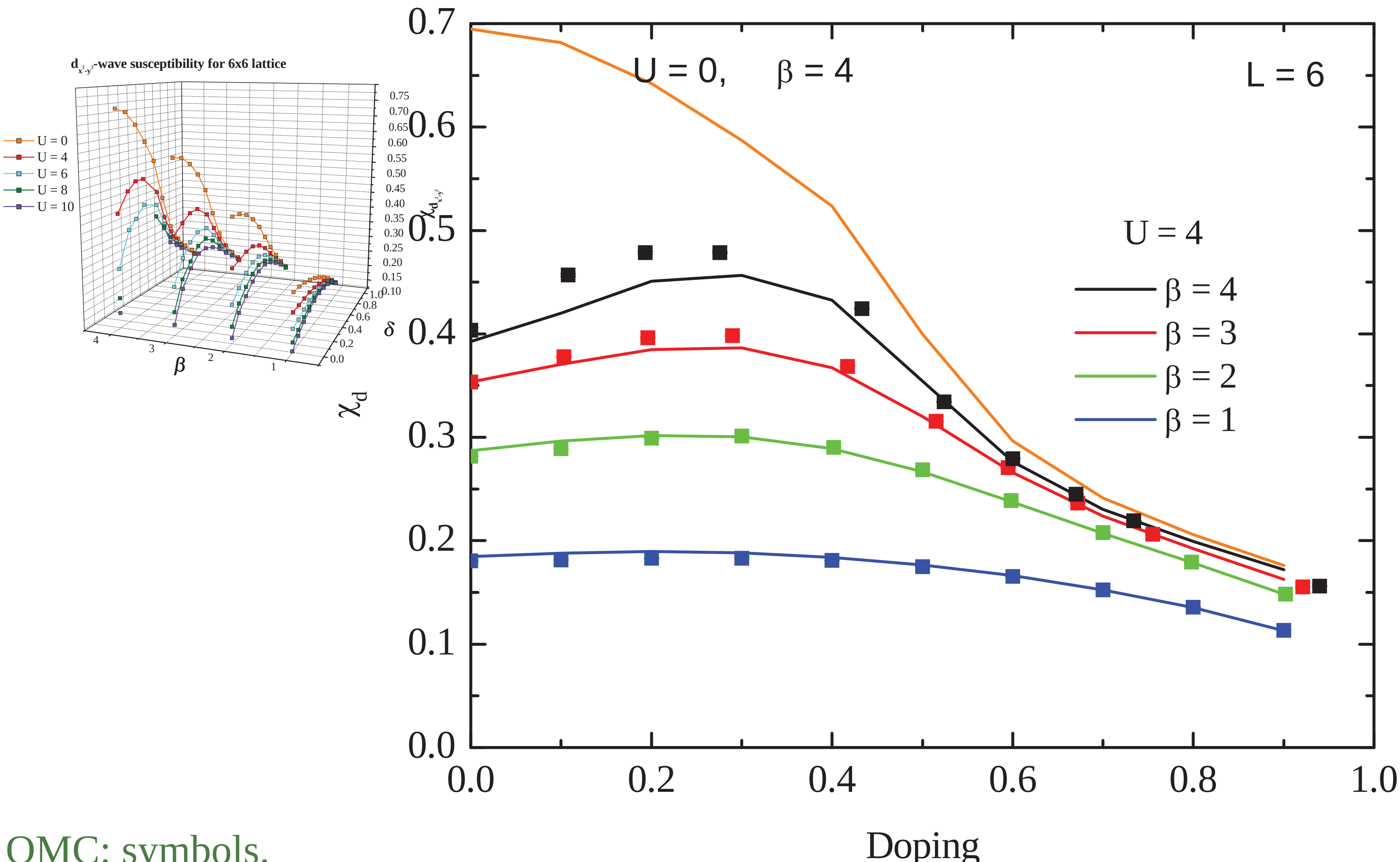


$$\boxed{\frac{\delta G}{\delta \eta} = GG\left(1 + \frac{\delta \Sigma}{\delta \eta}\right)} \qquad G = \frac{1}{G_0^{-1} - \eta - \Sigma}$$

$$\chi_d = \frac{\delta G}{\delta \eta} \sim$$

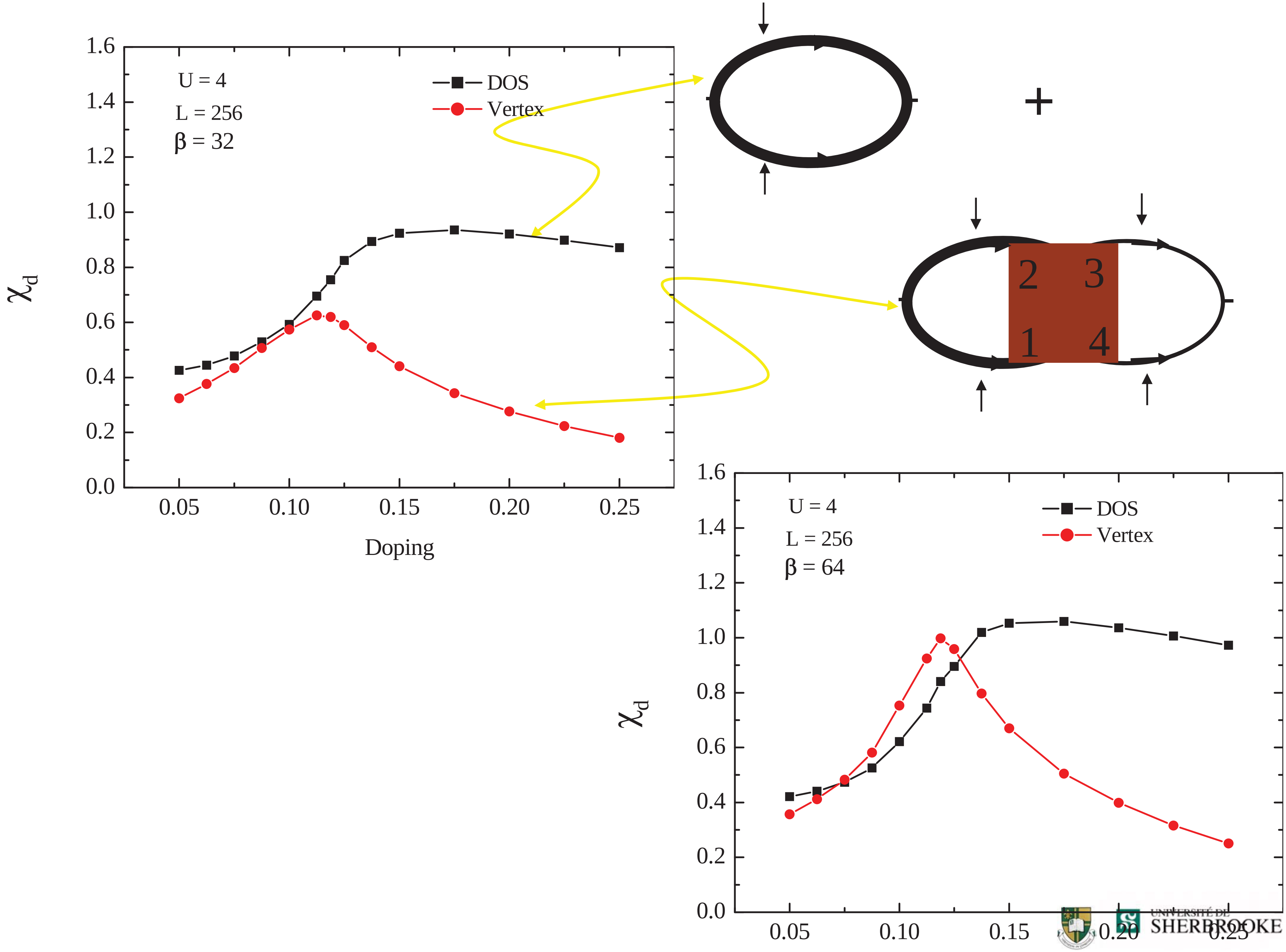


Σ for spin fluctuations, in the presence of off-diagonal source field



QMC: symbols.
Solid lines analytical.

Kyung, Landry, A.-M.S.T. PRB (2003)



U = 4
L = 256
β = 32
DOS
Vertex
χ_d
Doping
0.05
0.10
0.15
0.20
0.25
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
+
2
3
1
4
U = 4
L = 256
β = 64
DOS
Vertex
χ_d

To do

- Calculate T_c for e-doped
- Include feedback of SC on AFM fluctuations
  - (explain correlation length near optimal doping)
- Take atomic limit as starting point to generalize to strong correlations?
- Generalize to broken symmetry states and multiband
- Generalize to longer range interaction
  - Davoudi, AMST PRB **74**, 035113 (2006); PRB **76**, (2007);

Merci

Thank you