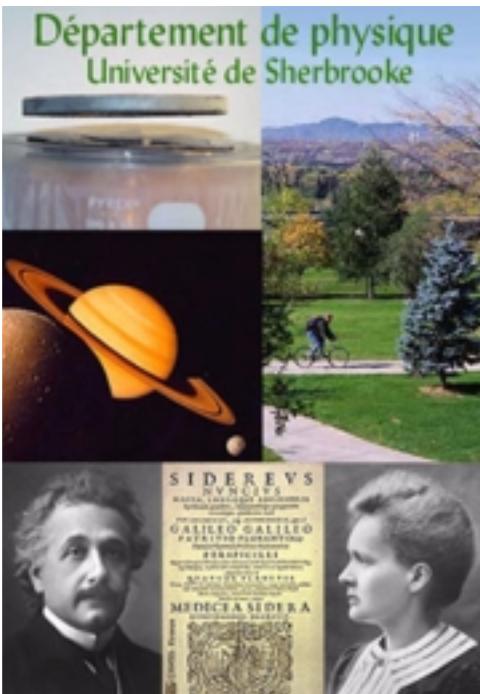
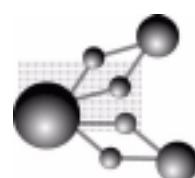


Electronic correlations



André-Marie Tremblay



CENTRE DE RECHERCHE SUR LES PROPRIÉTÉS
ÉLECTRONIQUES
DE MATÉRIAUX AVANCÉS



Sponsors:



Acknowledgements:

Steve Allen (PhD)

Bumsoo Kyung (postdoc)

Yury Vilk (now at Chicago)

Samuel Moukouri (postdoc)

Liang Chen (now at U. Ottawa)

François Lemay (PhD)

David Poulin

Hugo Touchette

1. Motivation

Theory of solids

$$H = \text{kinetic} + \text{Coulomb}$$

- Many new ideas and concepts needed for progress
(Born-Oppenheimer, H-F, Bands...)
- Successfull program
 - Semiconductors, metals
 - Magnets
- Is there anything left to do?
 - Unexplained materials: High T_c, Organics...
 - Strong correlations:
strong interactions, low dimension

Outline

1. Motivation

2. The standard approaches :

- Quasiparticles, Fermi surface, Fermi liquid
- Fermi liquids and phase transitions
- Heisenberg and related

3. Experimental evidence for failure :

- $d=1$ spin-charge separation
- $d=2$ disappearing act of Fermi surface

4. Theoretical reasons for failure :

- Effects of strong coupling
- Effects of low d in weak to intermediate coupling

5. The Hubbard model

6. A non-perturbative approach ($U > 0$ and $U < 0$)

- Proof that it works
- How it works

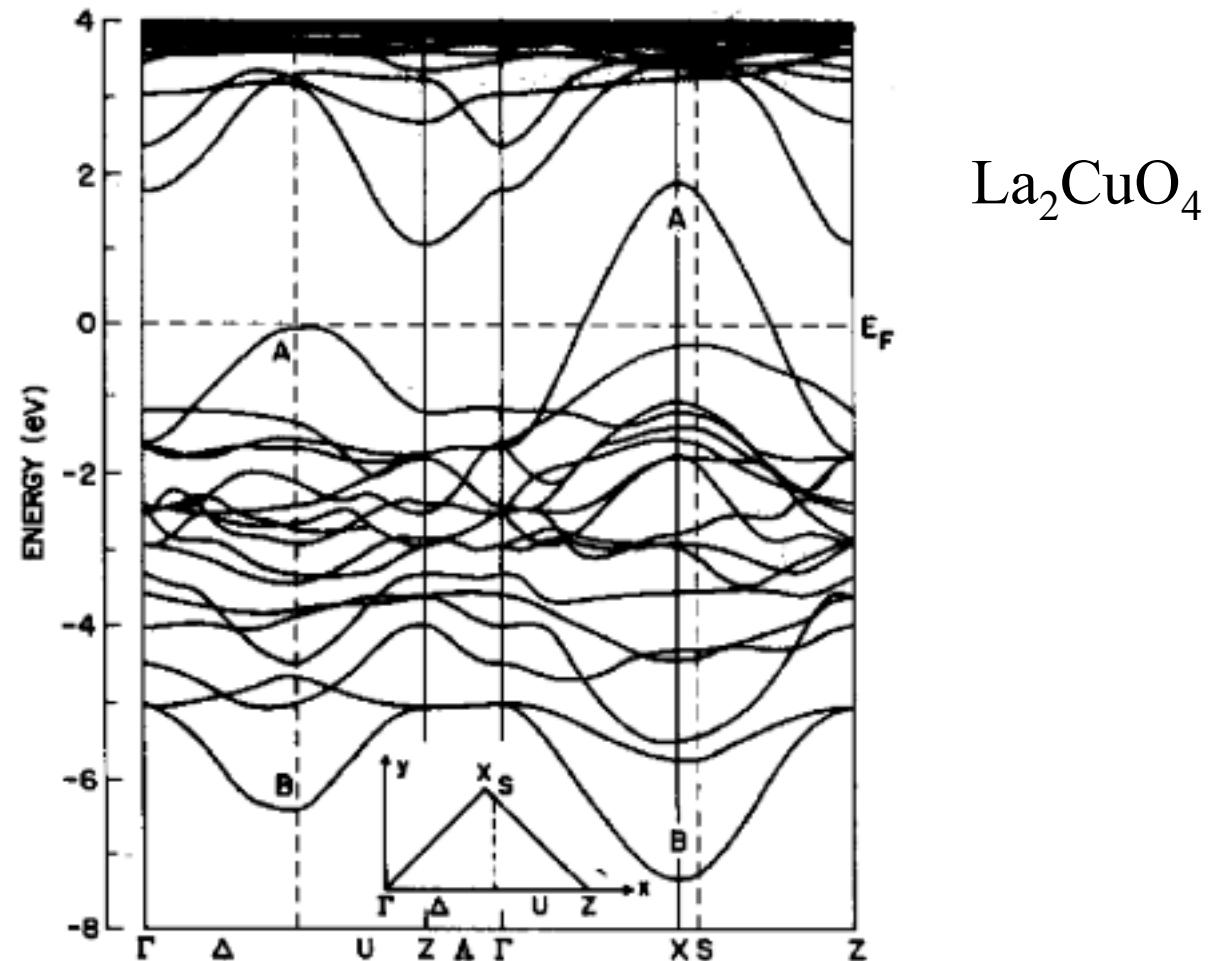
7. Results:

- Mechanism for pseudogap
- Spectral weight rearrangement

8. Conclusion.

2. The standard approaches :

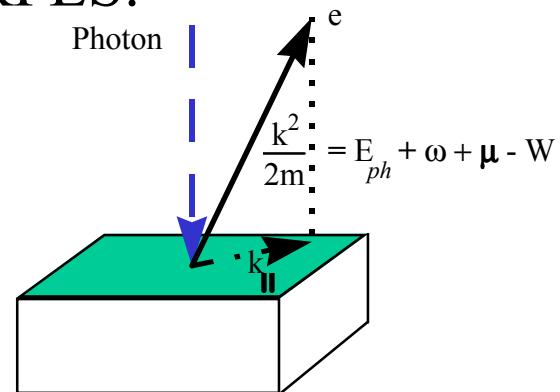
A. Quasiparticles, Fermi surface and Fermi liquids
- LDA (Nobel prize 1998)



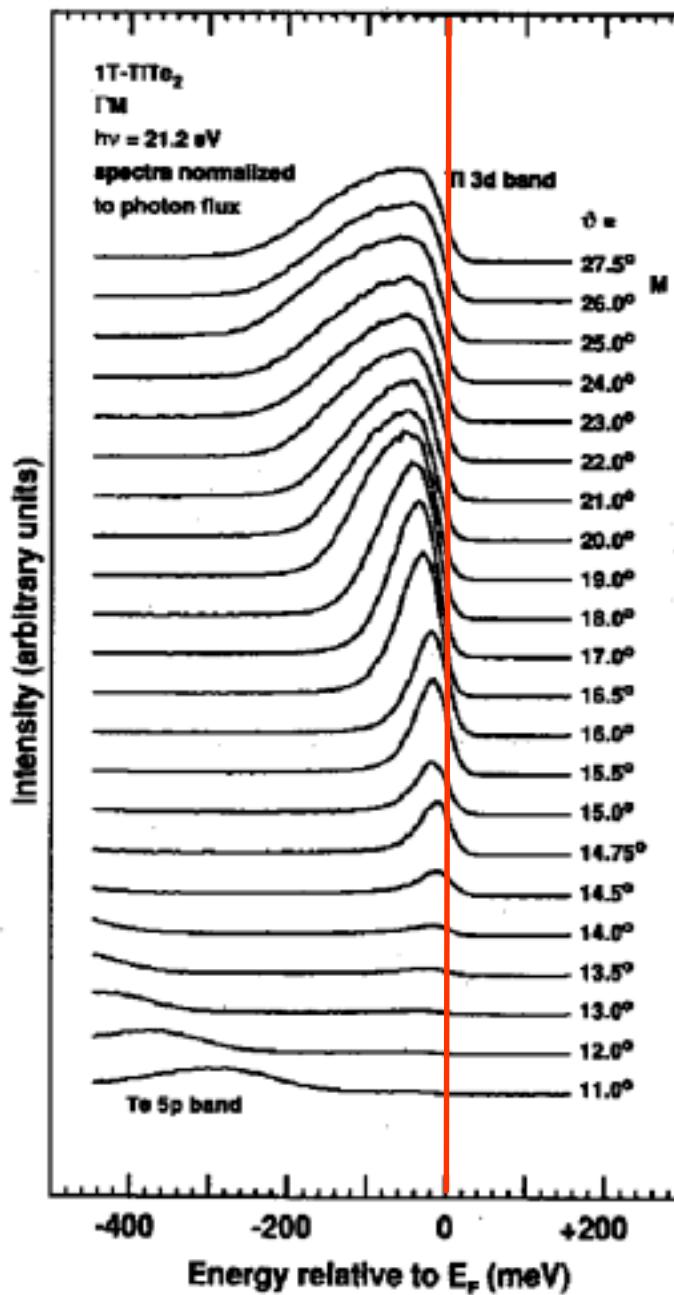
L.F. Mattheiss, Phys. Rev. Lett. 58, 1028 (1987).

2. The standard approaches :

- Matrix elements of H in LDA basis
 - In practice, from general considerations:
 - Short range
 - Single Slater determinant not eigenstate
 - Phase space + Pauli restricts possible scatterings:
 - Quasiparticles m^* , effective fields,
- «See» the quasiparticles with ARPES:



R. Claessen, R.O.
Anderson, J.W. Allen,
C.G. Olson, C.
Janowitz, W.P. Ellis,
S. Harm, M. Kalning,
R. Manzke,
and M. Skibowski,
Phys. Rev. Lett. 69,
808 (1992).



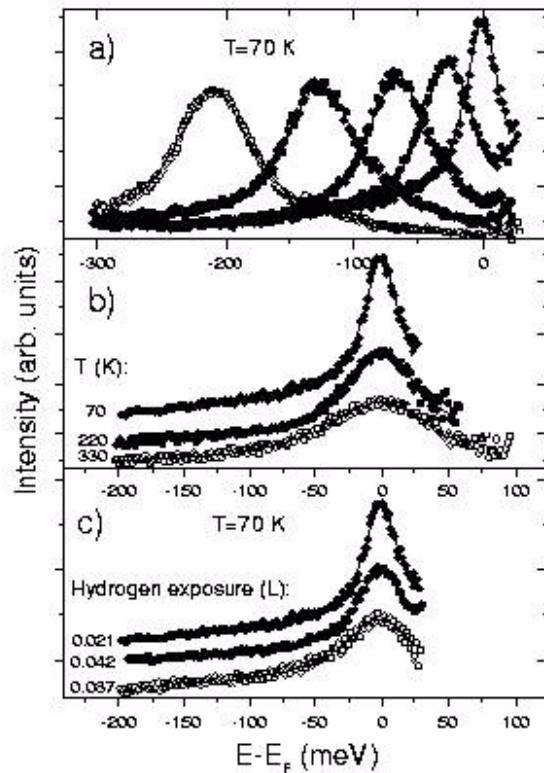


FIG. 2. Spectral intensity as a function of binding energy for constant emission angle, normalized to the experimentally determined Fermi cut-off. Data are symbols, while lines are fits to the Lorentzian peaks with a linear background. The dependence on the binding energy (a), temperature (b), and hydrogen exposure (c) is shown.

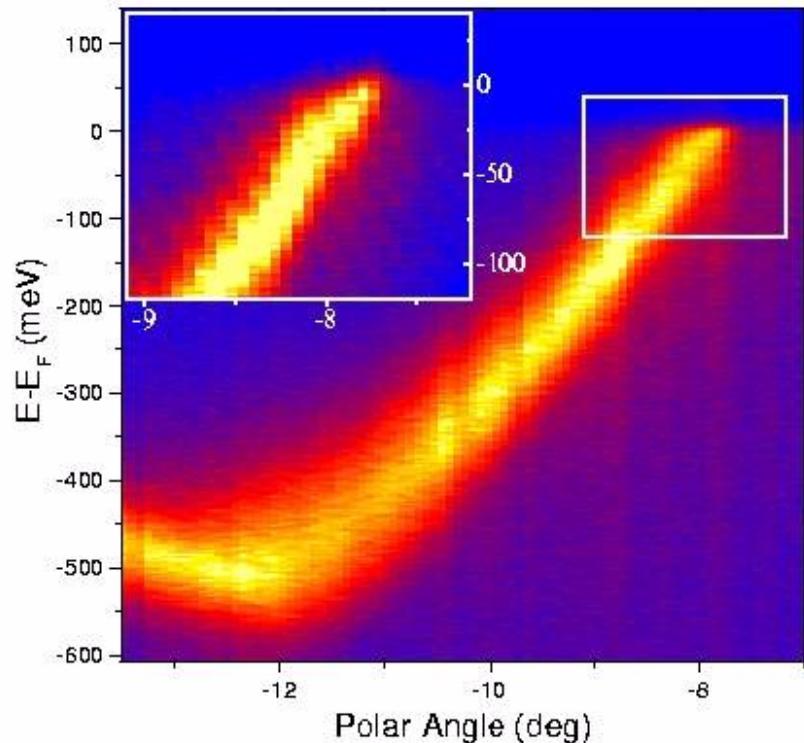


FIG. 1. ARPES intensity plot of the Mo(110) surface recorded along the $\bar{\Gamma} - \bar{N}$ line of the SBZ at 70 K. Shown in the inset is the spectrum of the region around k_F taken with special attention to the surface cleanliness.

T. Valla, A. V. Fedorov, P. D. Johnson, and S. L. Hulbert
P.R.L. **83**, 2085 (1999).

2. The standard approaches :

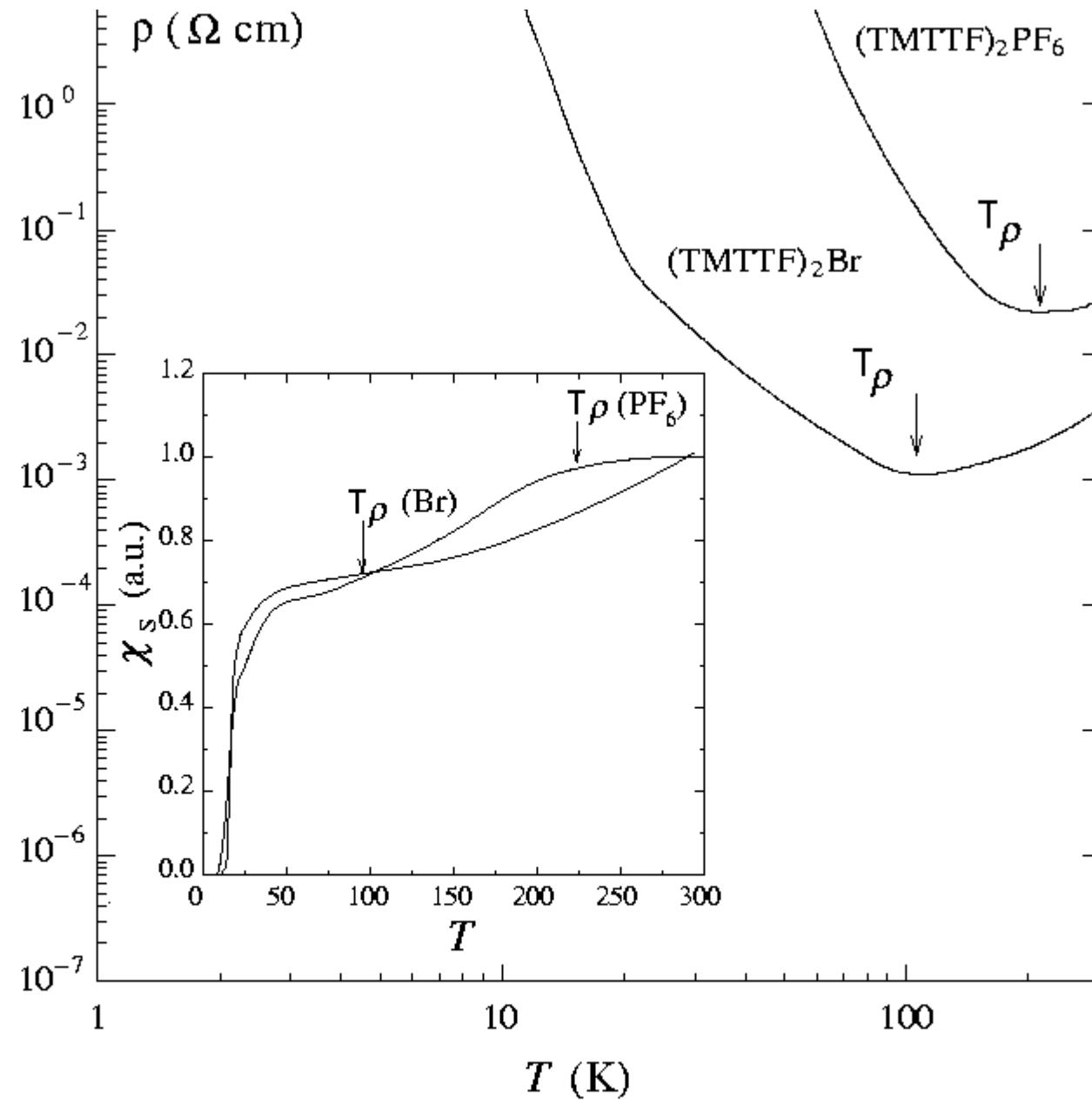
B. Thermodynamics and phase transitions

- Thermodynamics of Fermi liquids
 - particle-hole excitations
- Phase transitions
$$\chi \sim N(0) / (1 + F_o^a)$$
- Superconducting transition

C. Heisenberg model and related models

- Band for *s-p*
- Localized (often) for *d-f*
 - Only spin degrees of freedom
 - Use symmetry to write H

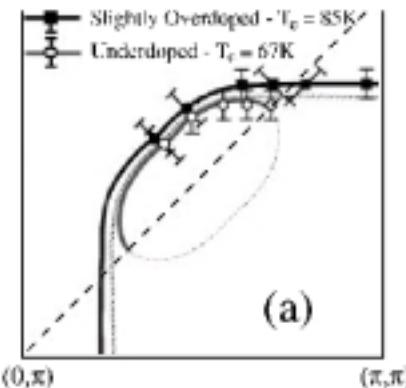
C. Bourbonnais
et al.
(cond-
mat/9903101).



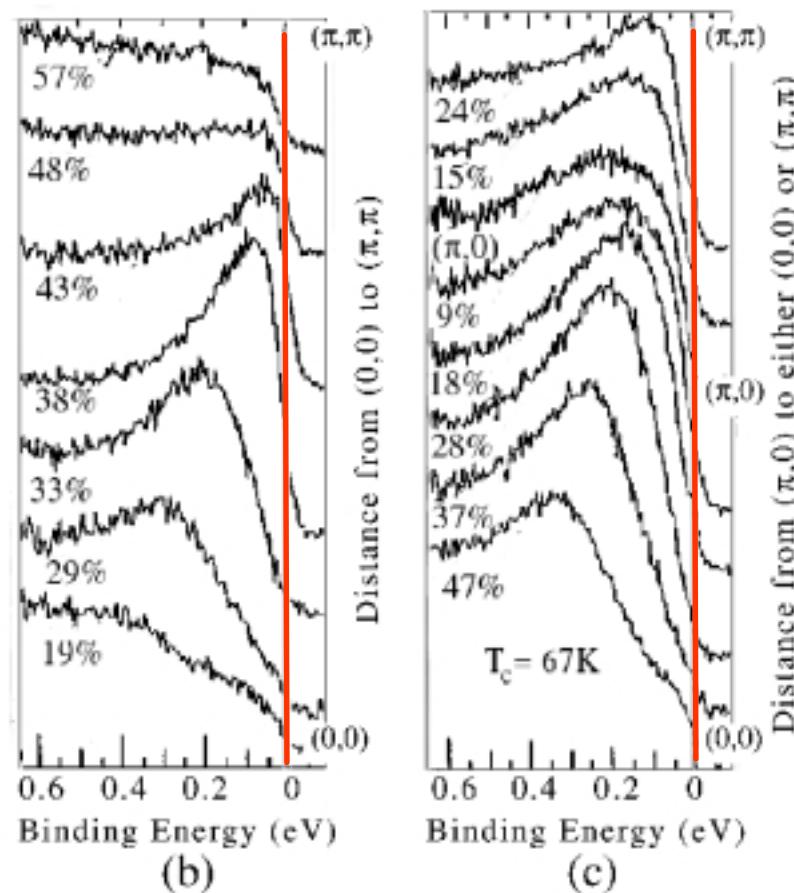
3. Experimental evidence for failure : - $d=1$ spin-charge separation

3. Experimental evidence for failure :

- $d=2$ partial vanishing act of the Fermi surface.

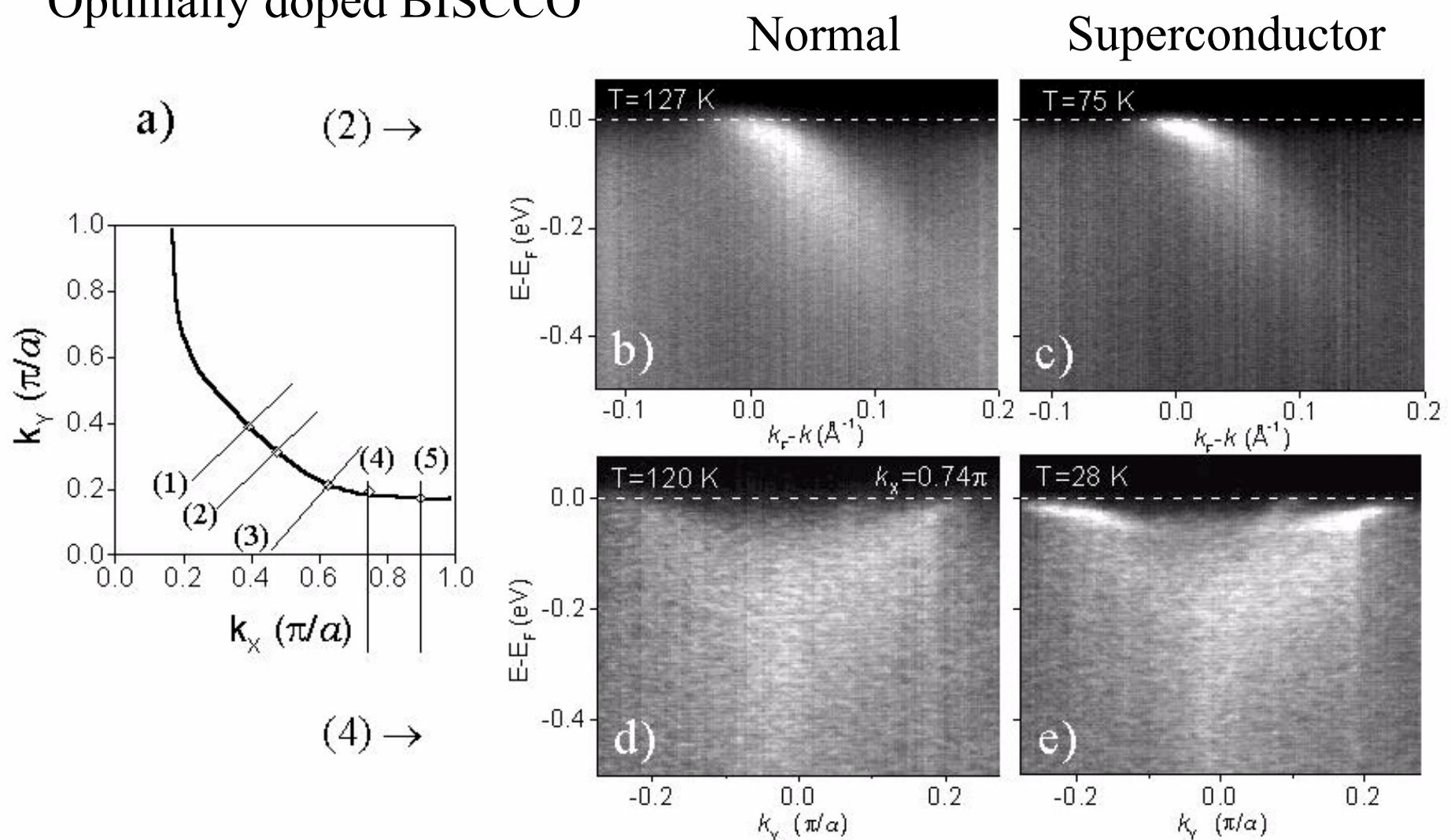


(a)



D.S. Marshall, D.S. Dessau, A.G.
Loeser, C.-H. Park,
A.Y. Matsuura, J.N. Eckstein, I.
Bozovic, P. Fournier,
A. Kapitulnik, W.E. Spicer, and
Z.X. Shen, Phys. Rev.
Lett. 76, 4841 (1996).

Optimally doped BISCCO



A. V. Fedorov, T. Valla, P. D. Johnson et al. P.R.L. **82**, 2179 (1999)

4. Theoretical reasons for failure :

- A. Strong interactions (localized states)
- B. Thermal and quantum fluctuations in $d = 2$

$d = 2$, Mermin-Wagner

$$(\nabla\theta)^2 \rightarrow q^2\theta_{\mathbf{q}}\theta_{-\mathbf{q}}$$

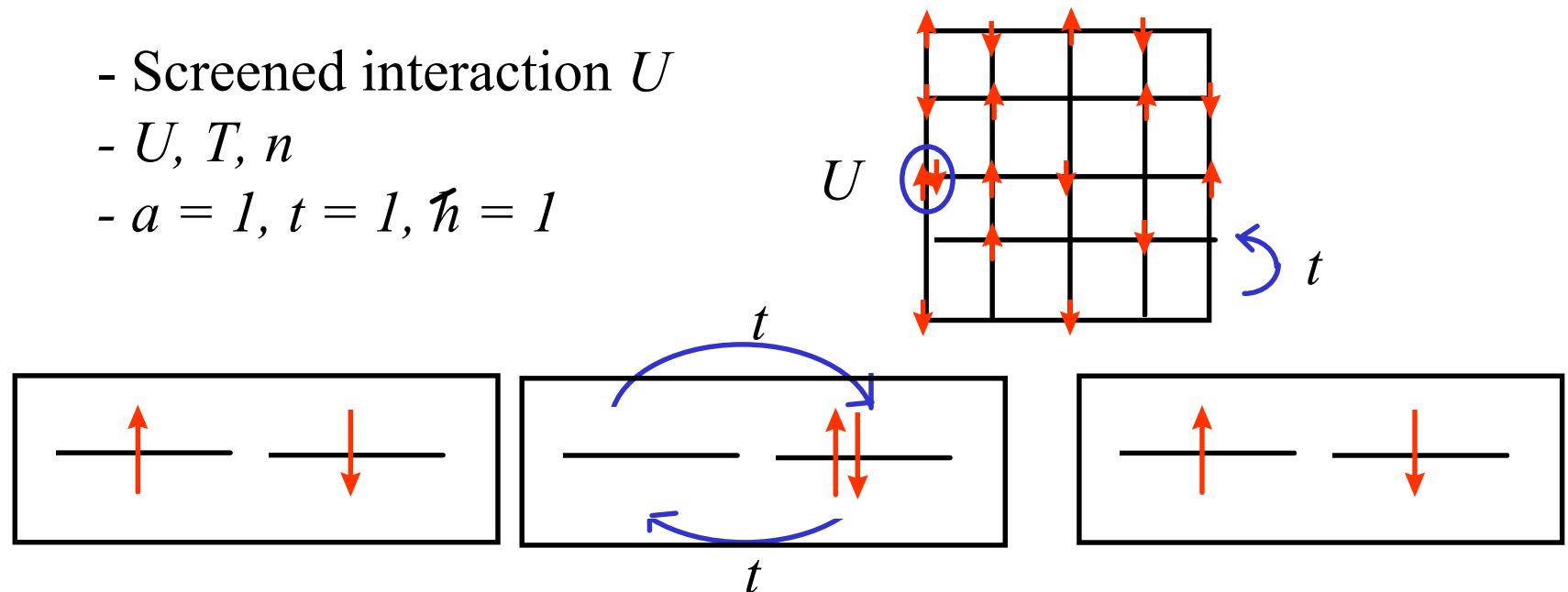
$$\langle\theta^2\rangle \propto \int d^2q \frac{kT}{q^2} \rightarrow \infty$$

$d = 1$: R.G., Bosonization, Conformal Field Theory...
 $d = 2$: Slave bosons, R.G., strong coupling p.t., TPSC

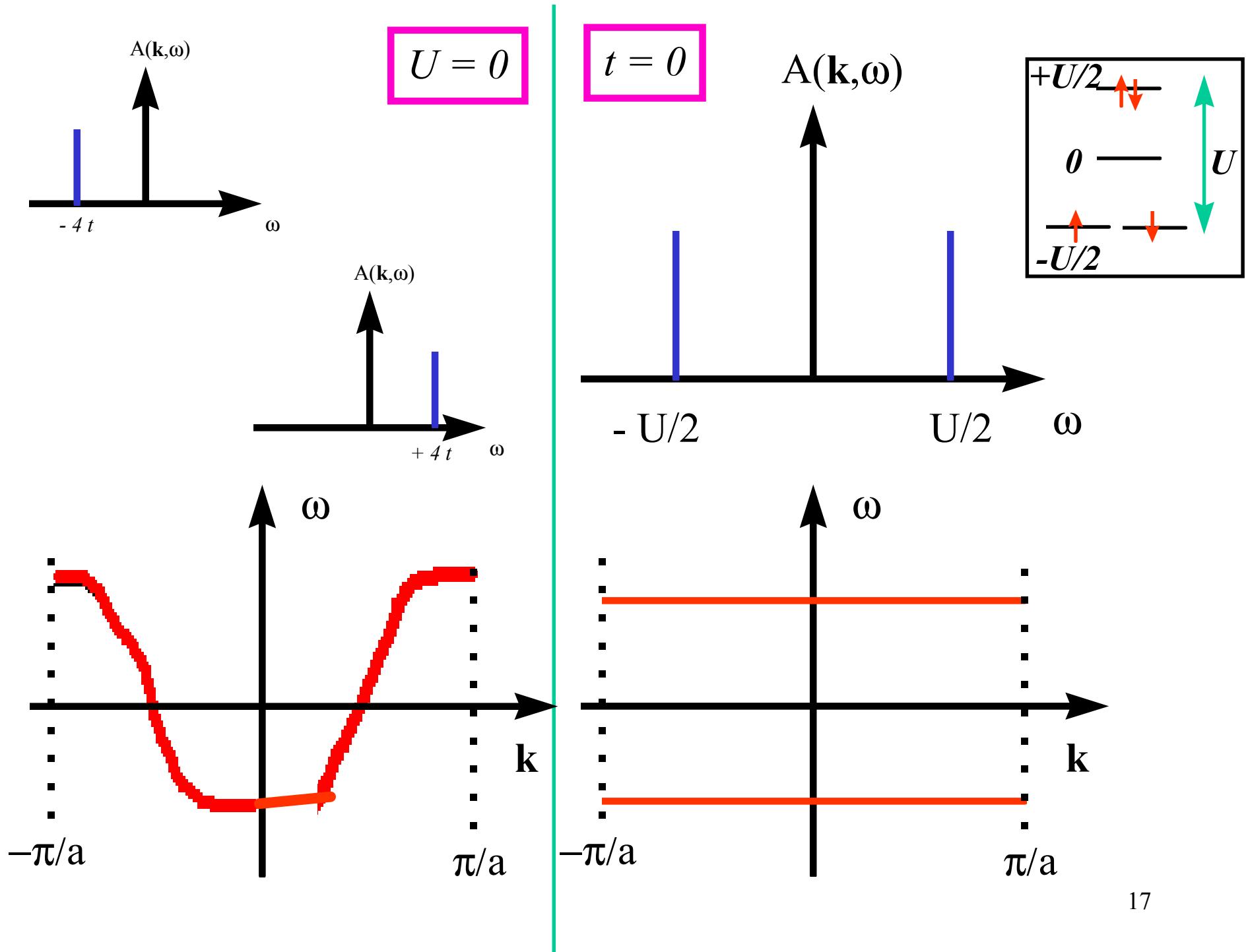
5. Hubbard model (Kanamori, Gutzwiller, 1963) :

$$H = - \sum_{\langle ij \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

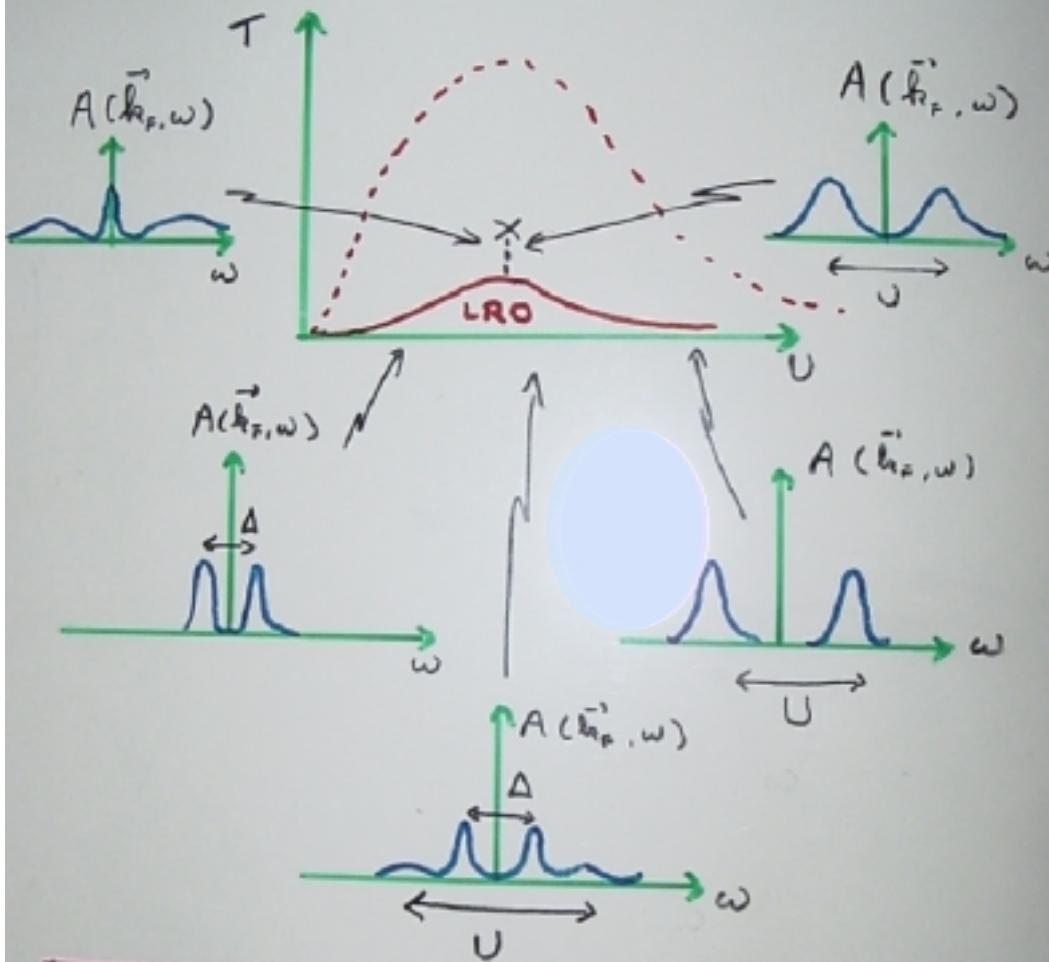
- Screened interaction U
- U, T, n
- $a = 1, t = 1, \hbar = 1$



- 2001 vs 1963: Numerical solutions to check analytical approaches



"Weak" vs "Strong" coupling ($d=\infty$)



Weak to intermediate coupling:

- Perturbation theory?
(RPA violates Pauli, to $O(U/\omega)^2$)
- Self-consistent approaches
- Are Fermi-liquid parameters calculable?

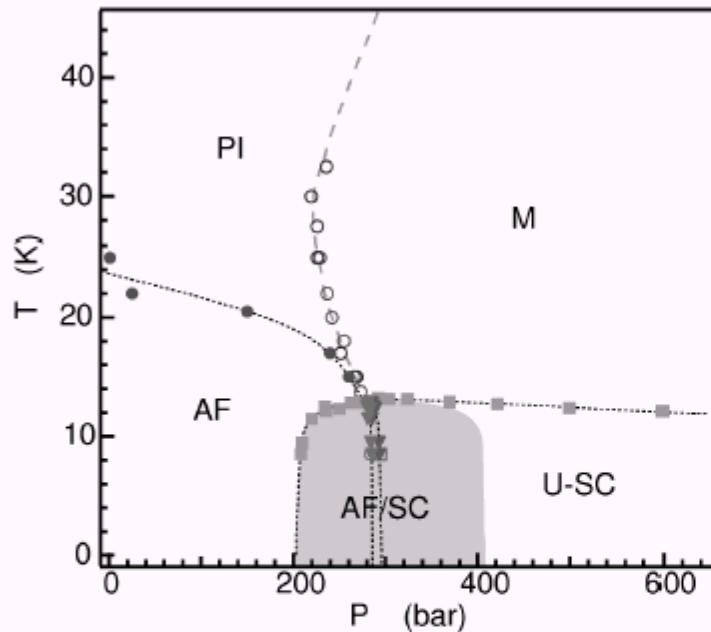


FIG. 1. Temperature vs pressure phase diagram of κ -Cl. The antiferromagnetic (AF) critical line $T_N(P)$ (dark circles) was determined from NMR relaxation rate while $T_c(P)$ for unconventional superconductivity (U-SC: squares) and the metal-insulator $T_{MI}(P)$ (MI: open circles) lines were obtained from the ac susceptibility. The AF-SC boundary (double-dashed line) is determined from the inflection point of $\chi'(P)$ and, for 8.5 K, from sublattice magnetization. This boundary line separates two regions of inhomogeneous phase coexistence (shaded area).

ture T_N is gradually suppressed under pressure with the value $dT_N/dP \approx -0.025$ K/bar for the pressure coefficient. Above 275 bar, there is no peak indicating the absence of a magnetic transition. A plateau of T_1^{-1} , however, persists up to 40 K or so, which marks a sizable enhancement due to short-range AF correlations.

An accurate determination of superconducting order in the phase diagram can be obtained from the ac susceptibility measurements as shown in Fig. 3 for selected temperature and pressure sweeps, respectively. In the high pressure domain above 400 bar, the $T_c(P)$ line below which there is a finite density of superconducting condensate slowly decreases in agreement with previous results ($dT_c/dP \approx -3.8$ K/kbar, squares in Fig. 1) [2]. As pressure is reduced below 400 bar, lower saturation levels are recorded indicating a gradual suppression of the superconducting order down to 200 bar where it vanishes; $T_c(P)$ thus crosses $T_N(P)$ and the regions of stability for SC and AF overlap.

S. Lefebvre, P. Wzietek, S. Brown,
C. Bourbonnais, D. Jérôme, C. Mézière,
M. Fourmigué, and P. Batail

For first part of this talk :

<http://www.physique.usherb.ca/~tremblay/articles/PiC.pdf>

6. A non-perturbative approach for both $U > 0$ and $U < 0$

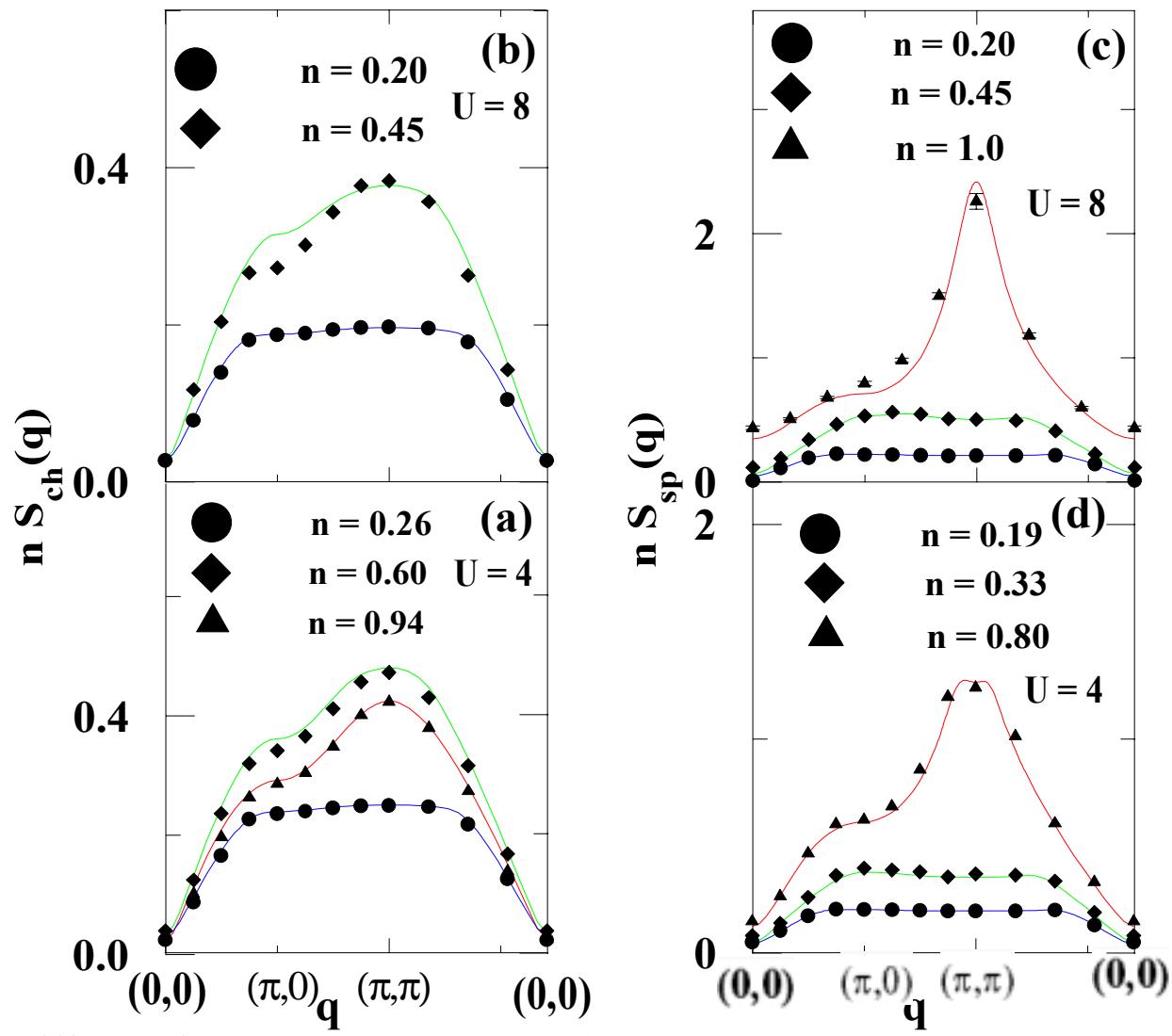
- Proofs that it works

$U > 0$

Notes:

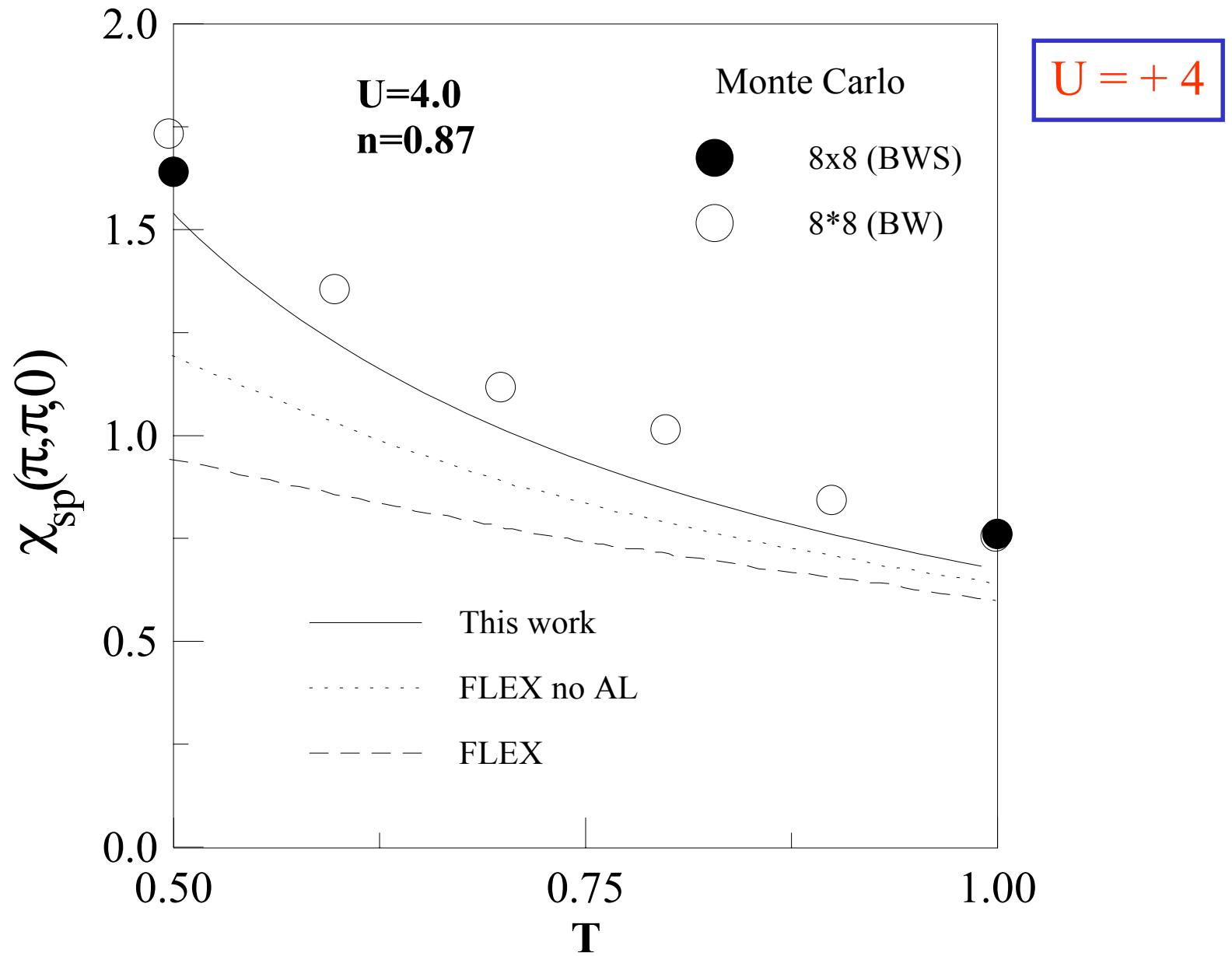
-F.L.
parameters

-Self also
Fermi-liquid



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

Proofs...

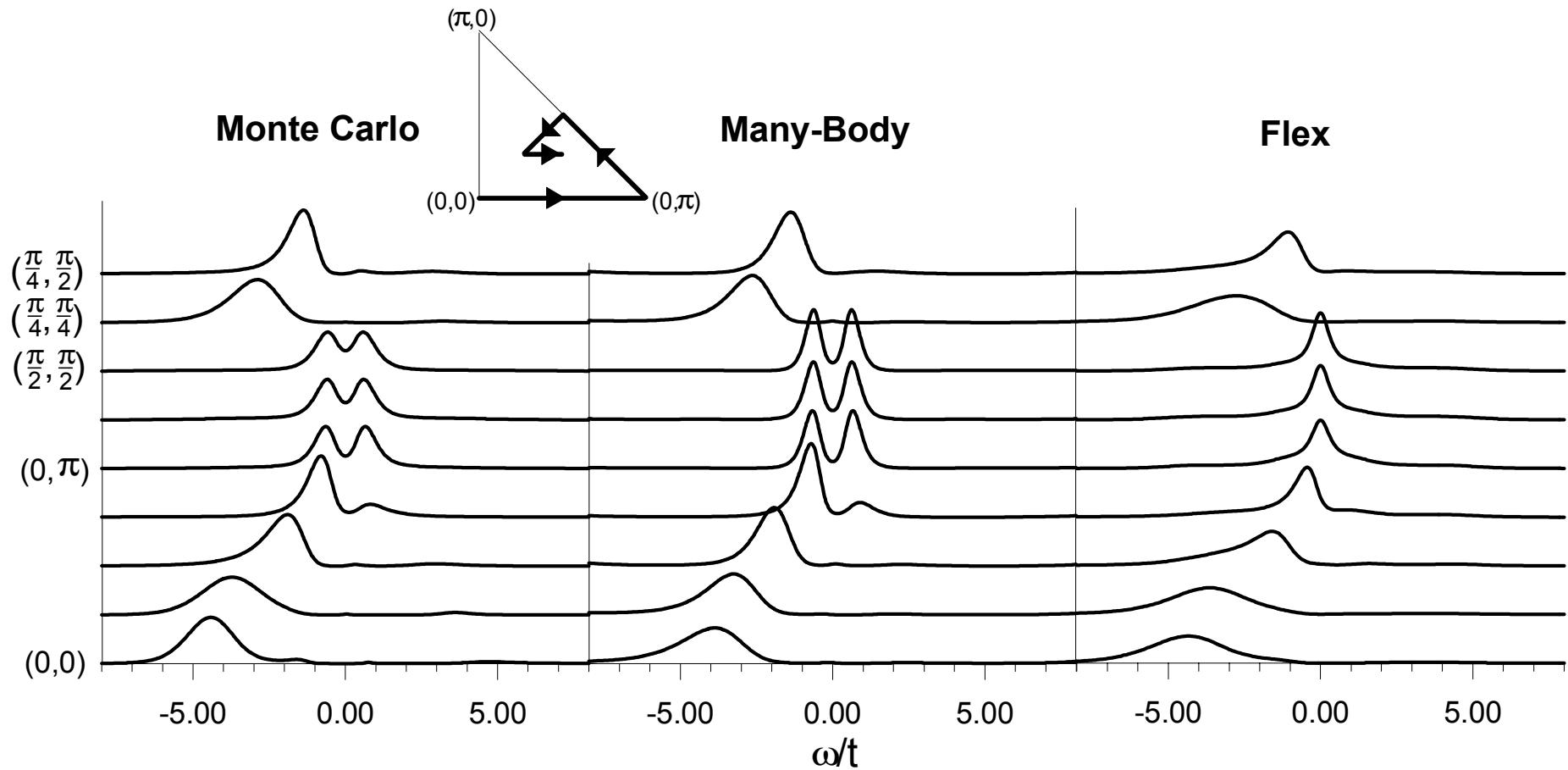


Calc.: Vilk, et al. J. Phys. I France, **7**, 1309 (1997).

QMC: Bulut, Scalapino, White, P.R. B **50**, 9623 (1994).

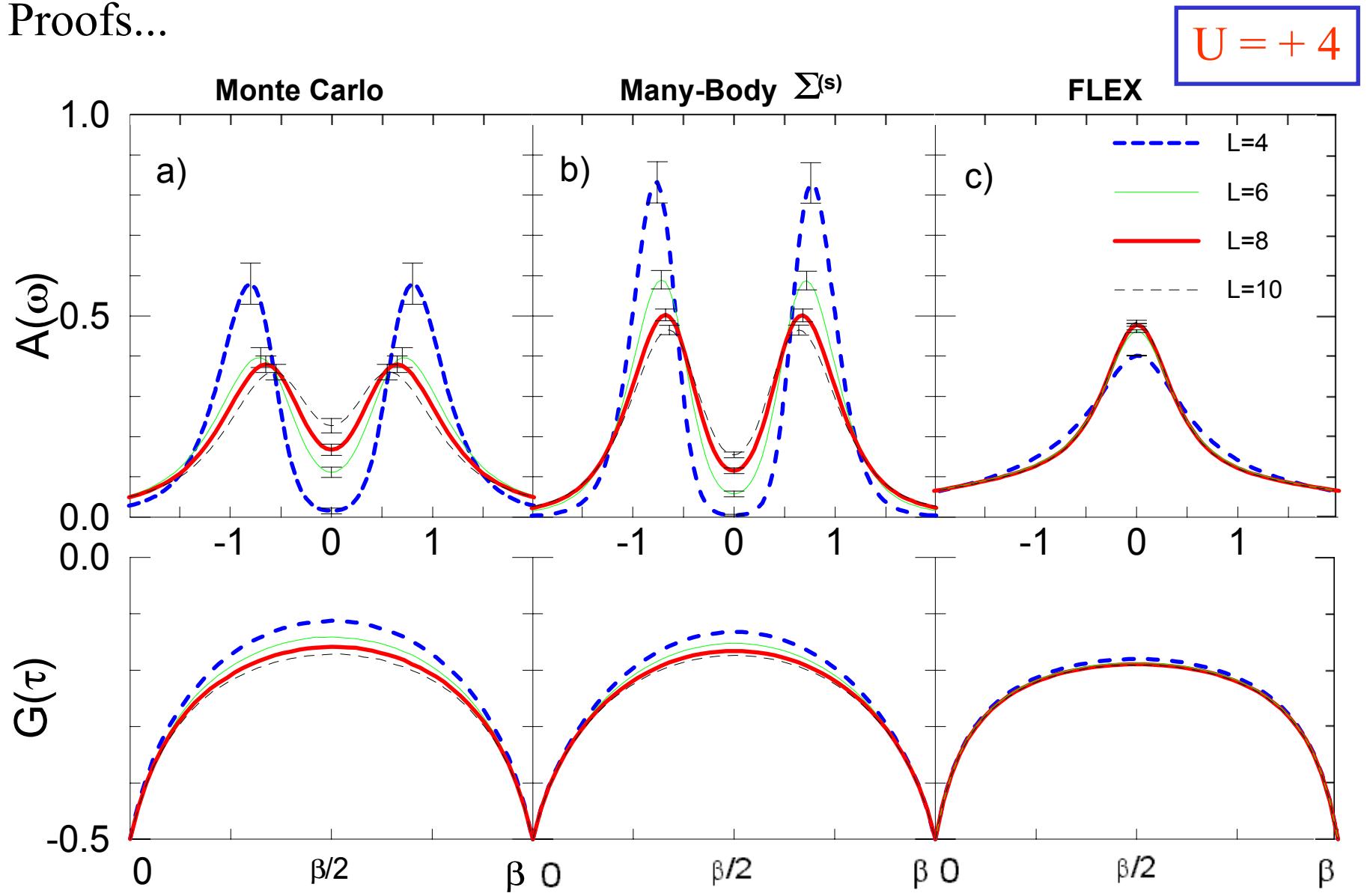
Proofs...

$U = +4$

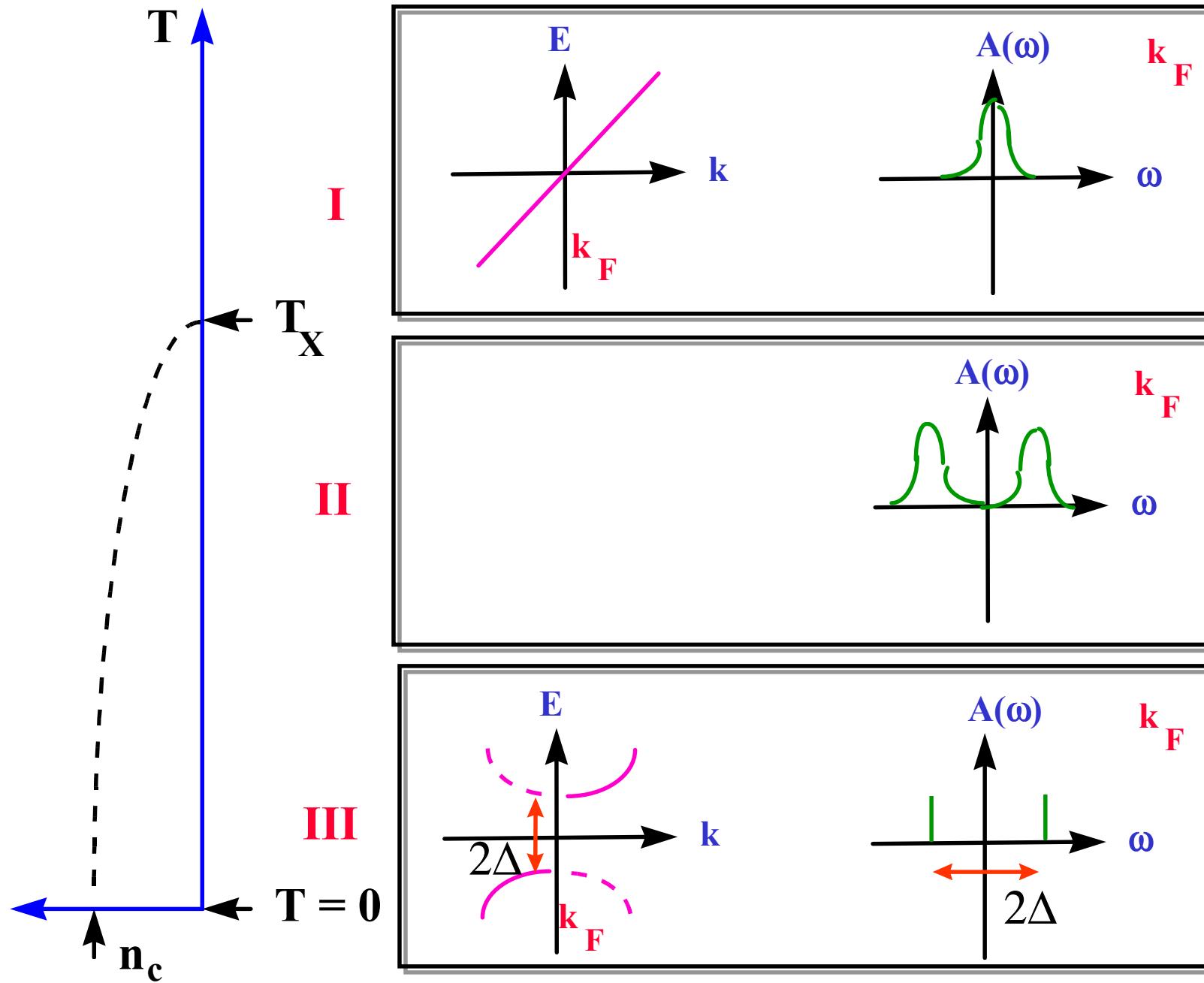


Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).

Proofs...



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



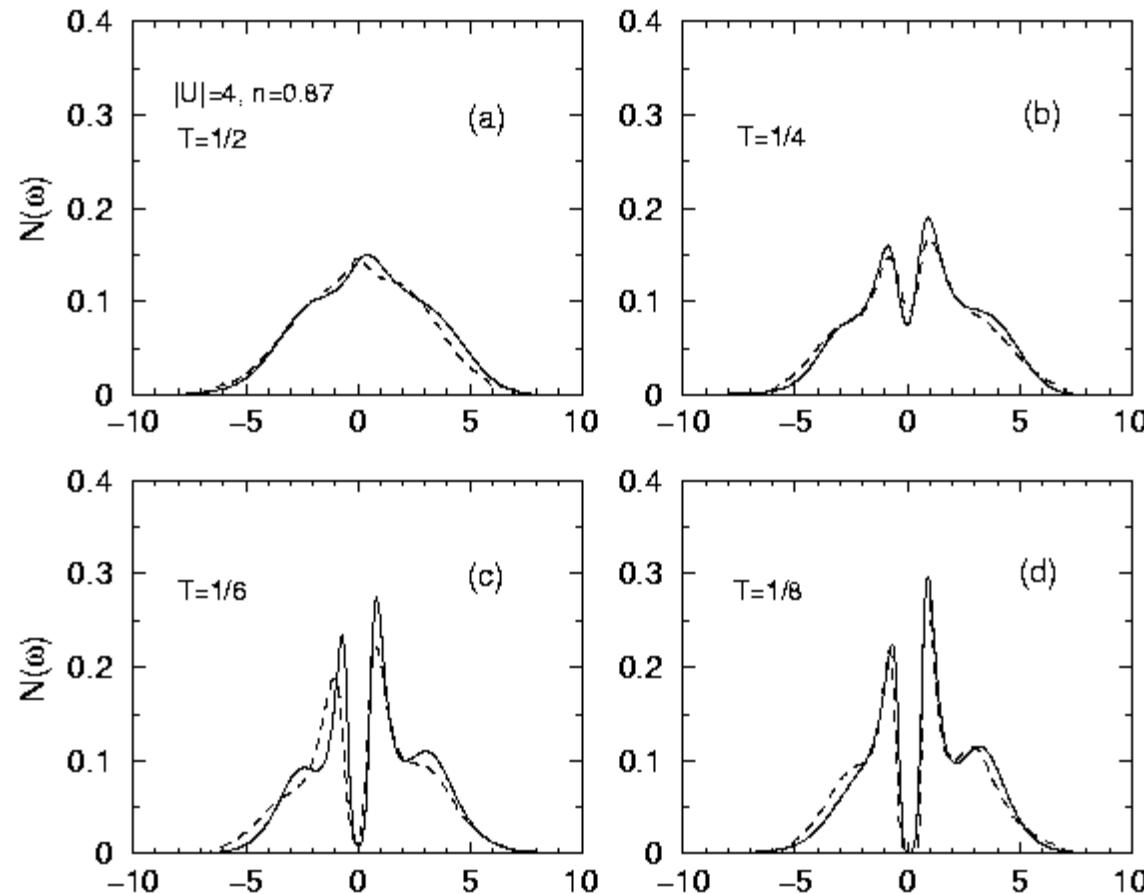
Moving to the attractive case....

U = - 4

Calc. : Kyung et al. cond-mat/0010001

QMC : Moreo, Scalapino, White, P.R. B. **45**, 7544 (1992) -----

Proofs...

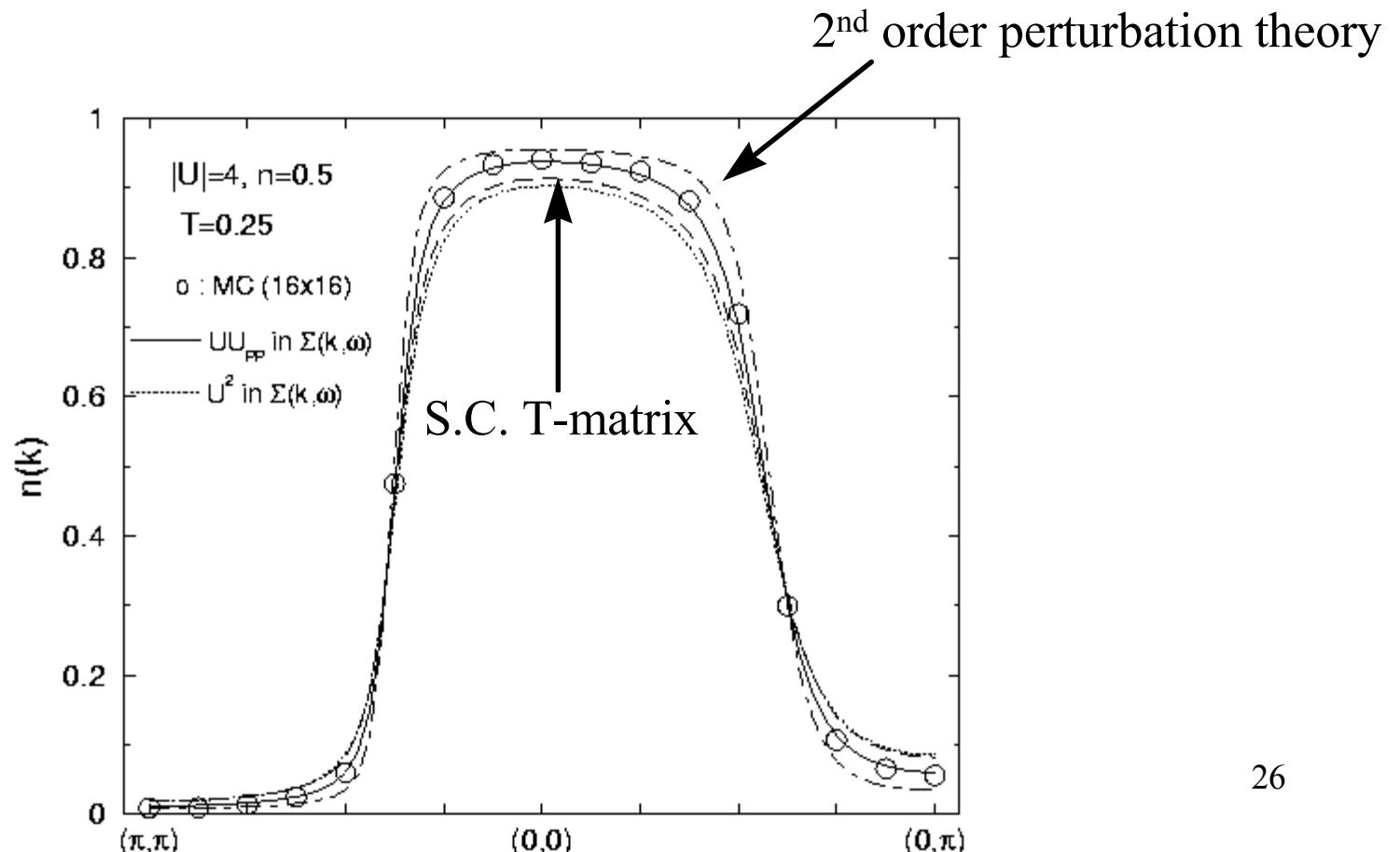


Proofs...

$$U = -4$$

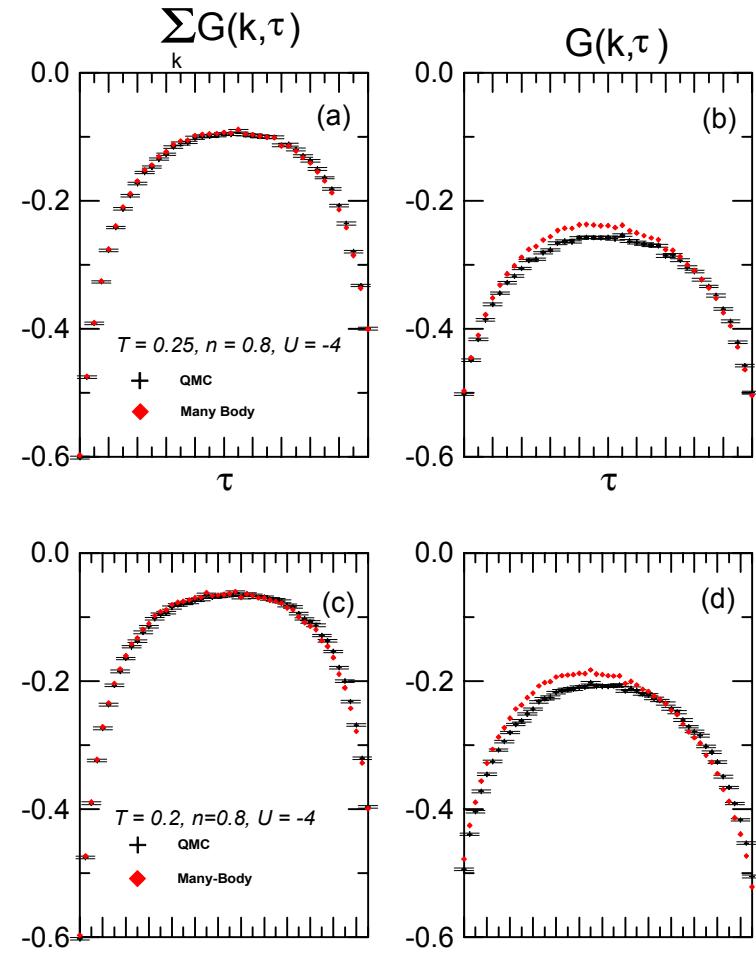
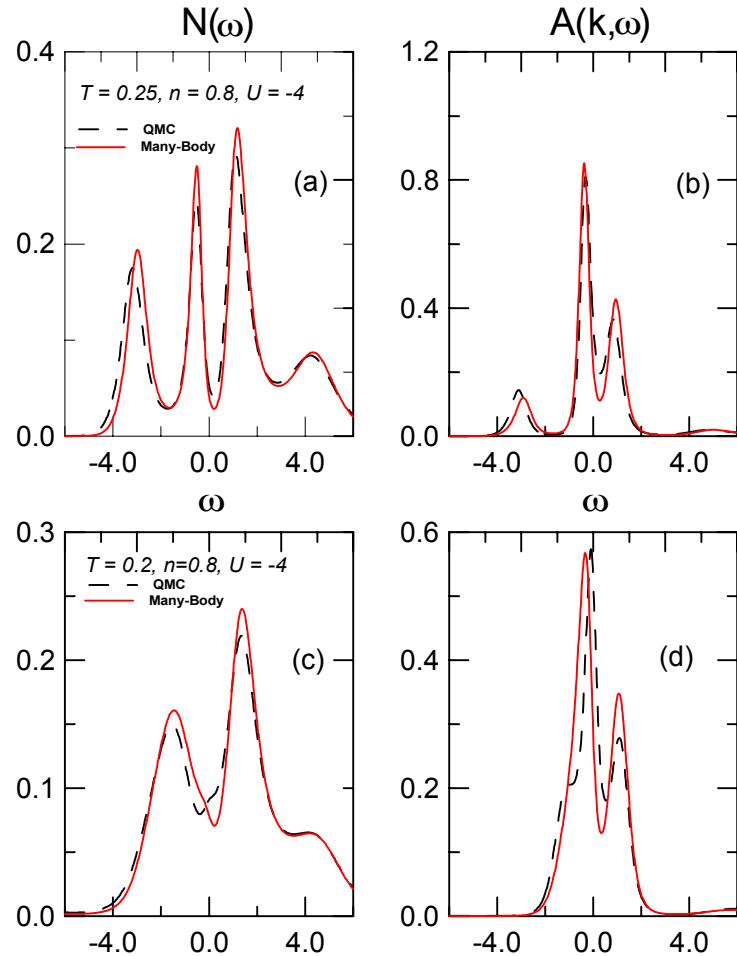
Calc. : Kyung et al. cond-mat/0010001

QMC : Trivedi and Randeria, P.R. L. 75, 312 (1995)



Proofs...

U = -4



How it works...

First step: Two-Particle Self-Consistent

$$\Sigma_{\sigma}^{(1)}(1, \bar{1}) G_{\sigma}^{(1)}(\bar{1}, 2) = A G_{-\sigma}^{(1)}(1, 1^+) G_{\sigma}^{(1)}(1, 2)$$

where A depends on external field and is chosen such that the exact result

$$\Sigma_{\sigma}(1, \bar{1}) G_{\sigma}(\bar{1}, 1^+) = U \langle n_{\uparrow} n_{\downarrow} \rangle$$

is satisfied. One finds

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

Functional derivative of $\langle n_{\uparrow} n_{\downarrow} \rangle / (\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle)$ drops out of spin vertex

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

How it works...

To close the system of equations, while satisfying conservation laws and the Pauli principle

$$\begin{aligned} \langle (n_{\uparrow} - n_{\downarrow})^2 \rangle &= \langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle - 2 \langle n_{\uparrow} n_{\downarrow} \rangle \\ \boxed{\frac{T}{N} \sum_{\tilde{q}} \frac{\chi_0(q)}{1 - \frac{1}{2} U_{sp} \chi_0(q)}} &= n - 2 \langle n_{\uparrow} n_{\downarrow} \rangle \end{aligned} \quad (1)$$

Recall

$$U_{sp} = U \frac{\langle n_{\uparrow} n_{\downarrow} \rangle}{\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle} \quad (2)$$

To have charge fluctuations that satisfy Pauli principle as well,

$$\boxed{\frac{T}{N} \sum_q \frac{\chi_0(q)}{1 + \frac{1}{2} U_{ch} \chi_0(q)}} = n + 2 \langle n_{\uparrow} n_{\downarrow} \rangle - n^2 \quad (3)$$

(Bonus: Mermin-Wagner theorem)

How it works...

Second step: improved self-energy

$$\Sigma_\sigma(1, \bar{1}) G_\sigma(\bar{1}, 2) = -U \left\langle \psi_{-\sigma}^\dagger(1^+) \psi_{-\sigma}(1) \psi_\sigma(1) \psi_\sigma^\dagger(2) \right\rangle_\phi$$

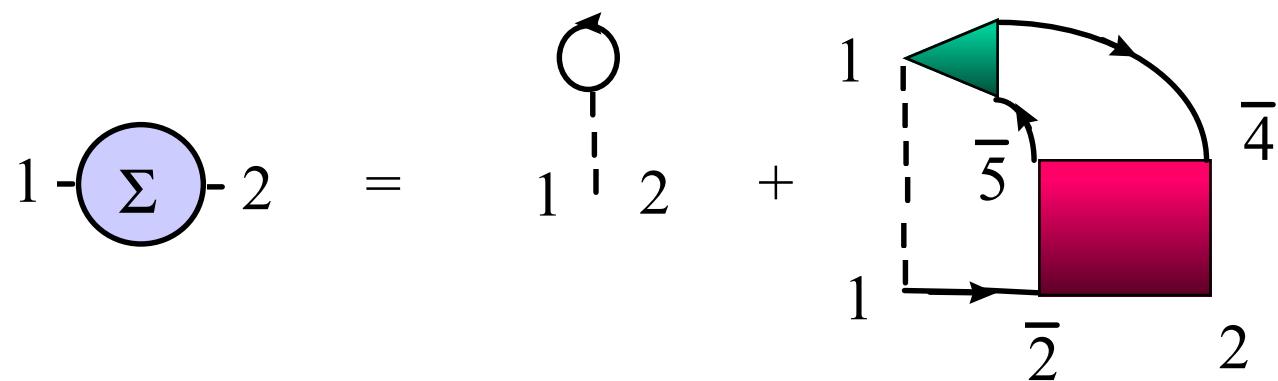
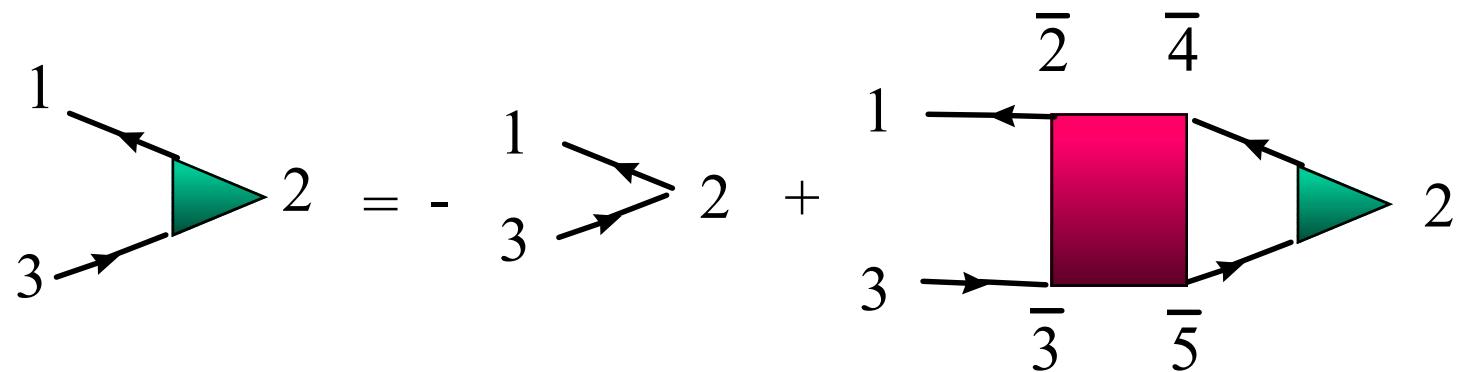
$$\Sigma_\sigma(1, \bar{1}) G_\sigma(\bar{1}, 2) = -U \left[\frac{\delta G_\sigma(1, 2)}{\delta \phi_{-\sigma}(1^+, 1)} - G_{-\sigma}(1, 1^+) G_\sigma(1, 2) \right]$$

Last term is Hartree Fock ($\lim \omega \rightarrow \infty$). Multiply by G^{-1} , replace lower energy part results of TPSC

$$\Sigma_\sigma^{(2)}(1, 2) = U G_{-\sigma}^{(1)}(1, 1^+) \delta(1 - 2) - U G^{(1)} \left[\frac{\delta \Sigma^{(1)}}{\delta G^{(1)}} \frac{\delta G^{(1)}}{\delta \phi} \right]$$

Transverse+longitudinal for crossing-symmetry

$$\Sigma_\sigma^{(2)}(k) = U n_{-\sigma} + \frac{U}{8} \frac{T}{N} \sum_q \left[3U_{sp} \chi^{(1)}(q) + U_{ch} \chi^{(1)}(q) \right] G_\sigma^{(1)}(k + q). \quad (4)$$



Results of the analogous procedure for $U < 0$

$$U_{pp} = U \frac{\langle (1 - n_\uparrow) n_\downarrow \rangle}{\langle 1 - n_\uparrow \rangle \langle n_\downarrow \rangle}. \quad (5)$$

$$\chi_p^{(1)}(q) = \frac{\chi_0^{(1)}(q)}{1 + U_{pp} \chi_0^{(1)}(q)} \quad (6)$$

$$\frac{T}{N} \sum_q \chi_p^{(1)}(q) \exp(-iqn0^-) = \langle \Delta^\dagger \Delta \rangle = \langle n_\uparrow n_\downarrow \rangle. \quad (7)$$

$$\Sigma^{(1)} \simeq \frac{U}{2} - \frac{U_{pp}(1 - n)}{2} \quad (8)$$

$$\Sigma_\sigma^{(2)}(k) = Un_{-\sigma} - U \frac{T}{N} \sum_q U_{pp} \chi_p^{(1)}(q) G_{-\sigma}^{(1)}(q - k) \quad (9)$$

Satisfies Pauli principle and generalization of f -sum rule

$$\int \frac{d\omega}{\pi} \text{Im} \chi^{(1)}(\mathbf{q}, \omega) = \langle [\Delta_{\mathbf{q}}(0), \Delta_{\mathbf{q}}^\dagger(0)] \rangle = 1 - n \quad ; \quad \forall \mathbf{q} \quad (10)$$

$$\int \frac{d\omega}{\pi} \omega \text{Im} \chi^{(1)}(\mathbf{q}, \omega) = \left[\frac{1}{N} \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} + \varepsilon_{-\mathbf{k}+\mathbf{q}}) (1 - 2 \langle n_{\mathbf{k}\uparrow} \rangle) \right] \quad (11)$$

$$-2 \left(\mu^{(1)} - \frac{U}{2} \right) (1 - n) \quad ; \quad \forall \mathbf{q} \quad (12)$$

Internal accuracy check (For both $U > 0$ and $U < 0$).

$$\frac{1}{2} \text{Tr} [\Sigma^{(2)} G^{(1)}] = \lim_{\tau \rightarrow 0^-} \frac{T}{N} \sum_k \Sigma_\sigma^{(2)}(k) G_\sigma^{(1)}(k) e^{-ik_n \tau} = U \langle n_\uparrow n_\downarrow \rangle$$

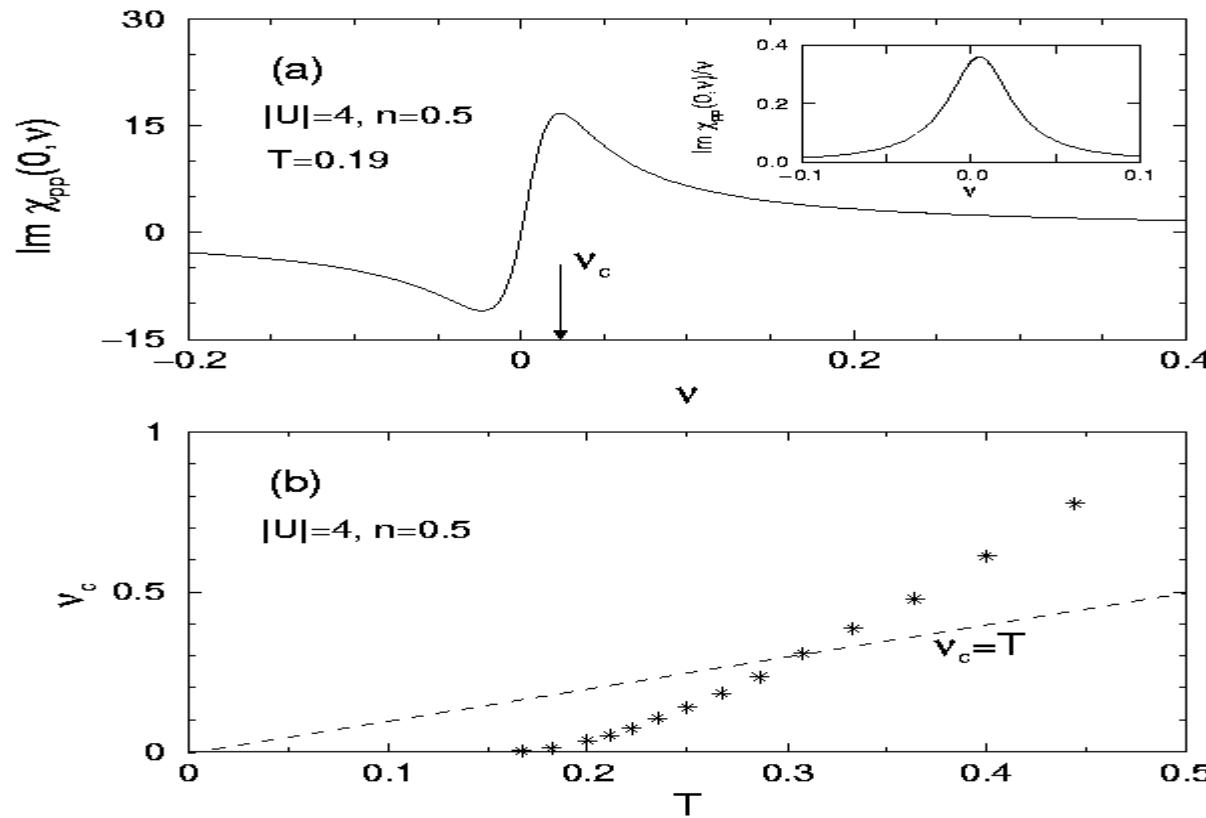
Check : $\text{Tr} [\Sigma^{(2)} G^{(1)}] \sim \text{Tr} [\Sigma^{(2)} G^{(2)}]$

7. Results:

- Mechanism for pseudogap

U = - 4

- (analogous to $U > 0$) : Vilk *et al.* Europhys. Lett. 33, 159 (1996)
Pines, Schmalian (98)
- Enter the renormalized-classical regime. N.B. $d = 2$

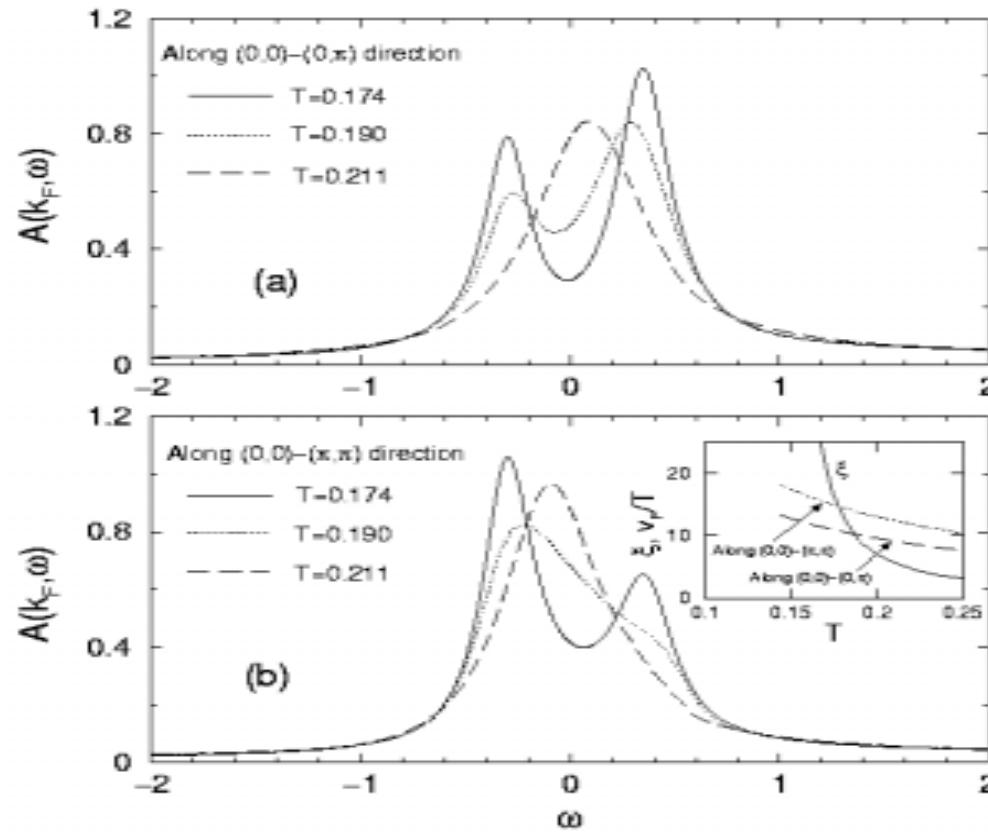


7. Results:

- Mechanism for pseudogap

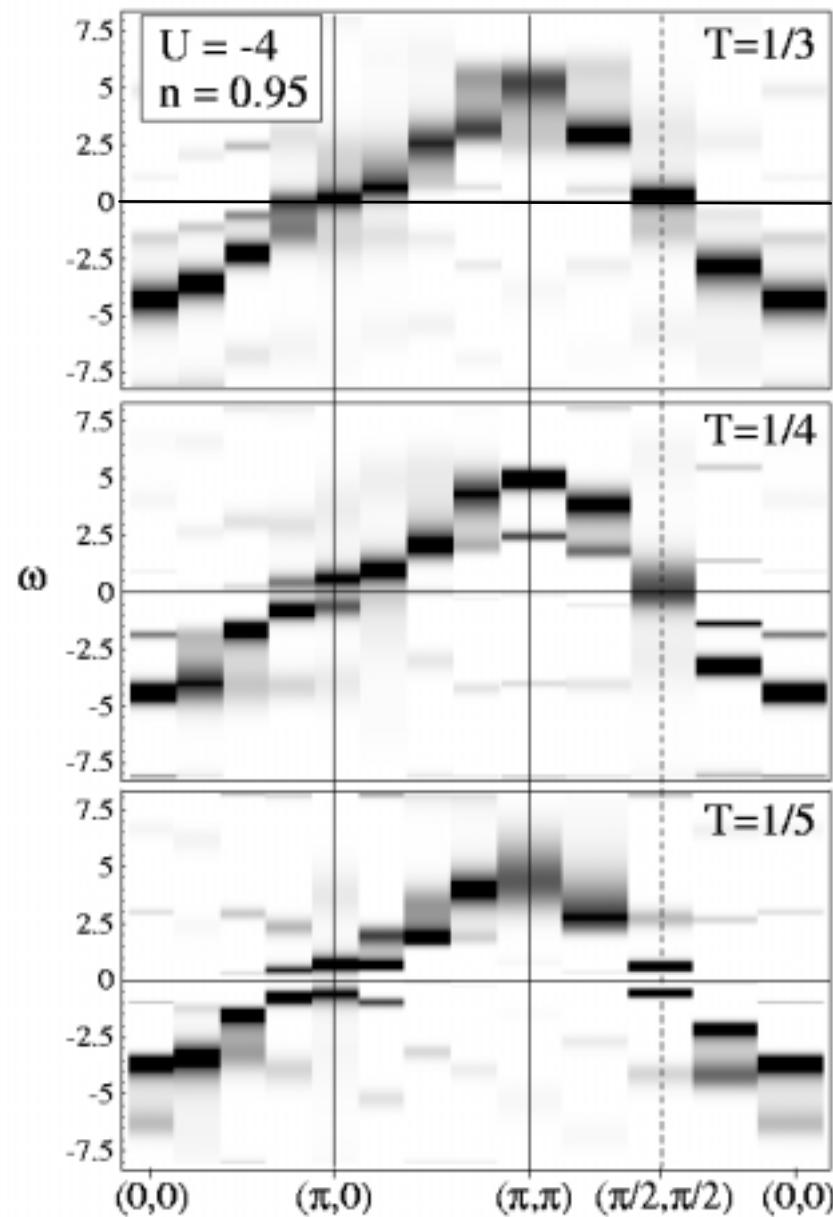
U = - 4

- Pairing correlation length larger than single-particle thermal de Broglie wavelength (v_F / T)



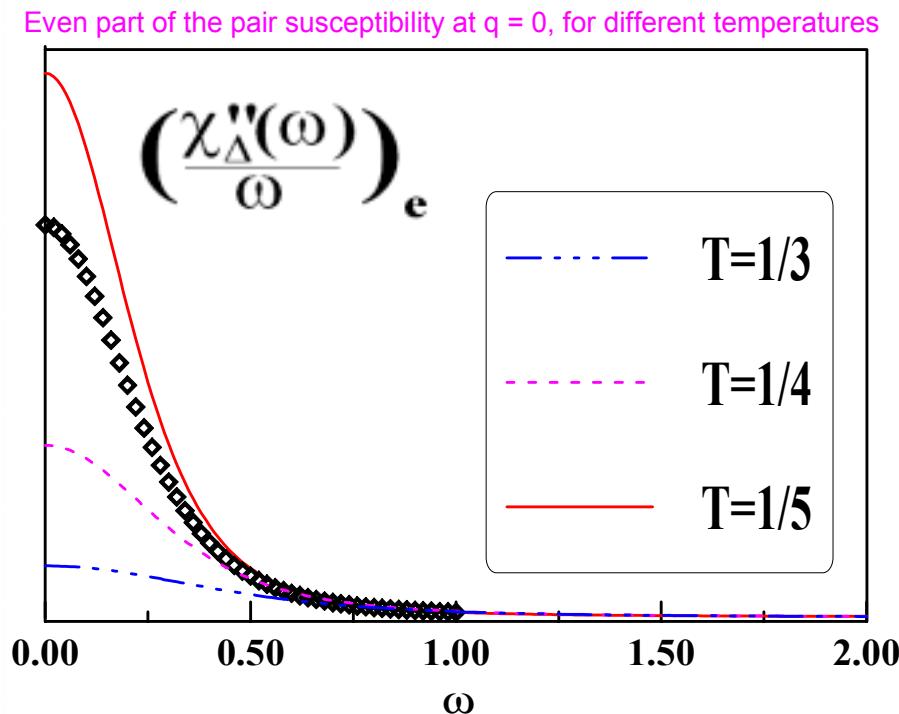
$$\xi \sim 1.3 \xi_{th}$$

Mechanism for pseudogap formation in the attractive model:



$U = -4$

$d = 2$ is crucial



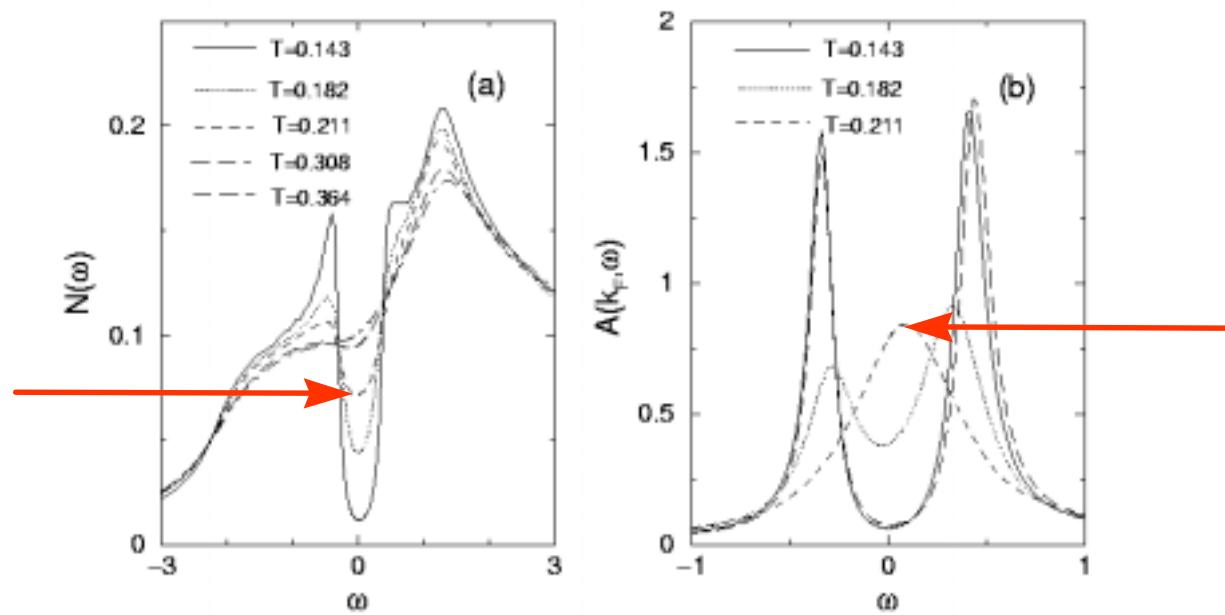
Allen, et al. P.R. L 83, 4128 (1999)
36

7. Results:

- Spectral weight rearrangement

$$U = -4$$

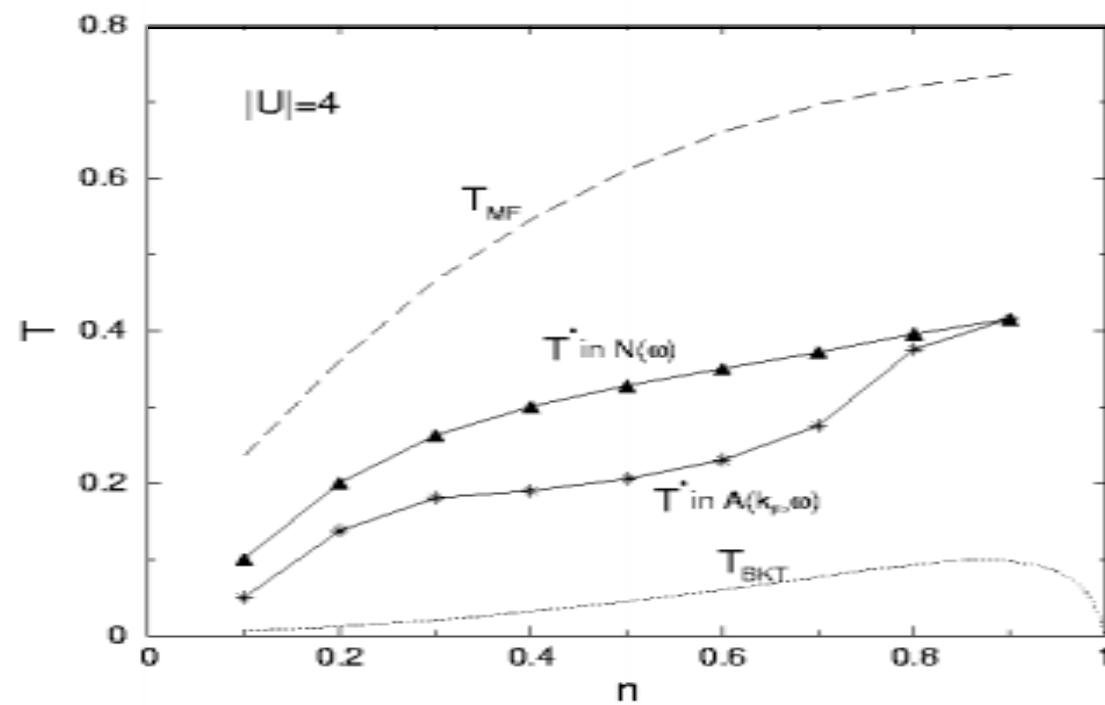
- Pseudogap appears first in total density of states
- Fills in instead of opening up
- Rearrangement over huge frequency scale compared with either T or ΔT . ($\Delta T \sim 0.03$, $T \sim 0.2$, $\Delta\omega \sim 1$)



7. Results:

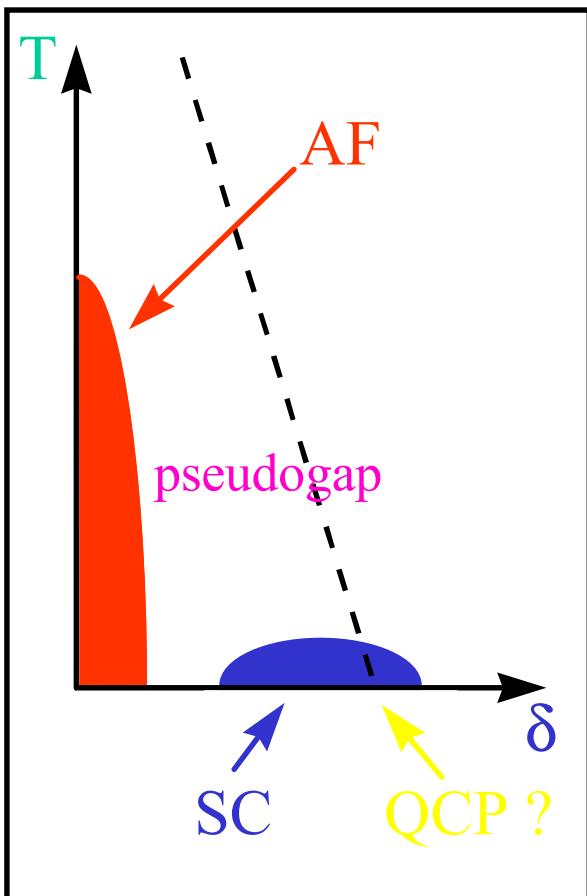
- Crossover diagram

$U = -4$

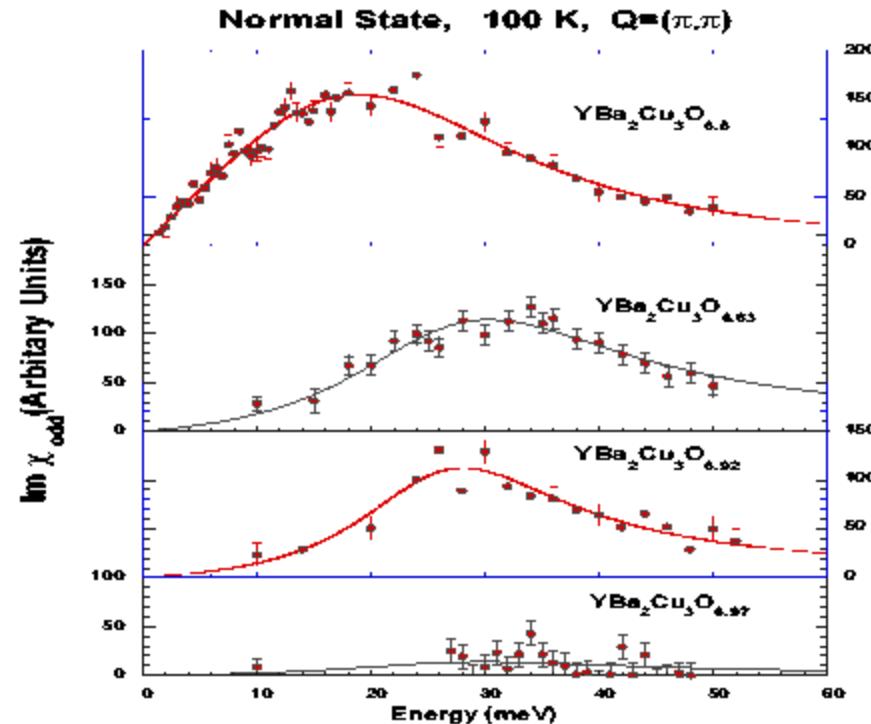


8. Conclusion :

$$U > 0$$



- Evidence against renormalized classical regime for spin fluctuations in pseudogap regime.

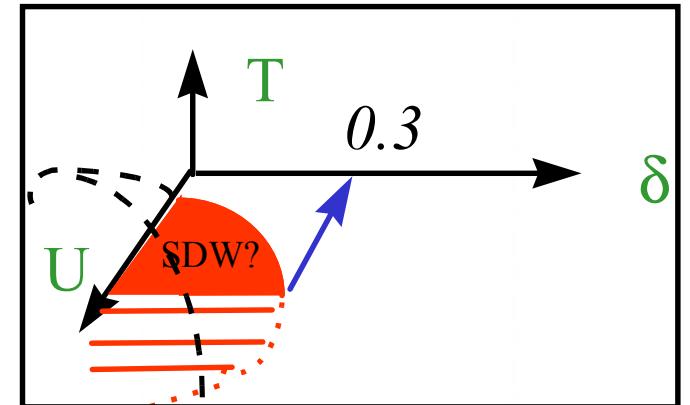


$U > 0$

- Quantum critical point, $d = 2$:

- Instability at incommensurate q
- Largest doping : 0.315

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

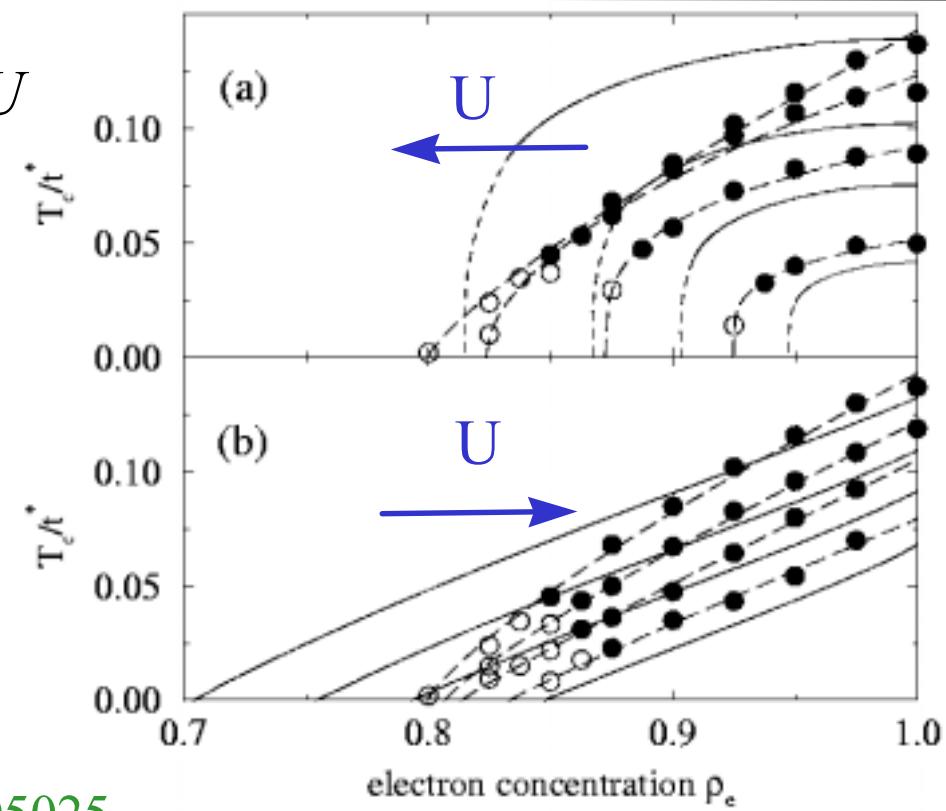


- Decreases with increasing U

$$U < W$$

$d = \text{infinity}$

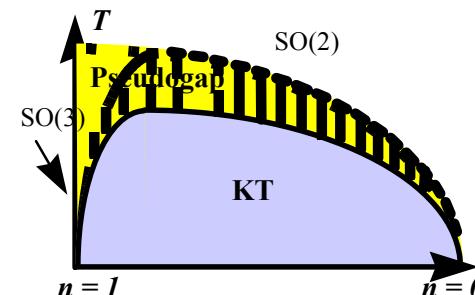
$$U > W$$



U < 0

Pairing-fluctuation induced pseudogap

- Slightly Overdoped High-Tc Superconductor $TlSr_2CaCu_2O_{6.8}$
Guo-qing Zheng *et al.*, P. R. L. **85**, 405 (2000)
 - Pseudogap in Knight shift and NMR relaxation strongly H dependent, contrary to underdoped (up to 23 T).
- Underdoped in a range $\Delta T \sim 15 K$ near T_c see evidence for renormalized classical regime (KT behavior).
Corson *et al.* Nature, **398**, 221 (1999).
- Higher symmetry group creates large range of T where there is a pseudogap.
Allen et al. P.R.L. **83**, 4128 (1999)



- How can we understand electronic systems that show both localized and extended character?
- Why do both organic and high-temperature superconductors show broken-symmetry states where mean-field-like quasiparticles seem to reappear?
- Why is the condensate fraction in this case smaller than what would be expected from the shape of the would-be Fermi surface in the normal state?
- Are there new elementary excitations that could summarize and explain in a simple way the anomalous properties of these systems?
- Do quantum critical points play an important role in the Physics of these systems?
- Are there new types of broken symmetries?
- How do we build a theoretical approach that can include both strong-coupling and $d = 2$ fluctuation effects?
- What is the origin of d-wave superconductivity in the high-temperature superconductors?