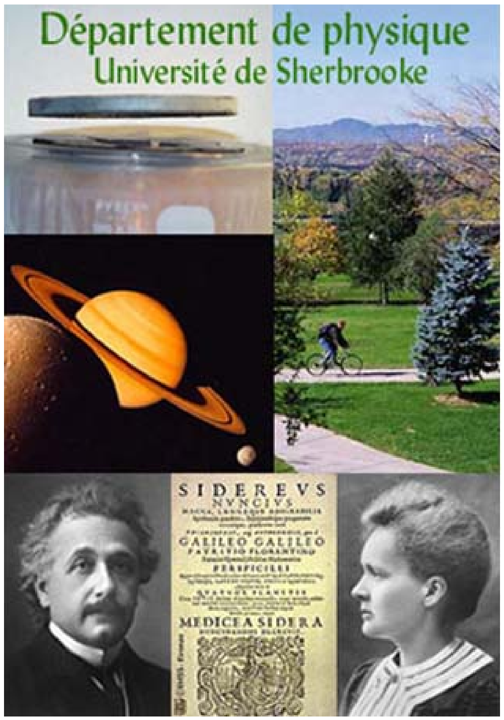

André-Marie Tremblay

CANADA RESEARCH CHAIRS
CHAIRES DE RECHERCHE DU CANADA

CENTRE DE RECHERCHE SUR LES PROPRIÉTÉS ÉLECTRONIQUES
DE MATÉRIAUX AVANCÉS

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INSTITUT DES MATÉRIAUX ET SYSTÈMES INTELLIGENTS
INTELLIGENT MATERIALS AND SYSTEMS INSTITUTE

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What is special about «*U* » in two dimensions.

What is new with U ?

What is wrong with U?

Outline

I- Motivation

- LDA + U, what to do with U.

II- Spin and charge fluctuations

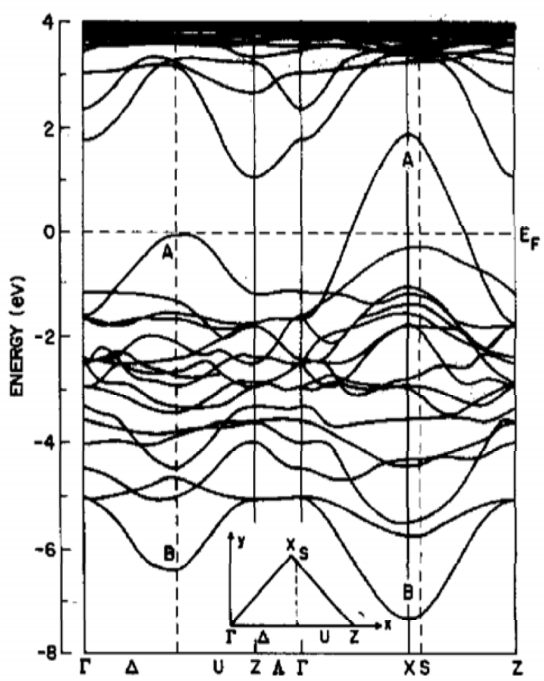
III- Self-energy effects

IV- Extensions

V- Conclusion

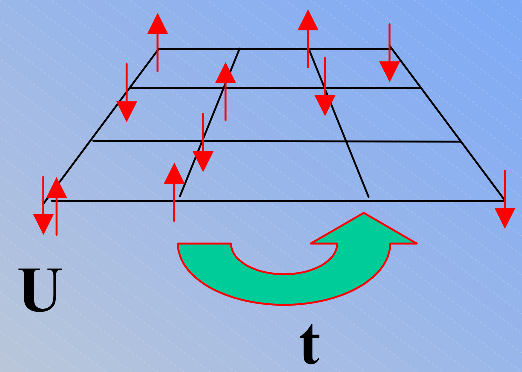
I- Motivation :
d-band materials, LDA + U

- Work in context of a « Hubbard » model.



- Screened interaction *U*
- *U, T, n (or δ=1-n)*
a = 1, t = 1

-Relevant parameter : *U/W*,
-*W = bandwidth.*



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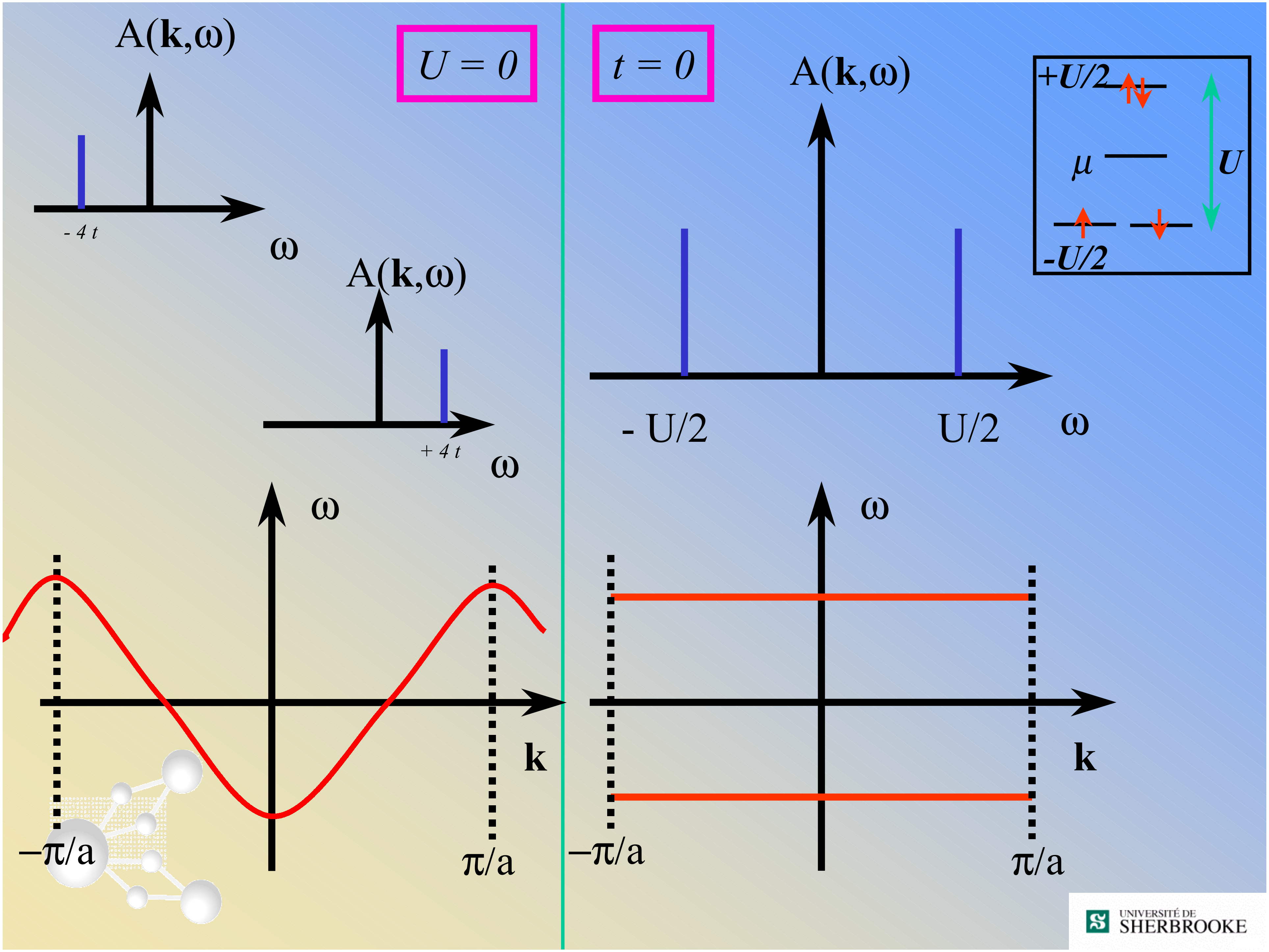
I-Motivation :
Lessons from DMFT, exact in d = infinity

- $U < W$, and $T < T_{coh}$ we have a « Fermi liquid ».
- $U > W$ we have a correlation driven (Mott) insulator (if frustration).
- There is a first-order phase transition between both phases.


U = 0
t = 0
A(k,ω)
- 4 t
ω
A(k,ω)
+ 4 t
ω
ω
k
–π/a
π/a
A(k,ω)
- U/2
U/2
ω
+U/2
μ
U
-U/2
ω
k
–π/a
π/a
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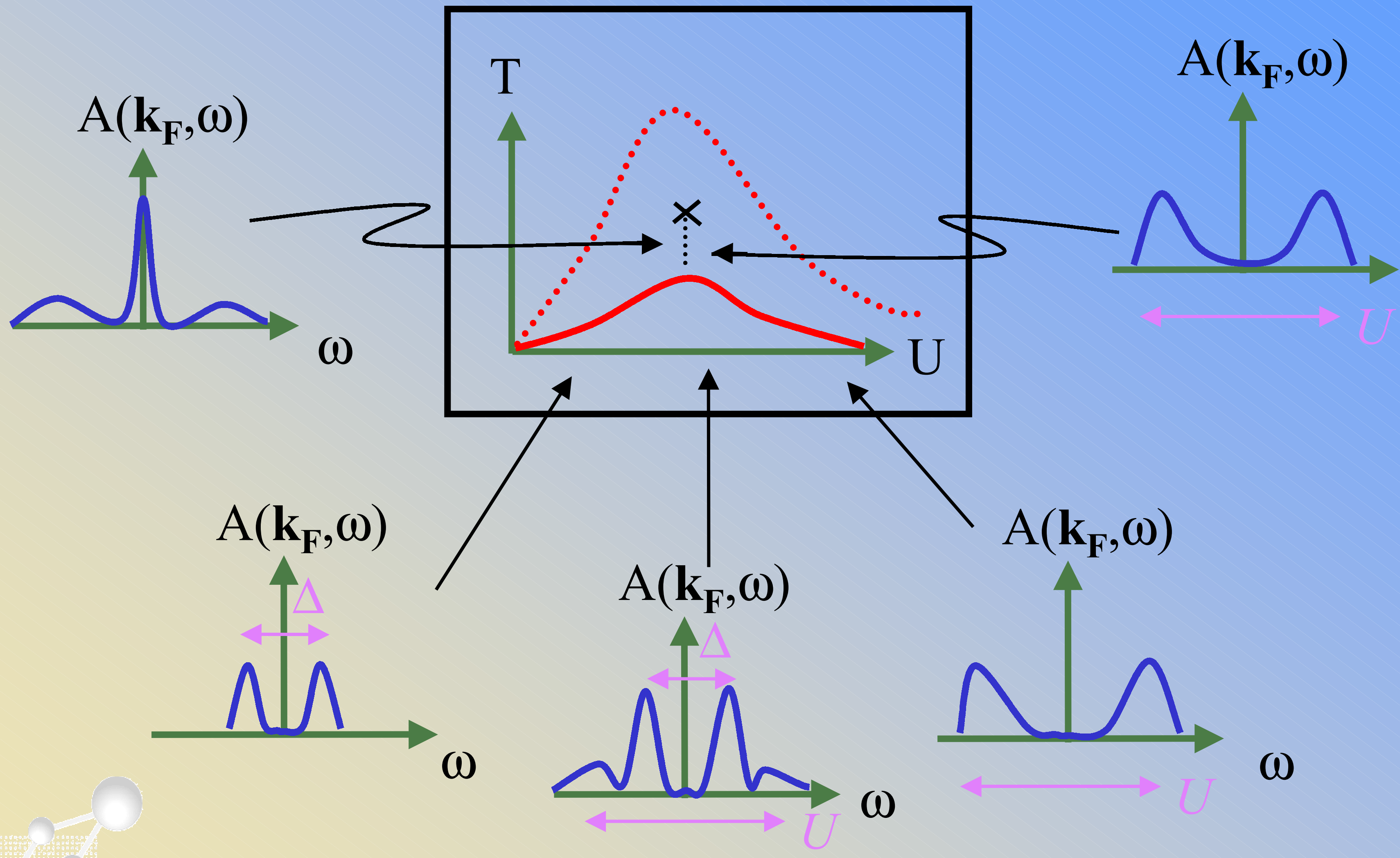
Weak vs *strong* coupling

Mott transition



I-Motivation: « Realistic theories ».
What is the effect of low dimension (of lattice)?

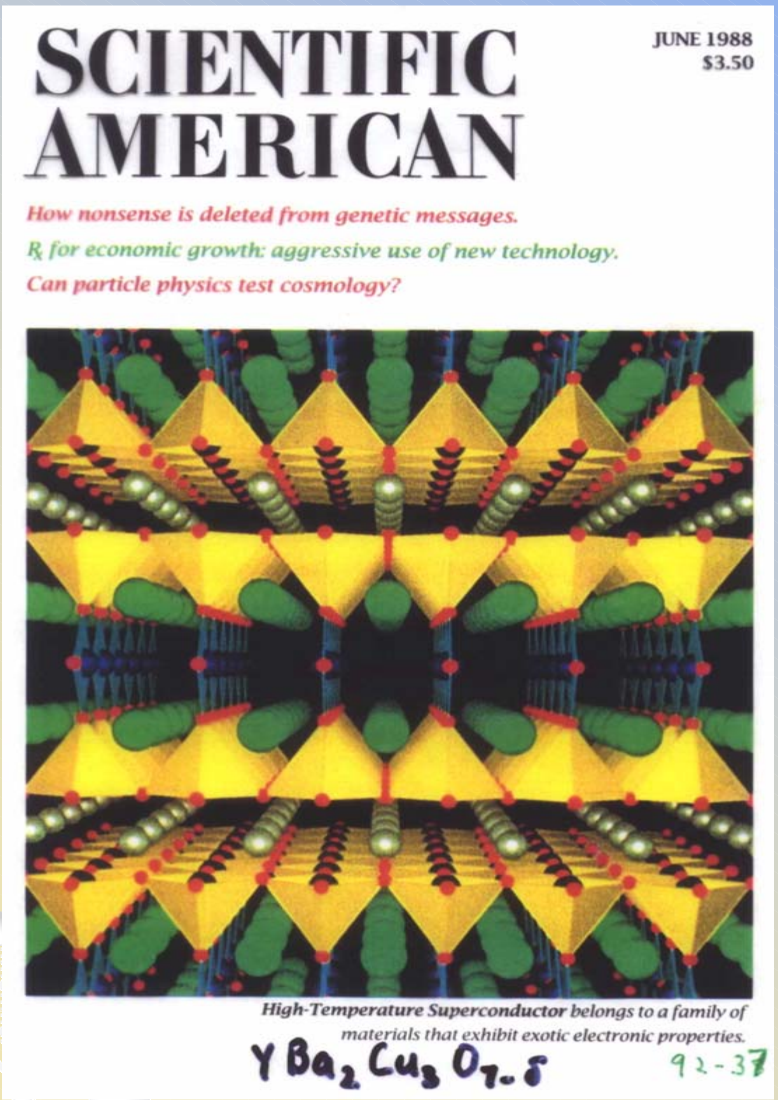
- On Fermi-liquid properties ?
- On Phase transitions ?

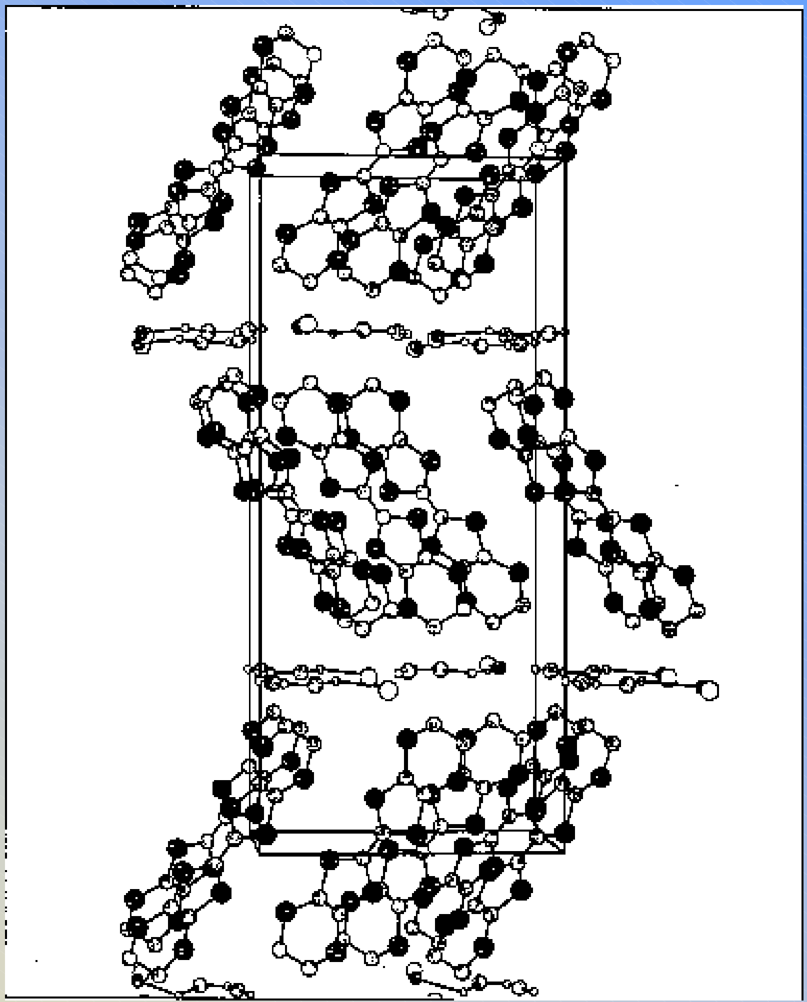
•Answer in $d = 1$: Enormous

–No symmetry breaking.

–No Fermi liquid (Luttinger liquid): spin-charge separation. …

I-Motivation:
Realistic theories in $d = 2$.





κ–$(BEDT)_2X$

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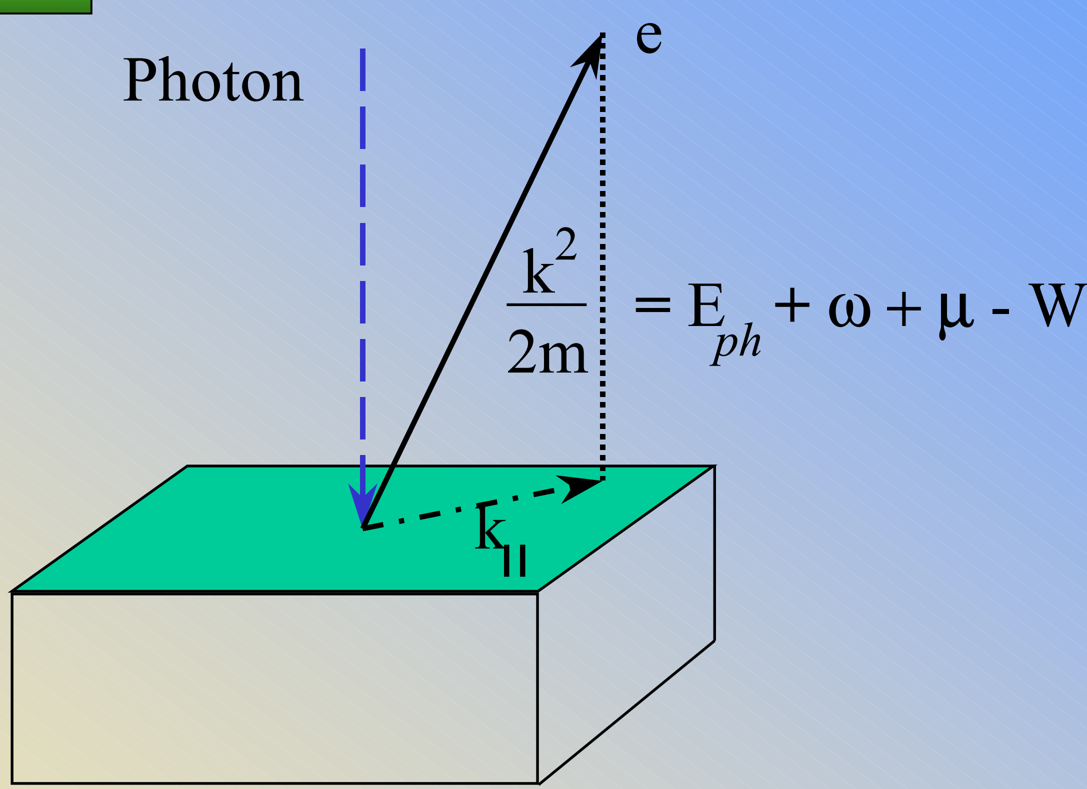
Measuring « band » properties

Photoemission



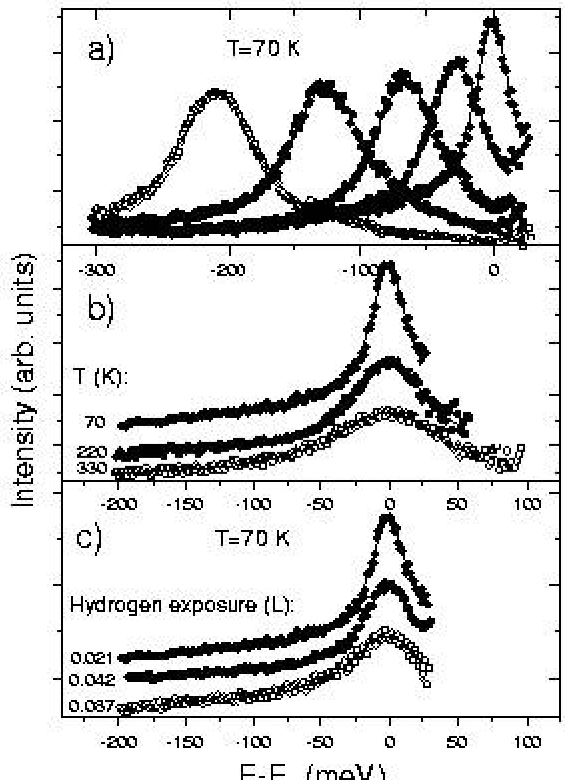


FIG. 2. Spectral intensity as a function of binding energy for constant emission angle, normalized to the experimentally determined Fermi cut-off. Data are symbols, while lines are fits to the Lorentzian peaks with a linear background. The dependence on the binding energy (a), temperature (b), and hydrogen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

taintics from the fits to peaks such as those shown in Fig. 2(a). The peak width shows a minimum at $\omega = 0$, a

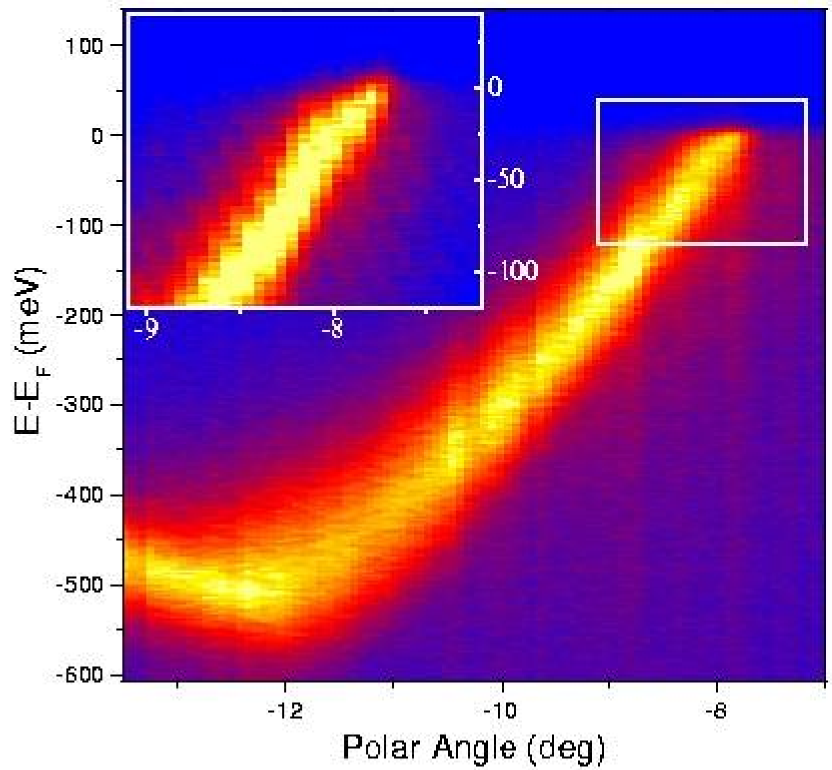


FIG. 1. ARPES intensity plot of the Mo(110) surfac recorded along the $\bar{\Gamma} - \bar{\mathrm{N}}$ line of the SBZ at 70 K Shown i the inset is the spectrum of the region around k_F taken wit special attention to the surface cleanliness.

Valla *et al*. P.R.L. **83**, 2085 (1999)

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Electron doped HTSC:

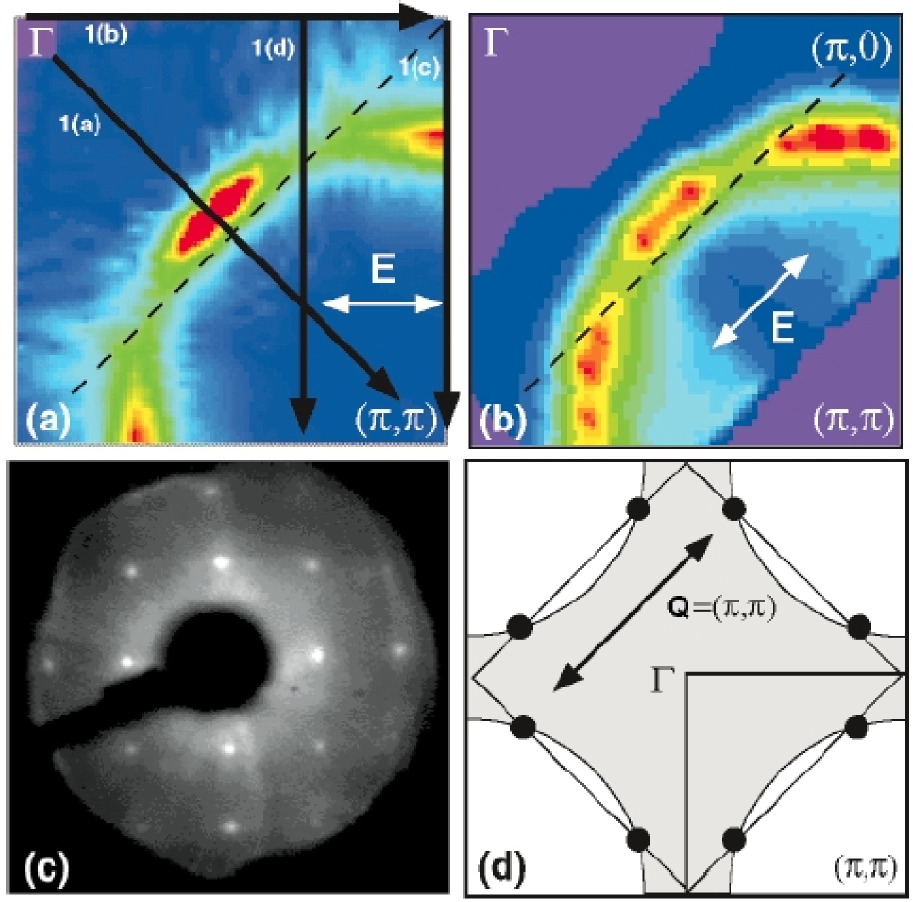

FIG. 2 (color). (a),(b) Fermi surface of the partial Brillouin zone of NCCO taken with $\hbar\omega = 16.5$ and 55 eV, respectively. The plotted quantity is a 30 meV integration about E_F of each EDC plotted as a function of $\vec{k}$. 16.5 eV data were taken over a Brillouin zone octant and symmetrized across the Γ to the (π, π) line, while the 55 eV data were taken over a full quadrant [6]. The polarization direction is denoted by the double ended arrow. The dotted line is the antiferromagnetic Brillouin zone boundary. (c) LEED spectra of NCCO cleaved *in situ* at 10 K. (d) Schematic showing only those regions of FS near the black circles can be coupled with a (π, π) scattering.

Armitage et al.
Phys. Rev. Lett.
87, 147003 (2001)

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I-Motivation:
Do we have accurate methods for $U < W$ and $d = 2$?

T-$TiTe_2$

$U / W = 0.8$

Perfetti, Grioni et al. Phys. Rev. B **64**, 115102 (2001)

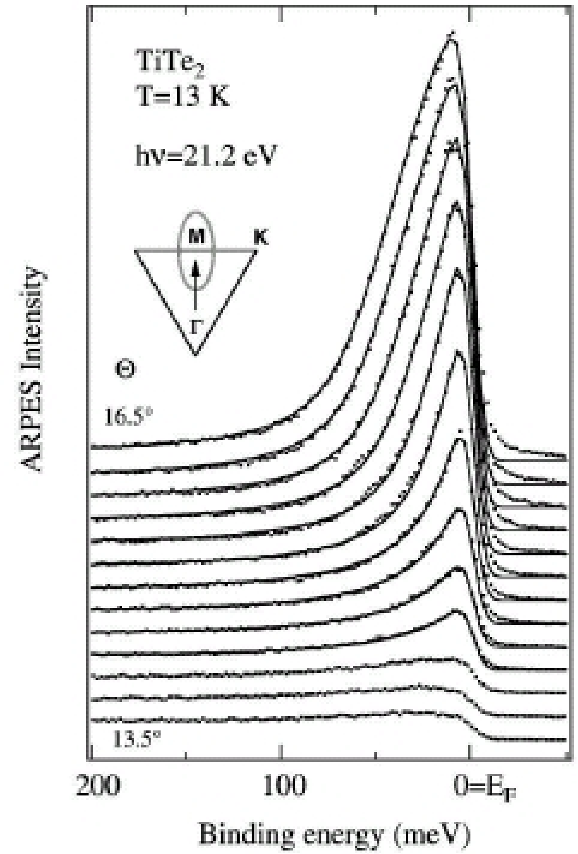

FIG. 1. High-resolution ARPES spectra of 1T-$TiTe_2$ measured near the Fermi surface crossing along the high-symmetry ΓM direction ($\theta = 0$ is normal emission). The lines are the results of Fermi liquid fits to the data with the parameters discussed in the text. The inset shows a portion of the Brillouin zone with the relevant ellipsoidal electron pocket.

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I-Motivation :
« Standard » methods for $U < W$ fail or are inaccurate.

- RPA + paramagnons

  (= GW for screened interaction *U*)
  - Predicts phase transitions that are prohibited by the Hohenberg-Mermin-Wagner-Coleman theorem (No continuous symmetry breaking in $d = 2$)
  - Does not satisfy the Pauli principle.

- « Conserving » approximations (Renormalized perturbation theory)
  - OK with Mermin-Wagner
  - Do not satisfy Pauli principle
  - Fail to reproduce the Physics to be described here.

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I-Motivation :
All is not so bad: Methods that work, but...

- Exact diagonalizations
  - Really small systems. Good for some ground-state properties, indications of broken symmetry.
  - Cluster perturbation theory. Sénéchal, cond-mat/0205044
- Finite *T*, Series expansion (Static quantities)
- Determinant quantum Monte Carlo
  - 16 x 16 is about maximum size.
  - « Negative sign problem » prevents simulations at very low temperature in interesting doping ranges.

I-Motivation: The point of view taken here, our goal

- QMC (BSSH algorithm) = « the truth »

•Develop « analytical approach » that agrees with QMC, wherever available, then

–Extend to regions inaccessible to QMC.

–Understand the physics

–Study more « realistic » models.

I-Motivation:
Extensions of DMFT in lower *d* are beginning

- « Quasi-one-d systems »
  - Biermann, Georges, Lichtenstein, Giamarchi, Phys. Rev. Lett, **87**, 276405 (2001).
- *d = 2* systems
  - C- DMFT (Kotliar *et al.*)
  - DCA (Jarrel *et al.*)

I-Motivation:
A new result from DCA in *d=2*

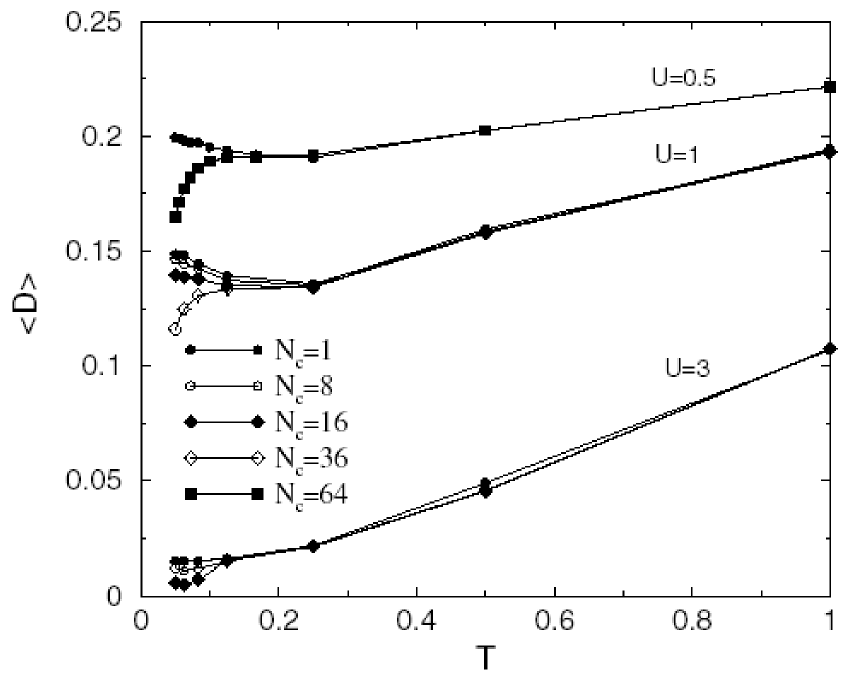

FIG. 1. The double occupancy D for $U = 0.5$, $U = 1$, and $U = 3$ for various N_c.

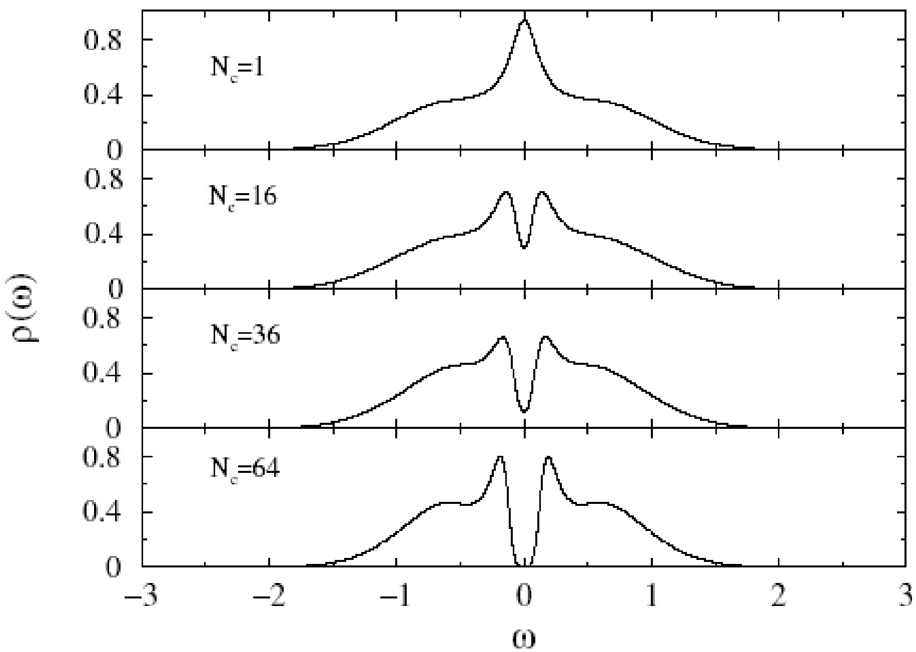

FIG. 2. The DOS $\rho(\omega)$ at $\beta = 32$ and $U = 1$.

Paramagnetic solution

S. Moukouri and M. Jarrell, Phys. Rev. Lett. 87, 167010 (2001).

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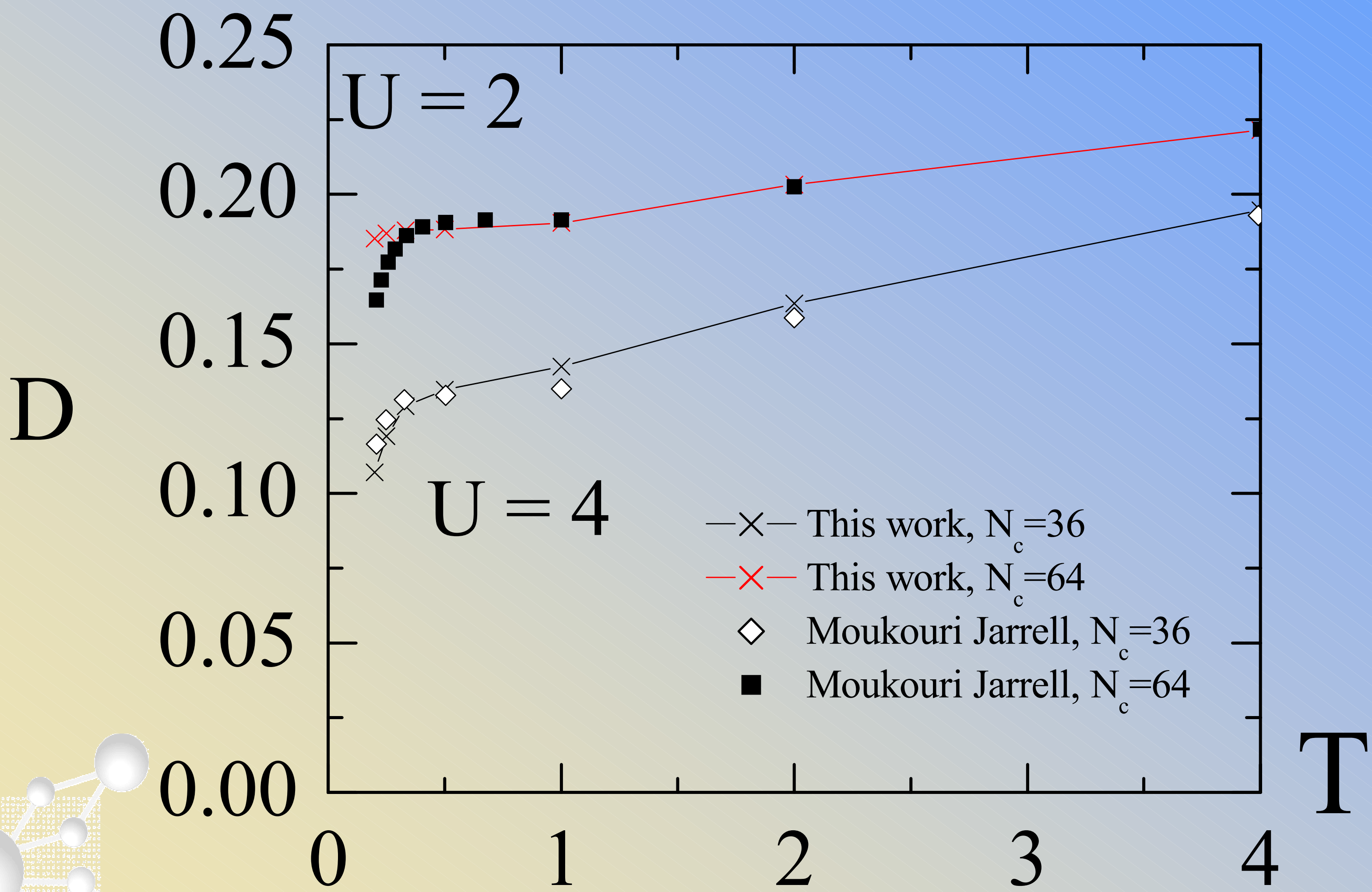
I-Motivation:
Understood by simple approach described here



I-Motivation: Understood by simple approach described here

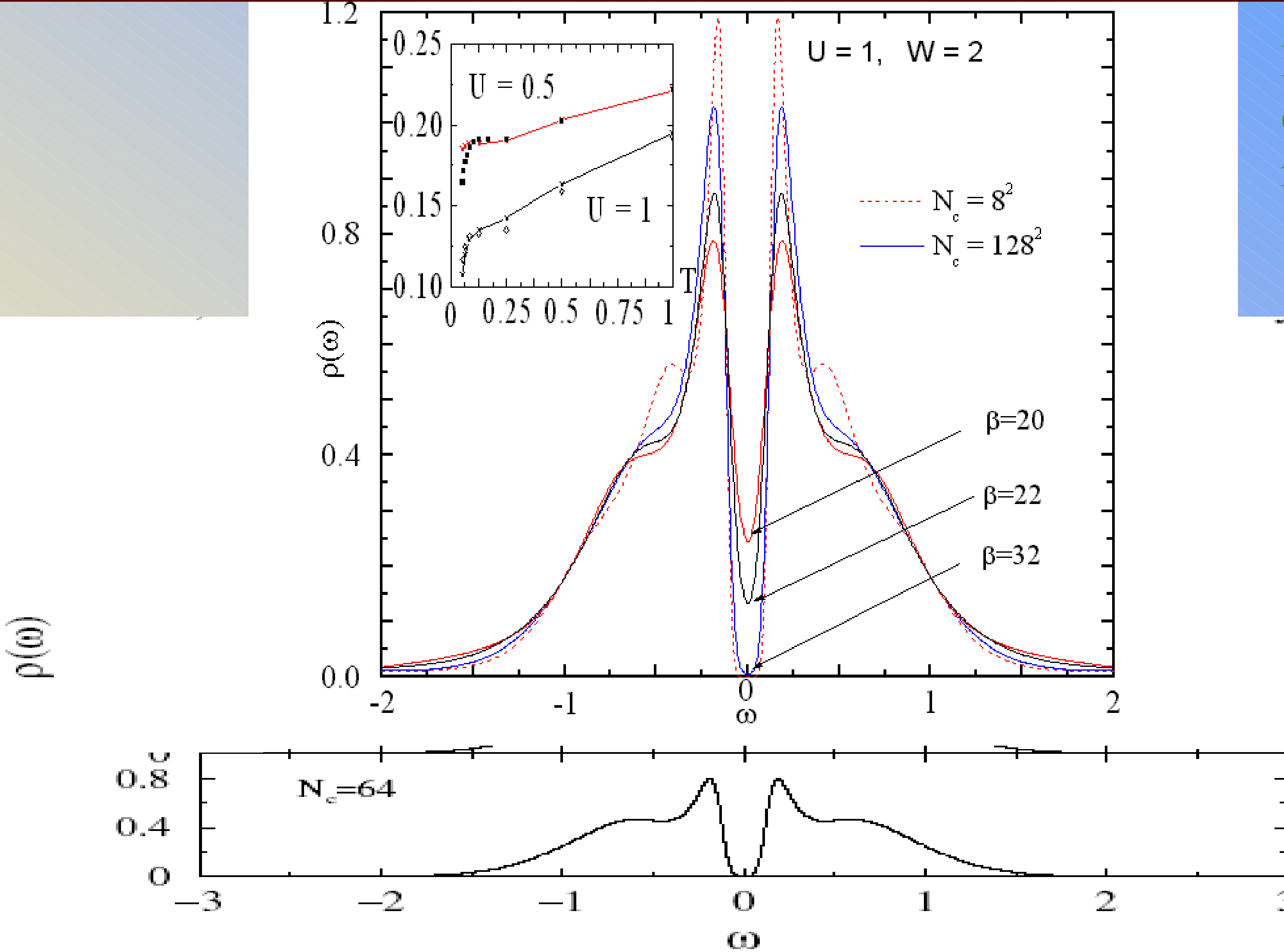


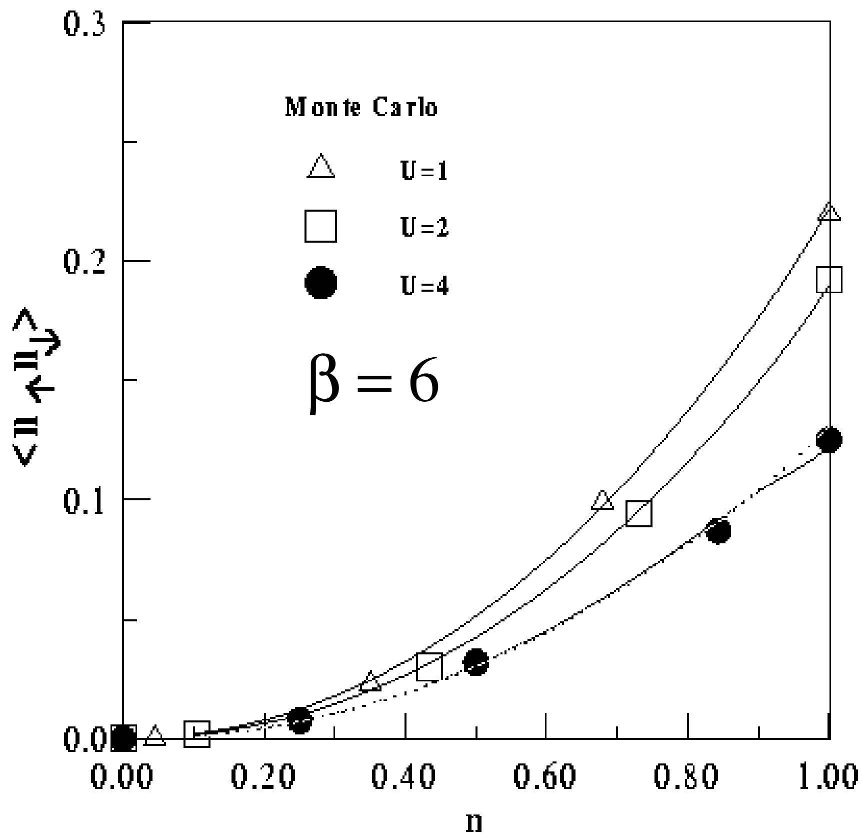
FIG. 2. The DOS $\rho(\omega)$ at $\beta = 32$ and $U = 1$.

Kyung et al. cond-mat/0112273

II- Spin and charge fluctuations:
-Proof that the method works.

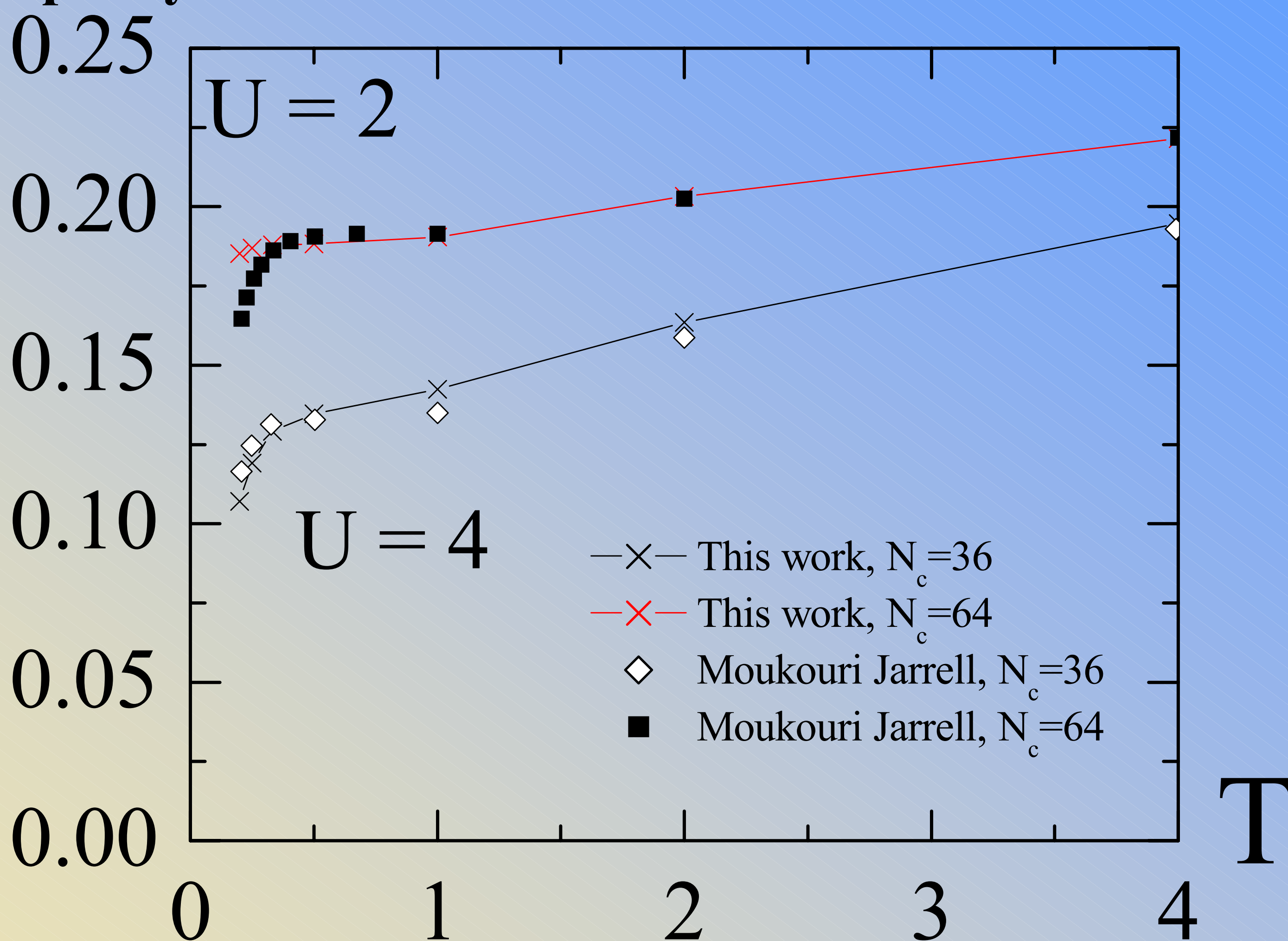
$$\left\langle (n_\uparrow - n_\downarrow)^2 \right\rangle = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle - 2\langle n_\uparrow n_\downarrow \rangle$$

- 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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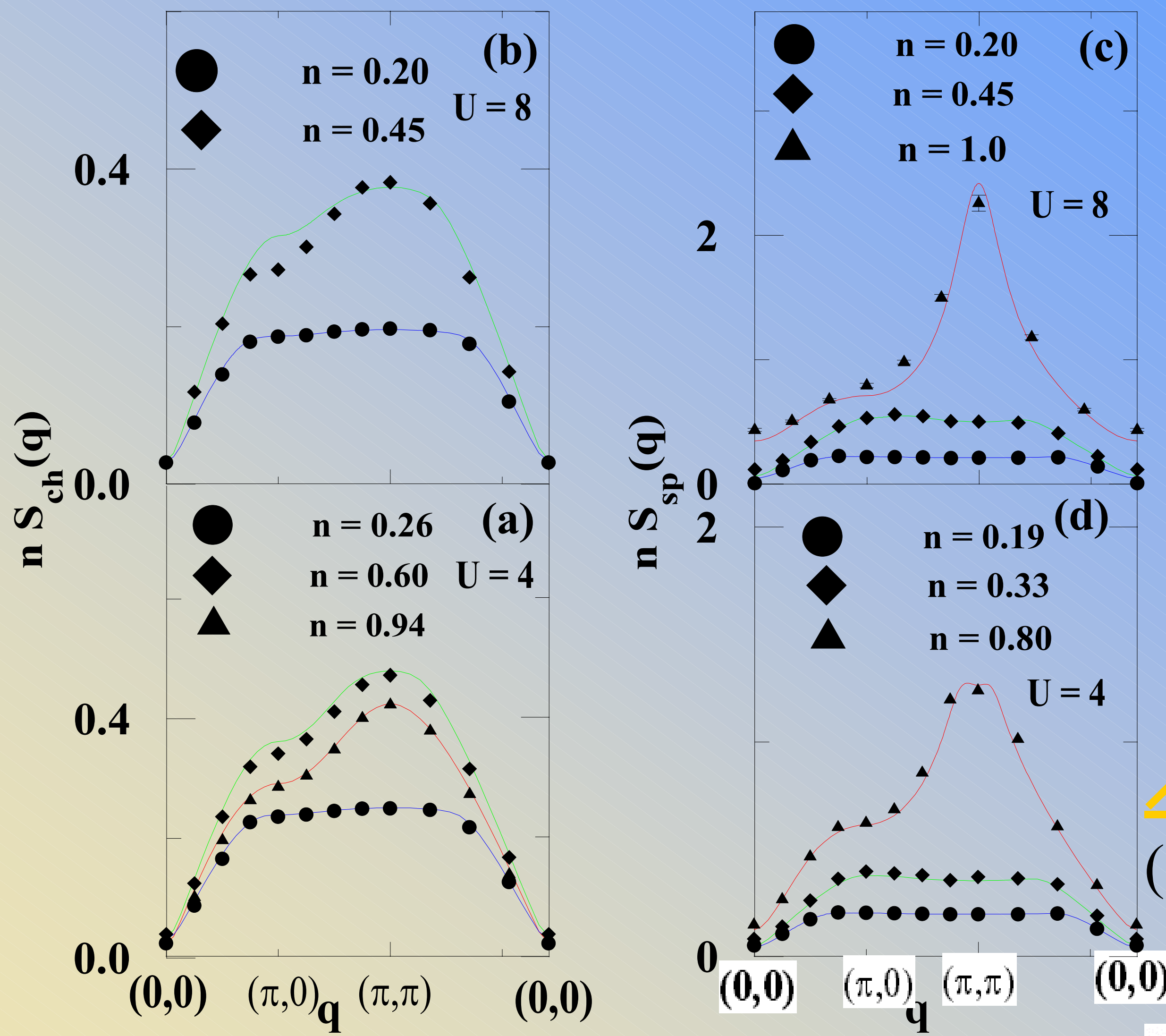
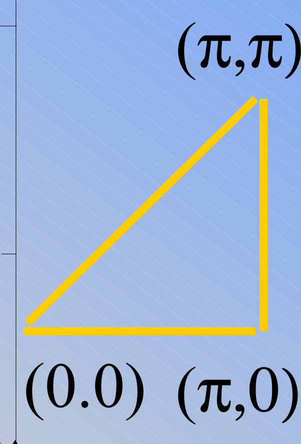
Notes:

-F.L. parameters

-Self also Fermi-liquid



U > 0



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

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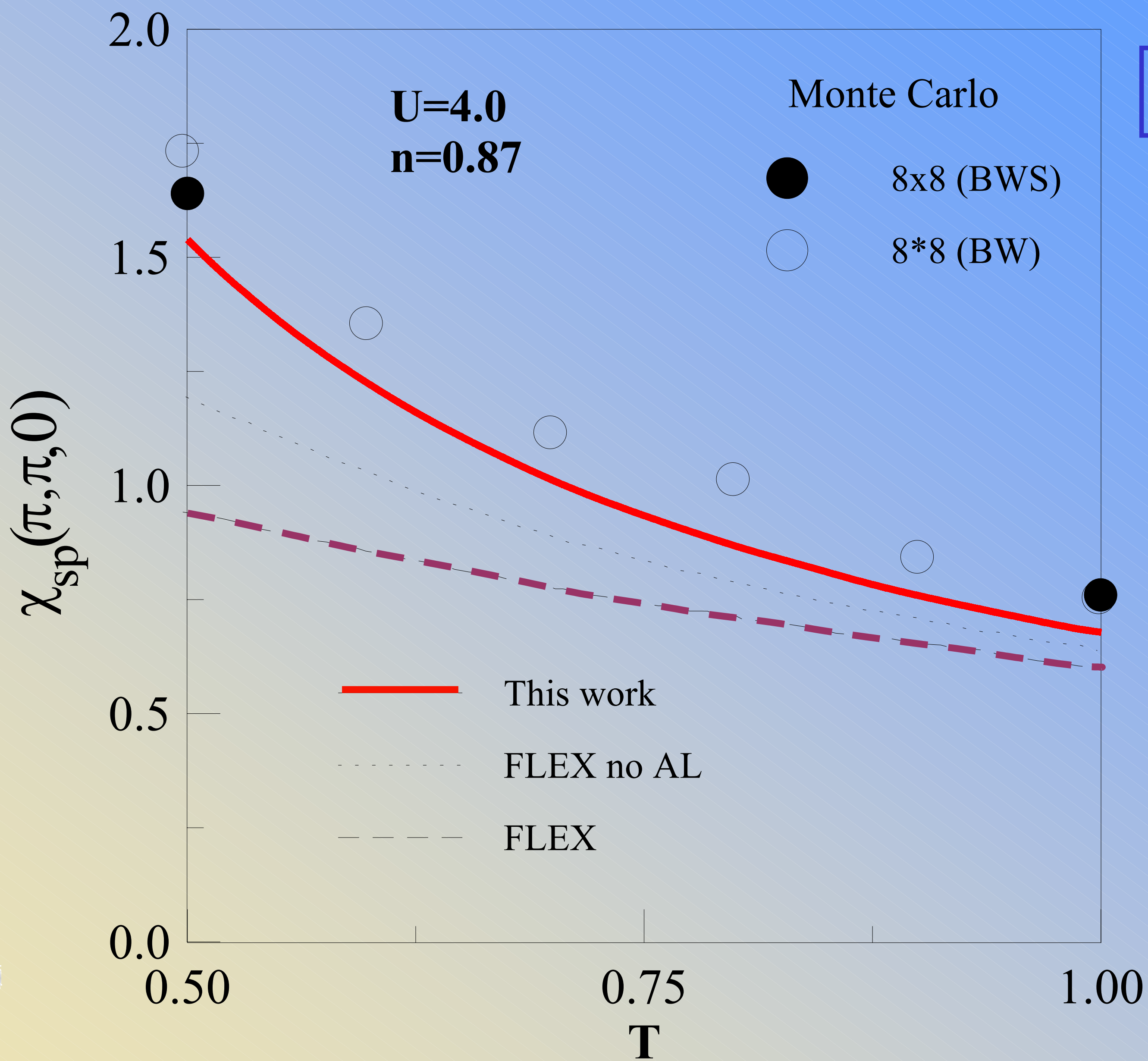
Proofs...

U = + 4



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

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

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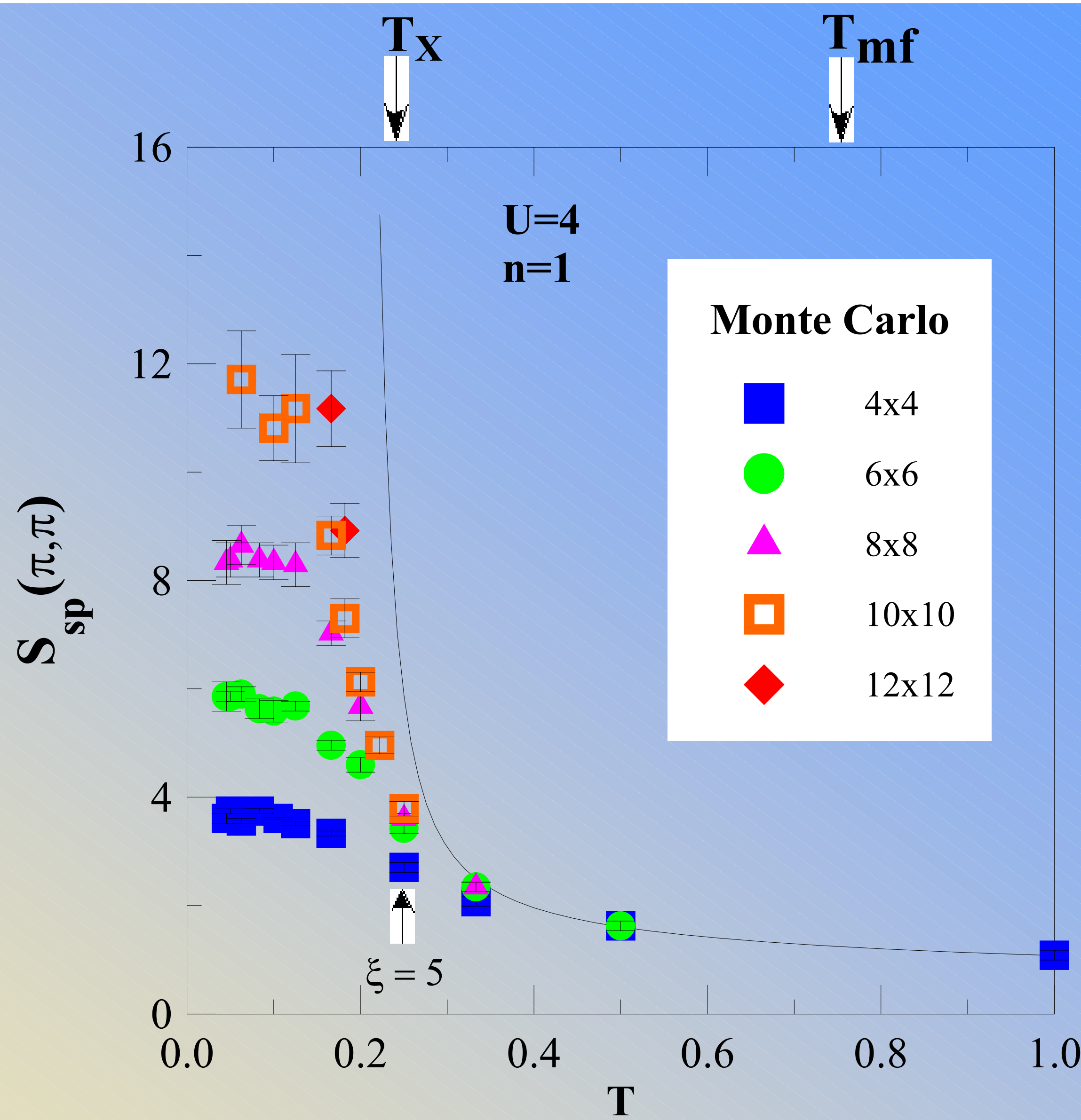
$$\xi \sim \exp\left(C(T)/T\right)$$



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)

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II-Spin and charge fluctuations
How do we do it?

- General philosophy
  - Drop diagrams
  - Impose constraints and sum rules and try to satisfy them.
    - Pauli principle
    - Conservation laws
    - Mermin-Wagner theorem

II-Spin and charge: Two-Particle Self-Consistent

Find $\langle n_\uparrow n_\downarrow \rangle$ from (a) fluctuation-dissipation theorem
(b)Pauli principle

$$U_{sp} = \frac{\delta \Sigma_\uparrow^{(1)}}{\delta G_\downarrow^{(1)}} - \frac{\delta \Sigma_\uparrow^{(1)}}{\delta G_\uparrow^{(1)}} = U \frac{\langle n_\uparrow n_\downarrow \rangle}{\langle n_\uparrow \rangle \langle n_\downarrow \rangle}.$$

N.B. Kanamori Brueckner

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

$$\frac{T}{N} \sum_q \frac{\chi_0(q)}{1 - \frac{1}{2} U_{sp} \chi_0(q)} = n - 2\langle n_\uparrow n_\downarrow \rangle$$

F.D.

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

RPA does not satisfy Pauli

II-Spin and charge: U_{sp} and U_{ch}

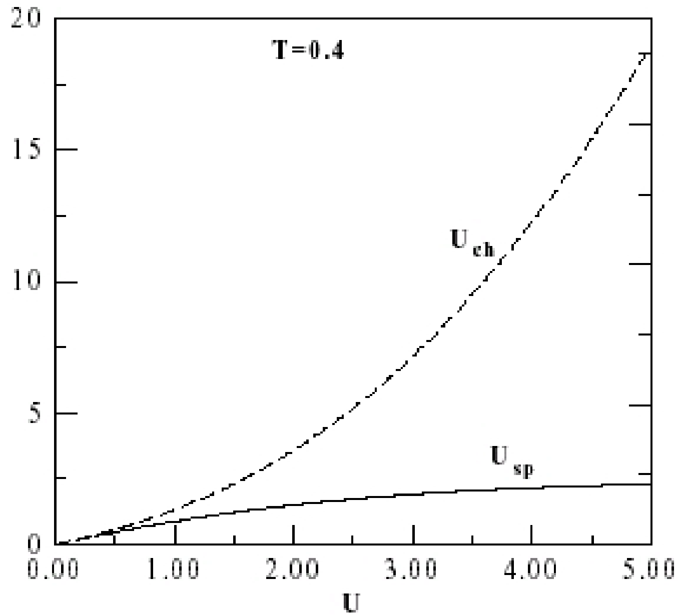


Fig. 2.

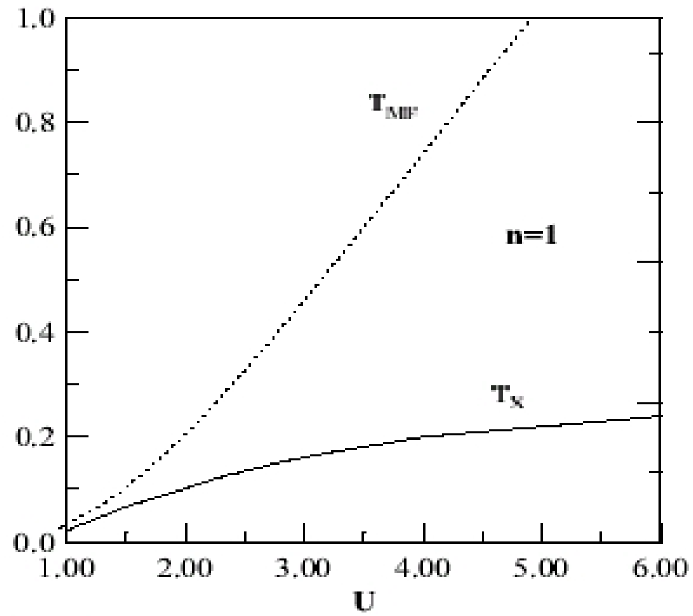


Fig. 3.

Fig. 2. — Dependence on U of the charge and spin effective interactions (irreducible vertices). The temperature is chosen so that for all U, it is above the crossover temperature. In this case, temperature dependence is not significant. The filling is $n = 1$.

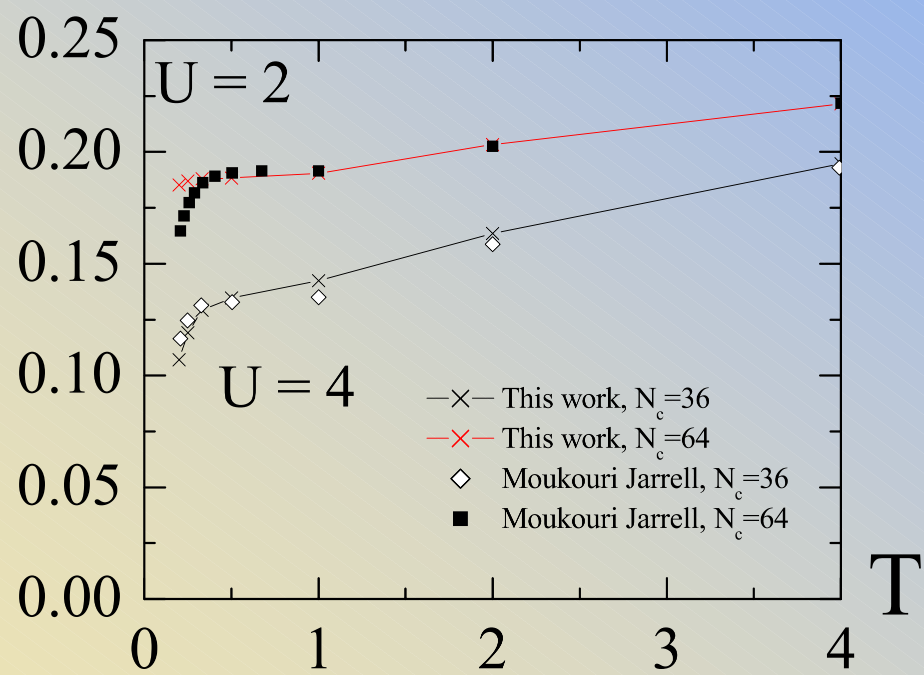
Fig. 3. — Crossover temperature at half-filling as function of U compared with the mean-field transition temperature.

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

II-Spin and charge: Mermin-Wagner

$$\frac{T}{N}\sum_{\tilde{q}} \frac{\chi_0(q)}{1-\frac{1}{2}\left(U\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}\right)\chi_0(q)} = n - 2\langle n_\uparrow n_\downarrow\rangle$$

•Note negative feedback and decrease in double occupancy when approach mean-field transition in *d = 2*



II-Spin and charge: Mermin-Wagner

$$\frac{T}{N}\sum_{\tilde{q}} \frac{\chi_0(q)}{1-\frac{1}{2}\left(U\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}\right)\chi_0(q)} = n - 2\langle n_\uparrow n_\downarrow\rangle$$

$$\frac{1}{((\mathbf{q}-\mathbf{Q}_d)^2+\xi^{-2})}$$

$$T\int \frac{d^d q}{(2\pi)^d}\,\frac{1}{q^2+\xi^{-2}} \propto n - 2\langle n_\uparrow n_\downarrow\rangle - C = C'$$

- Converges even when ξ = infinity when $d > 2$.
- In $d = 2$,

$$\xi \sim \exp\left(\frac{C'(T)}{T}\right)$$

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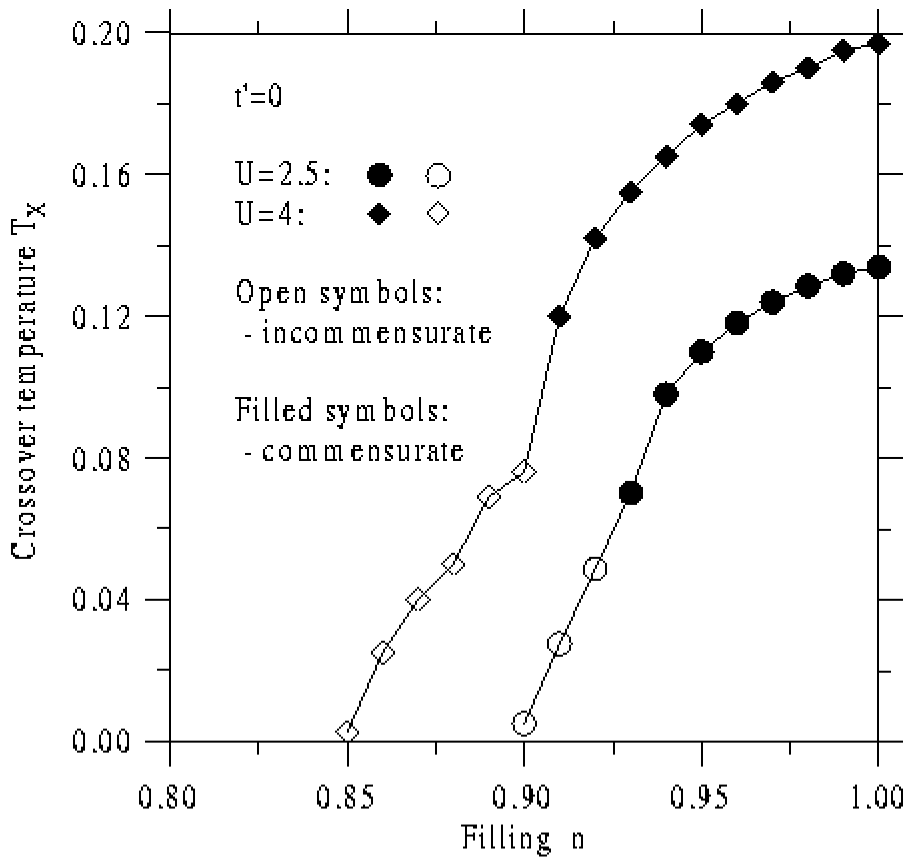
II-Spin and charge:
« Crossover » diagram

Quite different from RPA
In RPA (Stoner) we have,
-Long range order
-Ferromagnetism at low dopings.



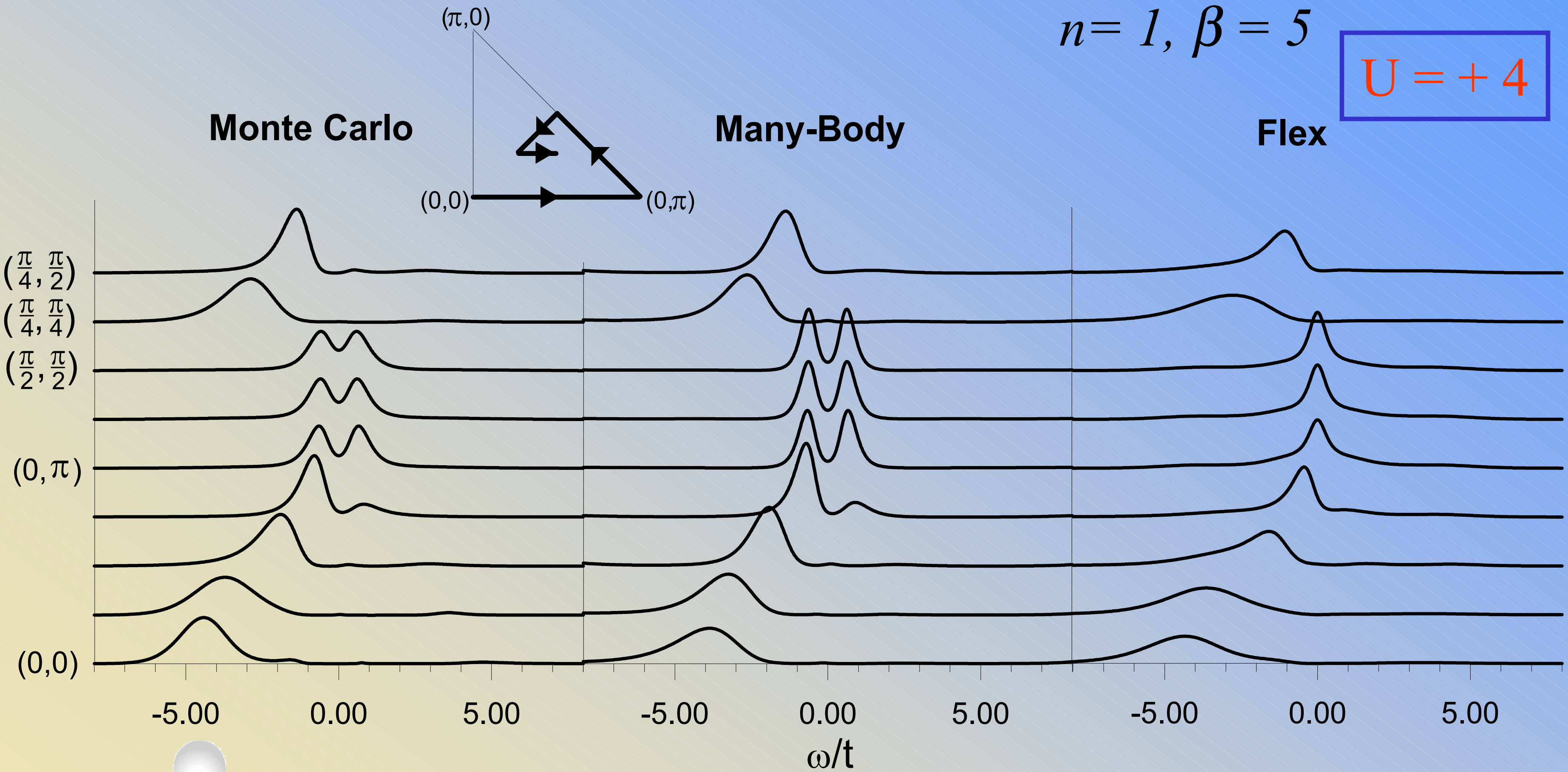
Vilk, et al. J. Phys. I France, **7**, 1309 (1997).
Vilk et al. P.R. B **49,** 13267 (1994)

III- Self-energy effects :

Proof that the method works

n= 1, β = 5

U = + 4



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

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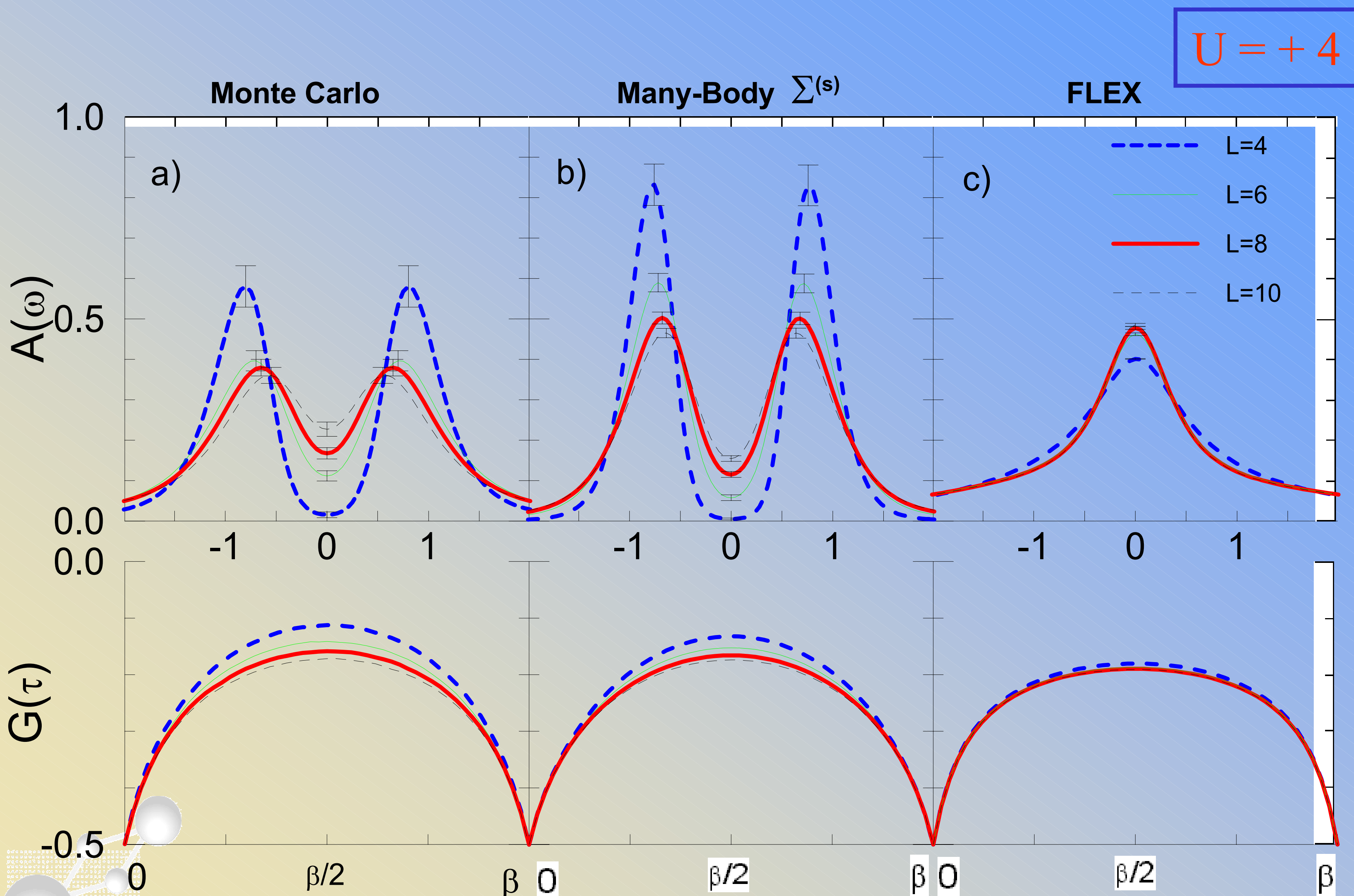
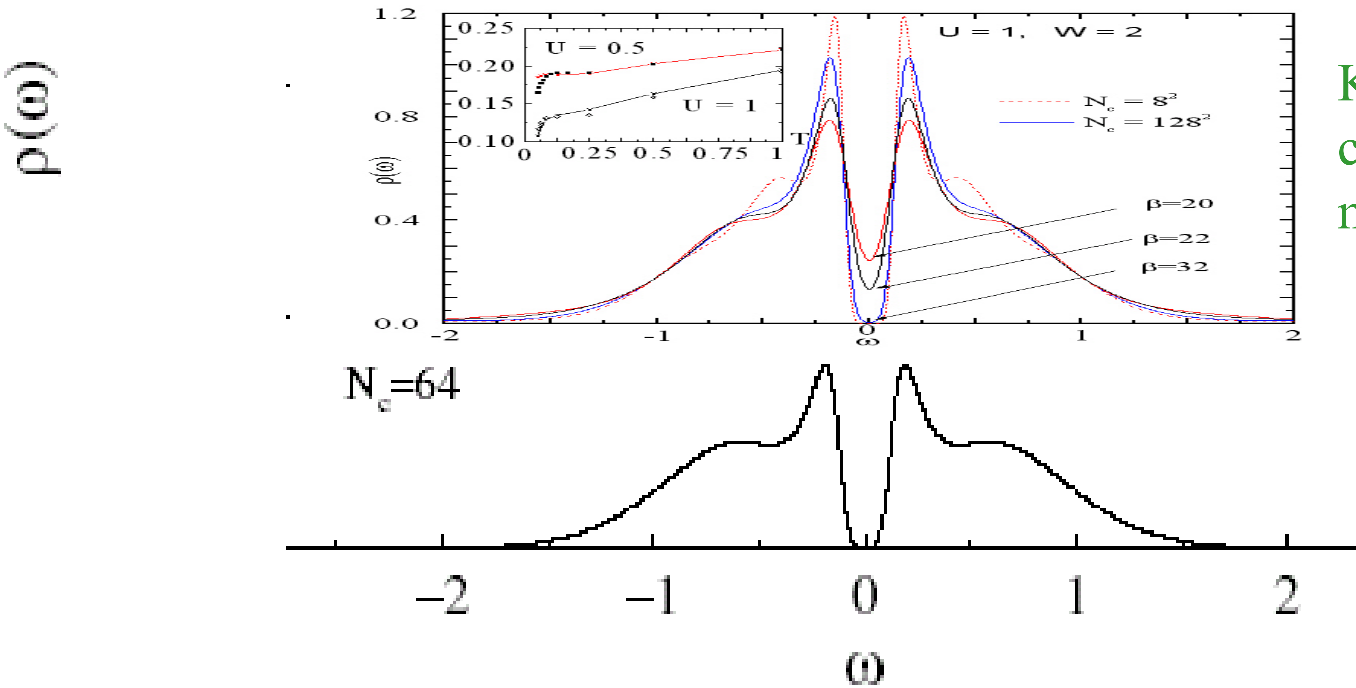


Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).

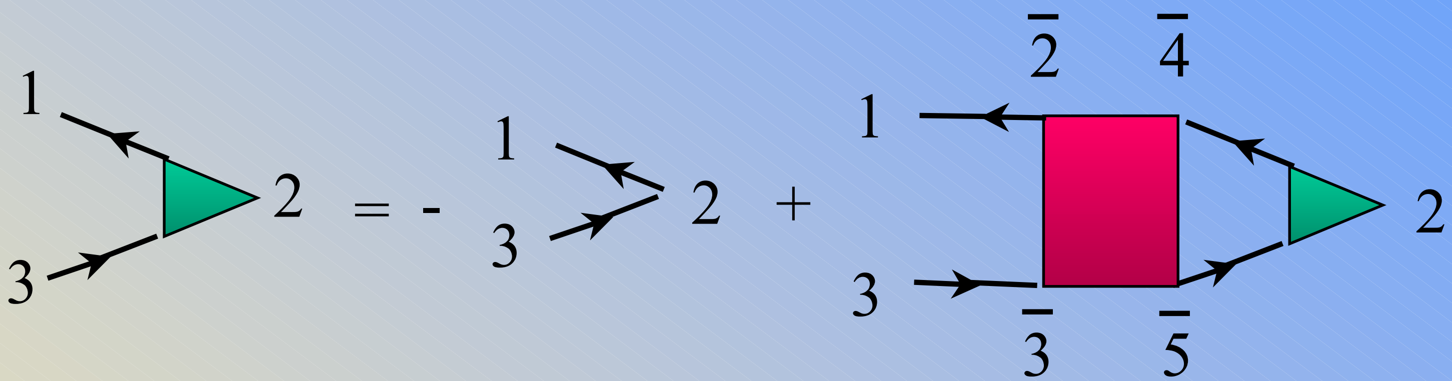


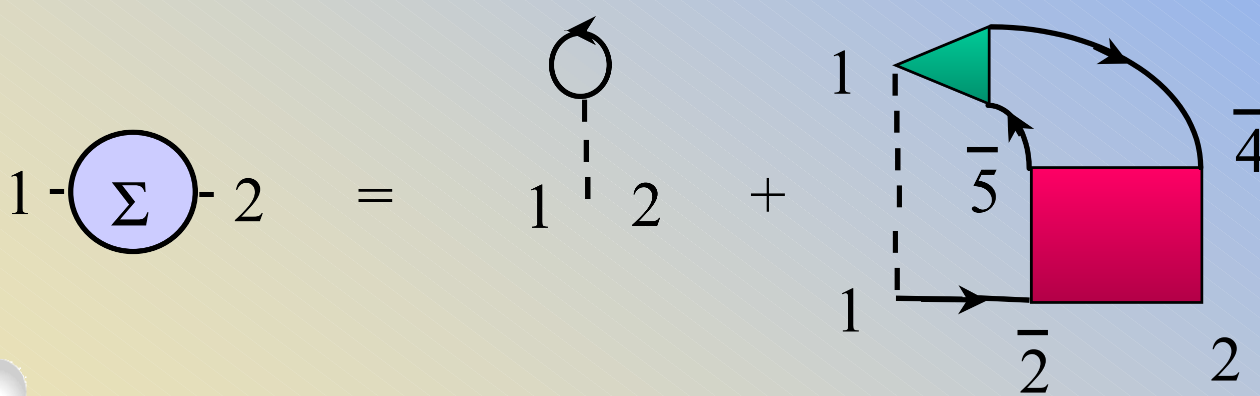
Kyung et al. cond-mat/0112273

FIG. 2. The DOS $\rho(\omega)$ at $\beta = 32$ and $U = 1$.

III- Self-energy effects :
How we do it…

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

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Improved self-energy (step (2))

$$\Sigma_{\sigma}^{(2)}(k)_{sym}$$

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

No « Migdal » theorem.

Consistency check

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

Not usually enforced by other approaches

Qualitatively new result:
effect of critical fluctuations on particles (RC regime)

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

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

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

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

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

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

in 3D: $\Sigma''^R(\mathbf{k}_F, 0) \propto -U(\ln \xi) / \left(\xi_{th}\xi_0^2\right)$

in 4D: quasiparticle survives up to T_c

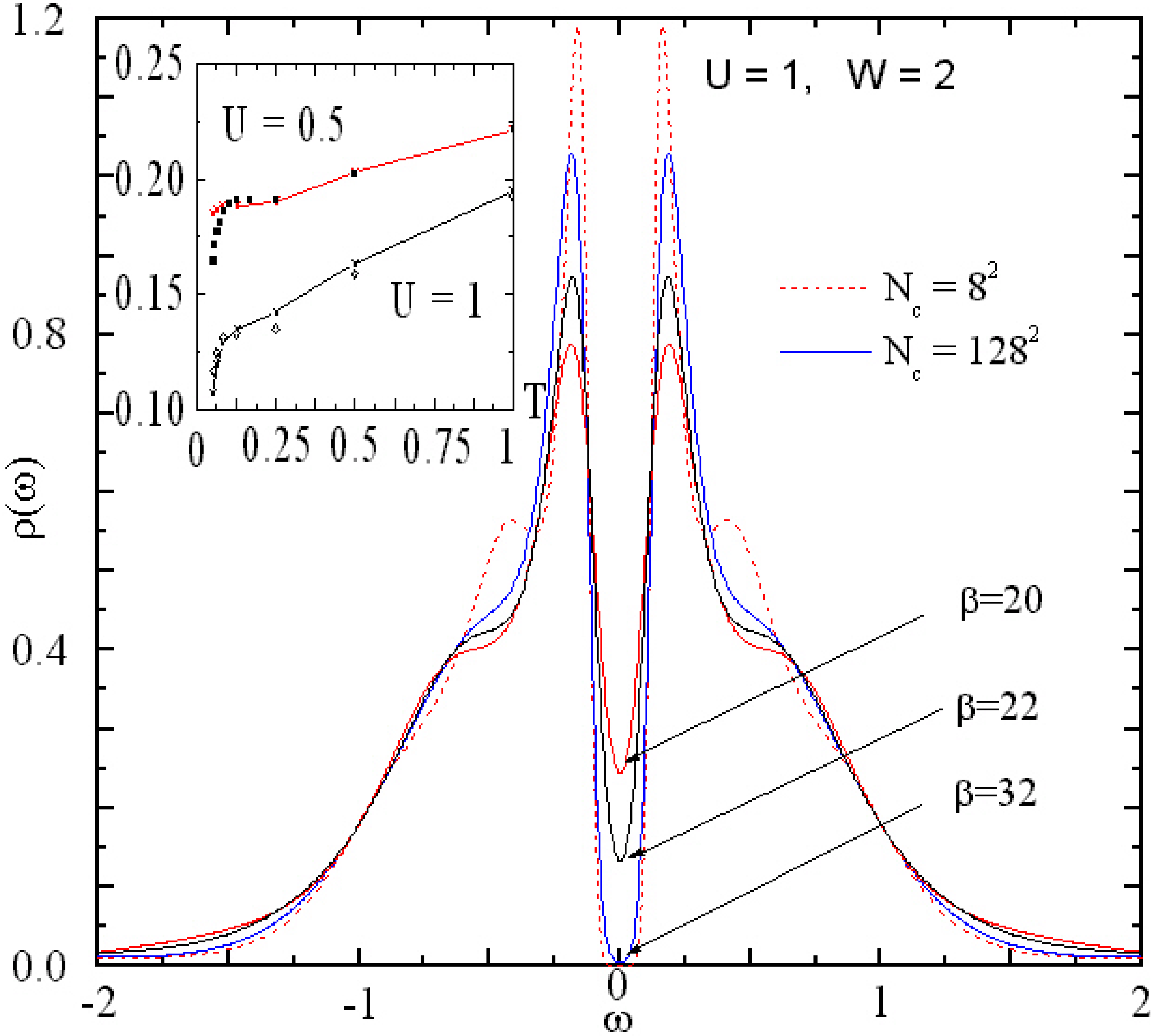
Y.M. Vilk and A.-M.S. Tremblay, J. Phys. Chem. Solids **56**, 1769 (1995).
Y.M. Vilk and A.-M.S. Tremblay, Europhys. Lett. **33**, 159 (1996);

Imaginary part: compare Fermi liquid, $\lim_{T\to 0} \Sigma_R''(\mathbf{k}_F, 0) = 0$

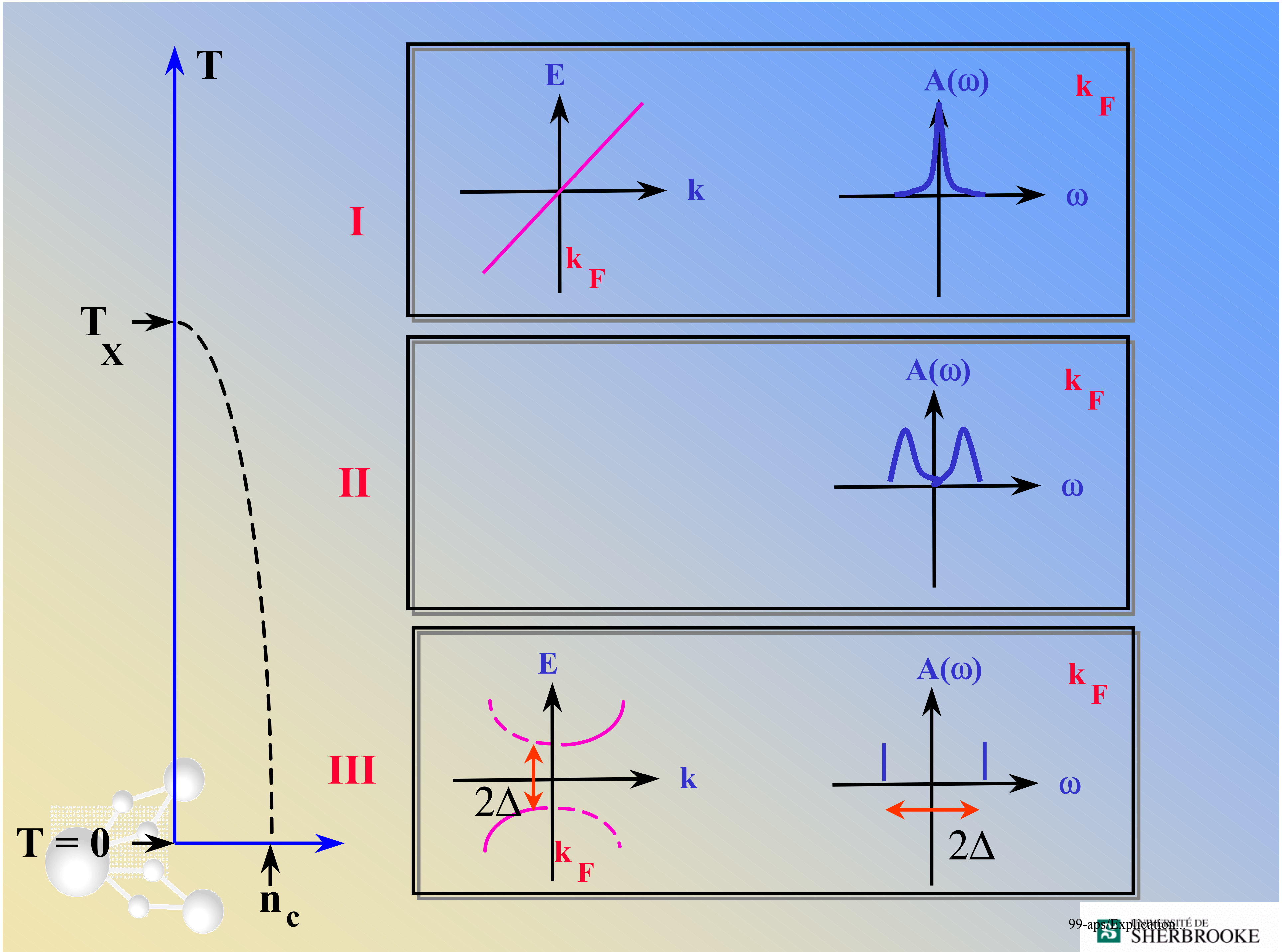
$$\Sigma_R''(\mathbf{k}_F, 0) \propto \frac{T}{v_F}\int d^{d-1}q_\perp \frac{1}{q_\perp^2 + \xi^{-2}} \propto \frac{T}{v_f}\xi^{3-d} \underset{d=2}{\propto} \frac{\xi}{\xi_{th}}$$

Why leads to pseudogap

$$A(\mathbf{k},\omega) = \frac{-2\Sigma_R''}{(\omega - \varepsilon_\mathbf{k} - \Sigma_R')^2 + \Sigma_R''^2}$$



U = 1, W = 2
U = 0.5
U = 1
T
0 0.25 0.5 0.75 1
0.25
0.20
0.15
0.10
$N_c = 8^2$
$N_c = 128^2$
β=20
β=22
β=32
1.2
0.8
0.4
0.0
ρ(ω)
-2
-1
0
1
2
ω


T
T_X
T = 0
n_c
I
II
III
E
k
k_F
A(ω)
ω
2Δ

IV-Extensions

- Works just as well in higher dimensions
  - *Néel temperature d=3*

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

- $U < 0$ and $U > 0$.

    Allen *et al.*, P.R. B 64, 075115 (2001).
    Kyung *et al.* P.R. B 64, 075116 (2001).

- Arbitrary-range hopping

    Veilleux et al. P.R.B. **52**, 16255 (1995).

- Pairing susceptibility

    Kyung et al. cond-mat/0205427
    Kyung et al. cond-mat/0204500

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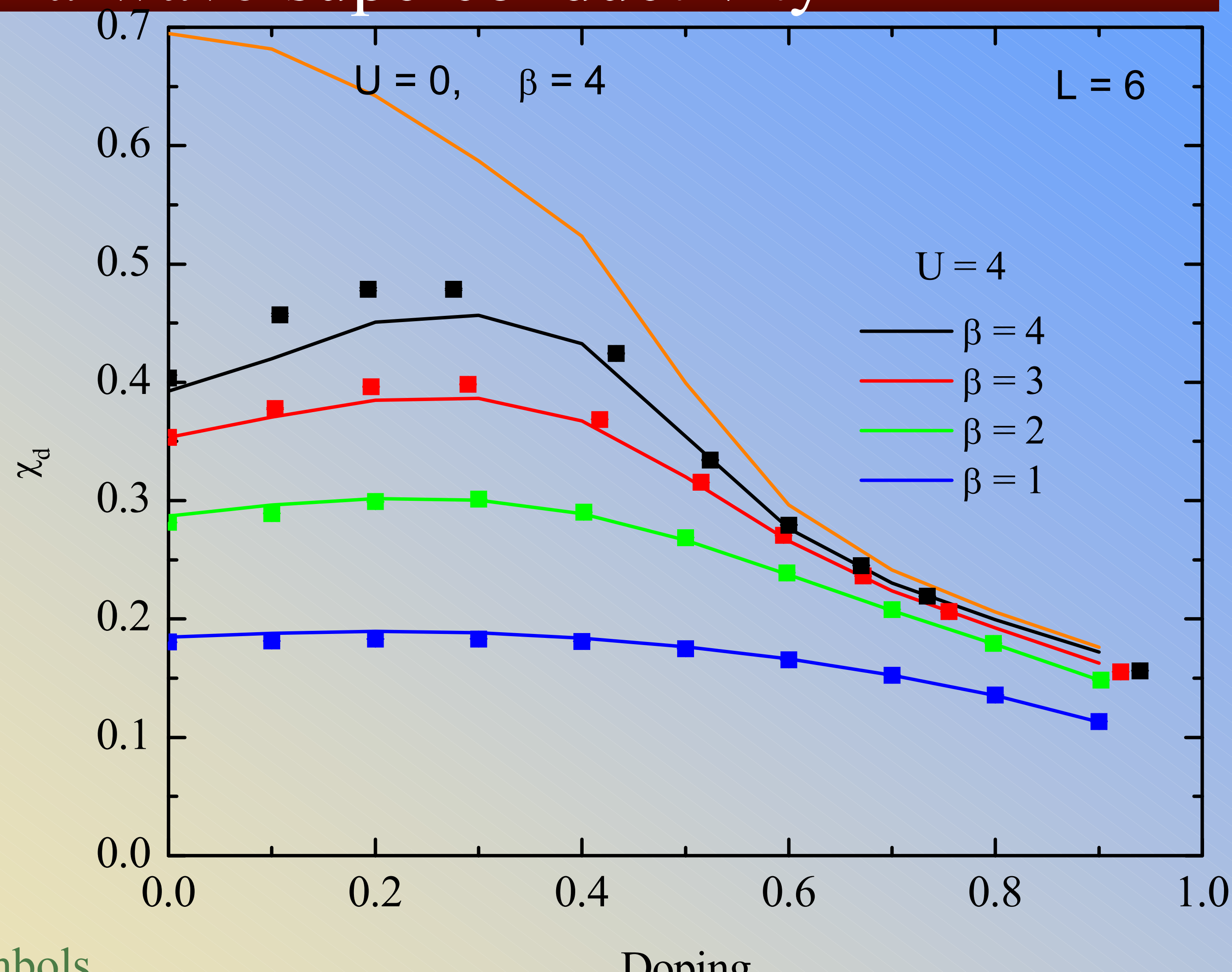
IV-Extensions:
d-wave superconductivity



QMC: symbols.
Solid lines analytical.

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

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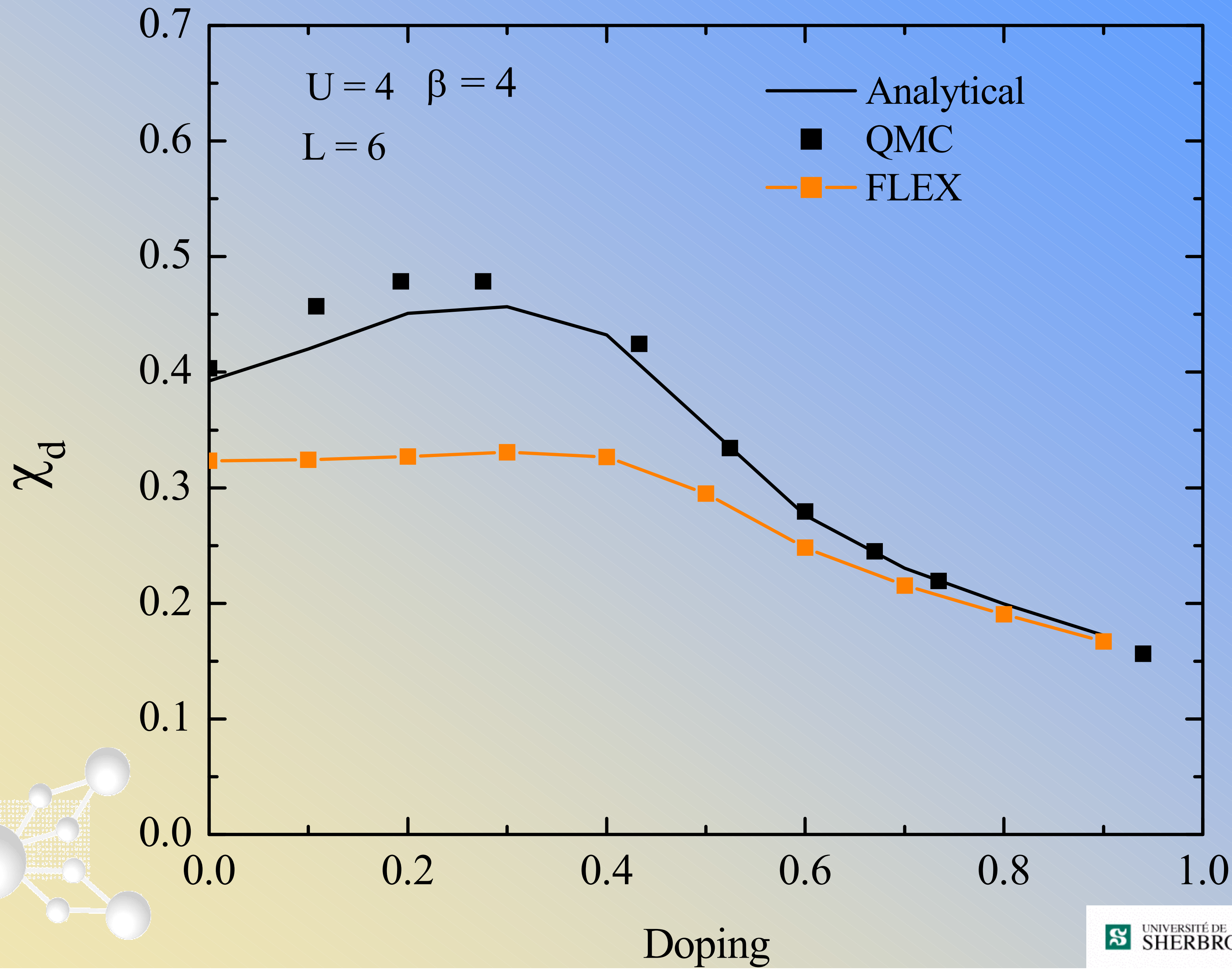

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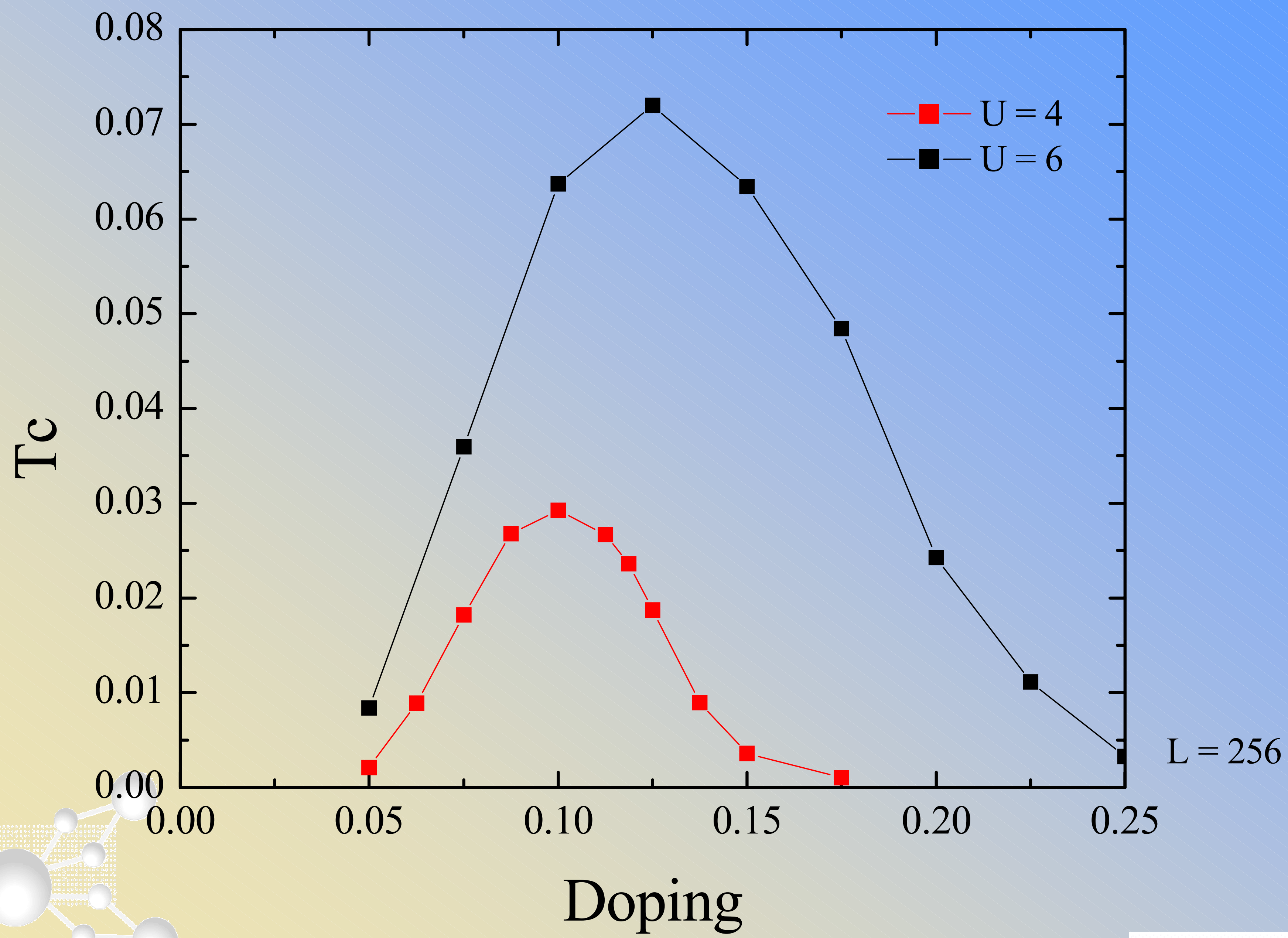

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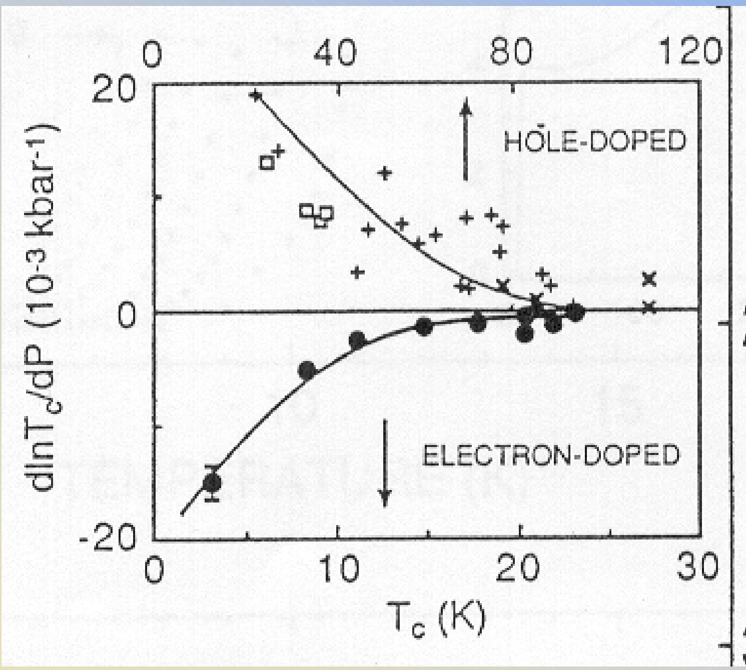
Electron doped:



M.B. Maple
MRS Bulletin,
June 1990

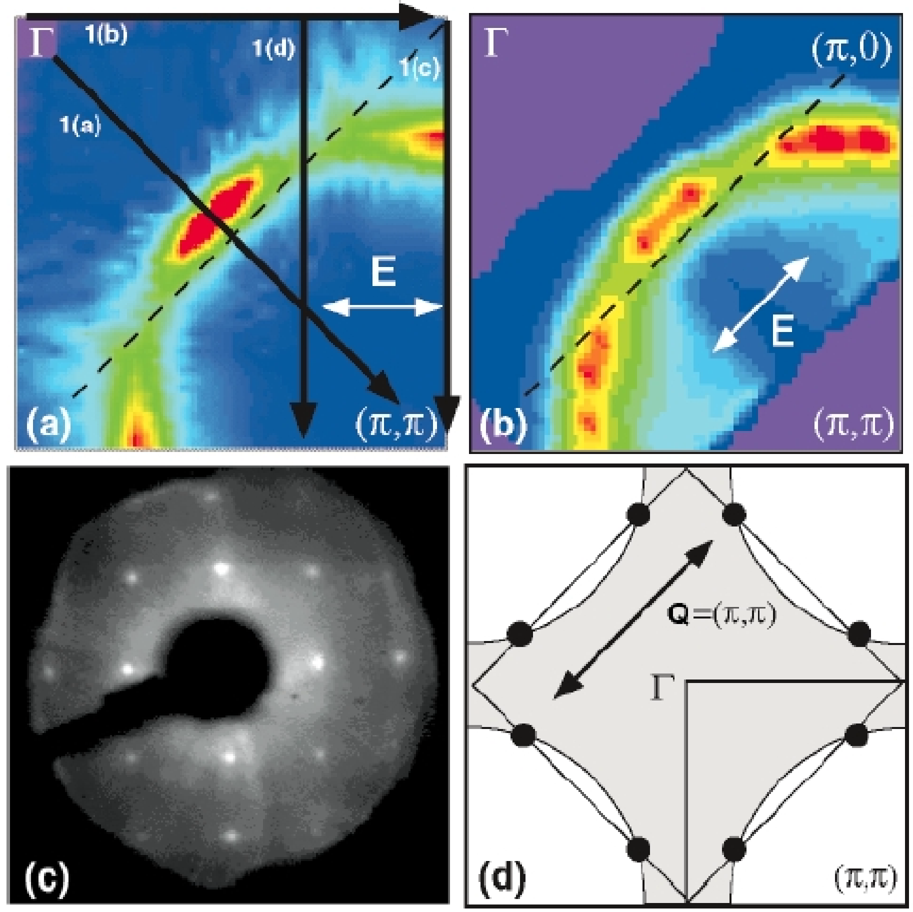


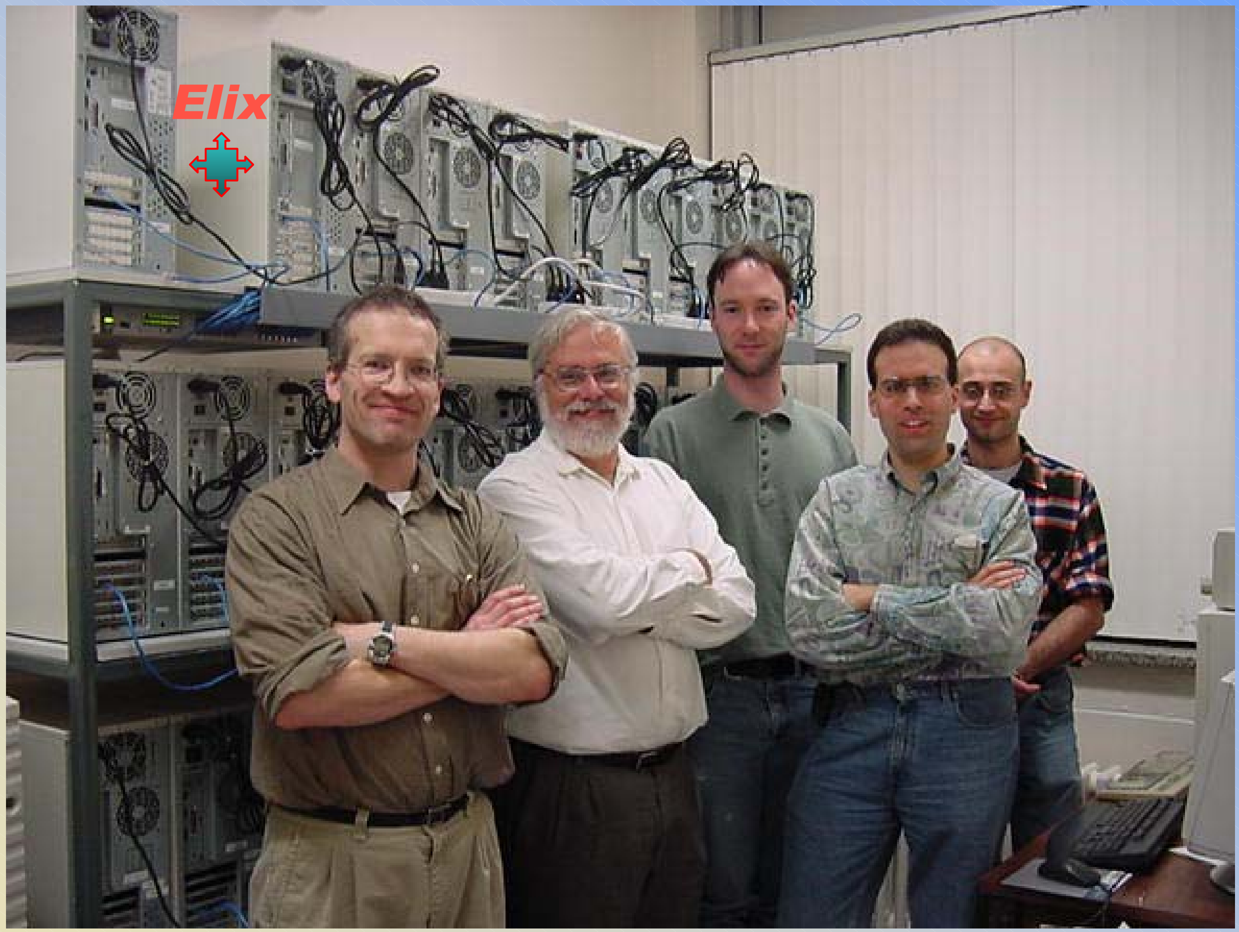
FIG. 2 (color). (a),(b) Fermi surface of the partial Brillouin zone of NCCO taken with $\hbar\omega$ = 16.5 and 55 eV, respectively. The plotted quantity is a 30 meV integration about E_F of each EDC plotted as a function of $\vec{k}$. 16.5 eV data were taken over a Brillouin zone octant and symmetrized across the Γ to the (π, π) line, while the 55 eV data were taken over a full quadrant [6]. The polarization direction is denoted by the double ended arrow. The dotted line is the antiferromagnetic Brillouin zone boundary. (c) LEED spectra of NCCO cleaved *in situ* at 10 K. (d) Schematic showing only those regions of FS near the black circles can be coupled with a (π, π) scattering.

Armitage et al.
Phys. Rev. Lett.
87, 147003 (2001)

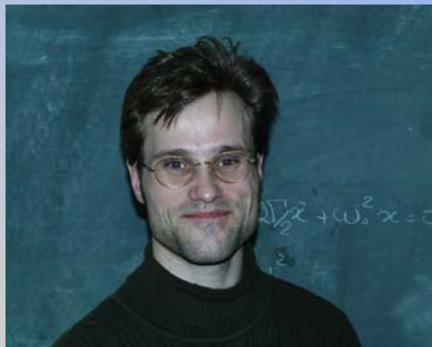
V-Summary and conclusion

- « Standard » approaches can give results that are qualitatively incorrect, even for $U/W < 1$.
- Preferable to forget diagrams and instead enforce Pauli, conservation, Mermin-Wagner…
- *TPSC* + self energy without Migdal is accurate (reproduces QMC and DCA))
- (1996) Physics: In $d=2$, precursors of the ordered phase make self-energy singular in both ω and $\mathbf{k}$.
- Recent advance : pairing susceptibility.
- Useful as a « cluster solver » in DMFT?

Michel Barrette Mehdi Bozzo-Rey



David Sénéchal A.-M.T. Alain Veilleux



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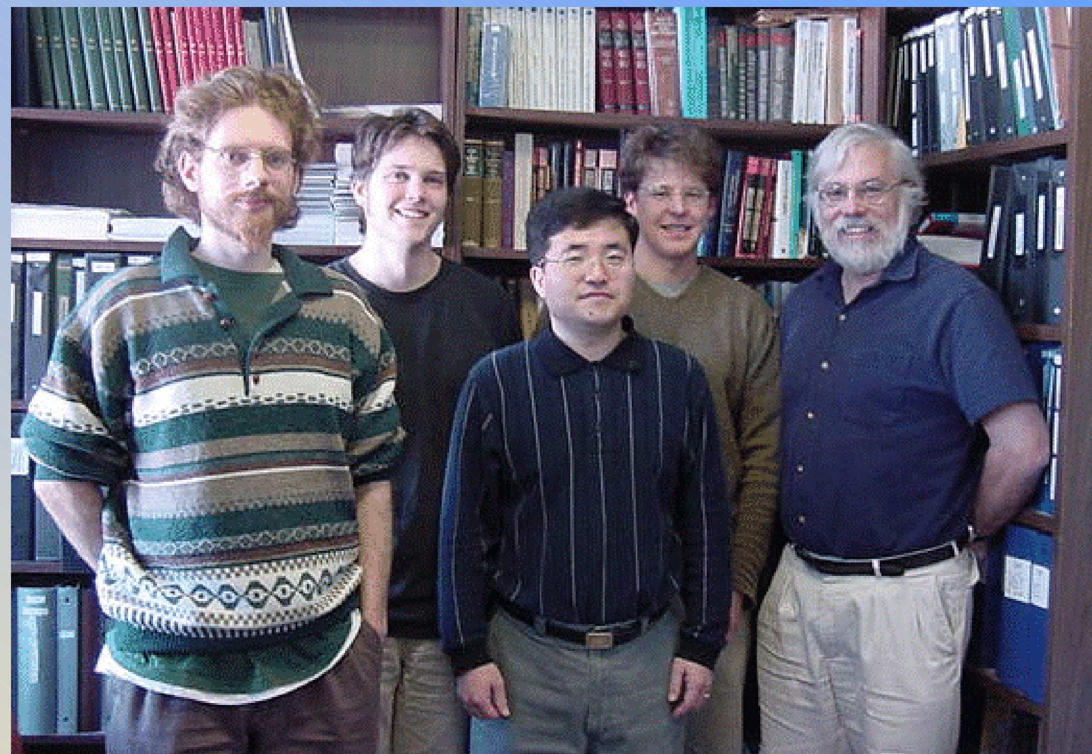

Jean-Séastien Landry A-M.T.

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C'est fini . . .

enfin