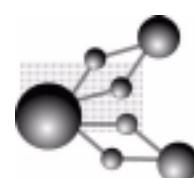


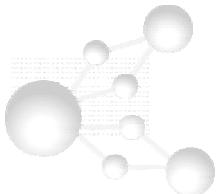
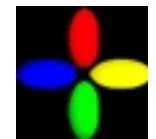
## André-Marie Tremblay



CENTRE DE RECHERCHE SUR LES PROPRIÉTÉS  
ÉLECTRONIQUES  
DE MATÉRIAUX AVANCÉS

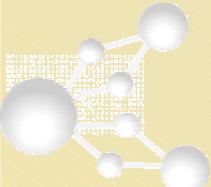


## Sponsors:



# Mathematics, Physics, and Computers : strongly correlated electrons in two dimensions as a case study.

- I. All is not well with the theory of solids
- II. A microscopic model
- III. Inching our way up the weak-coupling regime.
- IV. What was the competition up to?
- V. Conclusion

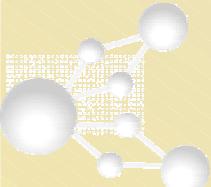


# I. All is not well with the theory of solids

Theory of solids

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

- Many new ideas and concepts needed for progress  
(Born-Oppenheimer, H-F, Bands...)
- Successful program
  - Semiconductors, metals *and superconductors*
  - Magnets
- Is there anything left to do?
  - Unexplained materials: High T<sub>c</sub>, Organics...
  - Strong correlations:  
strong interactions, low dimension  
strong fluctuations

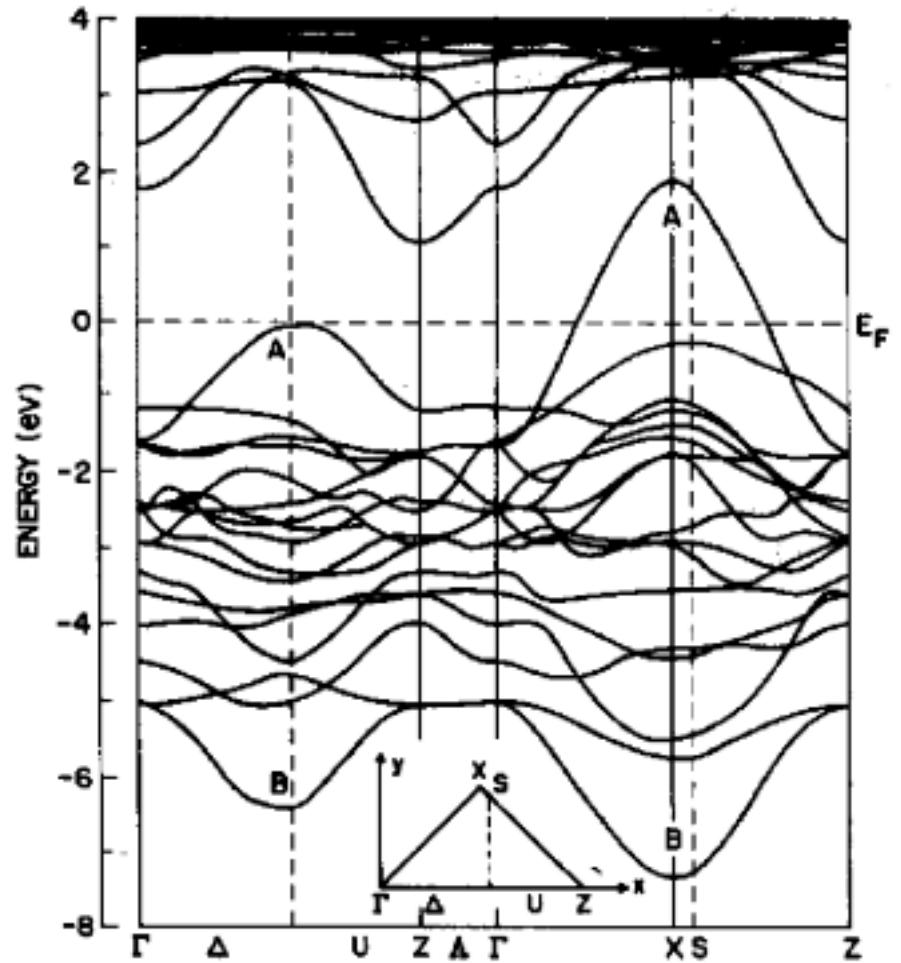


## The standard approaches :

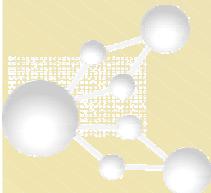
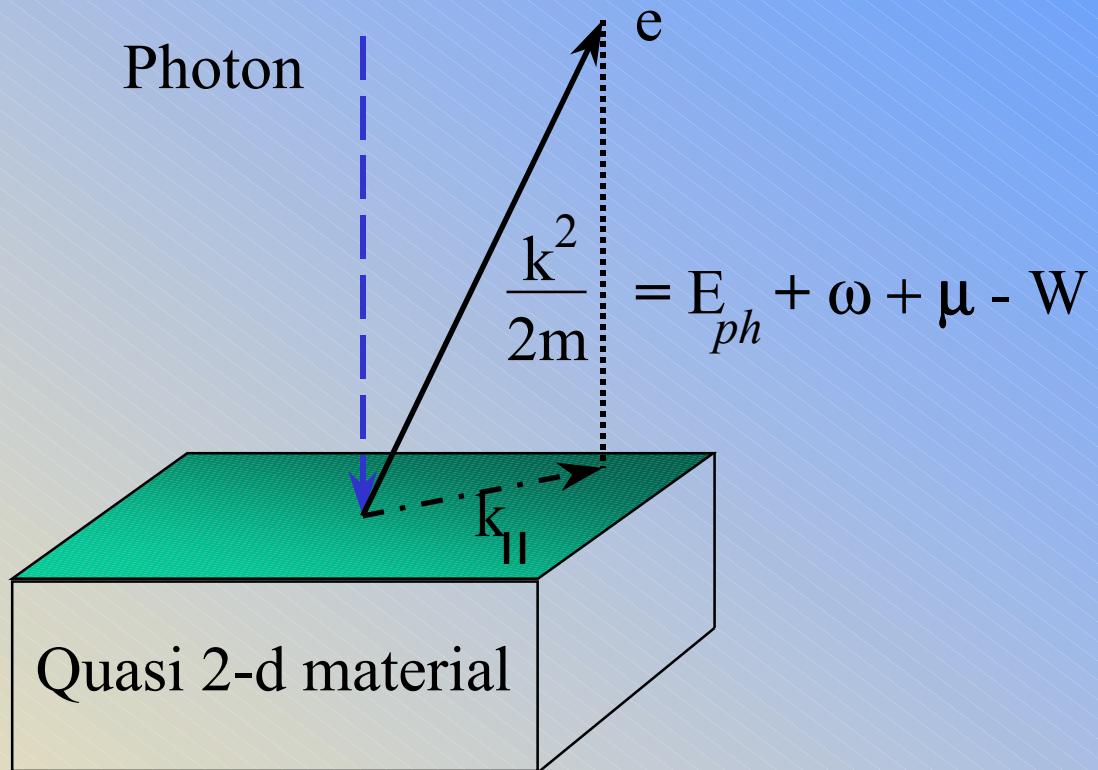
Quasiparticles, Fermi surface  
and Fermi liquids  
- LDA (Nobel prize 1998)



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



## Angle-Resolved Photoemission (ARPES)



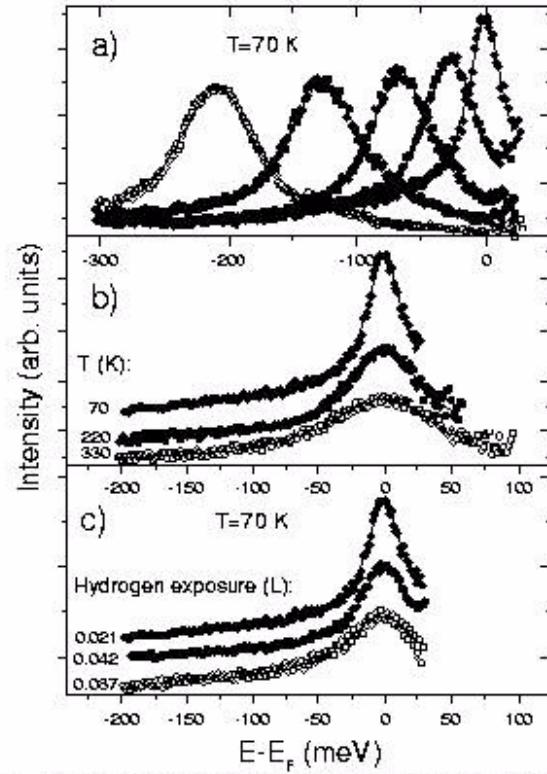


FIG. 2. Spectral intensity as a function of binding energy for constant emission angle, normalized to the experimentally determined Fermi cut-off. Data are symbols, while lines are fits to the Lorentzian peaks with a linear background. The dependence on the binding energy (a), temperature (b), and hydrogen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

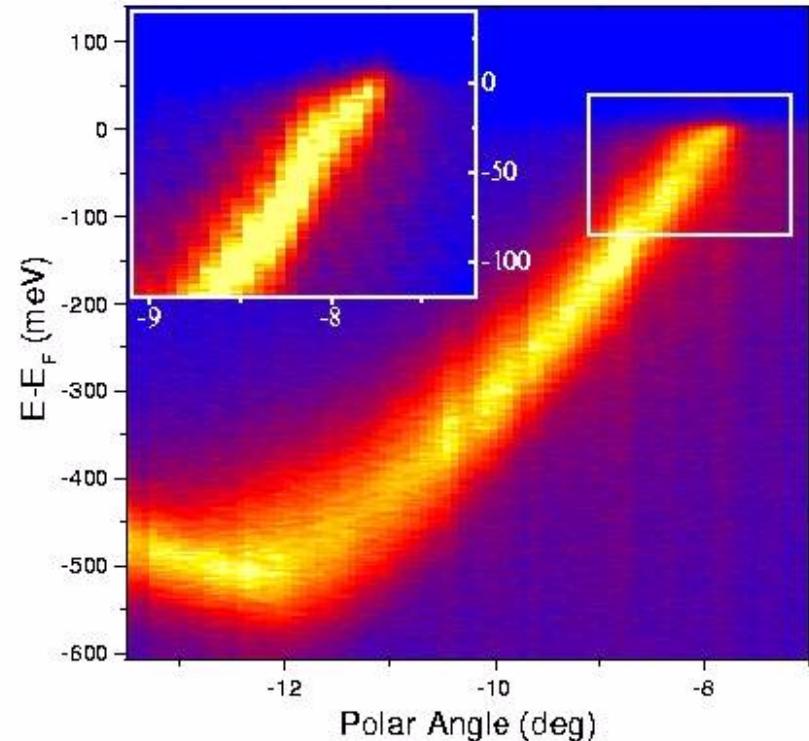


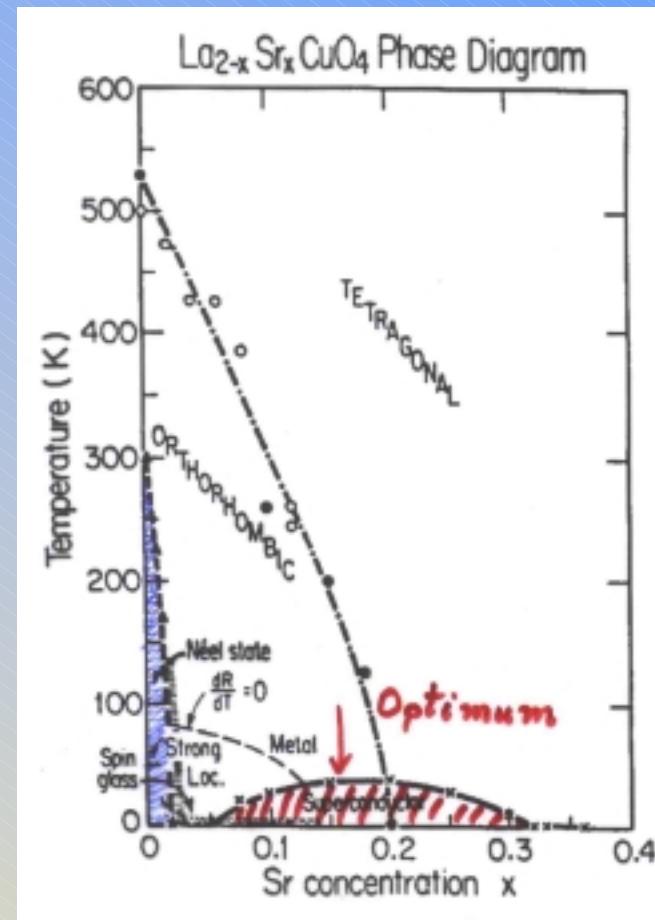
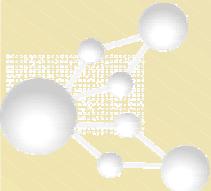
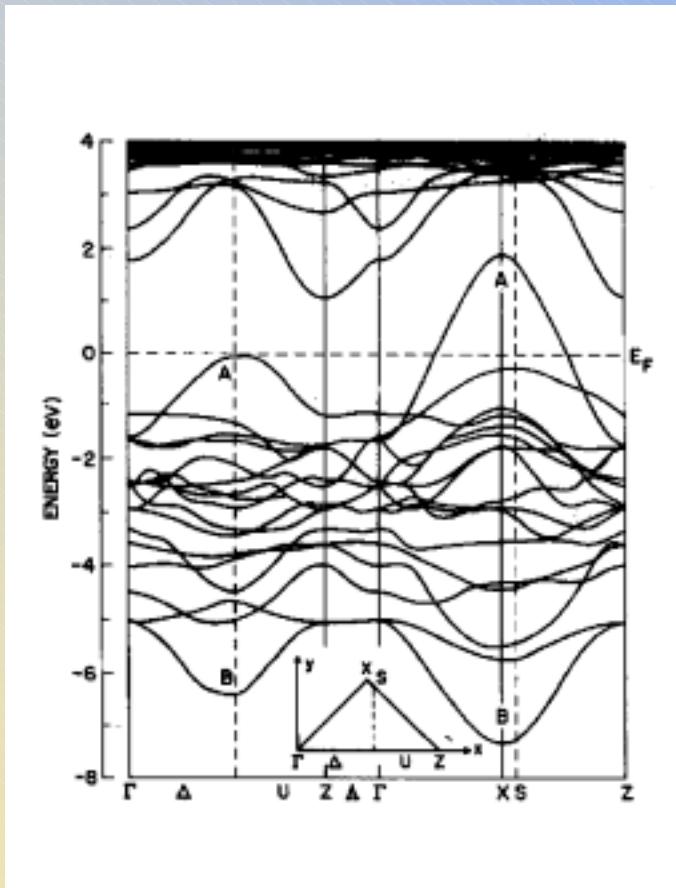
FIG. 1. ARPES intensity plot of the Mo(110) surface recorded along the  $\bar{\Gamma} - \bar{N}$  line of the SBZ at 70 K. Shown in the inset is the spectrum of the region around  $k_F$  taken with special attention to the surface cleanliness.

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



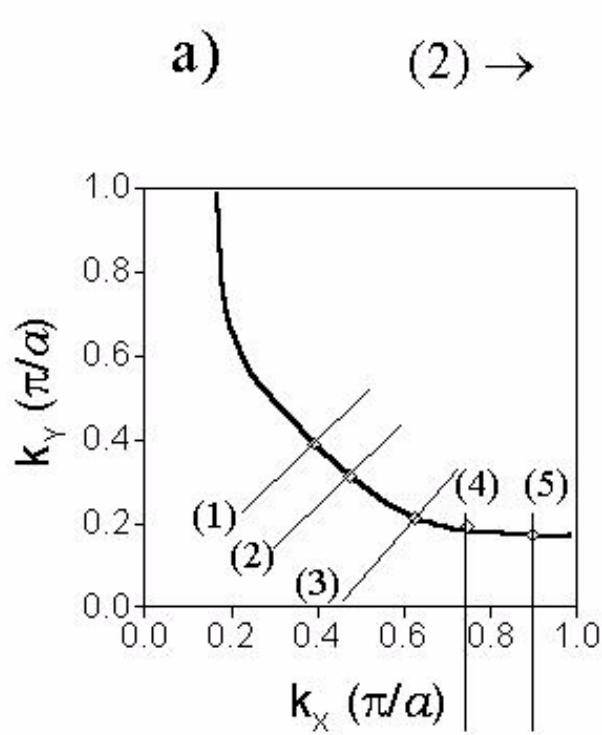
$n = 1,$

Metal according to band  
AFM insulator in reality

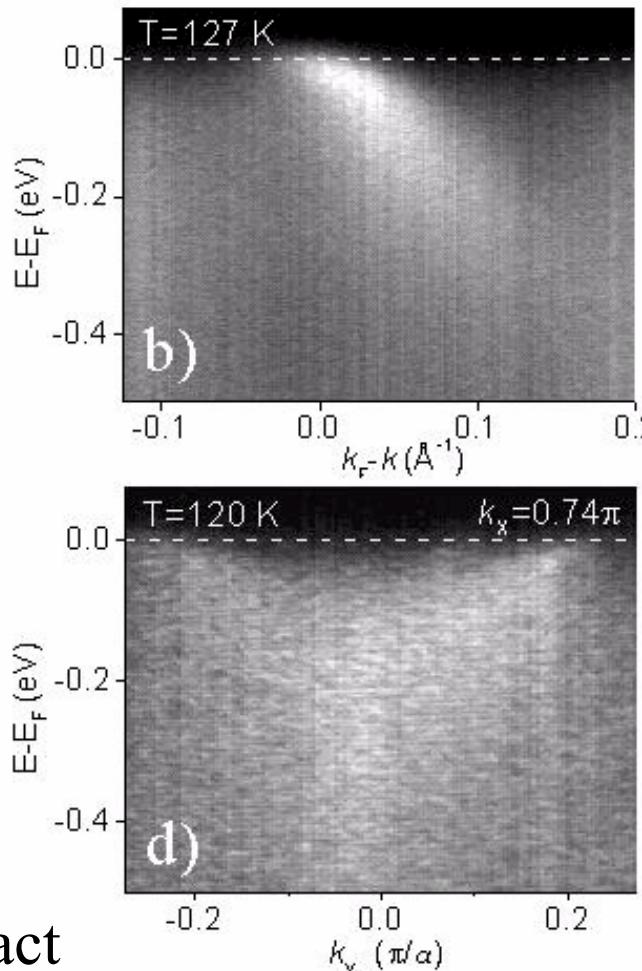


# Optimally doped BISCCO

Normal



(4) →



-  $d=2$  partial vanishing act  
of the Fermi surface away  
from  $n = 1$ .

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

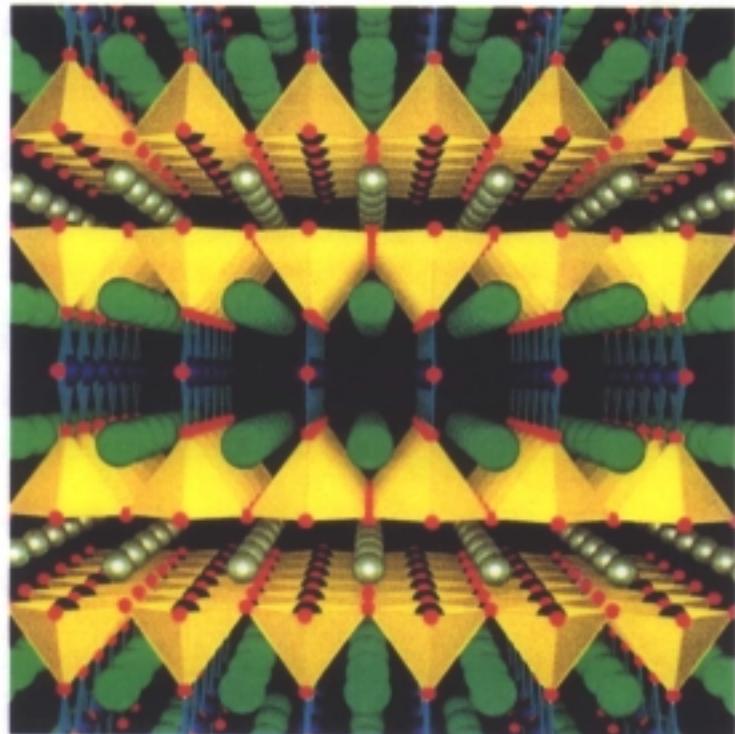
## II. A microscopic model

# SCIENTIFIC AMERICAN

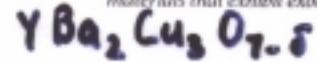
*How nonsense is deleted from genetic messages.*

*R for economic growth: aggressive use of new technology.*

*Can particle physics test cosmology?*

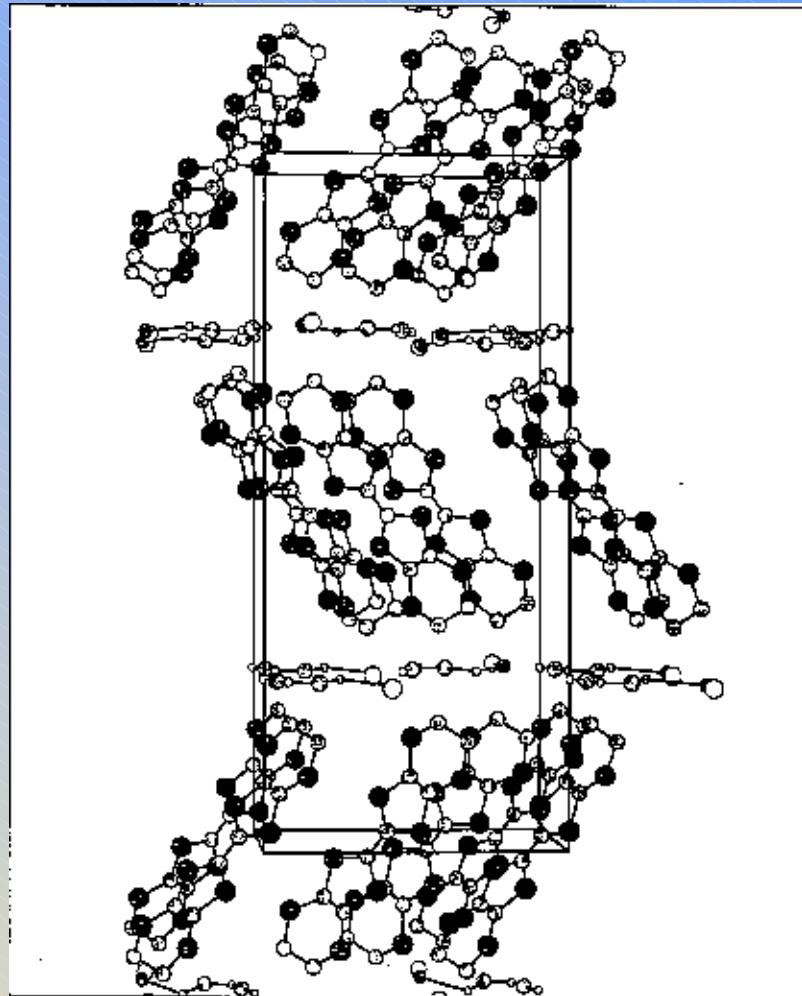


High-Temperature Superconductor belongs to a family of  
materials that exhibit exotic electronic properties.



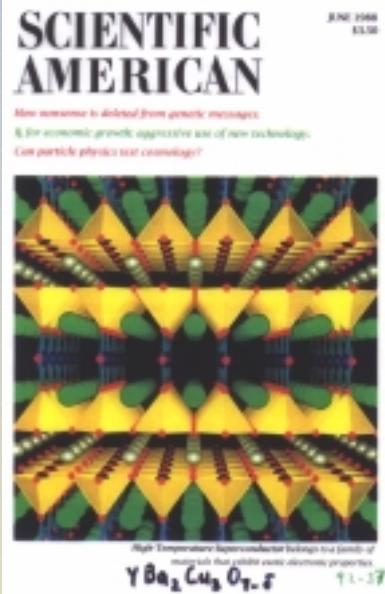
92-37

JUNE 1988  
\$3.50

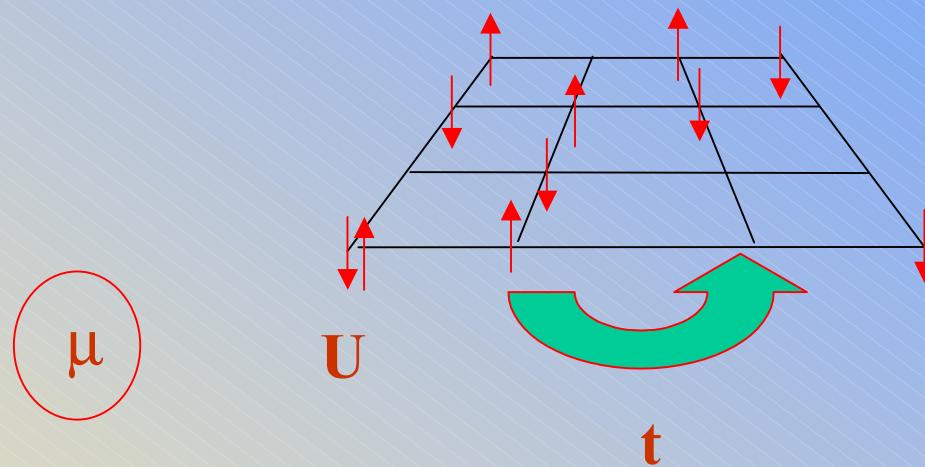


$\kappa\text{-(BEDT)}_2\text{X}$

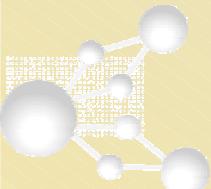




## Simplest microscopic model for $Cu O$ planes.



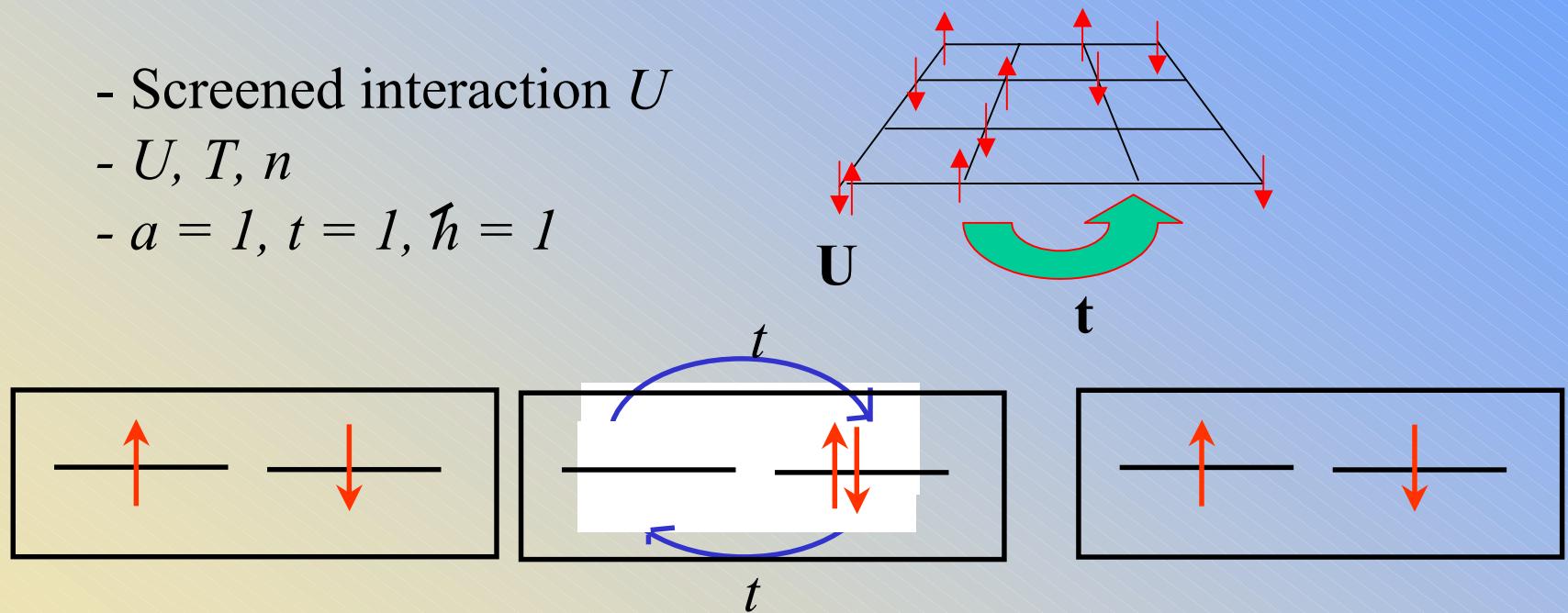
- Size of Hilbert space :  $4^N$  ( $N = 16$ )
- Compute 
$$\frac{\text{Tr}[\mathcal{O} e^{[-H/k_B T]}]}{\text{Tr}[e^{[-H/k_B T]}]}$$



## Hubbard model (Kanamori, Gutzwiller, 1963) :

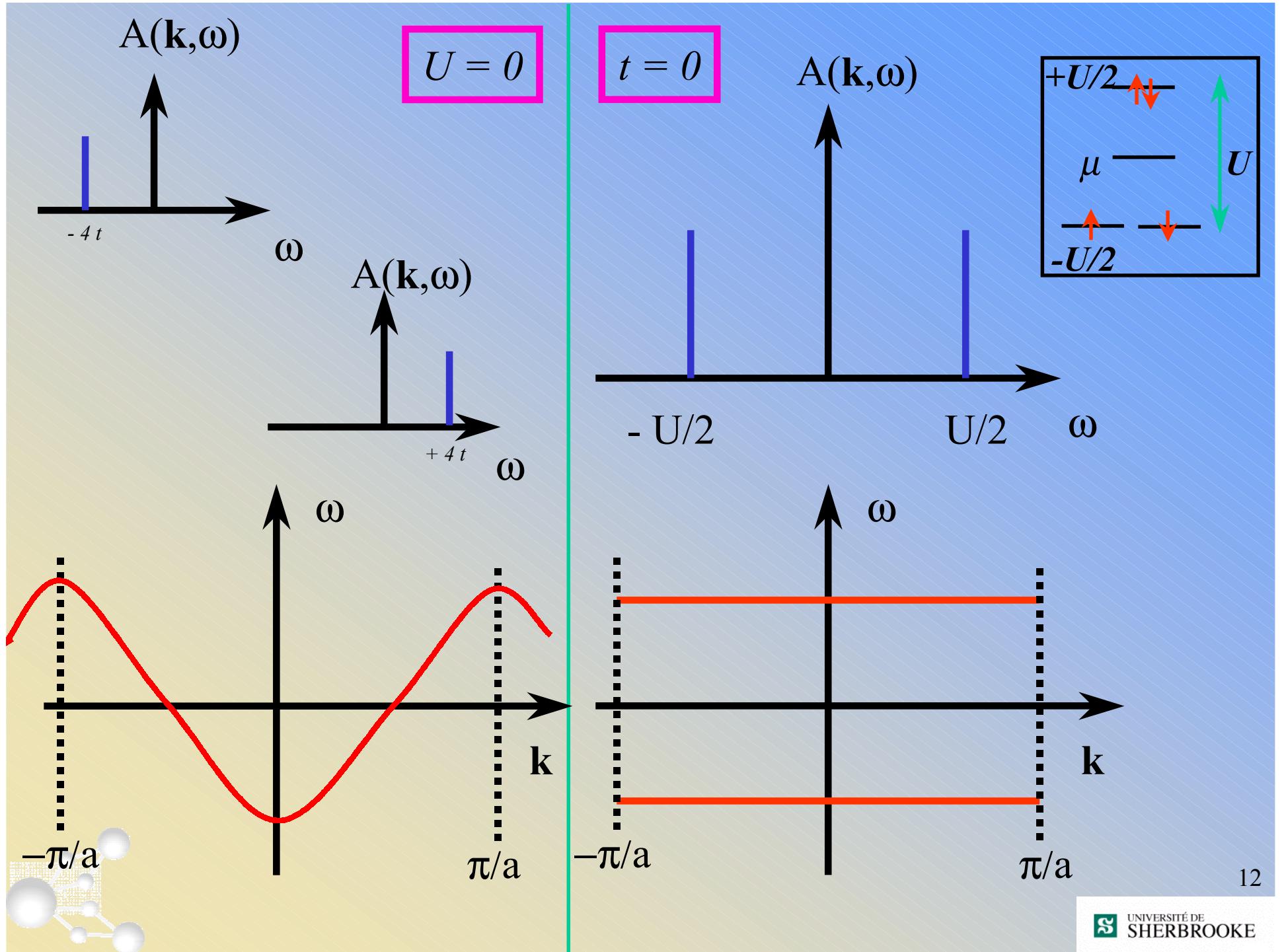
$$H = - \sum_{\langle ij \rangle \sigma} t_{i,j} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

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

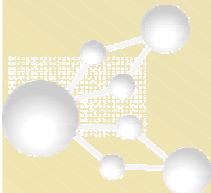
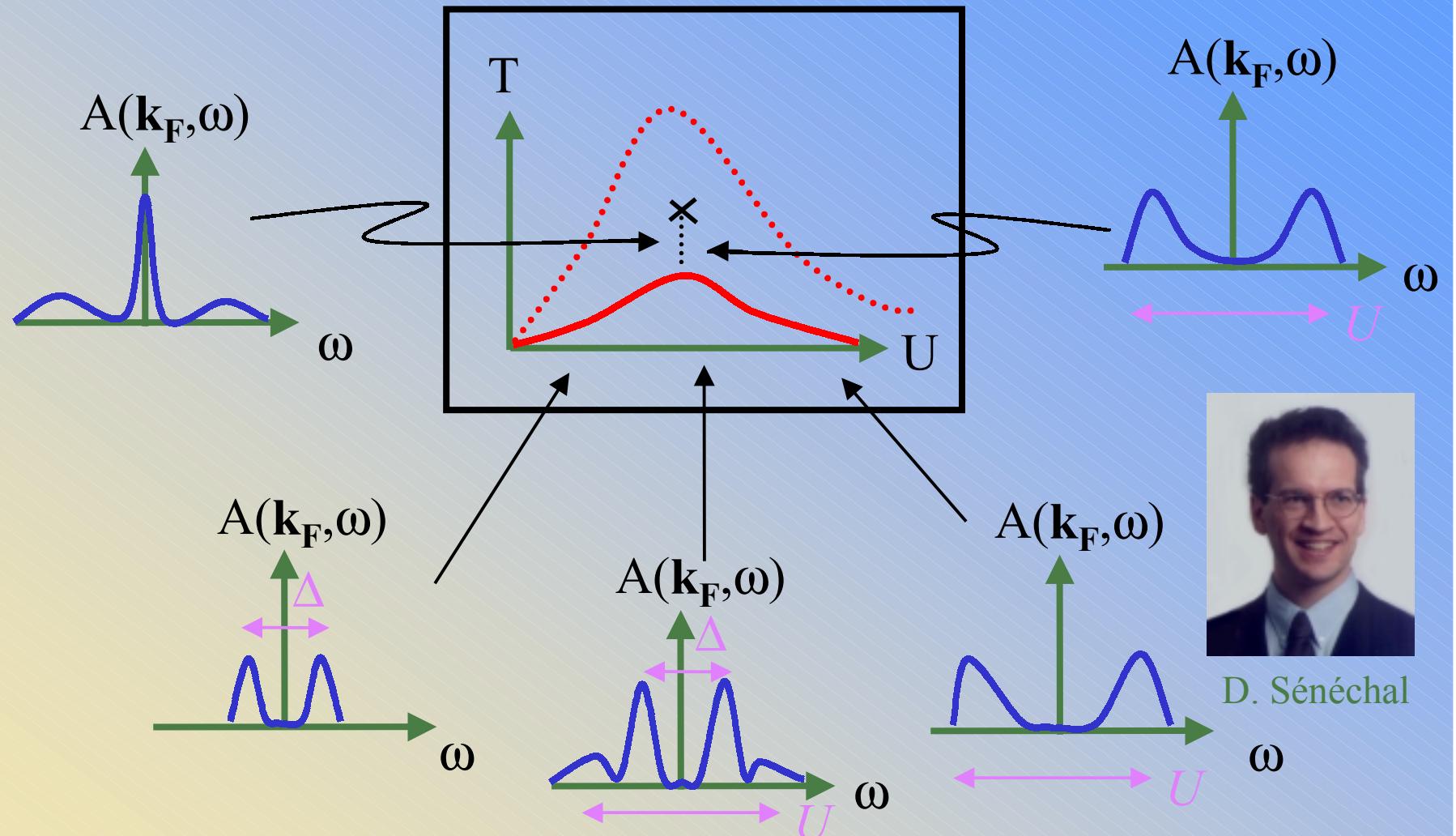


- 2001 vs 1963: Numerical solutions to check analytical approaches





## *Weak vs strong coupling*



### III. Inch our way up the weak coupling regime

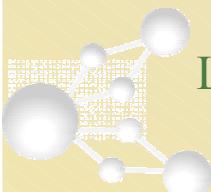
•QMC

•André Reid, Christian Boily, Hugues Nélisse

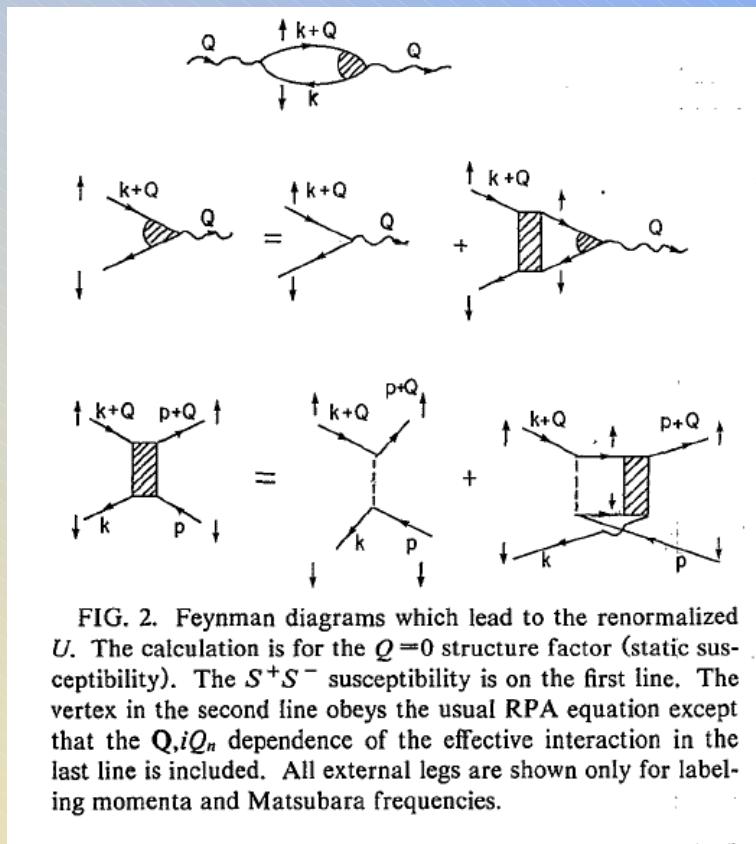
Liang Chen



Claude Bourbonnais

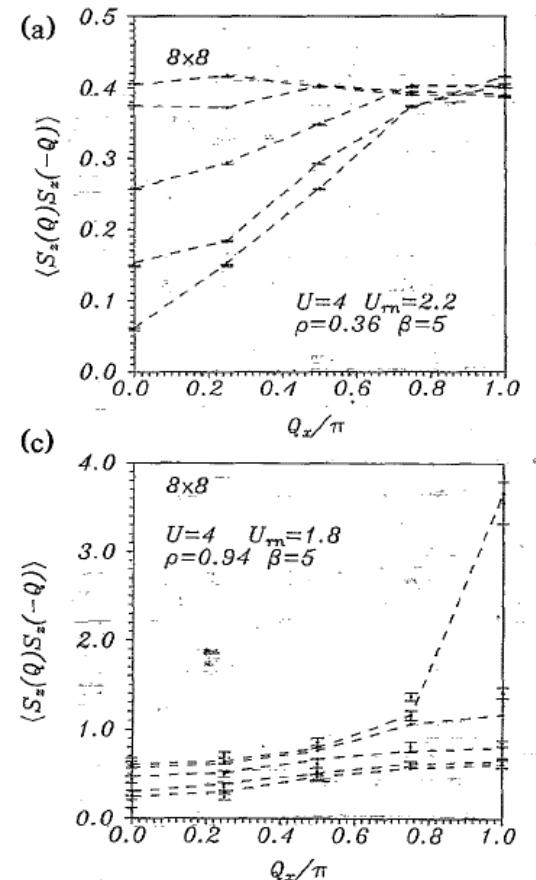


L. Chen, C. Bourbonnais, T. Li, and A.-M. S. Tremblay  
 Phys. Rev. Lett. 66, 369-372 (1991)



NUMBER 3

PHYSICAL REV



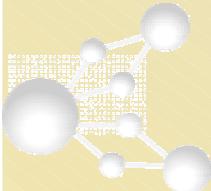
magnetic structure factor of the Hubbard model for  $8 \times 8$  RPA with a renormalized value  $U_m$  of the interaction for  $Q_y = \pi$ , with a change of  $\pi/4$  between every line. various fillings, while (d) shows a different value of  $U$  of Ref. 14 instead of RPA.

- **Problems:**

- Cannot compute charge structure factor with satisfactory accuracy
- Predicts a finite  $T$  antiferromagnetic phase transition in  $d = 2$
- Contradicts Mermin-Wagner theorem

$$(\nabla \theta)^2 \rightarrow q^2 \theta_q \theta_q \rightarrow k_B T \quad \langle \theta^2 \rangle \alpha \int d^2 q \frac{k_B T}{q^2} \rightarrow \infty$$

---



- Yury Vilk, 1993

- Forget diagrams

- Keep RPA form since satisfies conservation laws



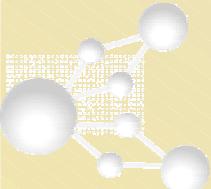
Yury Vilk

- Determine renormalized interaction from sum-rule (Singwi)

- (Double-occupancy determined self-consistently)

- Get the charge fluctuations from Pauli principle

→ • Mermin-Wagner theorem automatically satisfied



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

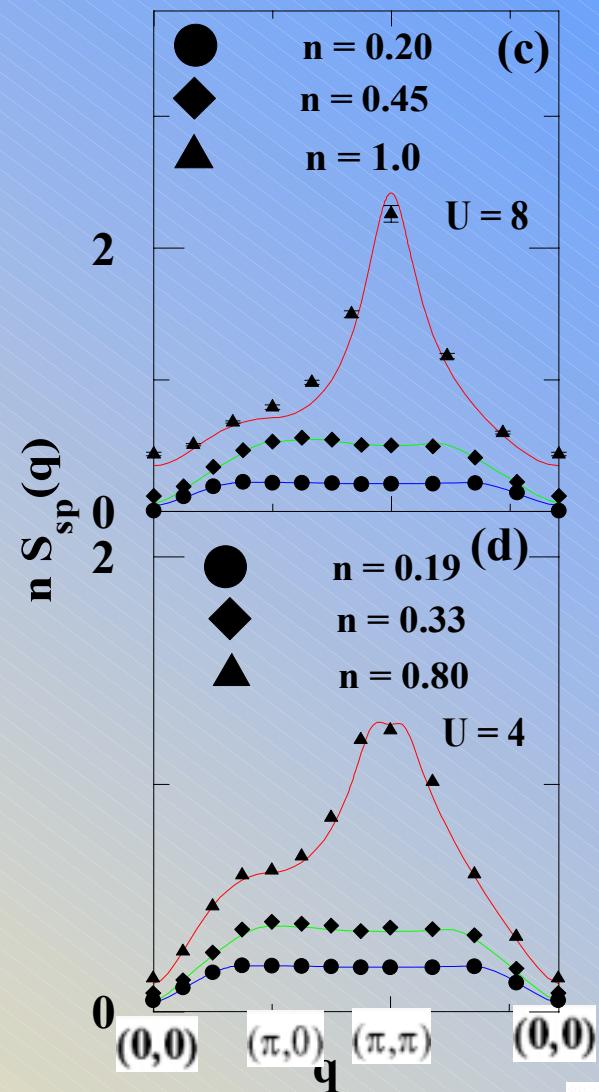
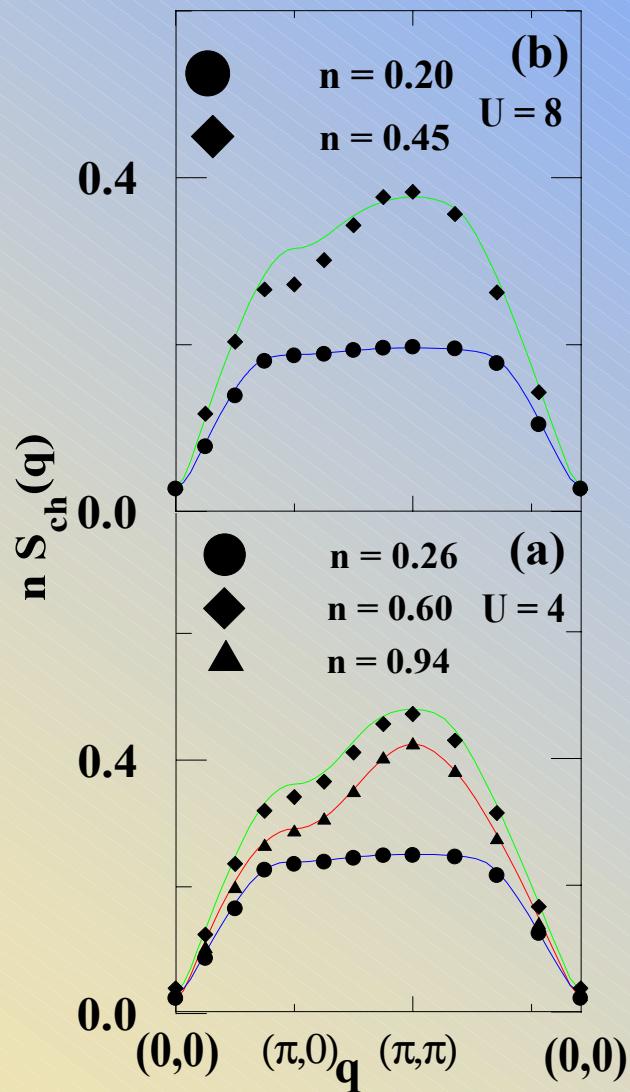
- Proofs that it works

$U > 0$

Notes:

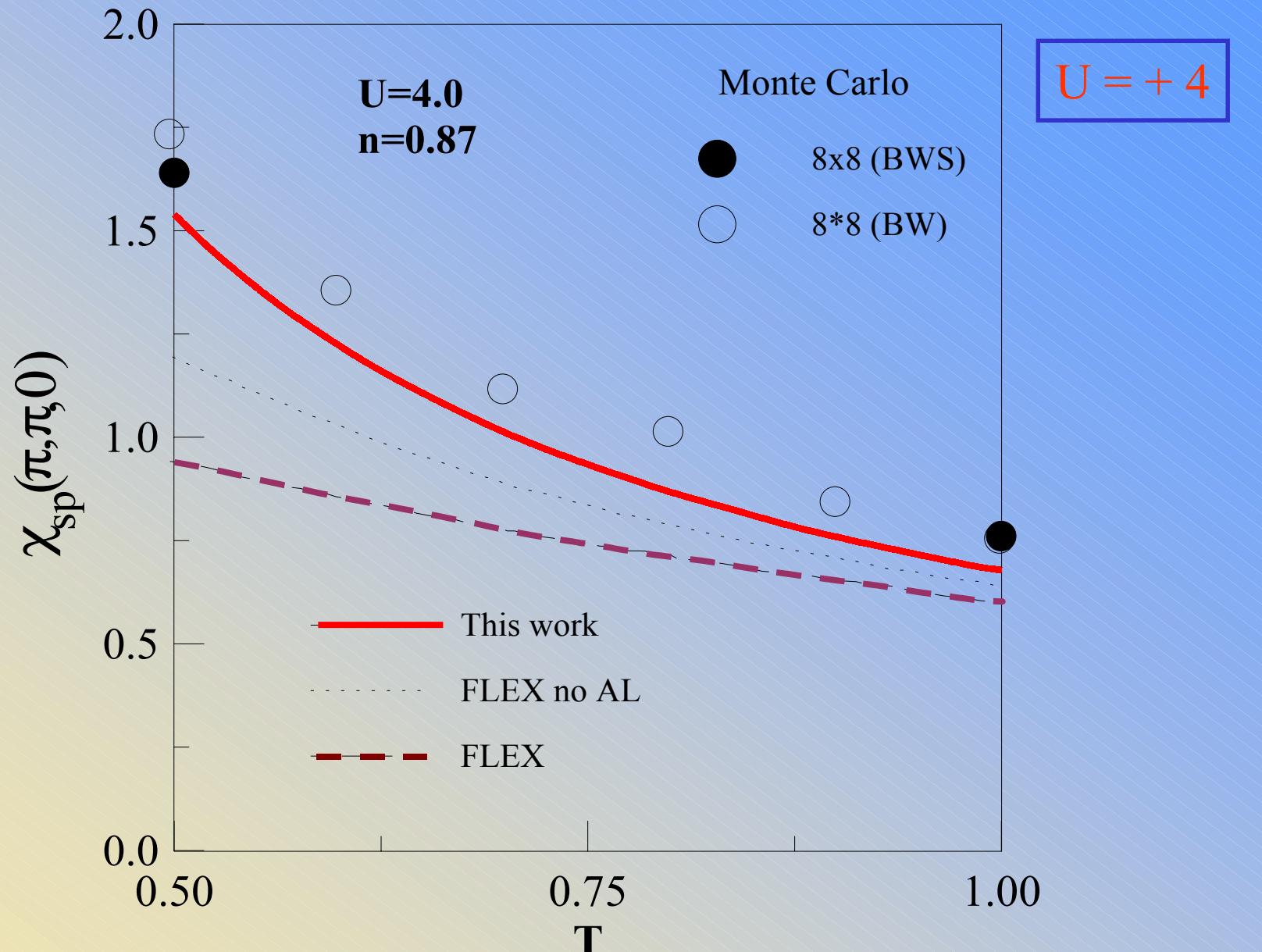
-F.L.  
parameters

-Self also  
Fermi-liquid



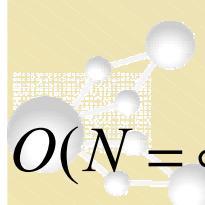
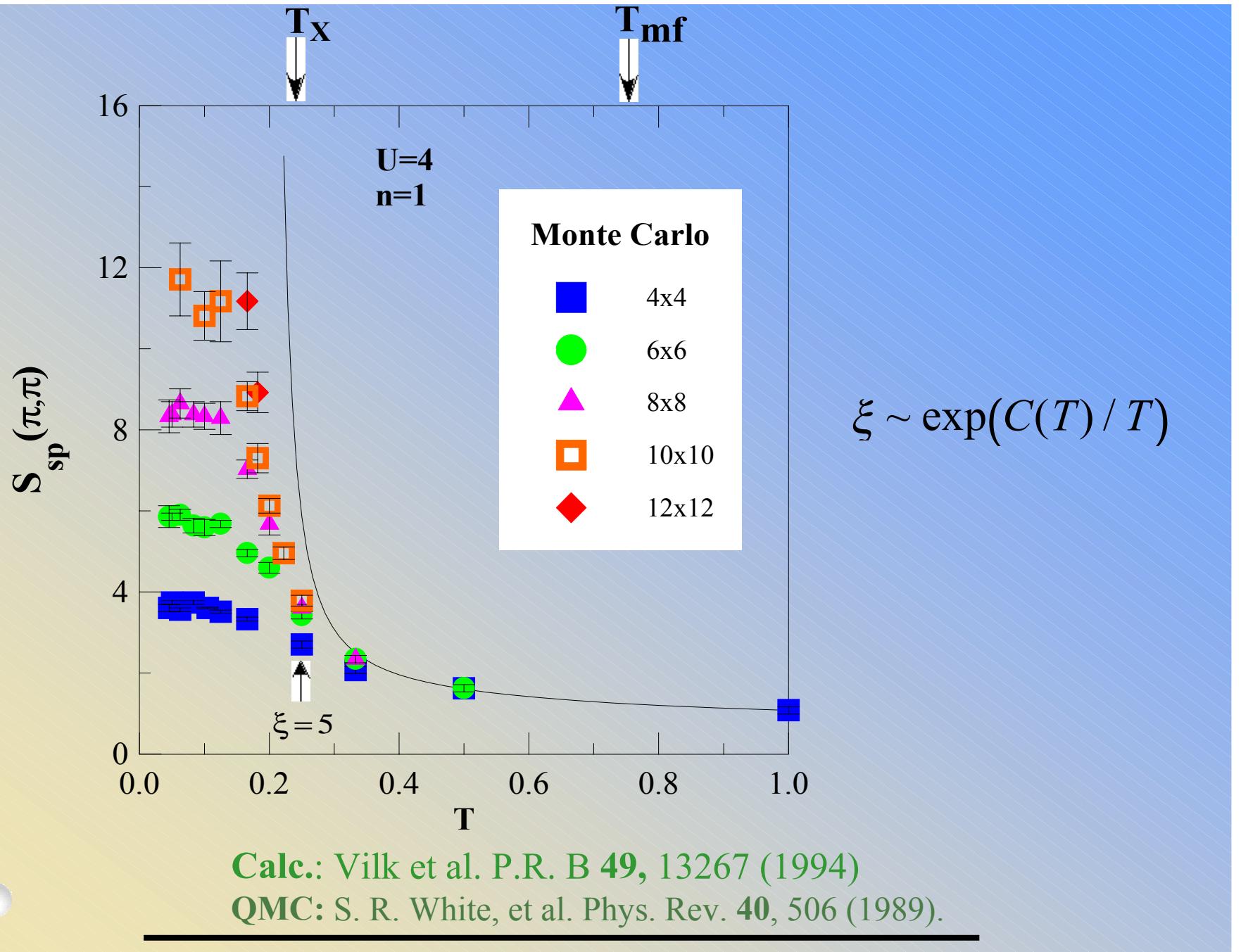
QMC + cal.: Vilk et al. P.R. B 49, 13267 (1994)

Proofs...



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

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



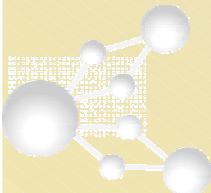
$O(N=\infty)$  A.-M. Daré, Y.M. Vilk and A.-M.S.T Phys. Rev. B **53**, 14236 (1996)

## What about single-particle properties? (Ruckenstein)

$$1 \rightarrow 2 = -1 \rightarrow 3 + 1 \rightarrow \bar{2} + 1 \rightarrow \bar{3} + 1 \rightarrow \bar{5}$$
$$1 - \Sigma - 2 = 1 \circlearrowleft 2 + 1 \rightarrow \bar{5} + 1 \rightarrow \bar{2}$$

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



# Quantitative agreement with QMC

Y. M. VILK *et al.*: DESTRUCTION OF FERMI-LIQUID QUASIPARTICLES ETC.

161

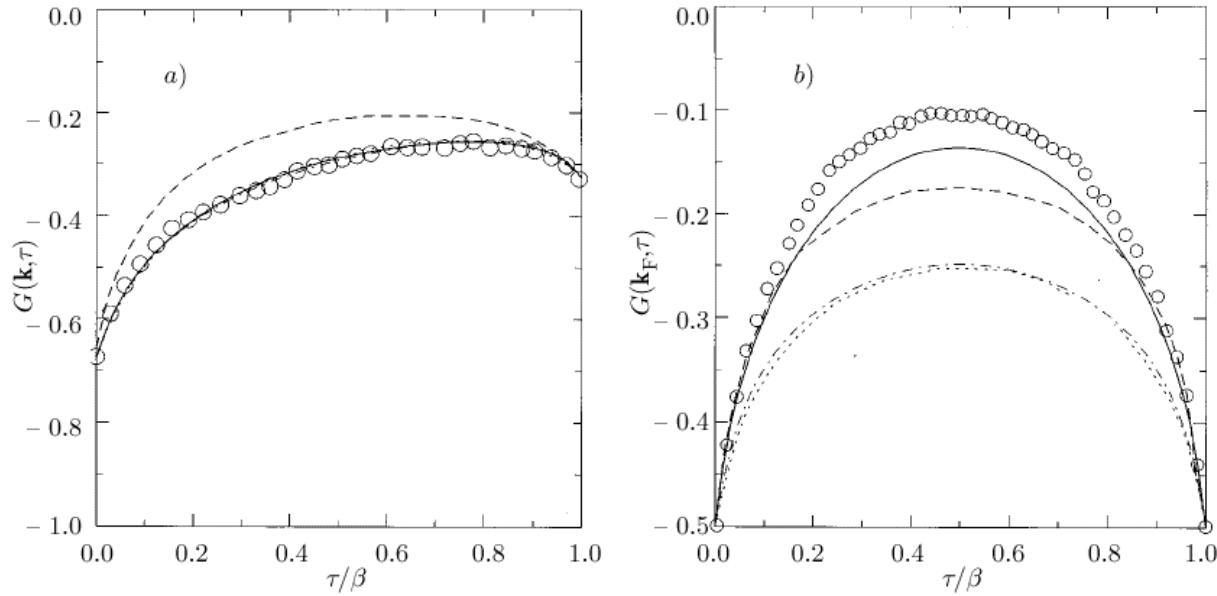
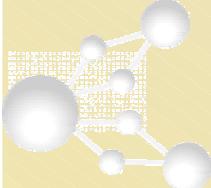


Fig. 1. – Comparison of our results for  $G(\mathbf{k}, \tau)$  (—) with Monte Carlo data (○), FLEX (---), parquet (- · - · -), and second-order perturbation theory (- · - · -), all on  $8 \times 8$  mesh with  $U = 4$ ,  $\mathbf{k}_F = (\pi, 0)$ . Monte Carlo data and results for FLEX and parquet are from ref. [4]. a)  $n = 0.875$ ,  $T = 0.25$ ; b)  $n = 1$ ,  $T = 0.17$ .



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

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

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

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

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

$$\Delta \epsilon \approx \nabla \epsilon_k \cdot \Delta k \approx v_F \hbar \Delta k = k_B T$$

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

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

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);

## IV. What was the competition up to?

FLEX

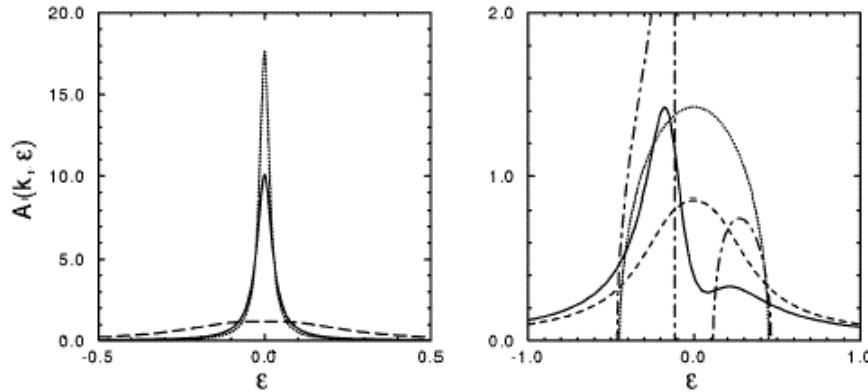


FIG. 1. Left: Spectral functions calculated in the FEA at  $T = 0.10$ , showing a dramatic reduction of spectral weight at the  $X$  point (on the Fermi surface) with a modest increase in  $U$  between  $T = 0.10$  and  $U = 1.0$  (dotted) and  $2.3$  (dashed). Also shown for  $U = 2.3$  (solid) is a calculation with only the second order skeleton diagram. Right: FEA spectral functions for  $\mathbf{k} = (0.891\pi, 0)$  (solid) and  $\mathbf{k} = (\pi, 0)$  (dashed) shown in comparison with those for the simple spin fluctuation model (long-dash-short-dashed and dotted, respectively) for  $\tilde{t}_{sp} = 0.05$ .

QMC

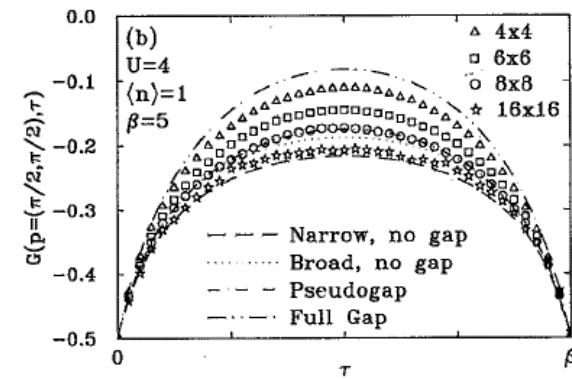
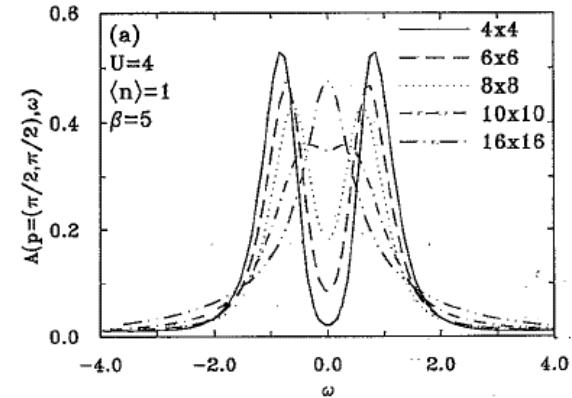


FIG. 1. (a) The spectral weight function  $A(p, \omega)$ , evaluated at  $p = (\pi/2, \pi/2)$  for different lattice sizes for  $U=4$  and  $\beta=5$ . (b) The Matsubara Green's function,  $G(p, \tau)$ , for  $\beta=5$  with  $U=4$  for different lattice sizes with reference curves for comparison obtained from a narrow spectrum with no gap (dashed line), a broad spectrum with no gap (dotted line), a pseudogap (dash-dot line), and a full gap (dashed-double-dotted line).

J. J. Deisz, D. W. Hess, and J. W. Serene  
Phys. Rev. Lett. 76, 1312-1315 (1996)

M. Vekic and S. R. White, Phys. Rev. B 47, 1160–1163 (1993)

## State of the art analytical tools

$$\Phi [G] = \text{Diagram showing two nodes connected by a dashed red line with clockwise arrows in each node}$$

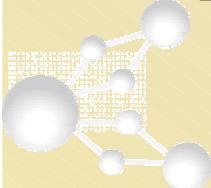
$$+ \frac{1}{2} \text{Diagram showing two nodes connected by a dashed red line with clockwise arrows in each node, plus a vertical dashed red line between them} + \dots$$

$$\Sigma [G] = \delta \Phi [G] / \delta G =$$

$$\text{Diagram showing a single node with a clockwise arrow, plus a horizontal black arrow pointing right, plus a vertical dashed red line between them} + \dots$$

$$\Gamma [G] = \delta \Sigma [G] / \delta G =$$

$$\text{Diagram showing two nodes connected by a dashed red line with clockwise arrows in each node}$$



## Advantages

- Thermodynamically consistent:

$$dF/d\mu = \text{Tr}[G]$$

- Satisfies Luttinger theorem

(Volume of Fermi surface at  $T = 0$  preserved)

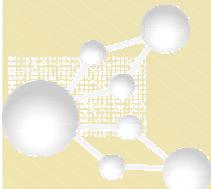
- Satisfies Ward identities (conservation laws):

$G_2(1,1;2,3)$  appropriately related to  $G(1,2)$

Gordon Baym, Phys. Rev. **127**, 1391 (1962).

N.E. Bickers and D.J. Scalapino, Annals of Physics, **193**, 206 (1989)

FLEX

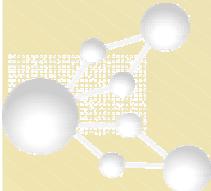


## Disdvantages

- Integration over coupling constant of potential energy does not give back the starting Free energy.
- The Pauli principle in its simplest form is not satisfied (It is used in defining the Hubbard model in the first place)
- There is an infinite number of conserving approximations (How do we pick up the diagrams?)
- Inconsistency:  
Strongly frequency-dependent self-energy, constant vertex



No Migdal theorem, so vertex corrections should be included



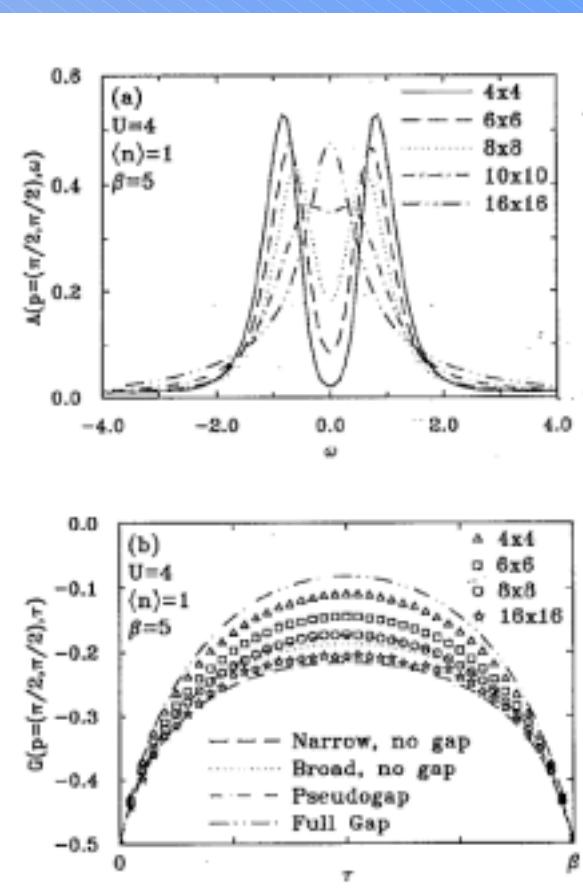
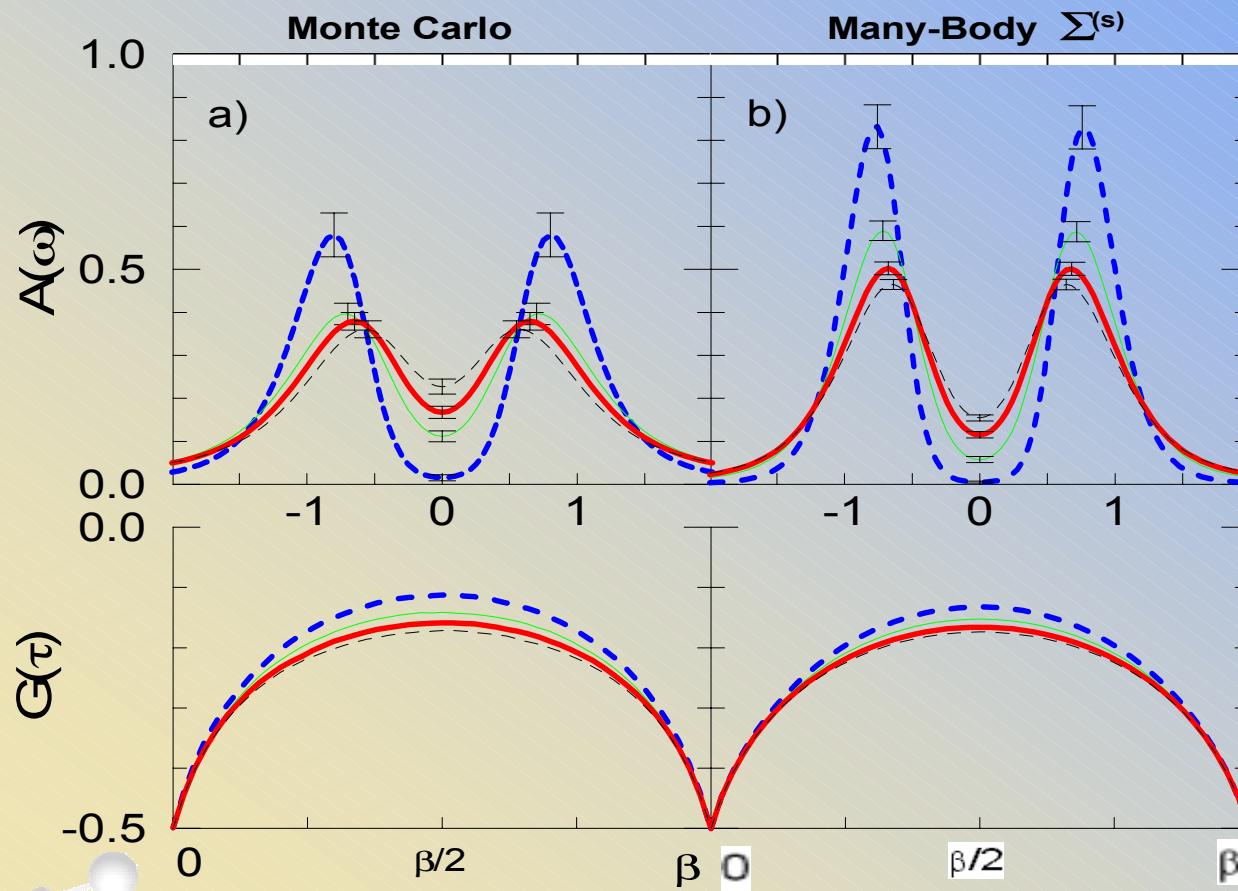
Back to us



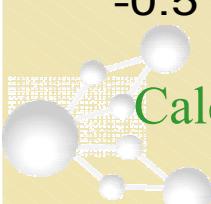
$U = +4$

H. Touchette

D. Poulin



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





S. Moukouri



F. Lemay



S. Allen

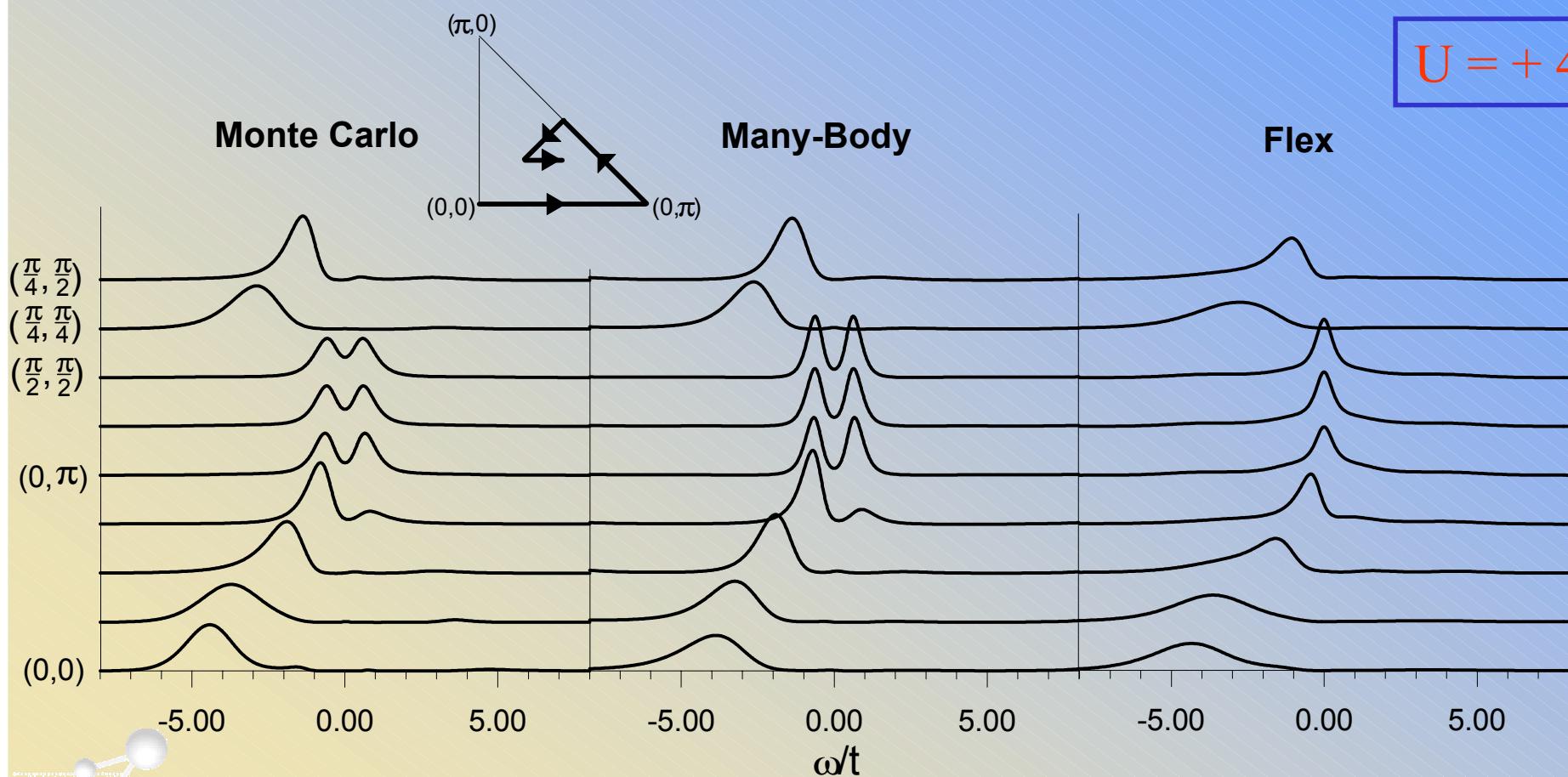


Y. Vilk

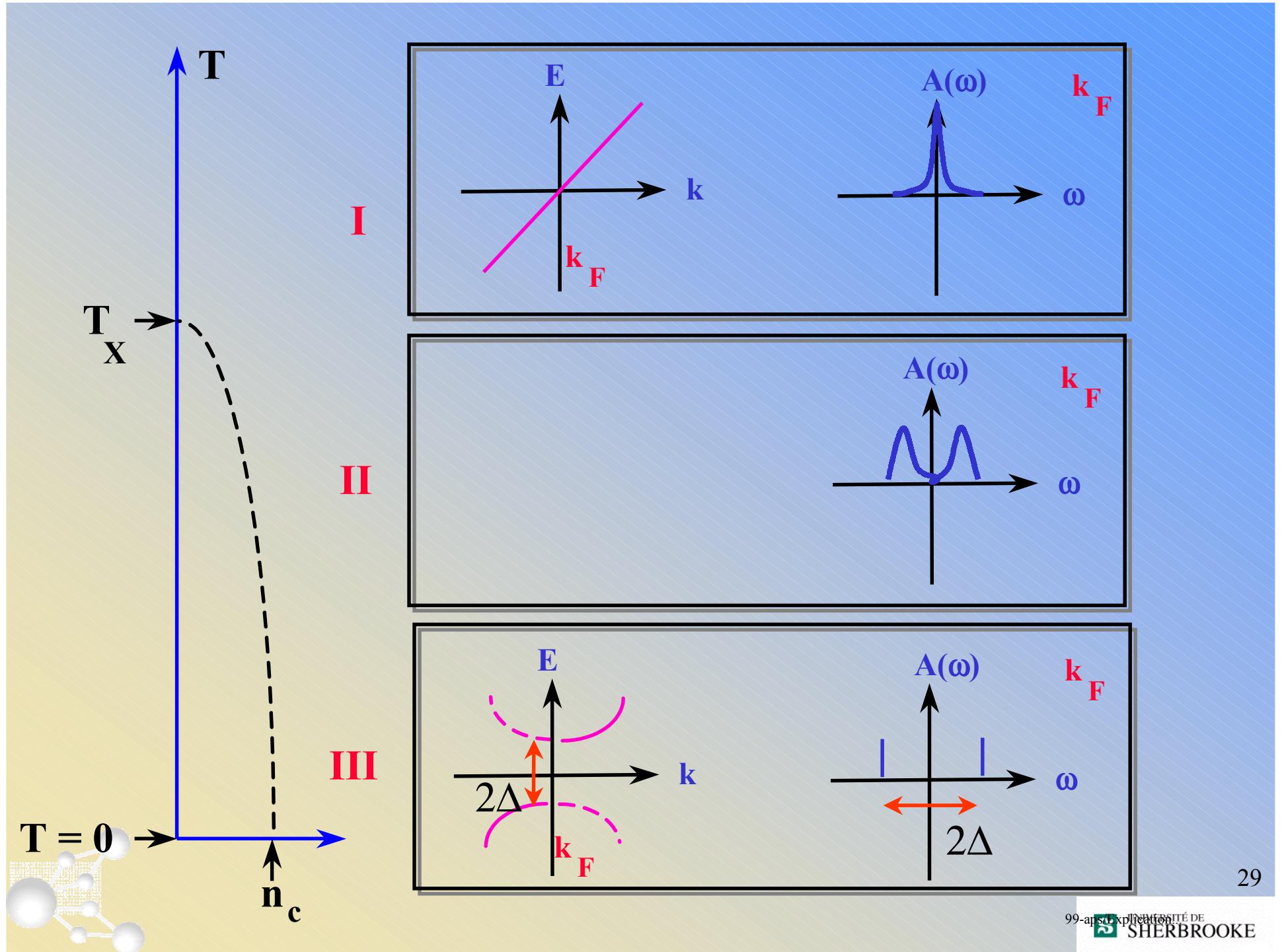


B. Kyung

$U = +4$



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



How it works...

## First step: Two-Particle Self-Consistent



$$\Sigma_{\sigma}^{(1)}(1, \bar{1}) G_{\sigma}^{(1)}(\bar{1}, 2) = A G_{-\sigma}^{(1)}(1, 1^+) G_{\sigma}^{(1)}(1, 2) \quad \text{S. Allen}$$

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

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

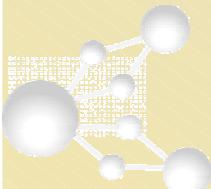
is satisfied. One finds

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

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



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



Y. Vilk

## How it works...

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

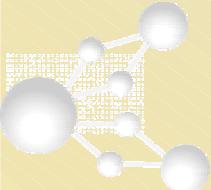
$$\begin{aligned} \left\langle (n_{\uparrow} - n_{\downarrow})^2 \right\rangle &= \langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle - 2 \langle n_{\uparrow} n_{\downarrow} \rangle \\ \boxed{\frac{T}{N} \sum_{\tilde{q}} \frac{\chi_0(q)}{1 - \frac{1}{2} U_{sp} \chi_0(q)}} &= n - 2 \langle n_{\uparrow}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

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

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

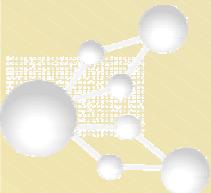
$$\Sigma_\sigma(1, \bar{1}) G_\sigma(\bar{1}, 2) = -U \left[ \frac{\delta G_\sigma(1, 2)}{\delta \phi_{-\sigma}(1^+, 1)} - G_{-\sigma}(1, 1^+) G_\sigma(1, 2) \right]$$

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

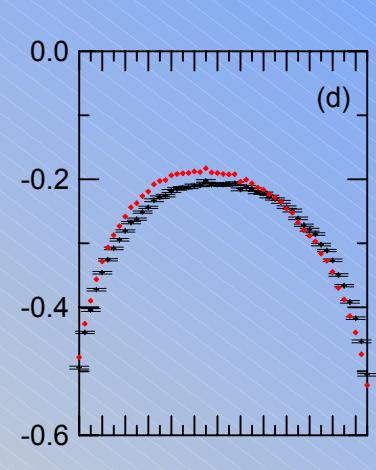
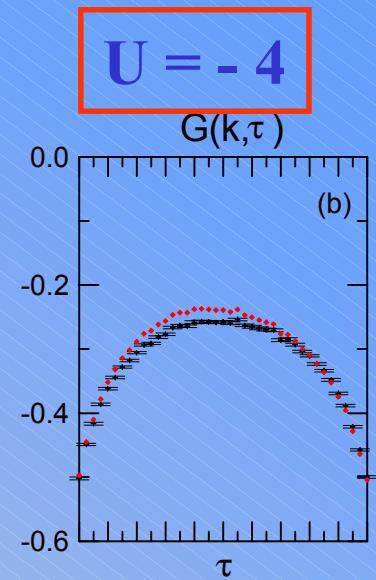
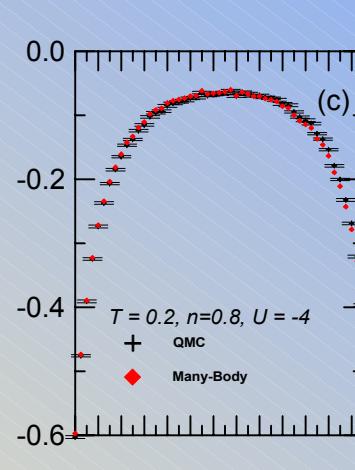
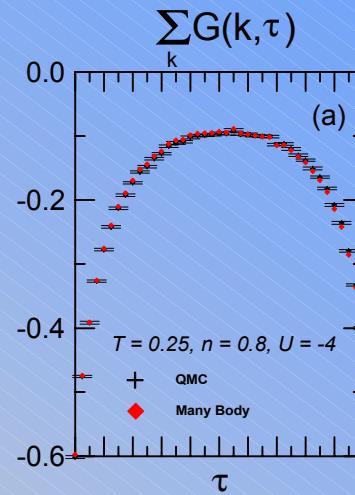
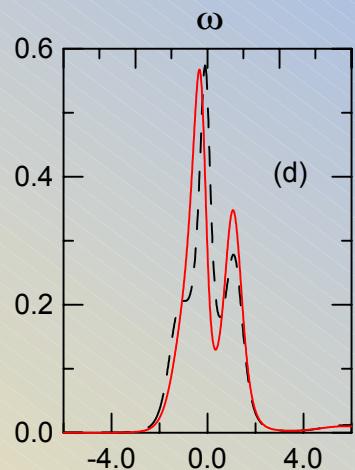
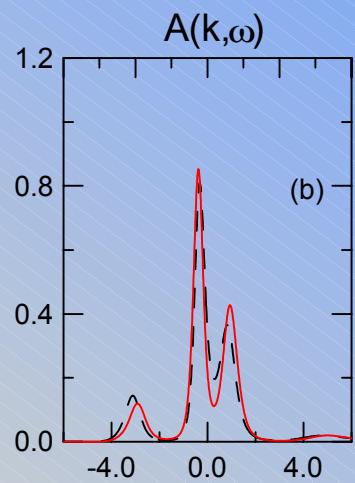
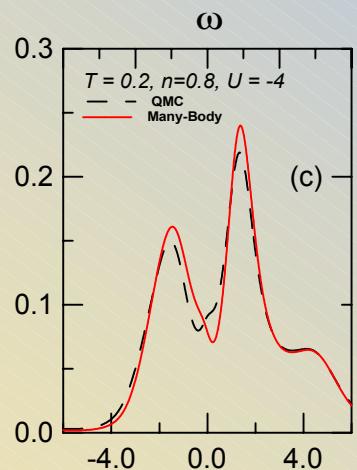
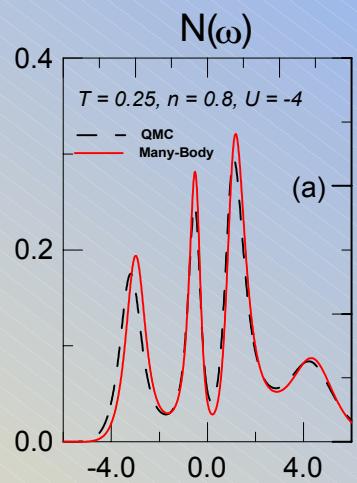
$$\boxed{\Sigma_\sigma^{(2)}(k) = U n_{-\sigma} + \frac{U}{8} \frac{T}{N} \sum_q \left[ 3U_{sp} \chi_{sp}^{(1)}(q) + U_{ch} \chi_{ch}^{(1)}(q) \right] G_\sigma^{(1)}(k + q).} \quad (4)$$



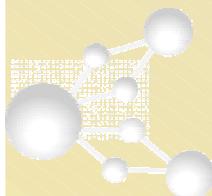
# Proof that generalization for $U < 0$ works



S. Allen

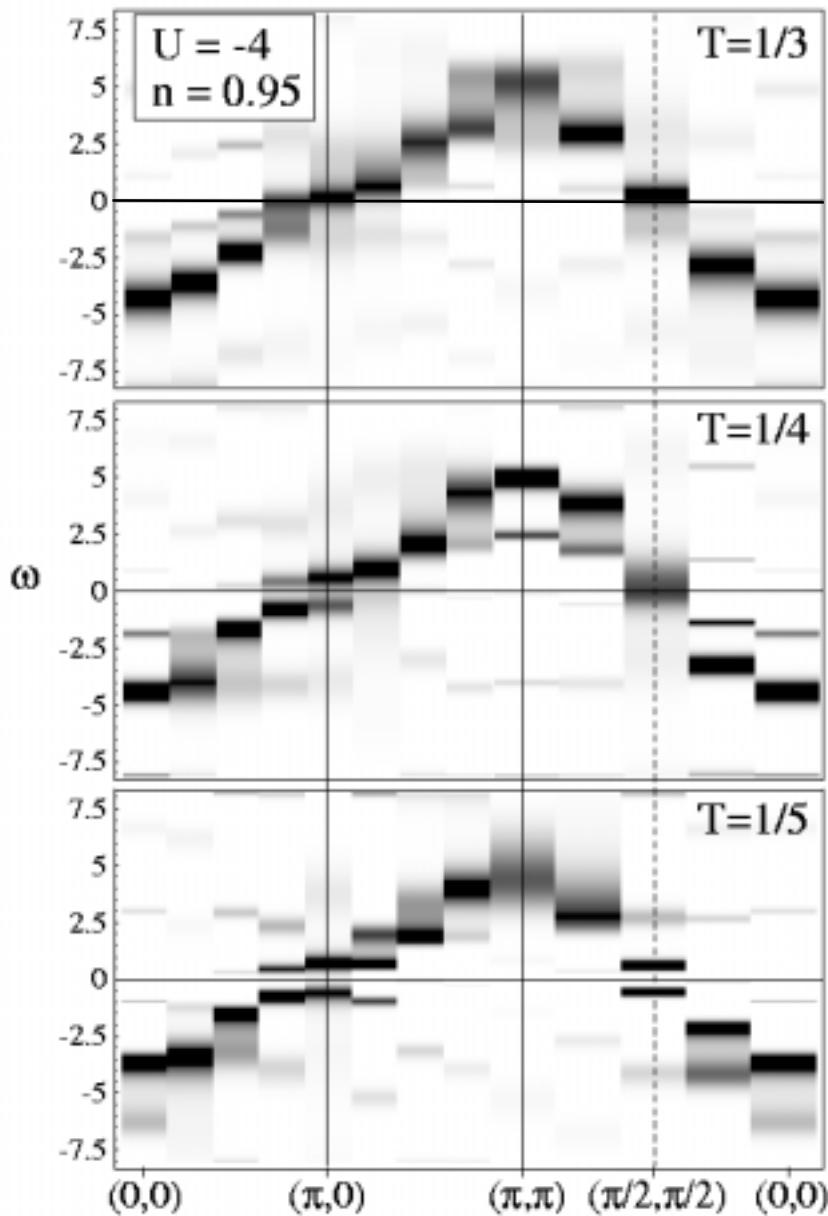


B. Kyung



Kyung et al. cond-mat/0010001

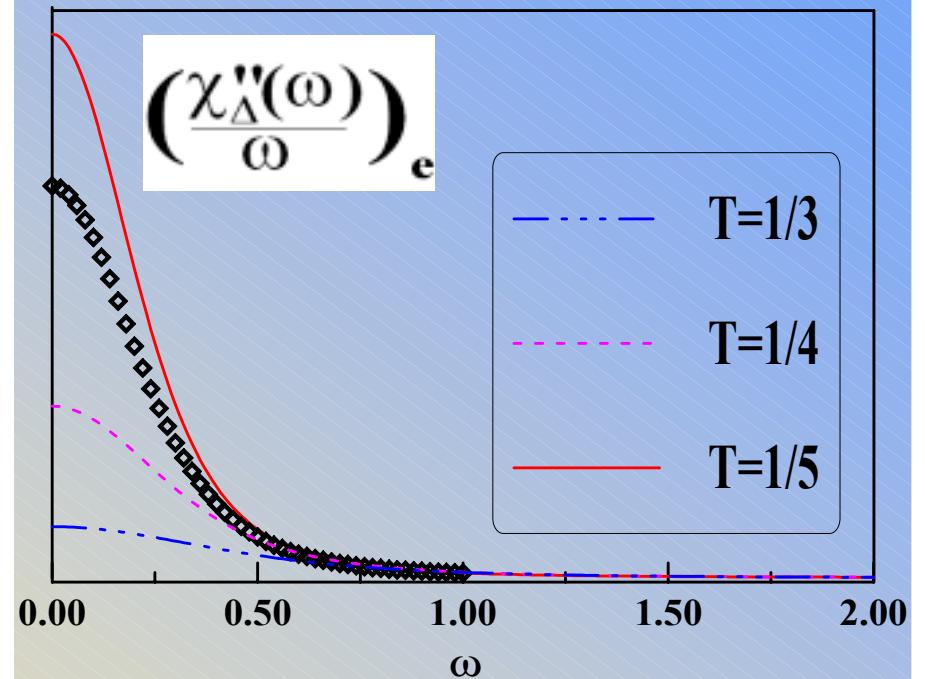
# Mechanism for pseudogap formation in the attractive model:



$U = -4$

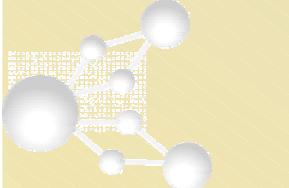
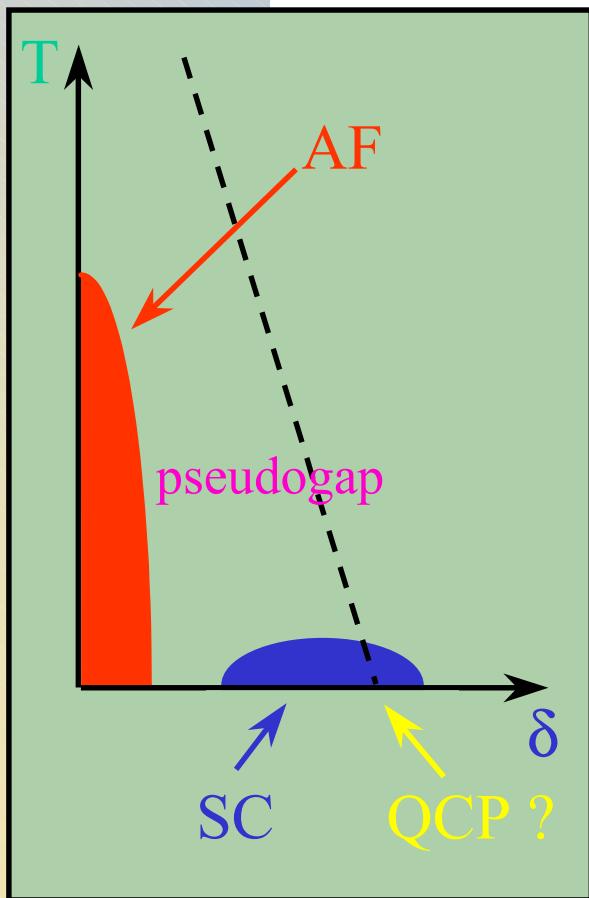
$d = 2$  is **crucial**

Even part of the pair susceptibility at  $q = 0$ , for different temperatures



Allen, et al. P.R. L 83, 4128 (1999) 34

$U > 0$



- Renormalized classical regime  
for spin fluctuations in pseudogap regime?

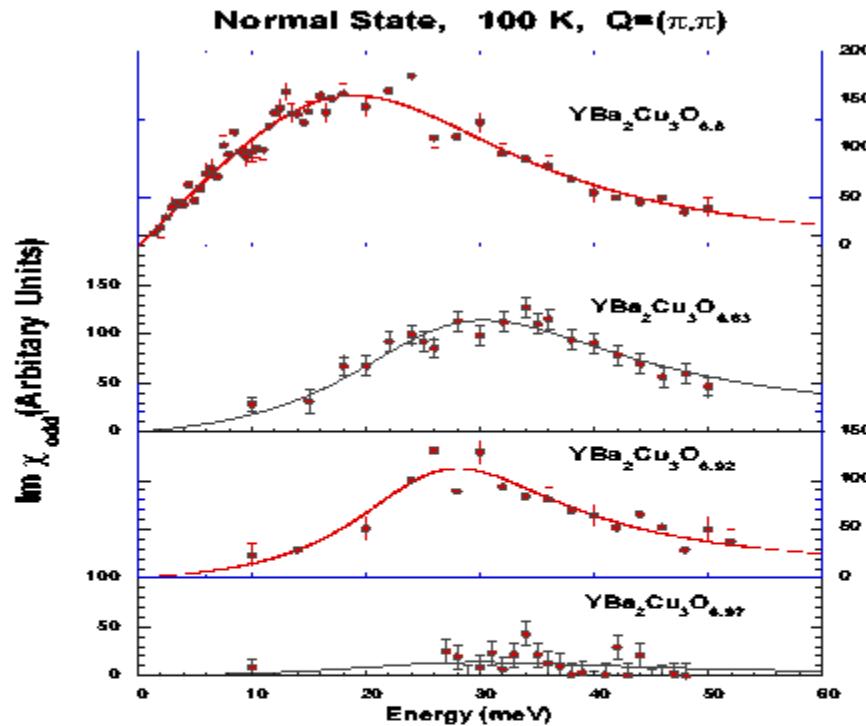


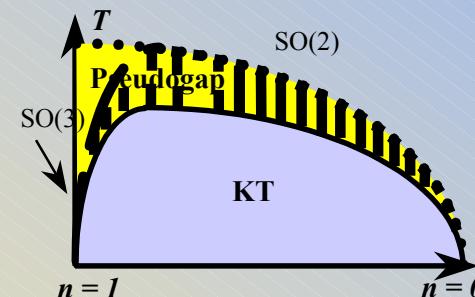
Figure 2: Normalized imaginary part of the spin susceptibility at the AF wavevector in the normal state, at  $T = 100$  K, for four oxygen contents in YBCO ( $T_c=15, 85, 91, 92.5$  K for  $x=0.5, 0.83, 0.92, 0.97$  respectively). These curves have been normalized to the same units using standard phonon calibration<sup>14</sup> (100 counts in the vertical scale roughly correspond to  $\sim 250 \mu_B^2/\text{eV}$  in absolute units) (from<sup>10</sup>).

Philippe Bourges cond-mat/0009373

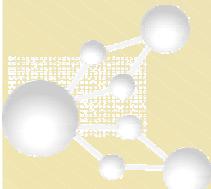
**U < 0**

## 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)

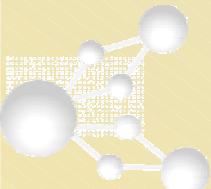


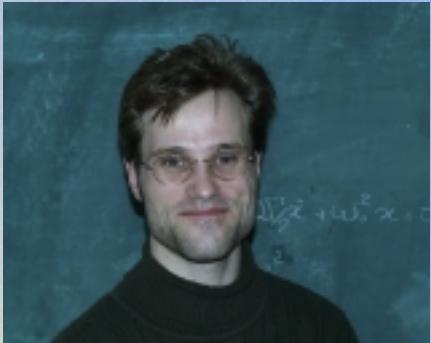
36



## V. Conclusion

- What is happening now?
  - Methods for thermodynamics and for crossed channels.
- Computers :
  - Small sizes, not all relevant parameter regimes are accessible
- Analytical studies :
  - No small parameter, no perfect approximation
- Limiting cases, physical intuition
  - Not always reliable





Steve Allen



François Lemay



David Poulin

Liang Chen



Yury Vilk



Bumsoo Kyung

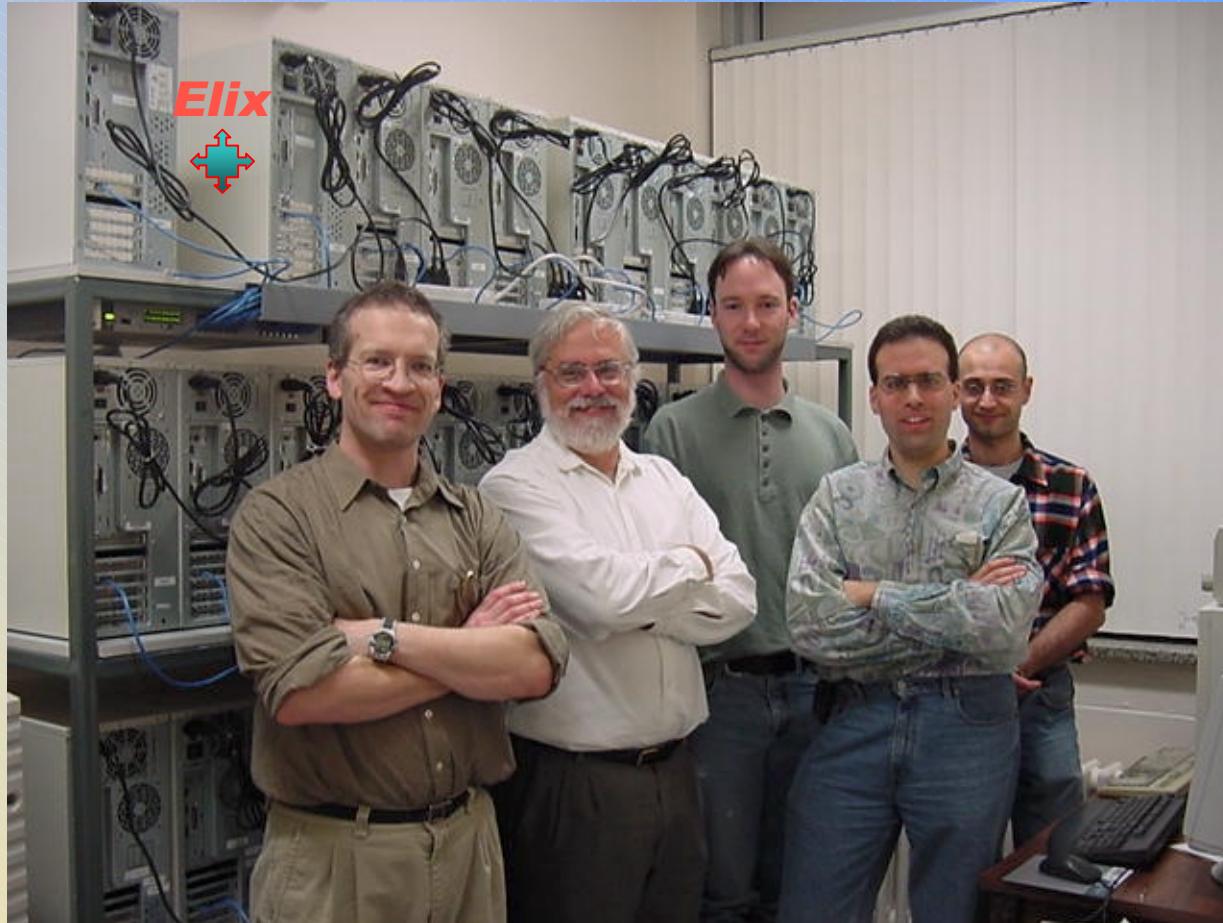
Samuel Moukouri

Hugo Touchette



Michel Barrette

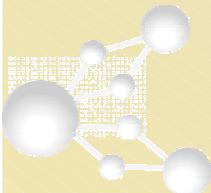
Mehdi Bozzo-Rey



David Sénéchal

A.-M.T.

Alain Veilleux





Claude Bourbonnais

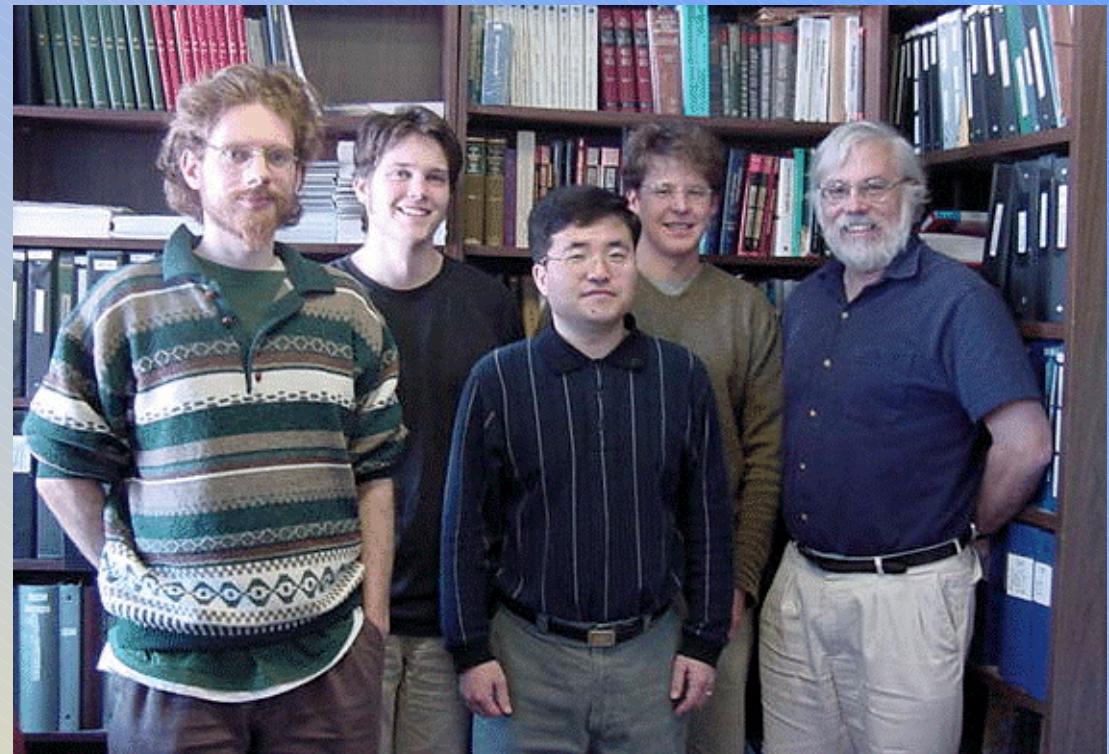


R. Côté



D. Sénéchal

Sébastien Roy    Alexandre Blais



Jean-Sébastien Landry

A-M.T.

Bumsoo Kyung

- 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?

