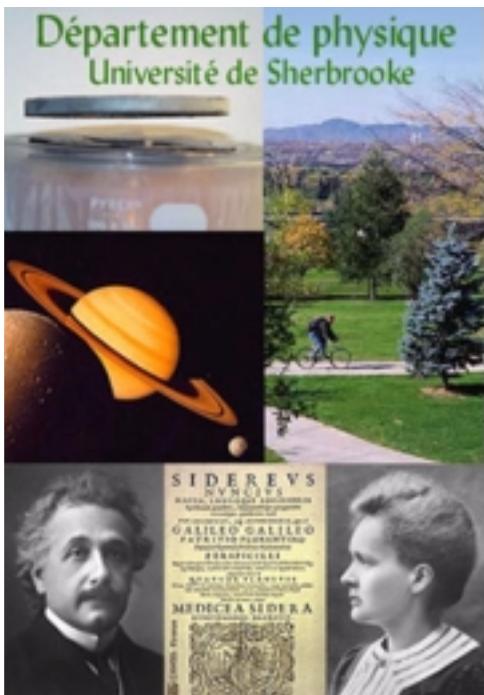
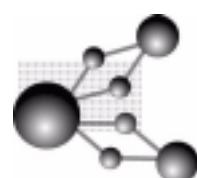


The standard model, from weak to intermediate coupling



André-Marie Tremblay



CENTRE DE RECHERCHE SUR LES PROPRIÉTÉS
ÉLECTRONIQUES
DE MATÉRIAUX AVANCÉS

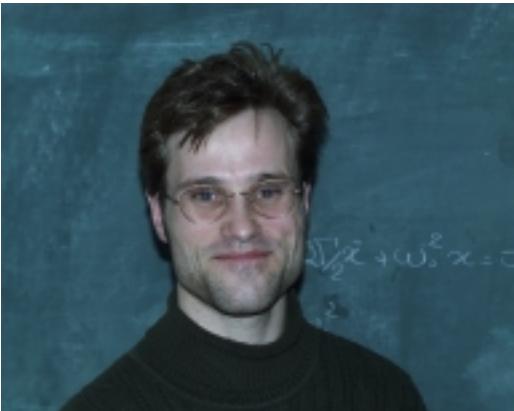


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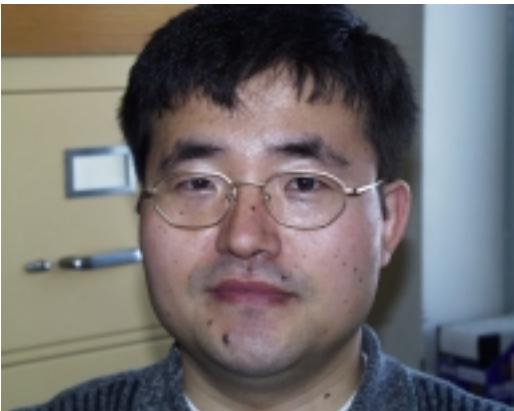


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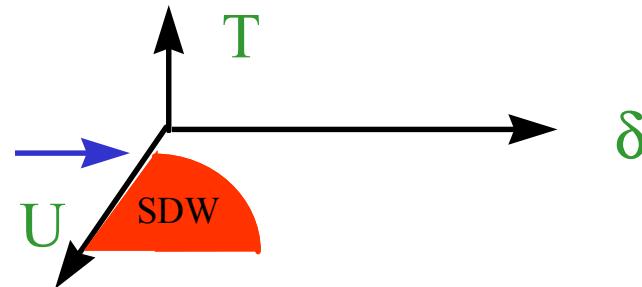


Hugo Touchette



1. Motivation

- Here, $-W < U < W$ with ($W = 8t$)
 - Relevant for high T_c where $U > W$?
 - A question of threshold (and continuity)



- Importance of quantitative predictions
 - Location of QCP
 - No ferromagnetism
- Effective $U < 0$ model may be not too strongly interacting
- Suppose we find new quasiparticles in strong coupling. How do we study residual interactions?
- Do we give up calculating Landau parameters?
 - How to predict when the theory is bad?
- Standard method gives qualitatively incorrect results⁴

Outline

1. Motivation

2. The standard approach :

- what it is
- a qualitatively incorrect result
- limitations of the approach

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

- Proof that it works
- How it works

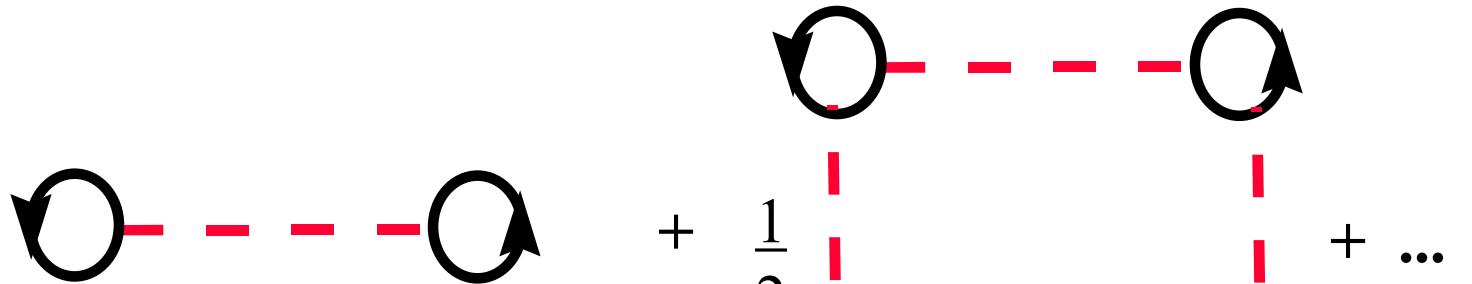
4. Results:

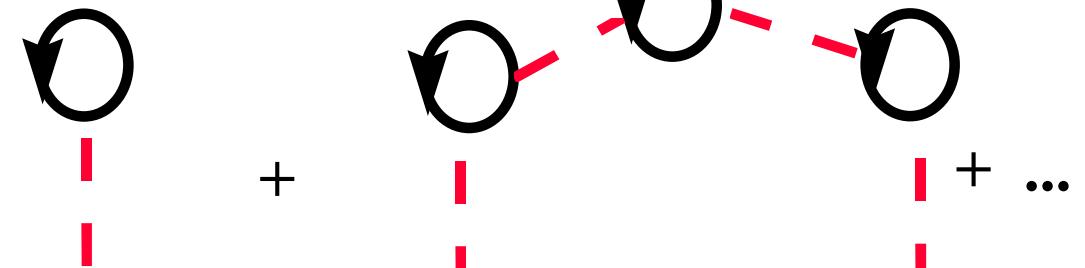
- Mechanism for pseudogap
- Spectral weight rearrangement

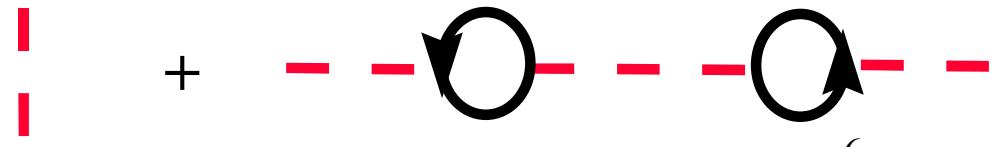
5. Conclusion.

2. The standard approach :

- what it is (FLEX, self-consistent T-matrix ...)

$$\Phi [G] = \text{Diagram} + \frac{1}{2} \text{Diagram} + \dots$$


$$\Sigma [G] = \delta \Phi [G] / \delta G = \text{Diagram} + \text{Diagram} + \dots$$


$$\Gamma [G] = \delta \Sigma [G] / \delta G = \text{Diagram} + \text{Diagram} - \dots$$


2. The standard approach :

- what it is (FLEX, self-consistent T-matrix ...)

- Thermodynamically consistent:

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

- Satisfies Luttinger theorem

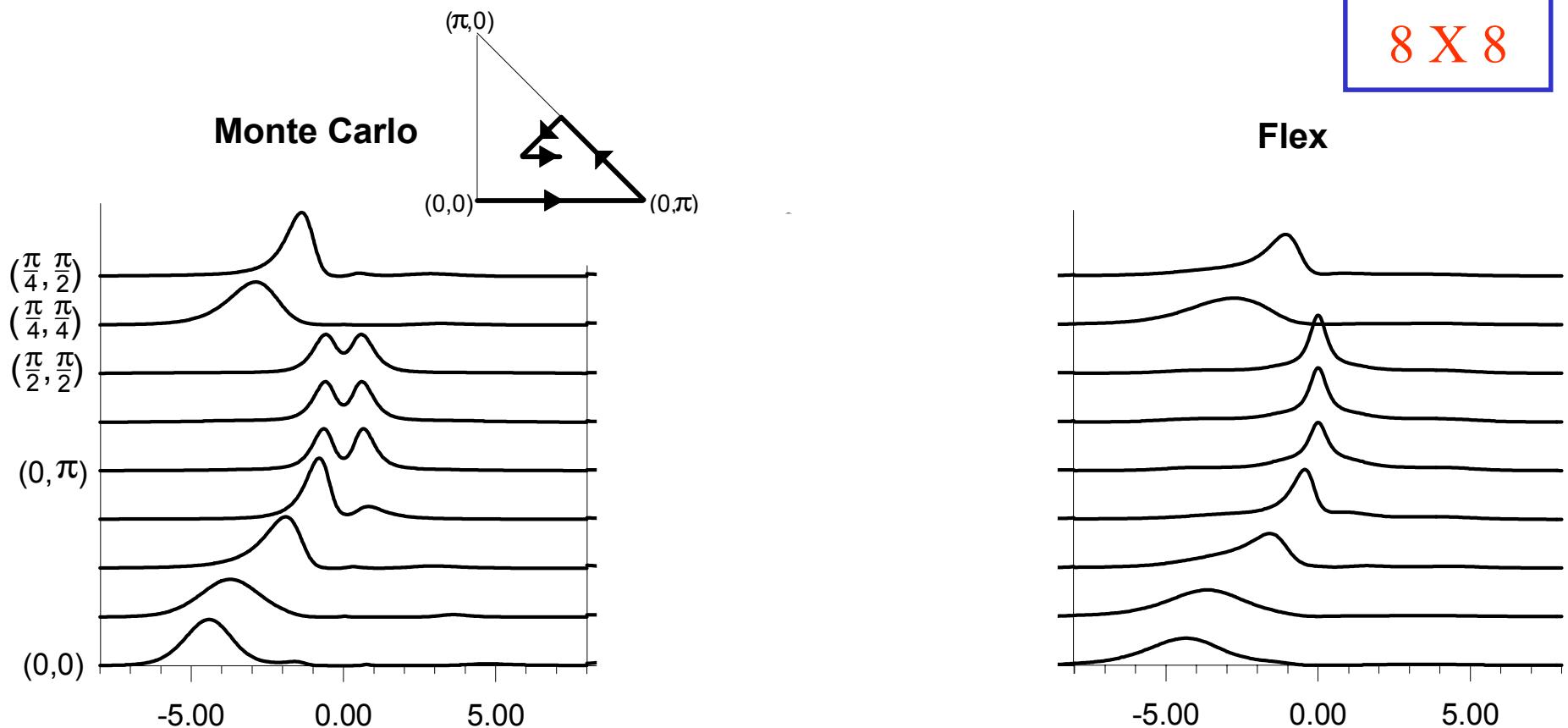
(Volume of Fermi surface at $T = 0$ preserved)

- Satisfies Ward identities (conservation laws):

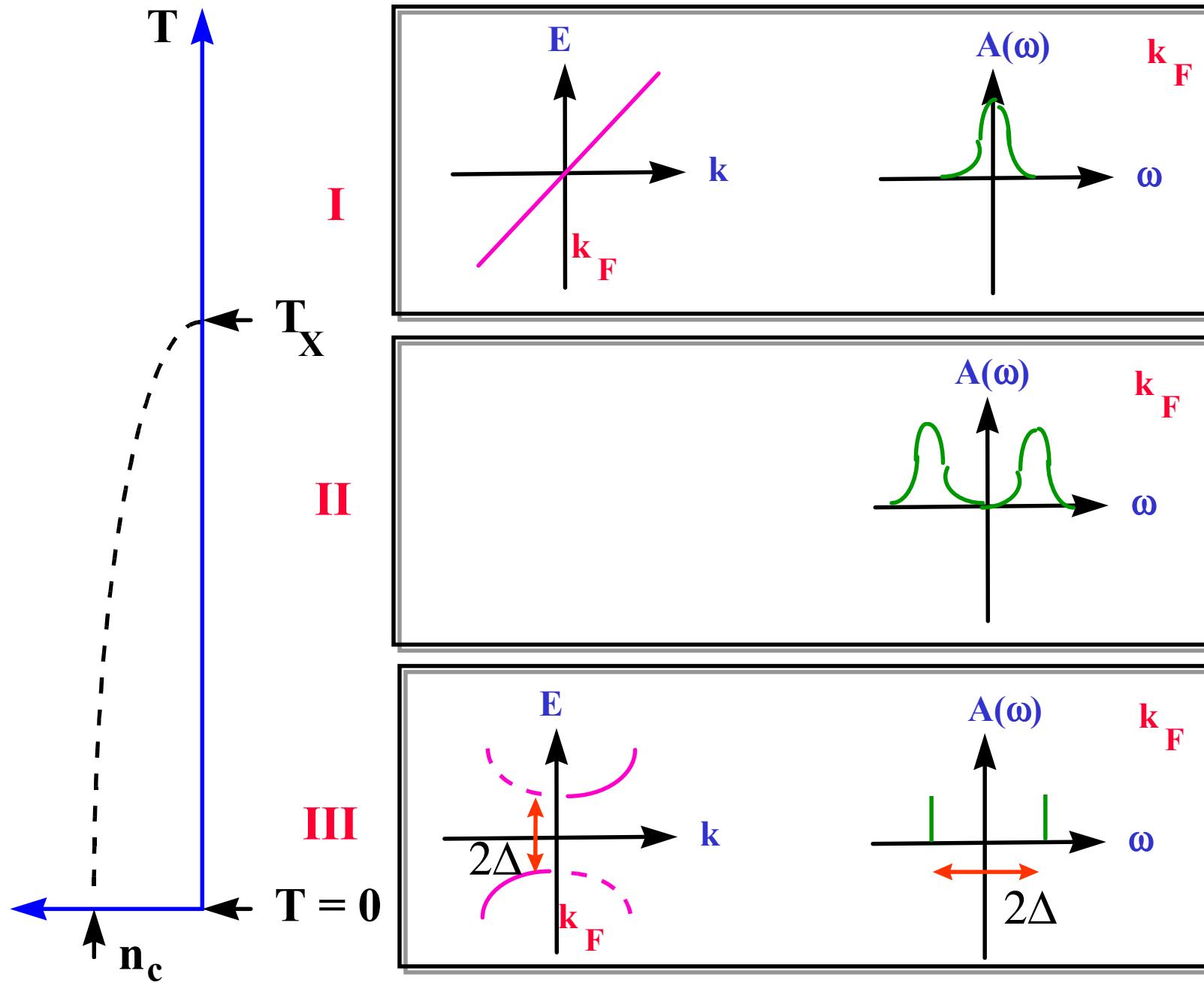
$G_2(1,1;2,3)$ appropriately related to $G(1,2)$

2. The standard approach :
 - a qualitatively incorrect result

U = + 4
 T = 0.2
 n=1
 8 X 8



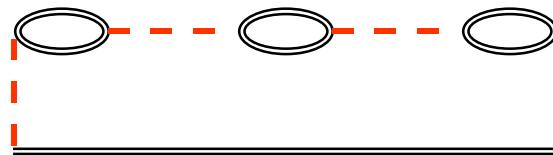
Calc. + QMC: Moukouri et al. P.R. B 61, 7887 (2000).



2. The standard approach :

- limitations of the approach

- 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

Singular



$$\Sigma(\mathbf{k}_F, ik_n) \approx \frac{U}{4} \frac{T}{N} \sum_{\mathbf{q}} U_{sp} \chi_{sp}(\mathbf{q}, 0) \frac{1}{ik_n - \tilde{\epsilon}_{\mathbf{k}+\mathbf{q}} - \Sigma(\mathbf{k}_F + \mathbf{q}, ik_n)}$$

$$\Sigma(ik_n) = \frac{\Delta^2}{ik_n - \Sigma(ik_n)}$$



$$\text{Re}\Sigma^R(\omega) = \frac{\omega}{2} - \frac{\omega}{2|\omega|} \theta(|\omega| - 2\Delta) (\omega^2 - 4\Delta^2)^{1/2}$$

$$\text{Im}\Sigma^R(\omega) = -\frac{1}{2} \theta(2\Delta - |\omega|) (4\Delta^2 - \omega^2)^{1/2}$$

Non Fermi-liquid but not singular at $\omega = 0$

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

2. The standard approach :

- problem...

- We do not know how to properly solve even the «standard model» for heavy fermions (Coleman).
- Lee-Rice-Anderson simpler approach seems qualitatively better, why?
- GW approach to improve band structure calculations?

3. An approach for both $U > 0$ and $U < 0$

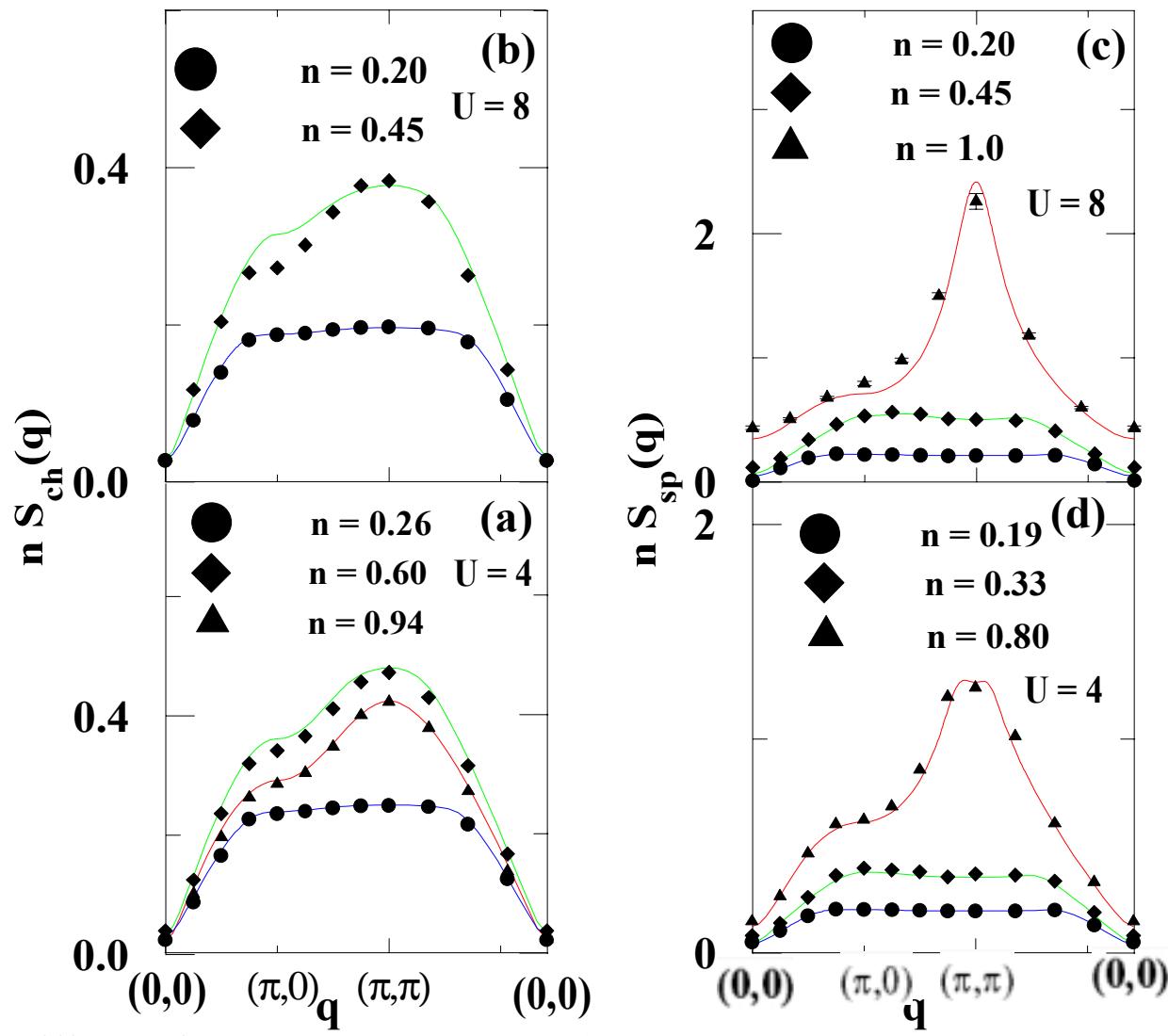
- Proofs that it works

$U > 0$

Notes:

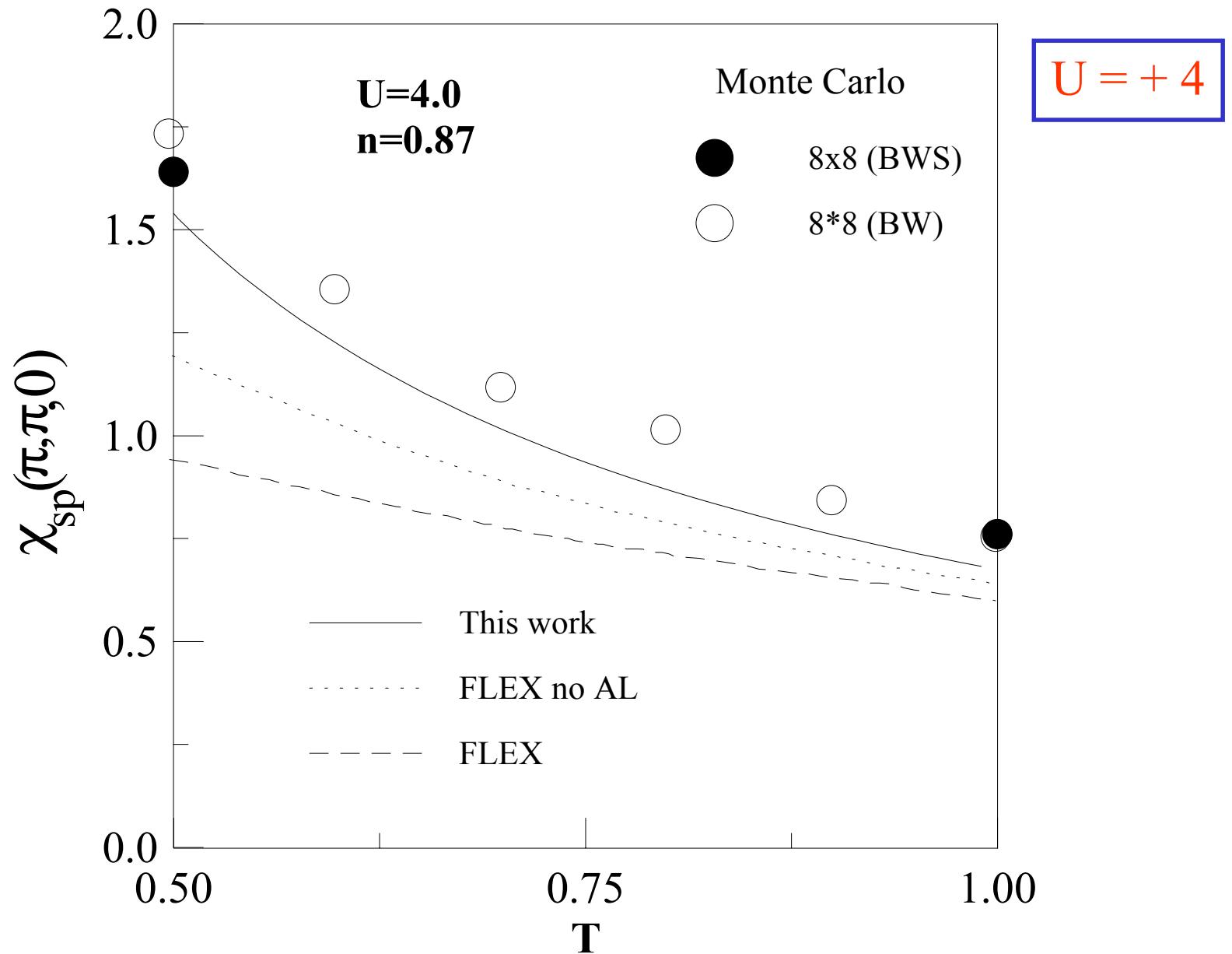
-F.L.
parameters

-Self also
Fermi-liquid



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

Proofs...

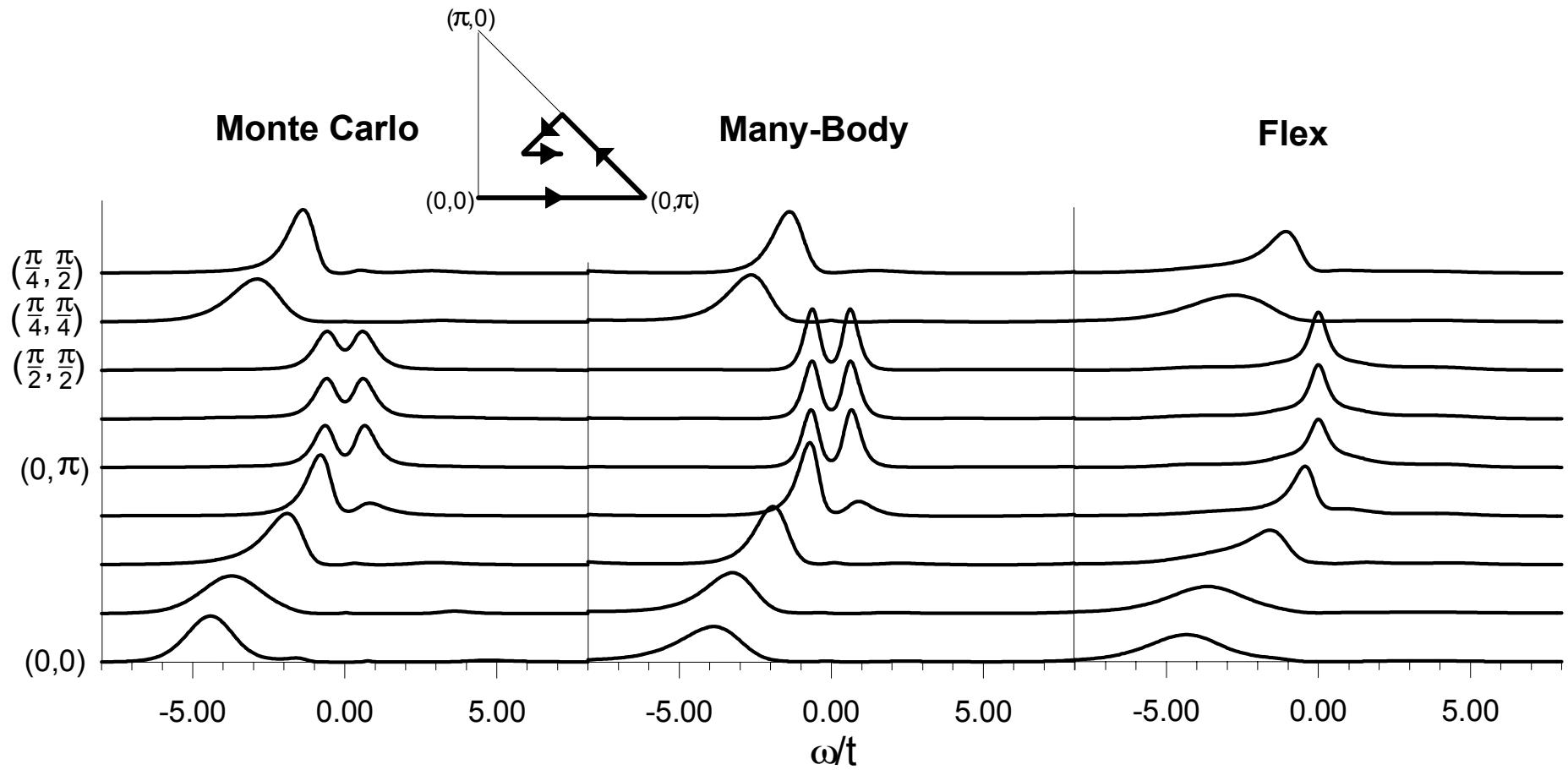


Calc.: Vilk, et al. J. Phys. I France, **7**, 1309 (1997).

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

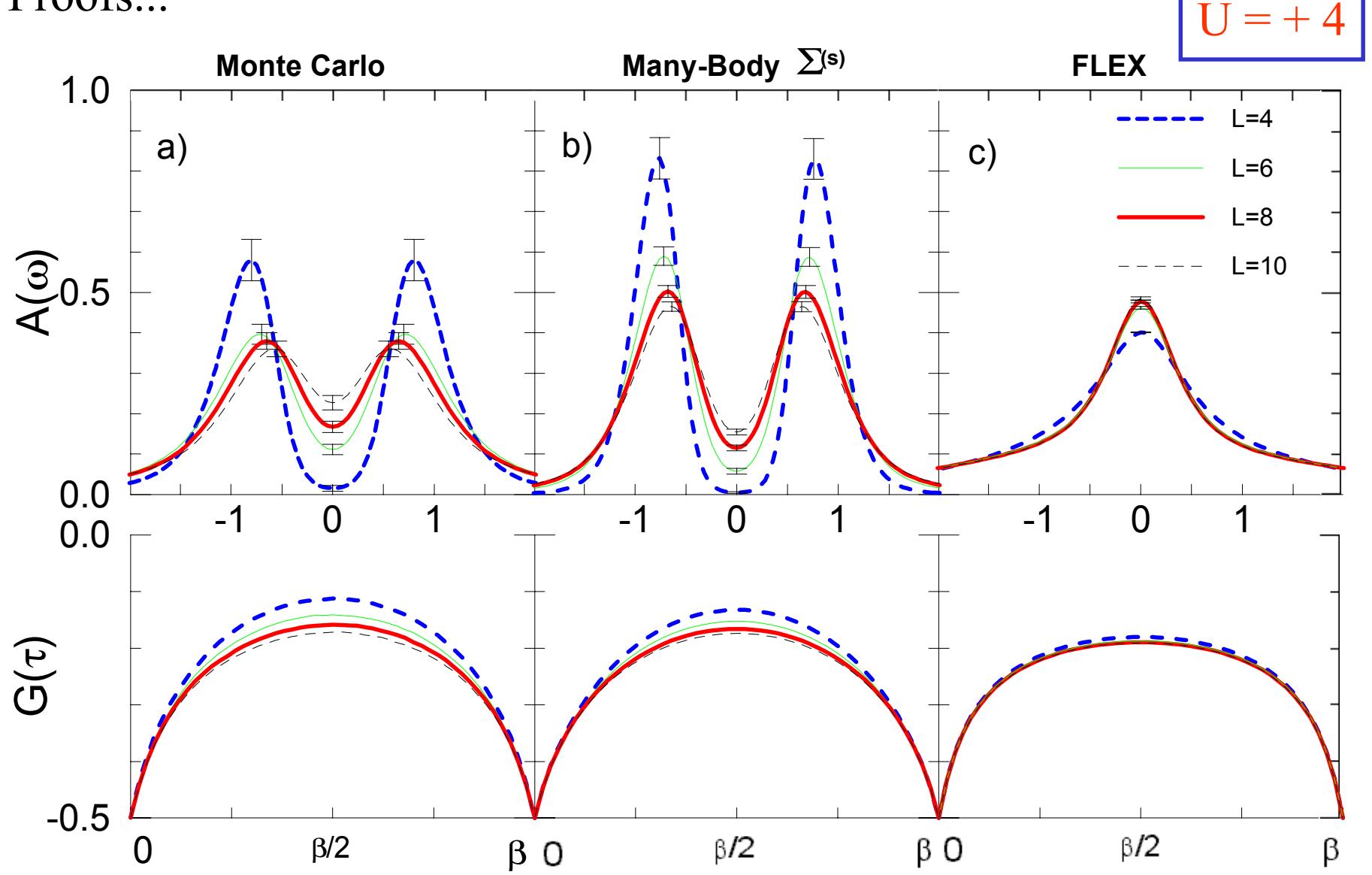
Proofs...

$U = +4$



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

Proofs...



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

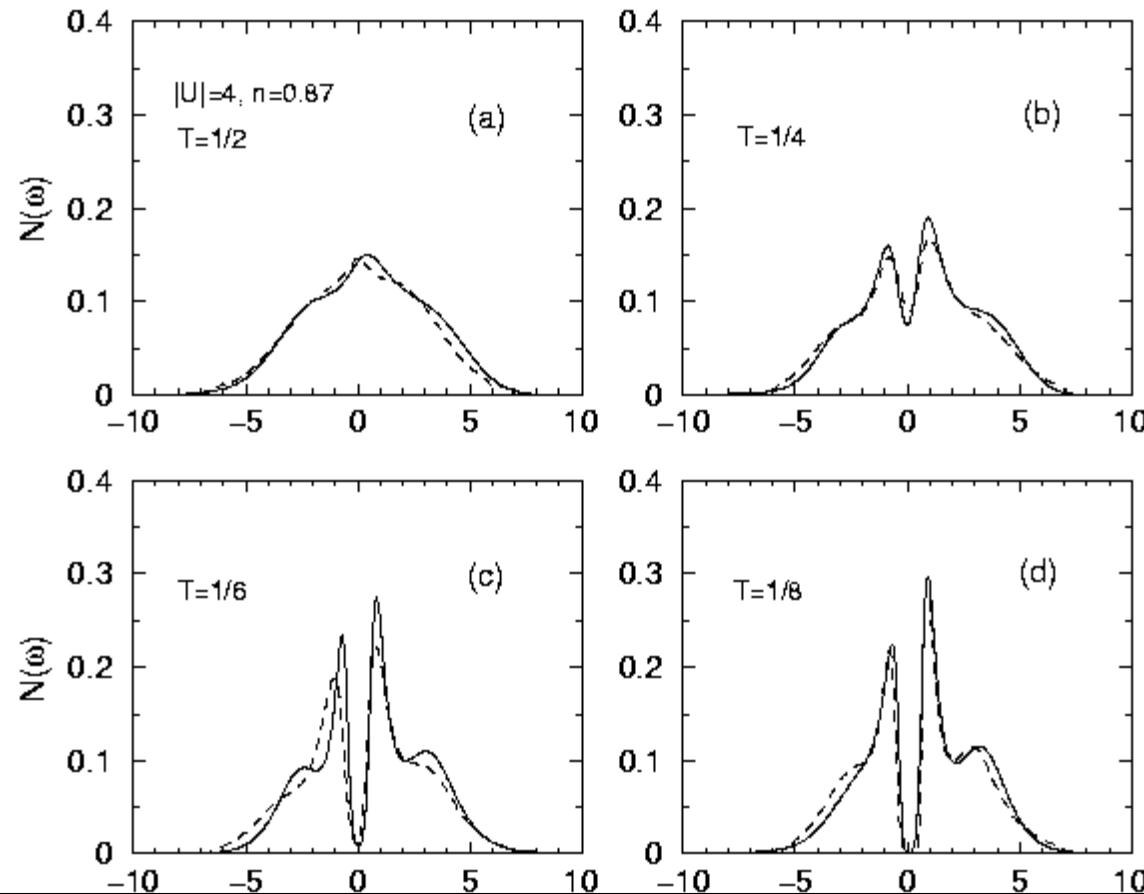
Moving to the attractive case....

U = - 4

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

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

Proofs...

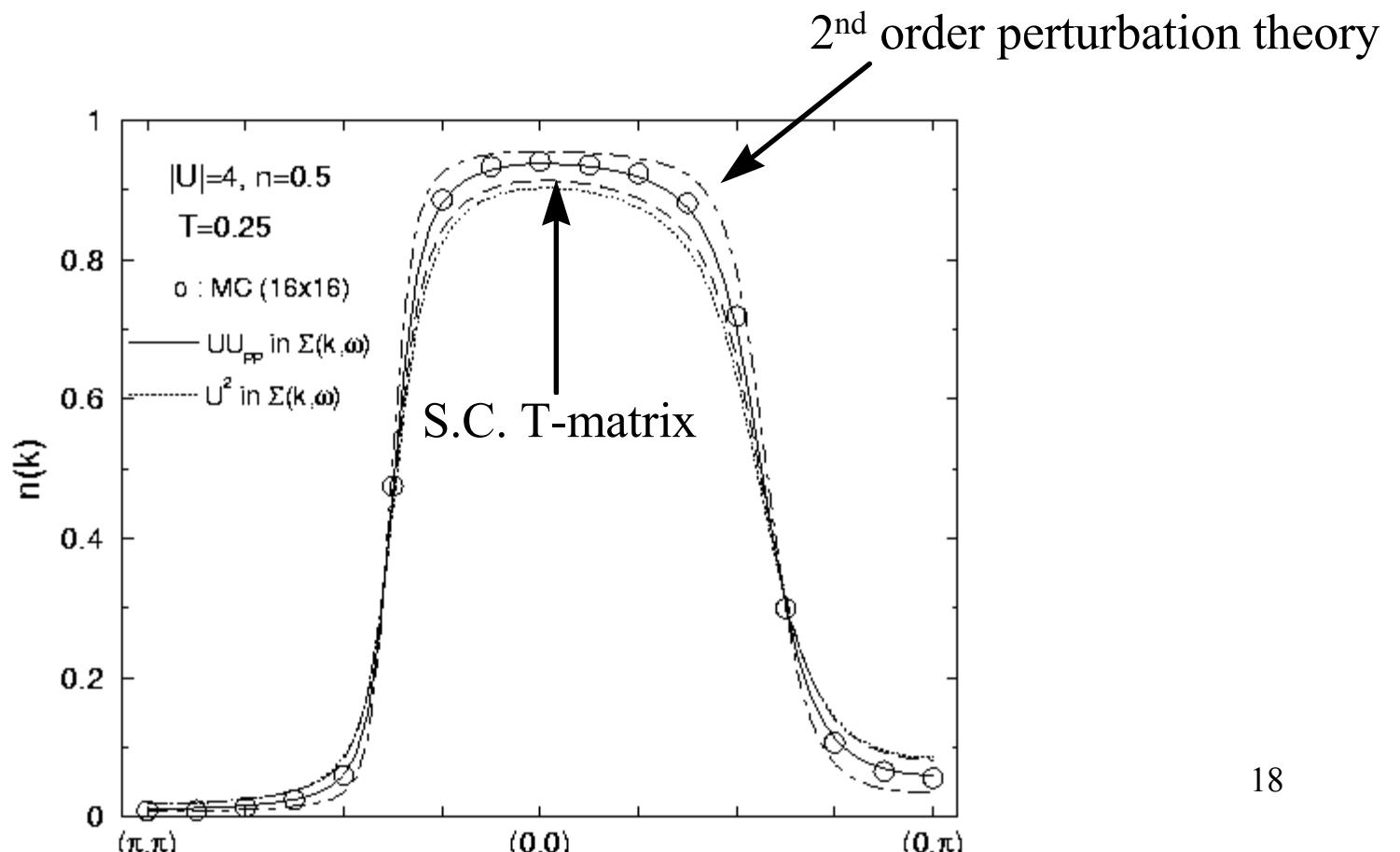


Proofs...

$$\boxed{\mathbf{U} = -4}$$

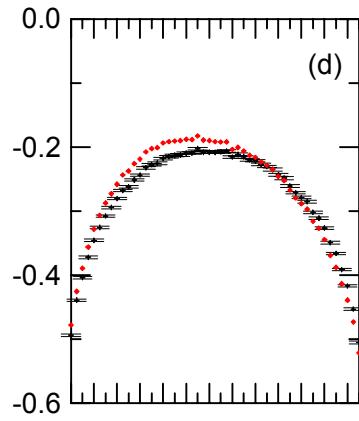
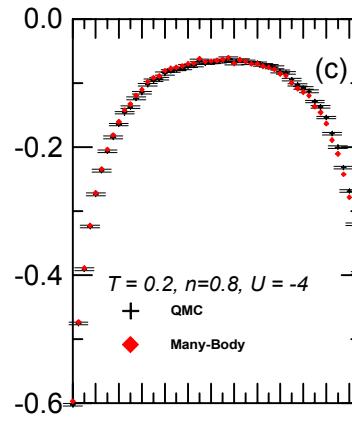
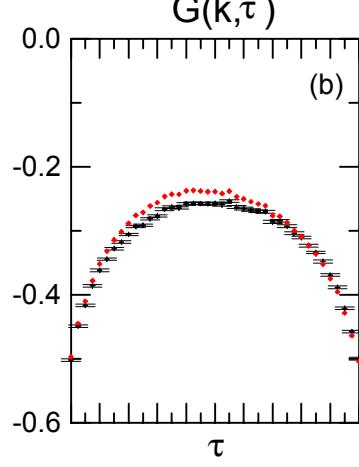
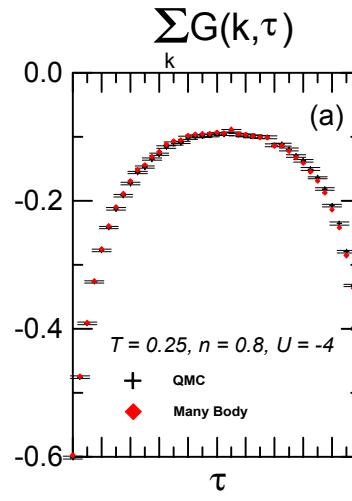
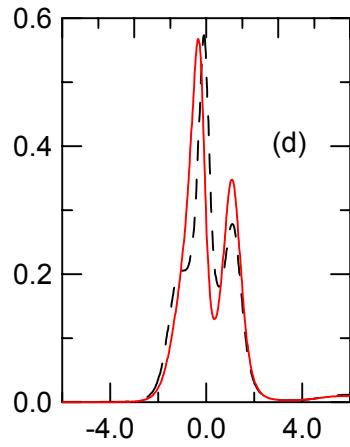
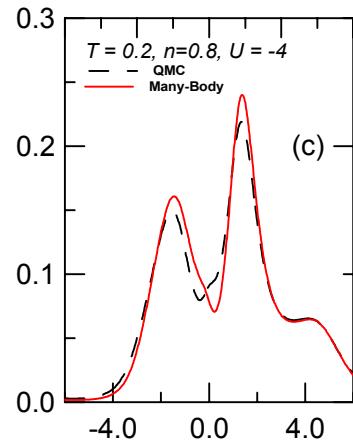
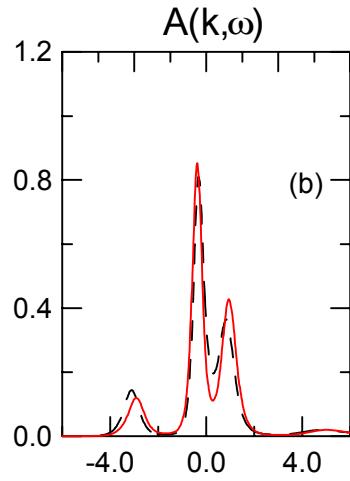
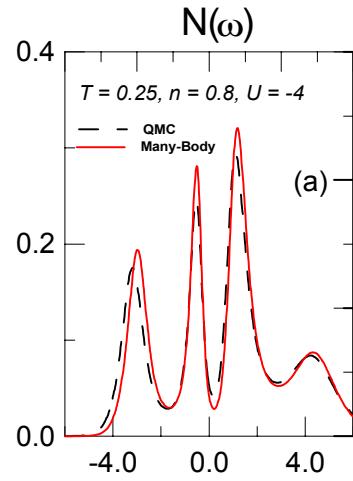
Calc. : Kyung et al. cond-mat/0010001

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



Proofs...

U = -4



3. An non-perturbative approach for both $U > 0$ and $U < 0$

Reminder: Generating function, with source field

$$Z[\phi] = \text{Tr} [T_\tau \left(e^{-\psi_{\bar{\sigma}}^\dagger(\bar{1})\phi_{\bar{\sigma}}(\bar{1},\bar{2})\psi_{\bar{\sigma}}(\bar{2})} \right)]$$

Propagator in the presence of the source field

$$G_\sigma(1, 2; \{\phi\}) = -\langle \psi_\sigma^\dagger(1) \psi_\sigma(2) \rangle_\phi = -\frac{\delta \ln Z[\phi]}{\delta \phi_\sigma(2, 1)}$$

Equation of motion and definition of self-energy

$$(G_0^{-1} - \phi) G = 1 + \Sigma G \quad ; \quad G^{-1} = G_0^{-1} - \phi - \Sigma$$

where, from the commutator of the interacting part of H :

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

Response functions :

$$GG^{-1} = 1$$

$$\frac{\delta G}{\delta \phi} G^{-1} + G \frac{\delta G^{-1}}{\delta \phi} = 0$$

Using $G^{-1} = G_0^{-1} - \phi - \Sigma$

$$\frac{\delta G}{\delta \phi} = -G \frac{\delta G^{-1}}{\delta \phi} G = G \hat{G} + G \frac{\delta \Sigma}{\delta \phi} G$$

Legendre transform of Z is $\Phi[G]$ and $\Sigma[G] = \delta \Phi[G] / \delta G$. We have the RPA equation in particle-hole channel, (or Bethe-Salpeter in particle-particle)

$$\frac{\delta G}{\delta \phi} = G \hat{G} + G \left[\frac{\delta \Sigma}{\delta G} \frac{\delta G}{\delta \phi} \right] G$$

Vertices appropriate for spin and charge responses

$$U_{sp} = \frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} - \frac{\delta \Sigma_\uparrow}{\delta G_\uparrow} \quad ; \quad U_{ch} = \frac{\delta \Sigma_\uparrow}{\delta G_\downarrow} + \frac{\delta \Sigma_\uparrow}{\delta G_\uparrow}$$

Hartree-Fock as an example of use of this formalism:

As an example, consider Hartree-Fock (N.B. all in external field ϕ . Take $\phi = 0$ at the end only.)

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

$$\Sigma_{\sigma}^H(1, 2) = U G_{-\sigma}^H(1, 1^+) \delta(1 - 2)$$

$$\frac{\delta \Sigma_{\uparrow}(1, 2)}{\delta G_{\downarrow}(3, 4)} = U n_{-\sigma} \delta(1 - 2) \delta(3 - 1) \delta(4 - 2)$$

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

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

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)

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 $U < 0$).

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

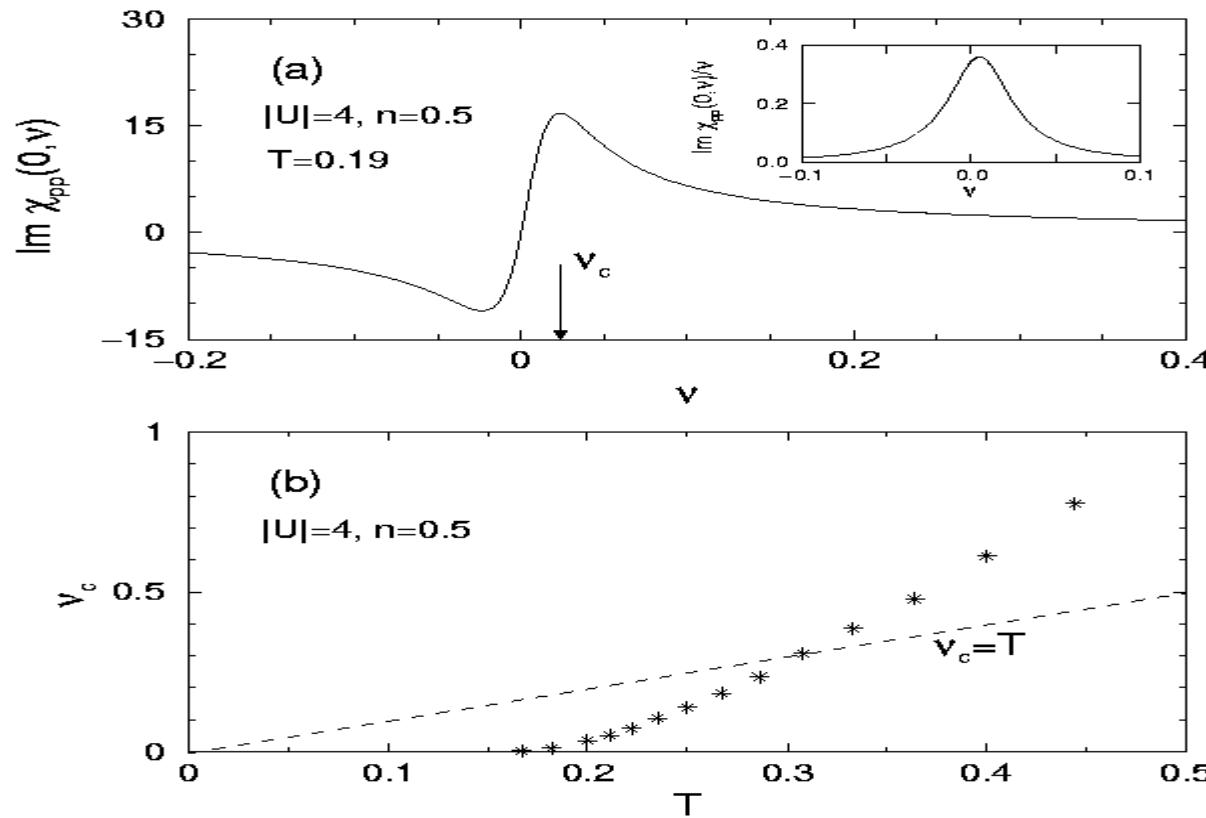
Check : $\text{Tr} [\Sigma^{(2)} G^{(1)}] \sim \text{Tr} [\Sigma^{(2)} G^{(2)}]$

4. 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. $d = 2$

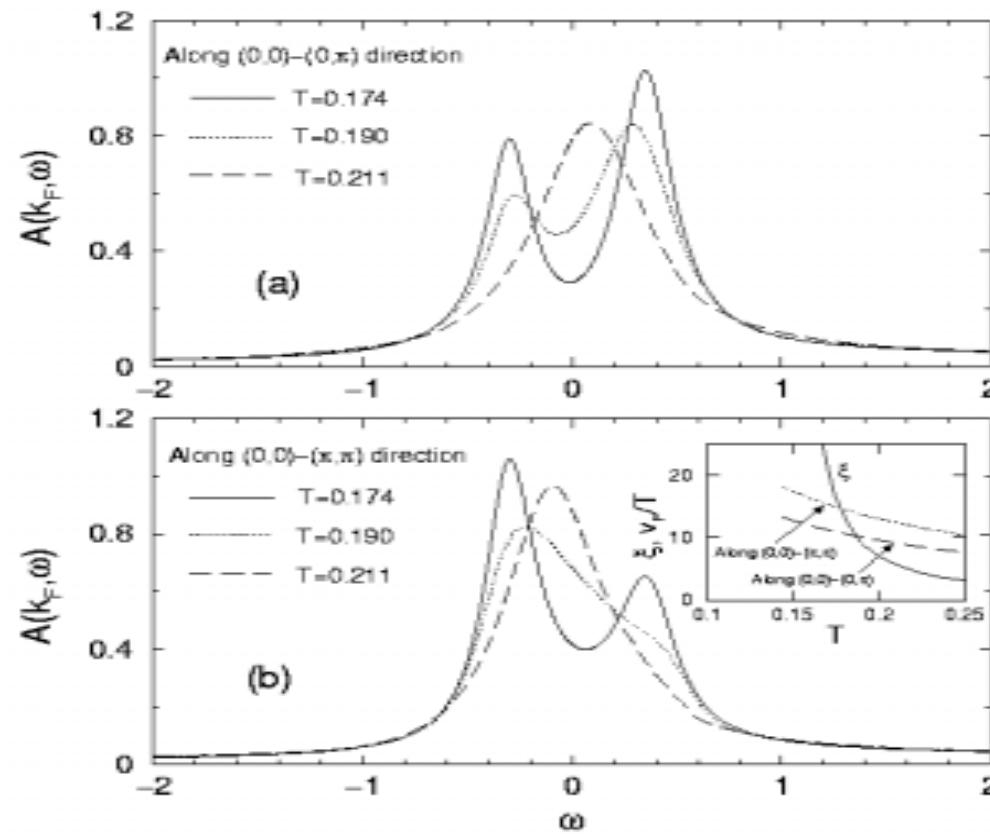


4. Results:

- Mechanism for pseudogap

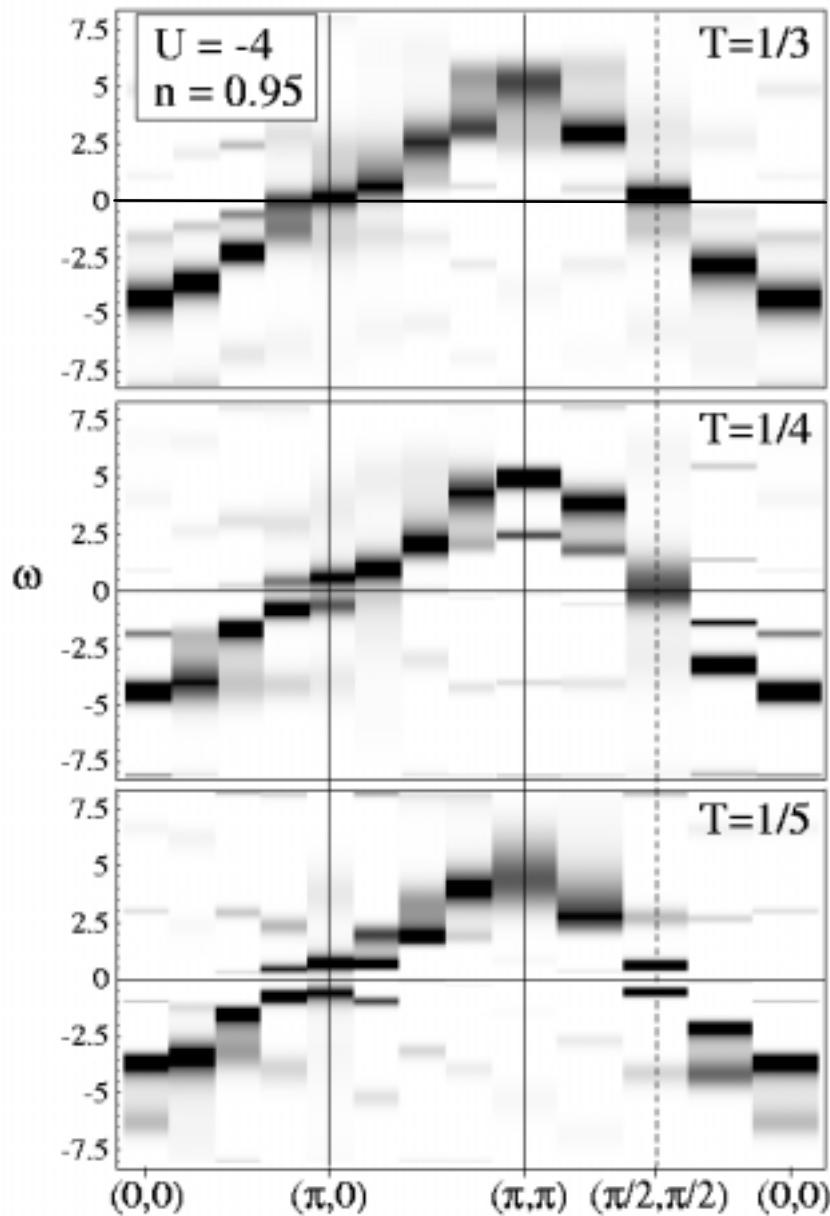
$U = -4$

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



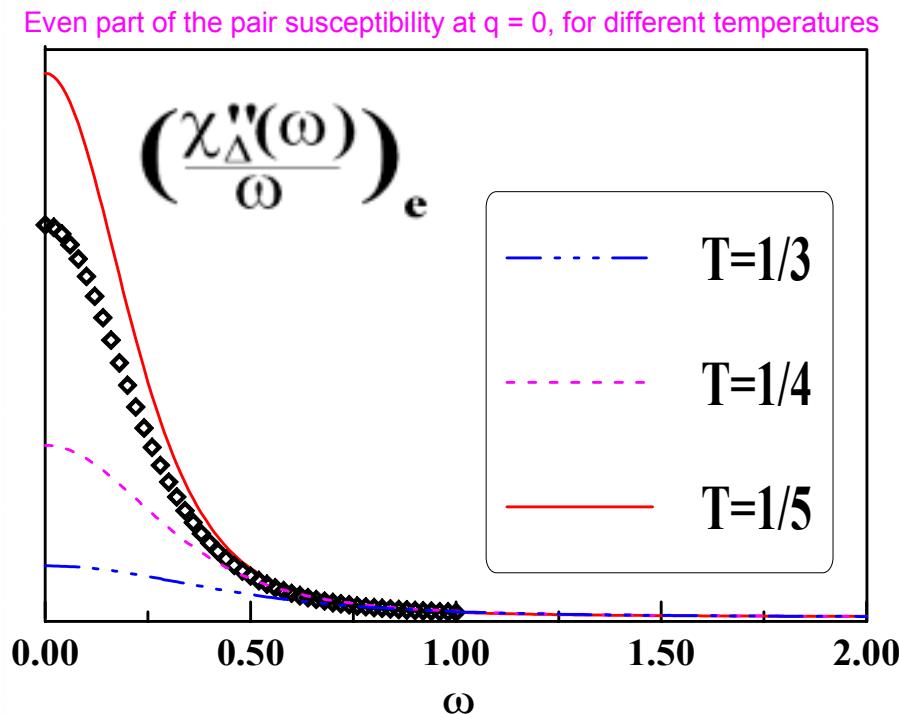
$$\xi \sim 1.3 \xi_{th}$$

Mechanism for pseudogap formation in the attractive model:



U = - 4

$d = 2$ is crucial



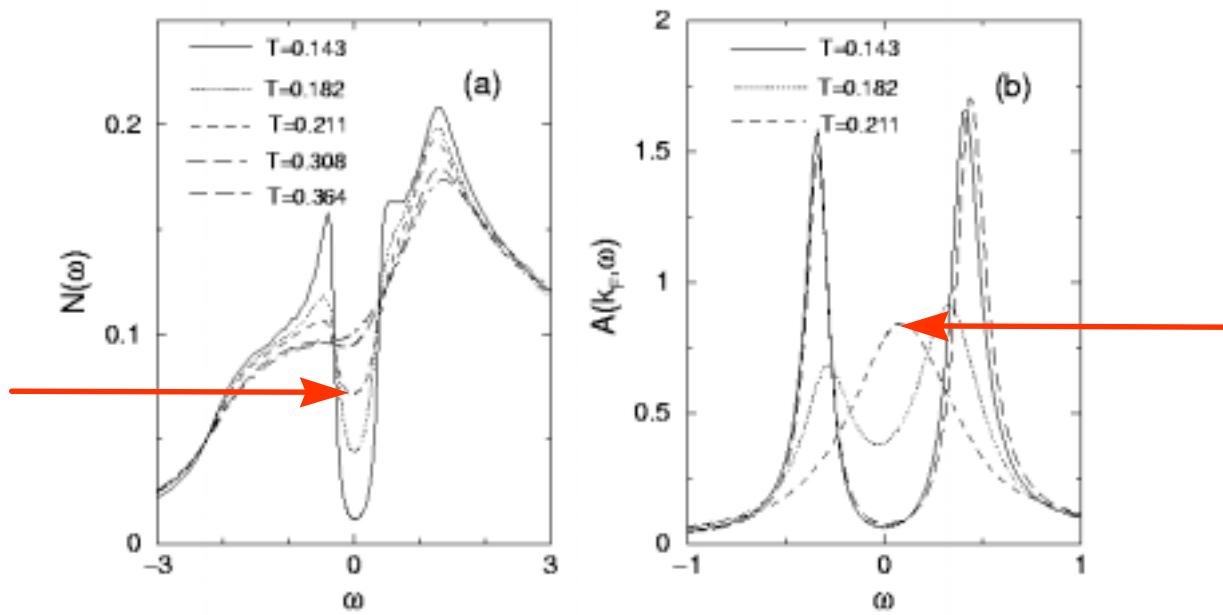
Allen, et al. P.R. L 83, 4128 (1999)
31

4. Results:

- Spectral weight rearrangement

$$U = -4$$

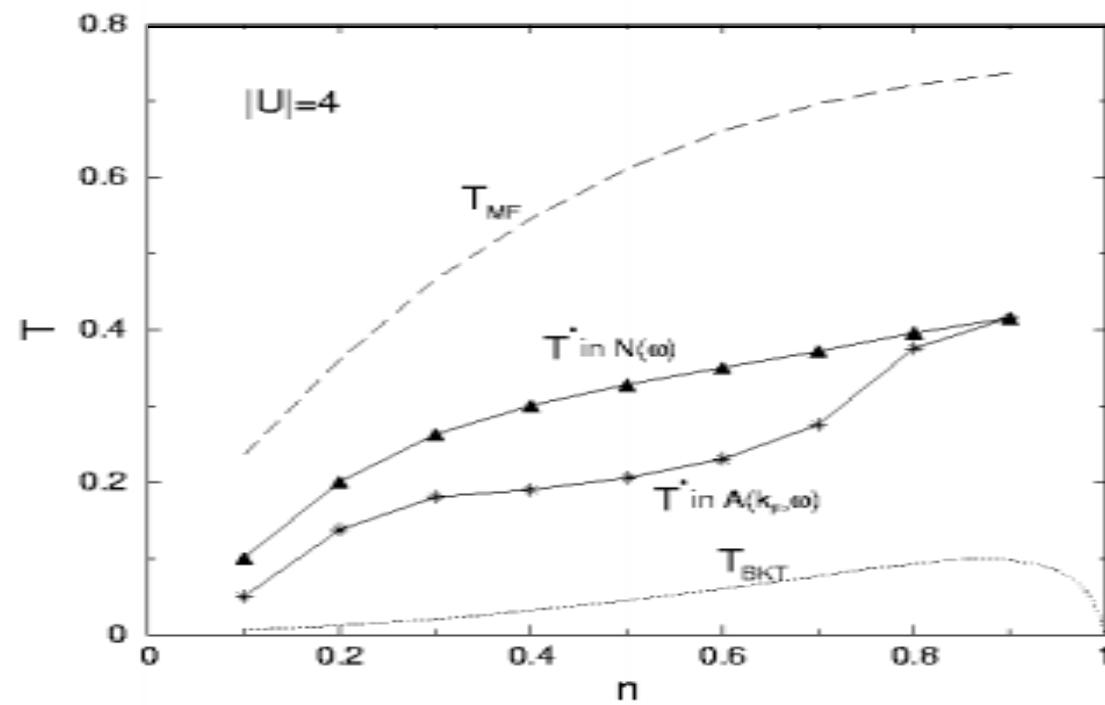
- Pseudogap appears first in total density of states
- Fills in instead of opening up
- Rearrangement over huge frequency scale compared with either T or ΔT . ($\Delta T \sim 0.03$, $T \sim 0.2$, $\Delta\omega \sim 1$)



4. Results:

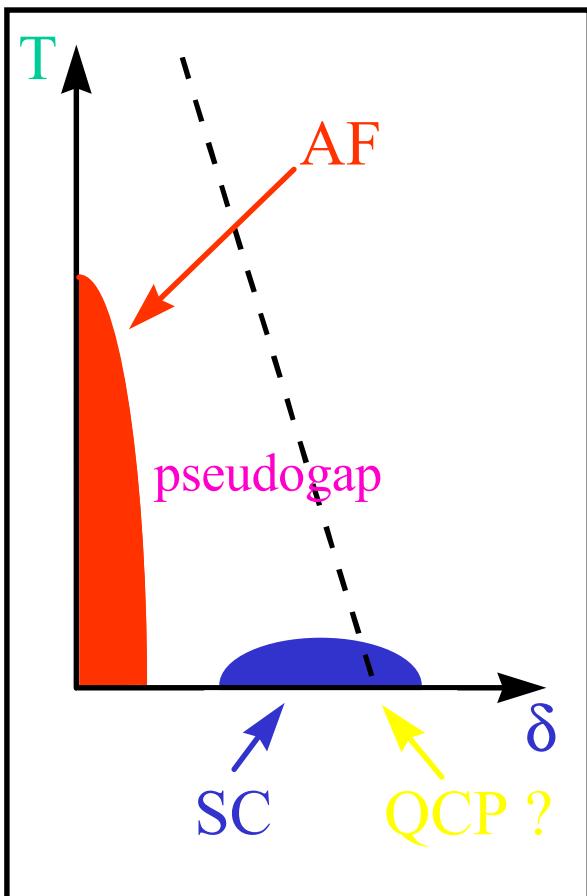
- Crossover diagram

$U = -4$



5. Conclusion :

$$U > 0$$



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

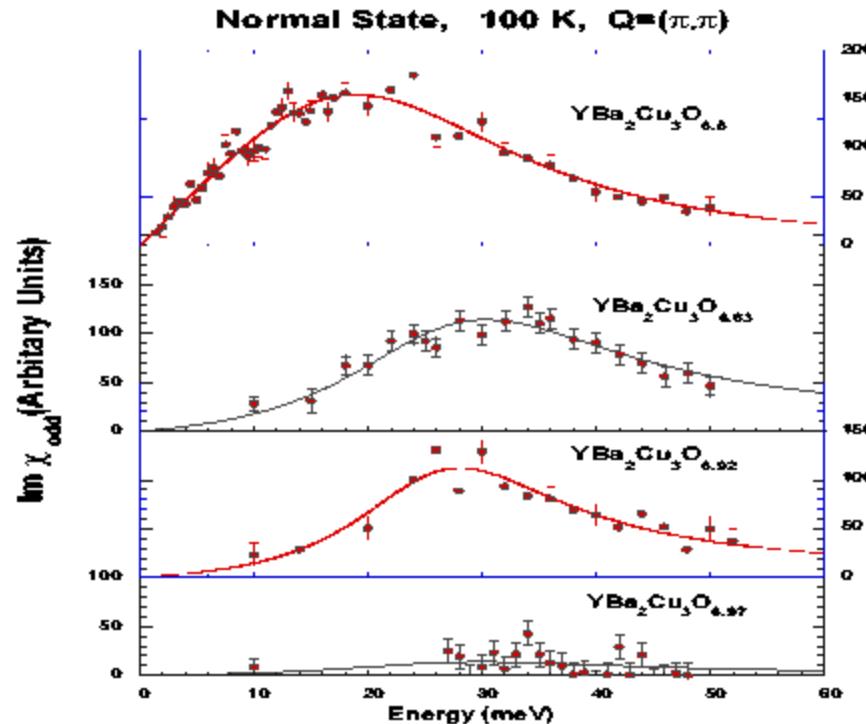


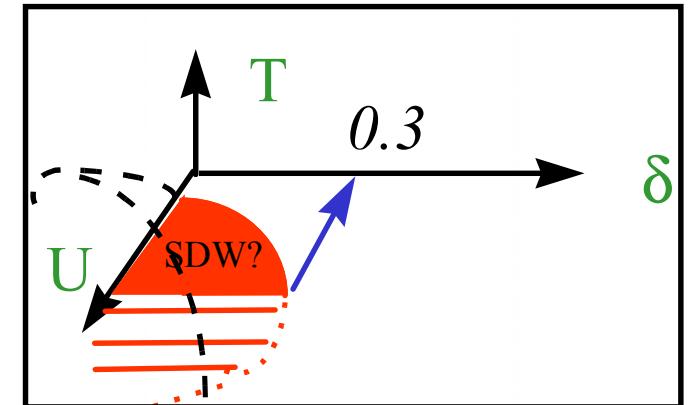
Figure 2: Normalized imaginary part of the spin susceptibility at the AF wavevector in the normal state, at $T = 100$ K, for four oxygen contents in YBCO ($T_c = 15, 85, 91, 92.5$ K for $x = 0.5, 0.83, 0.92, 0.97$ respectively). These curves have been normalized to the same units using standard phonon calibration¹⁴ (100 counts in the vertical scale roughly correspond to $\sim 350 \mu_B^2/eV$ in absolute units) (from¹⁰).

$U > 0$

- Quantum critical point, $d = 2$:

- Instability at incommensurate q
- Largest doping : 0.315

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

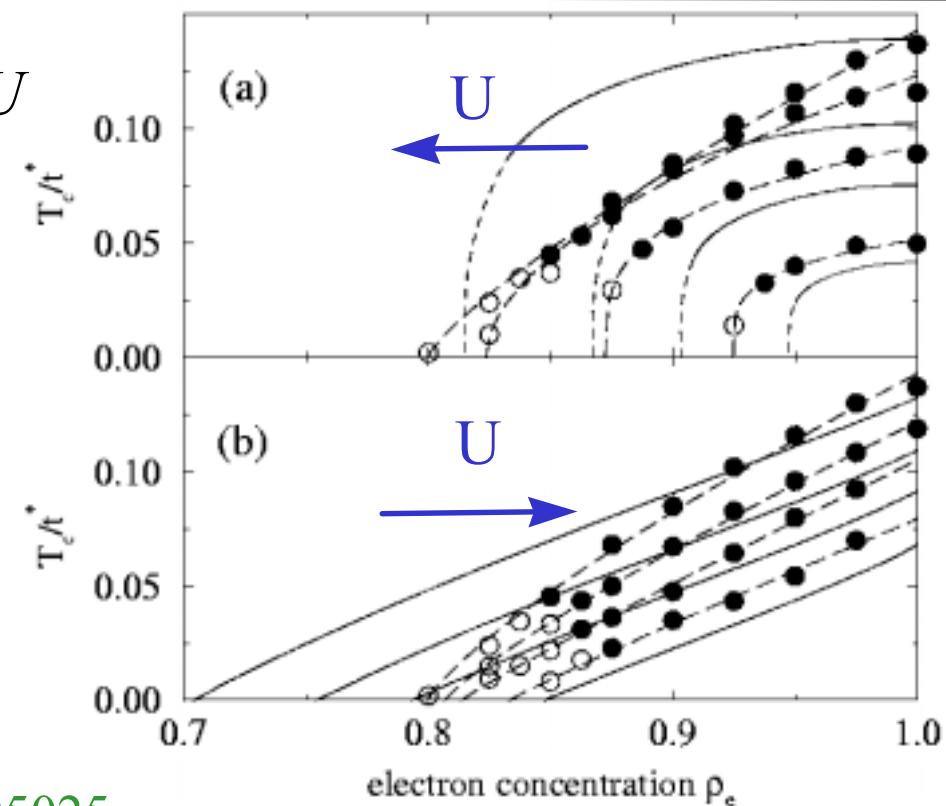


- Decreases with increasing U

$$U < W$$

$d = \text{infinity}$

$$U > W$$



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)

