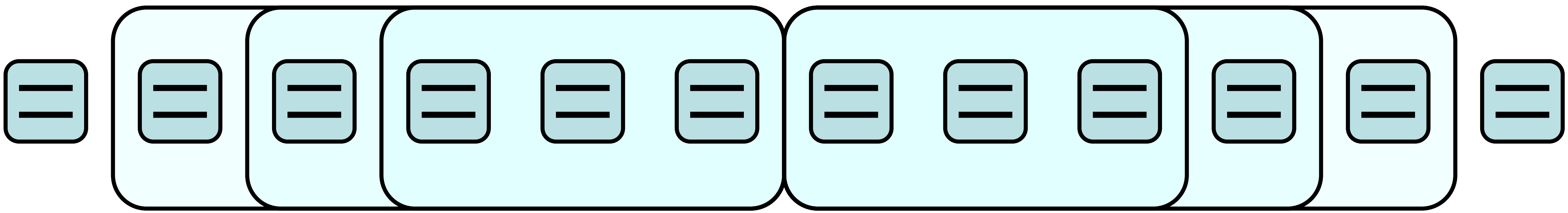
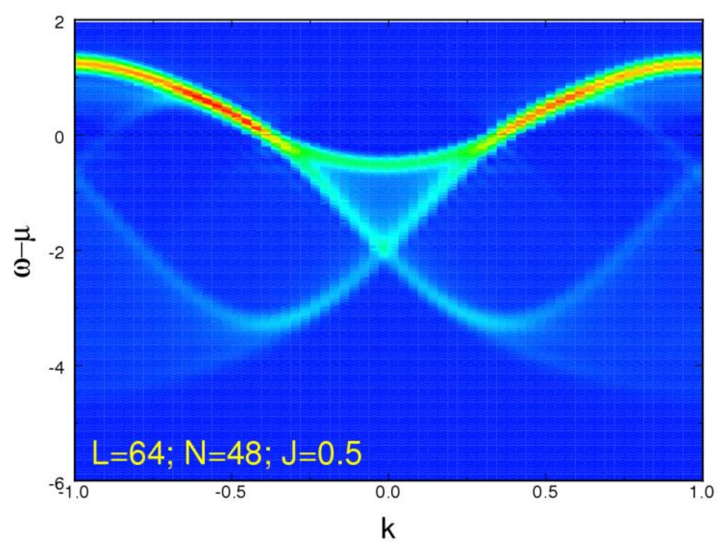
Toward a unified description of spin-incoherent behavior at finite-T and zero-T

Adrian Feiguin





Toward a unified description of spin-incoherent behavior at finite-T and zero-T

Outline:

- Spin-charge separation
- Spin-incoherent behavior
- The factorized wave function
- Thermofield/ancilla representation
- Finite Temperature state
- SILL behavior in the **ground state** of strongly correlated systems

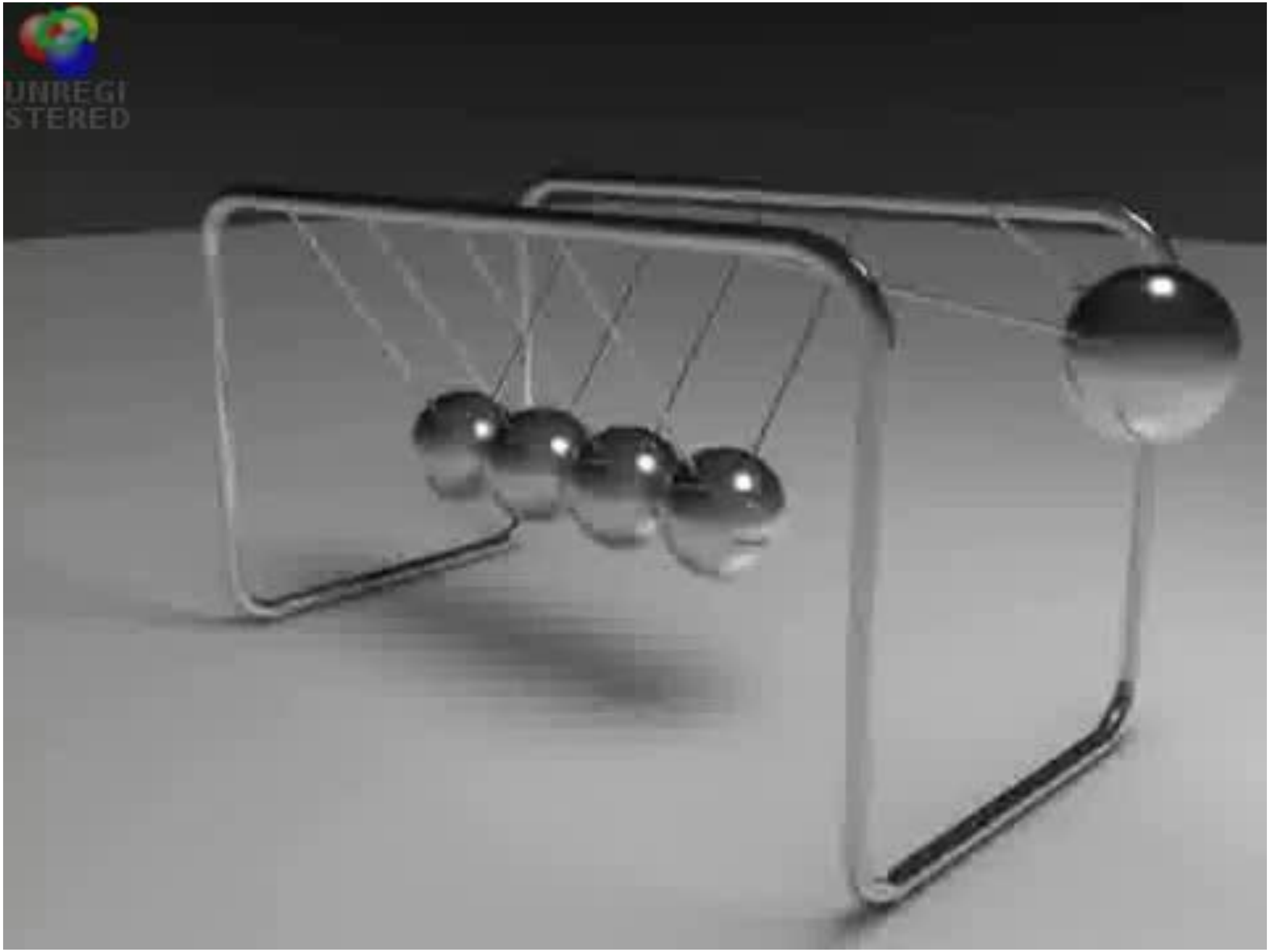
Collaborators:

Greg Fiete (U.T. Austin**)**
M. Soltanieh-ha (Northeastern)

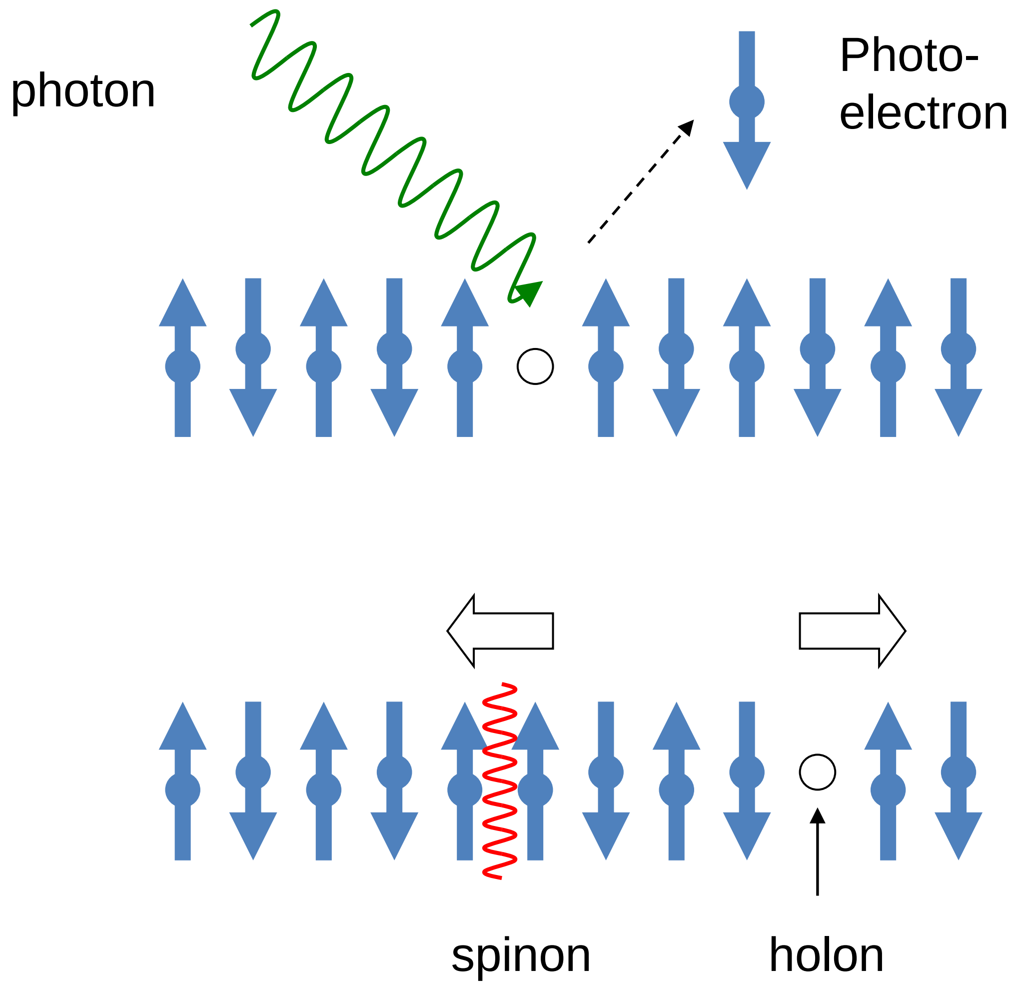
References:

AEF and G. Fiete: Phys. Rev. B 81, 075108 (2010)
AEF and G. Fiete: Phys. Rev. Lett. (2011)
M. Soltanieh-ha and AEF: PRB (accepted); arXiv: 1210.0982

Why is 1-D special?



Spin-charge separation



The excitations don't carry the same quantum numbers as the original electron $\rightarrow$ zero quasi-particle weight

Hubbard and t-J model

Hubbard model:

$$H = \boxed{-t \sum_{i=1,\sigma}^{L-1} \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + h.c. \right)} + \boxed{U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow}}$$

Kinetic energy

On-site interaction

Large U

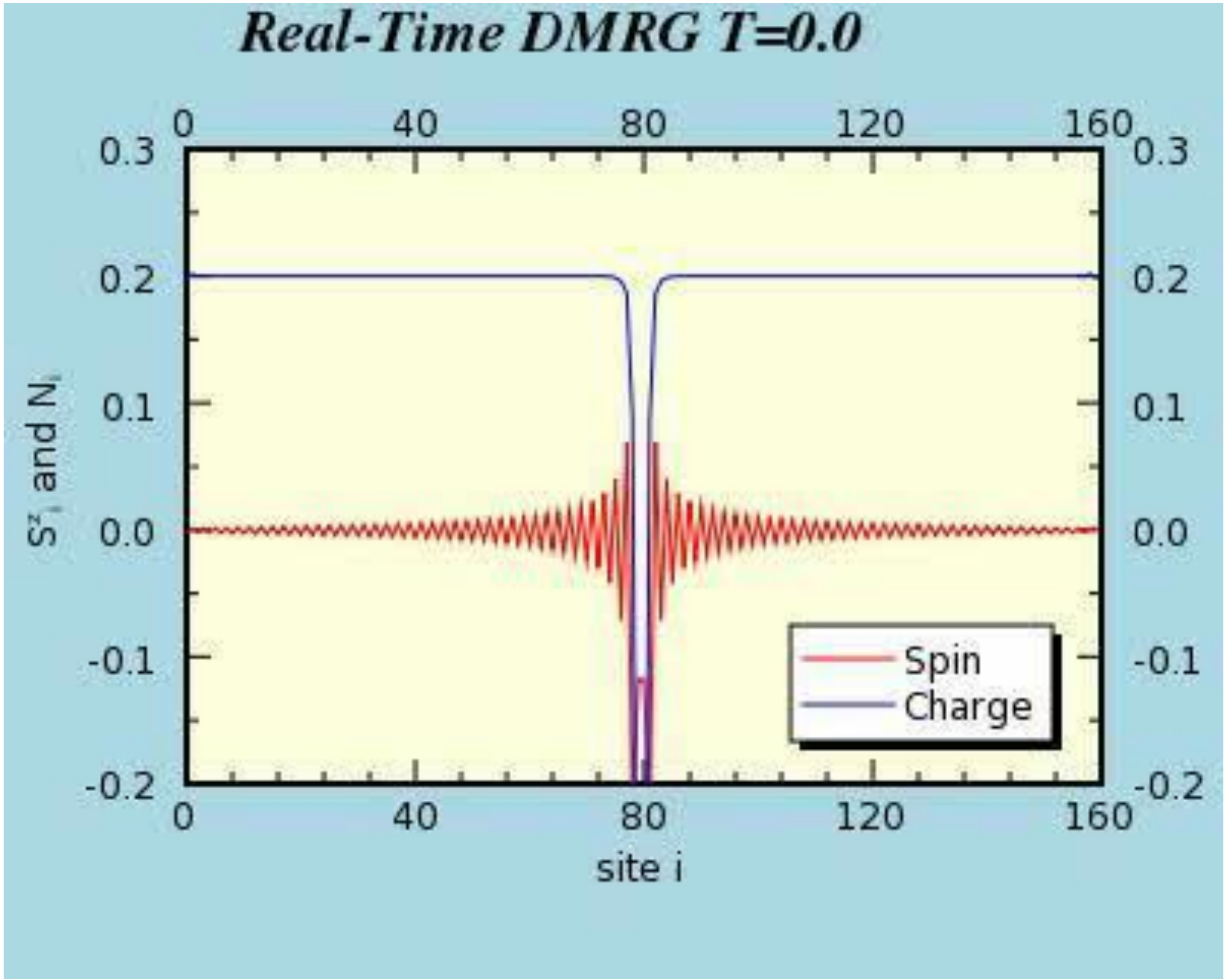
t-J model (no double occupancy):

$$H = -t \sum_{i=1,\sigma}^{L} \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + \mathrm{h.c.} \right) + \boxed{J \sum_{i=1}^{L} \vec{S}_i \vec{S}_{i+1}}$$

Heisenberg

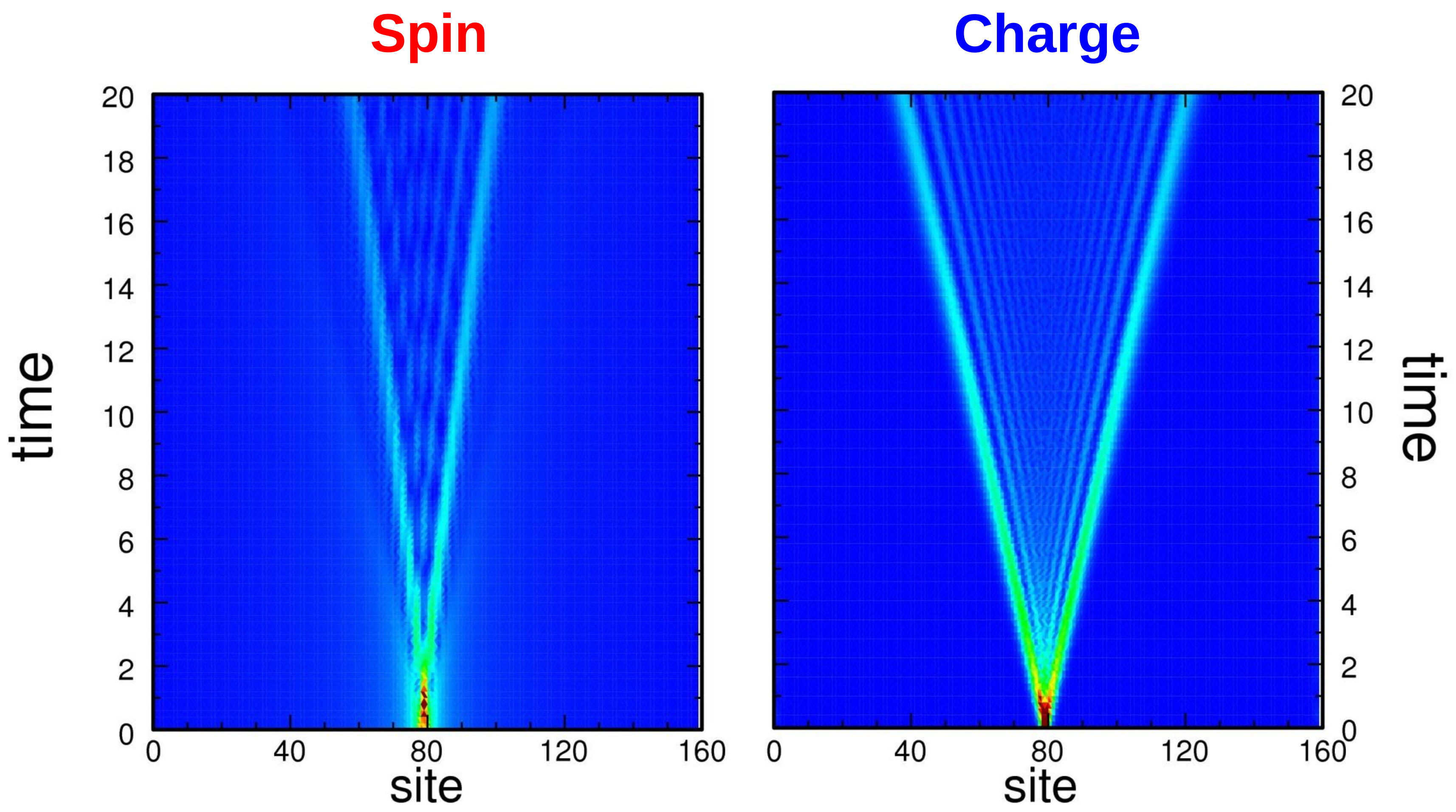
Real-time simulation

Half-filled Hubbard model (L=160, U=4)



See for instance E. Jagla, K. Hallberg and C. Balseiro, PRB (93), and C. Kollath, U. Schollwock, and W. Zwerger, PRL (05)

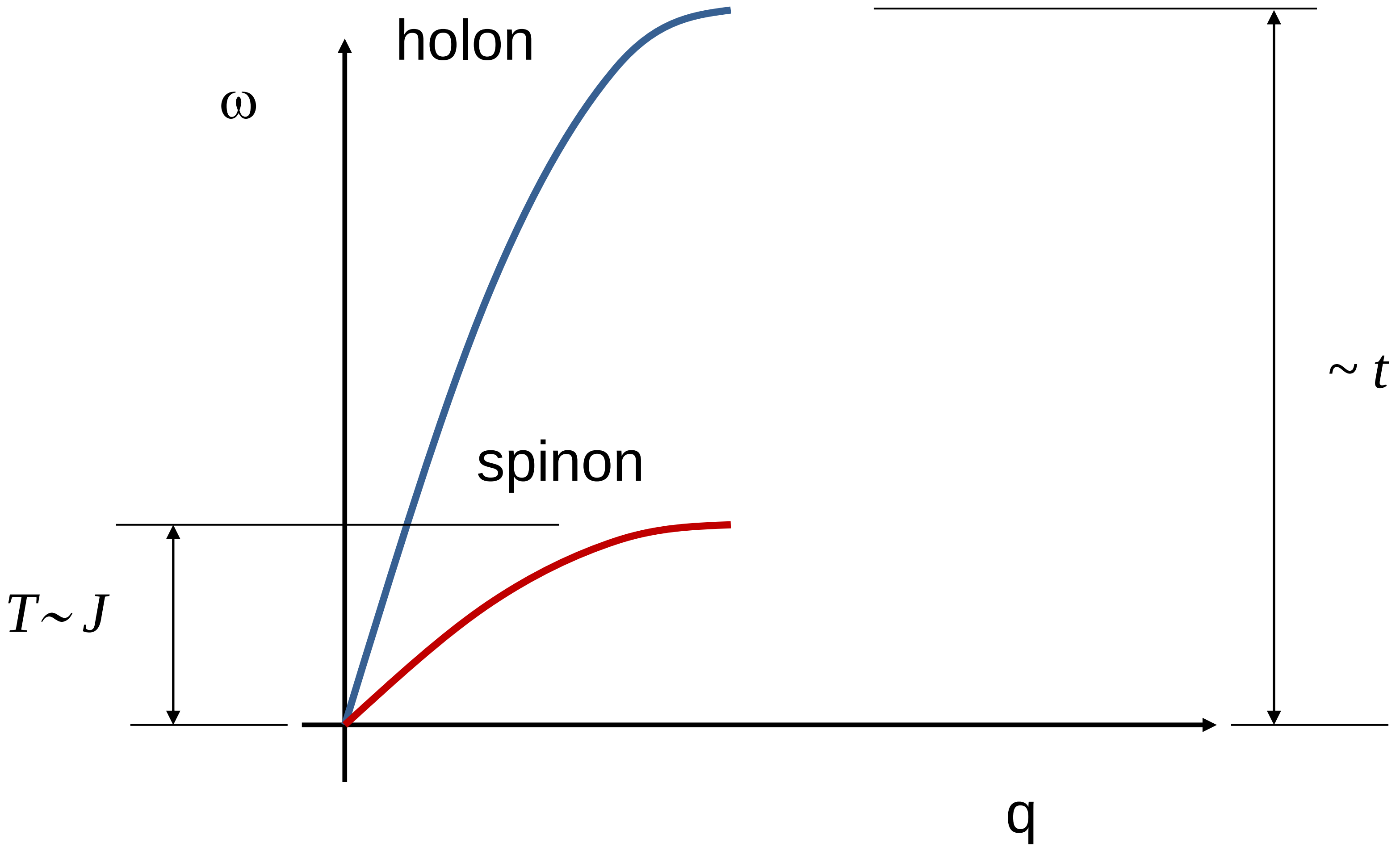
Lightcones



Spin and charge propagate with different velocities

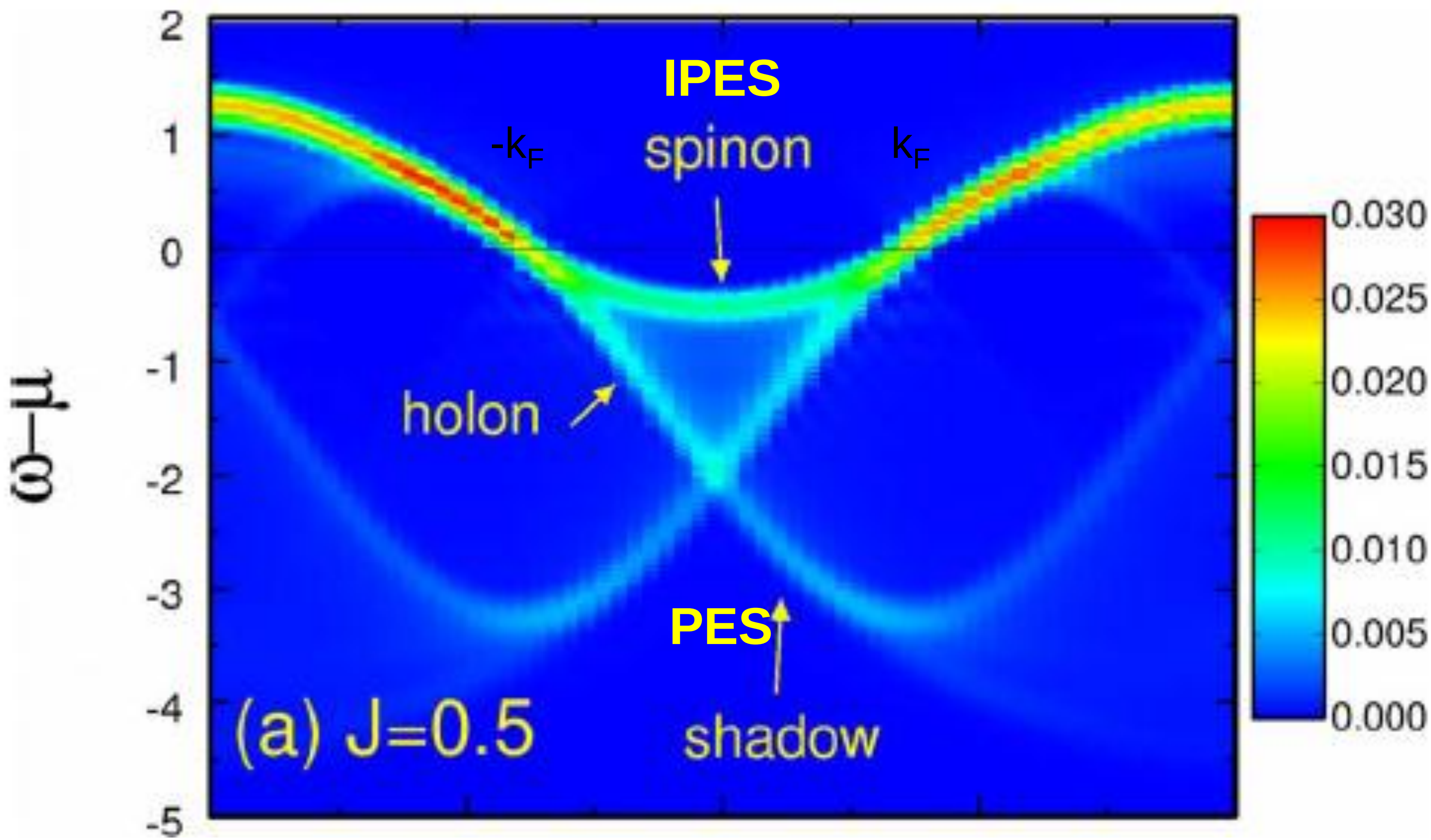
See for instance E. Jagla, K. Hallberg and C. Balseiro, PRB (93), and C. Kollath, U. Schollwock, and W. Zwerger, PRL (05)

Spin and charge excitations

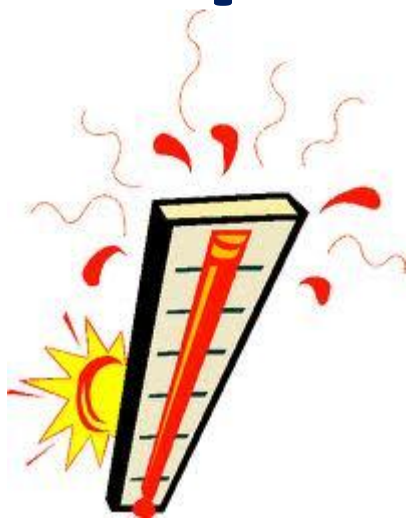


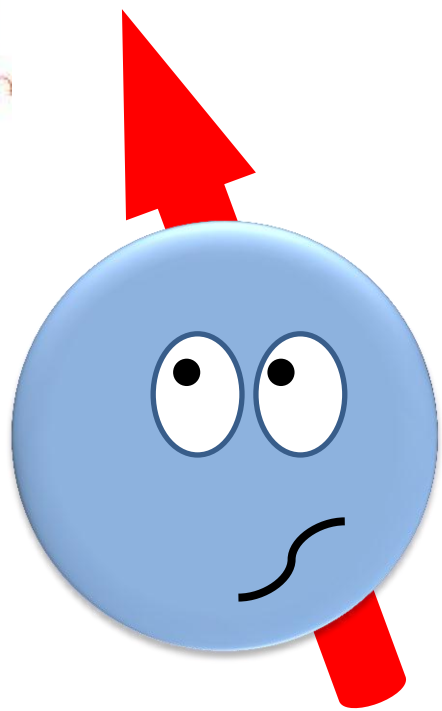
ARPES at T=0

1D t-J model (J=0.5)

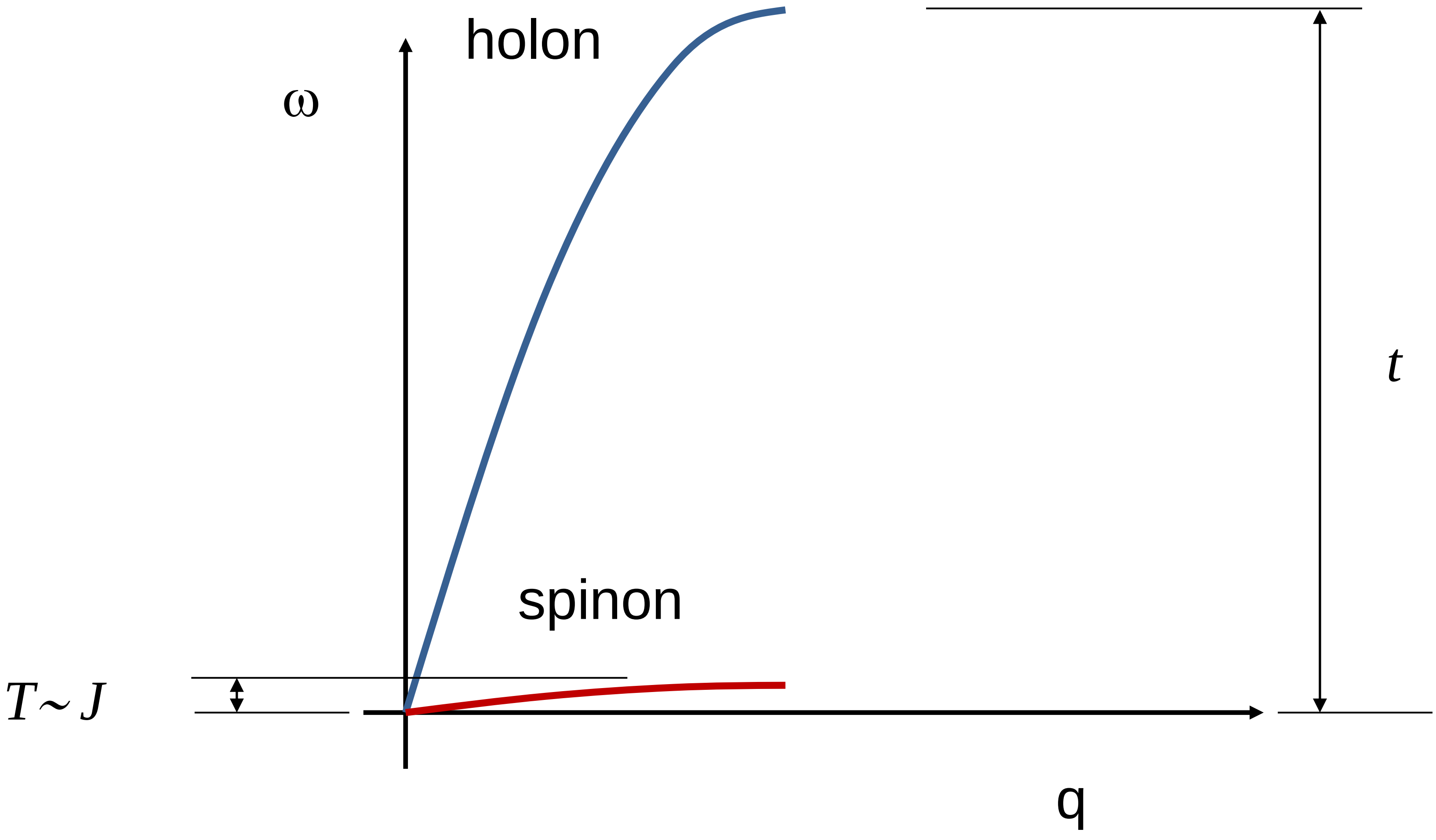


Finite temperature physics





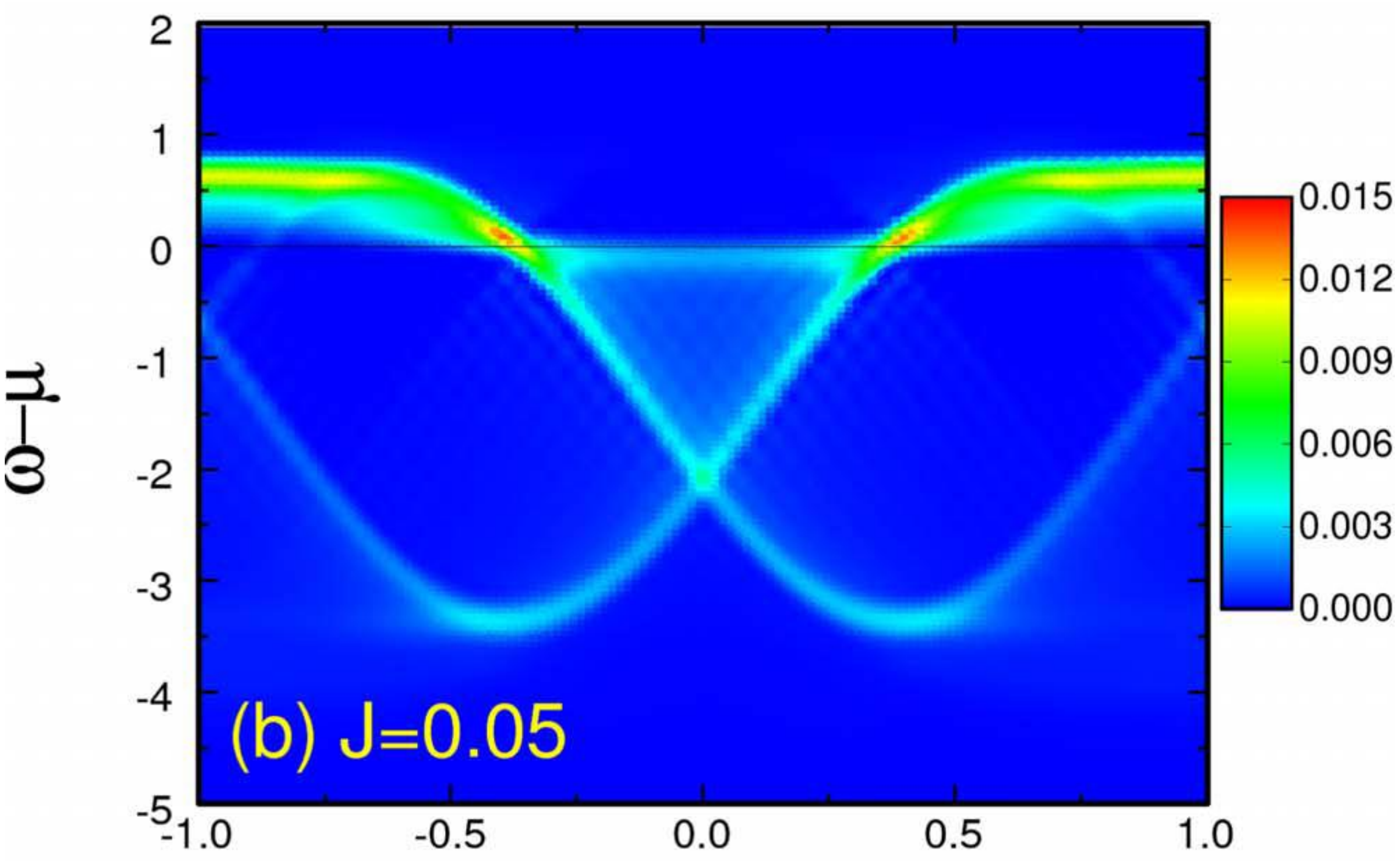
Spin incoherent behavior



See G. Fiete, RMP (07); B. Halperin, J. Appl. Phys (05), Cheianov and Zvonarev (04)

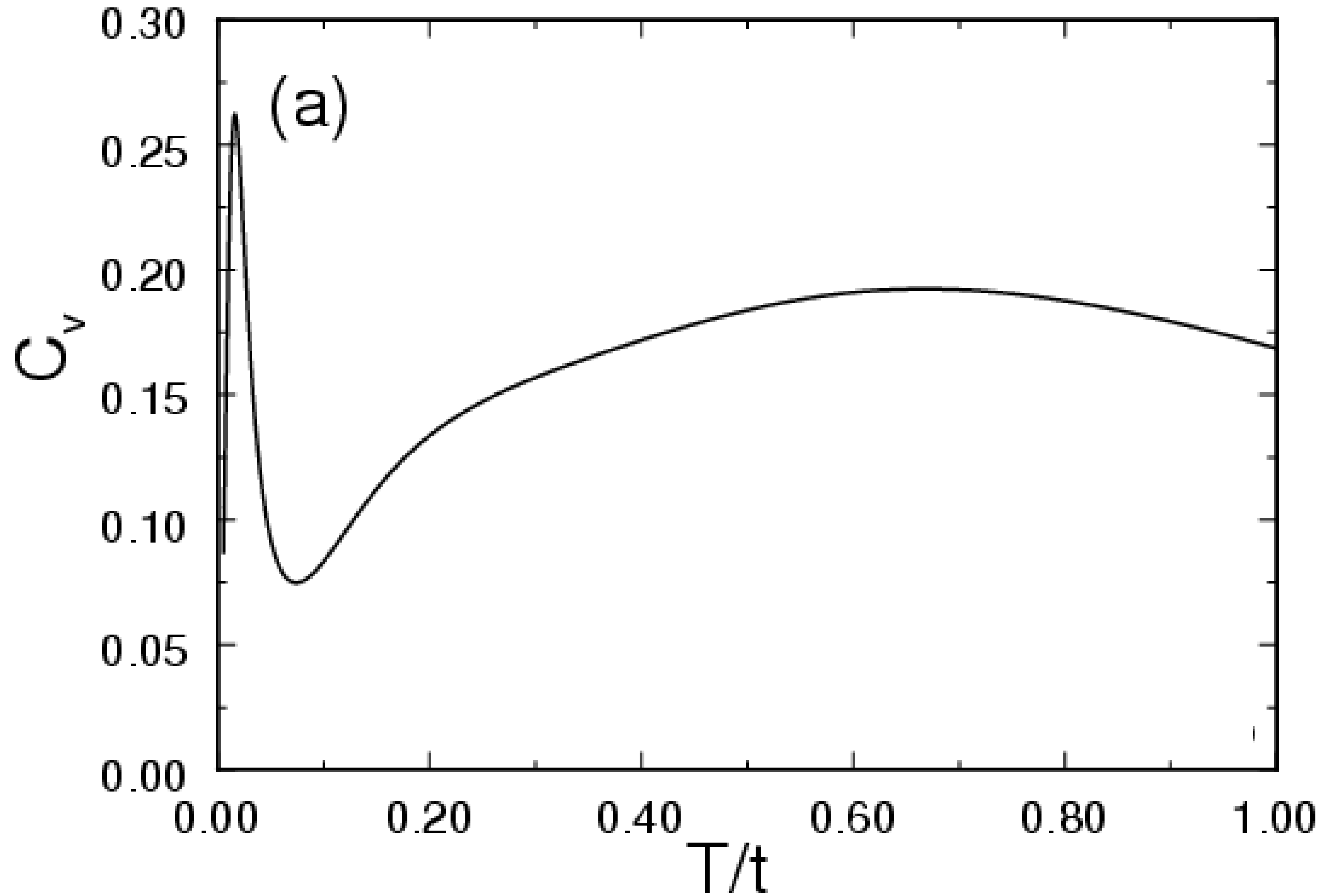
ARPES at T=0

1D t-J model (J=0.05)



Results: Thermodynamics

J=0.05; L=32, N=24; n=0.75

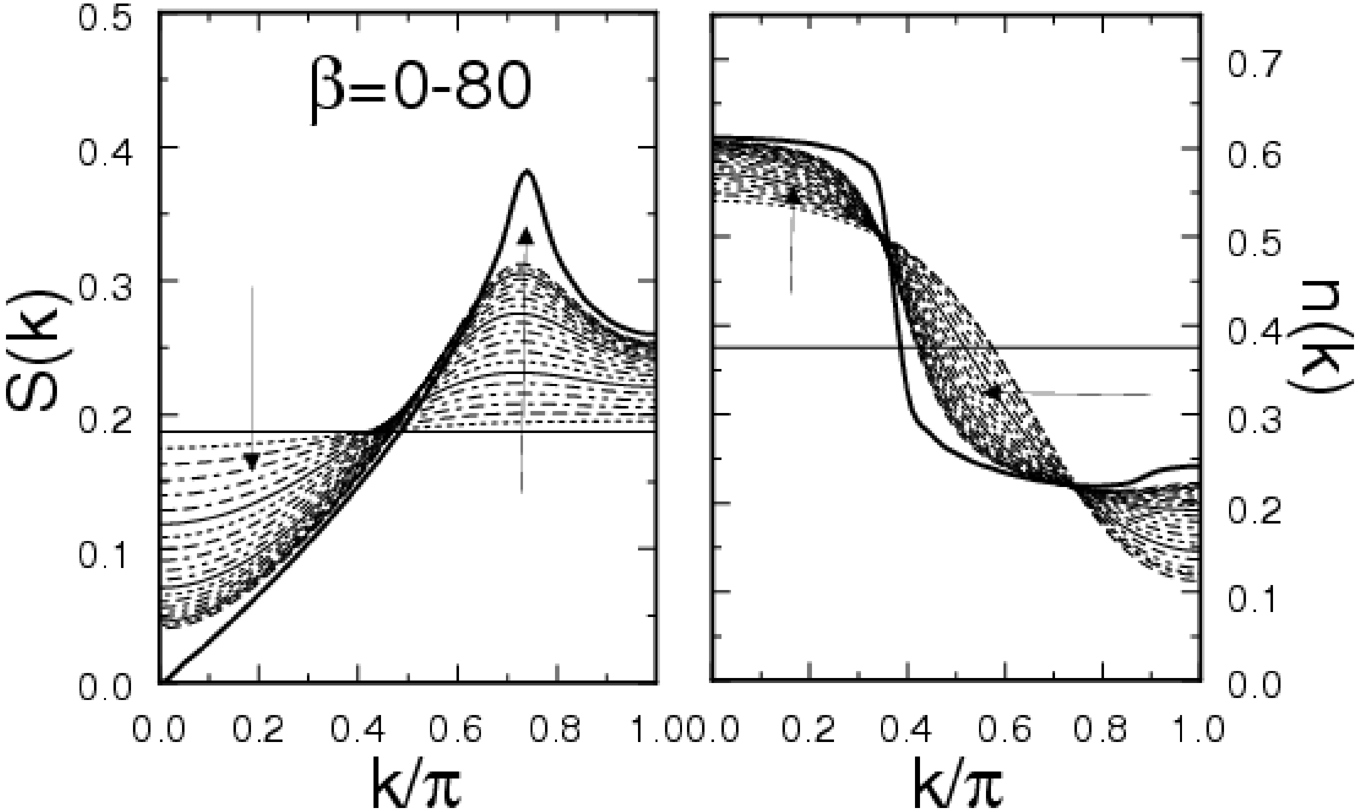


Correlation functions

J=0.05; L=32, N=24; n=0.75

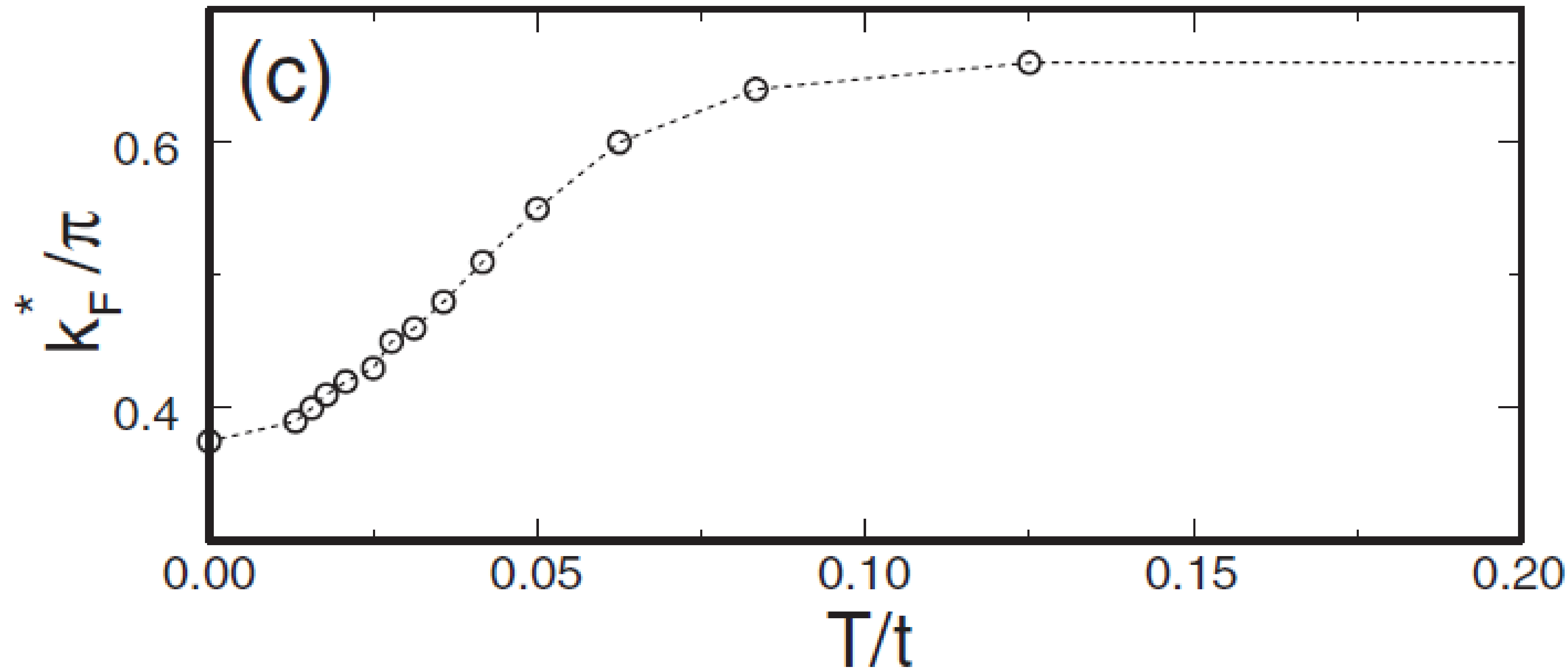
Spin structure factor

Momentum distribution



Fermi momentum

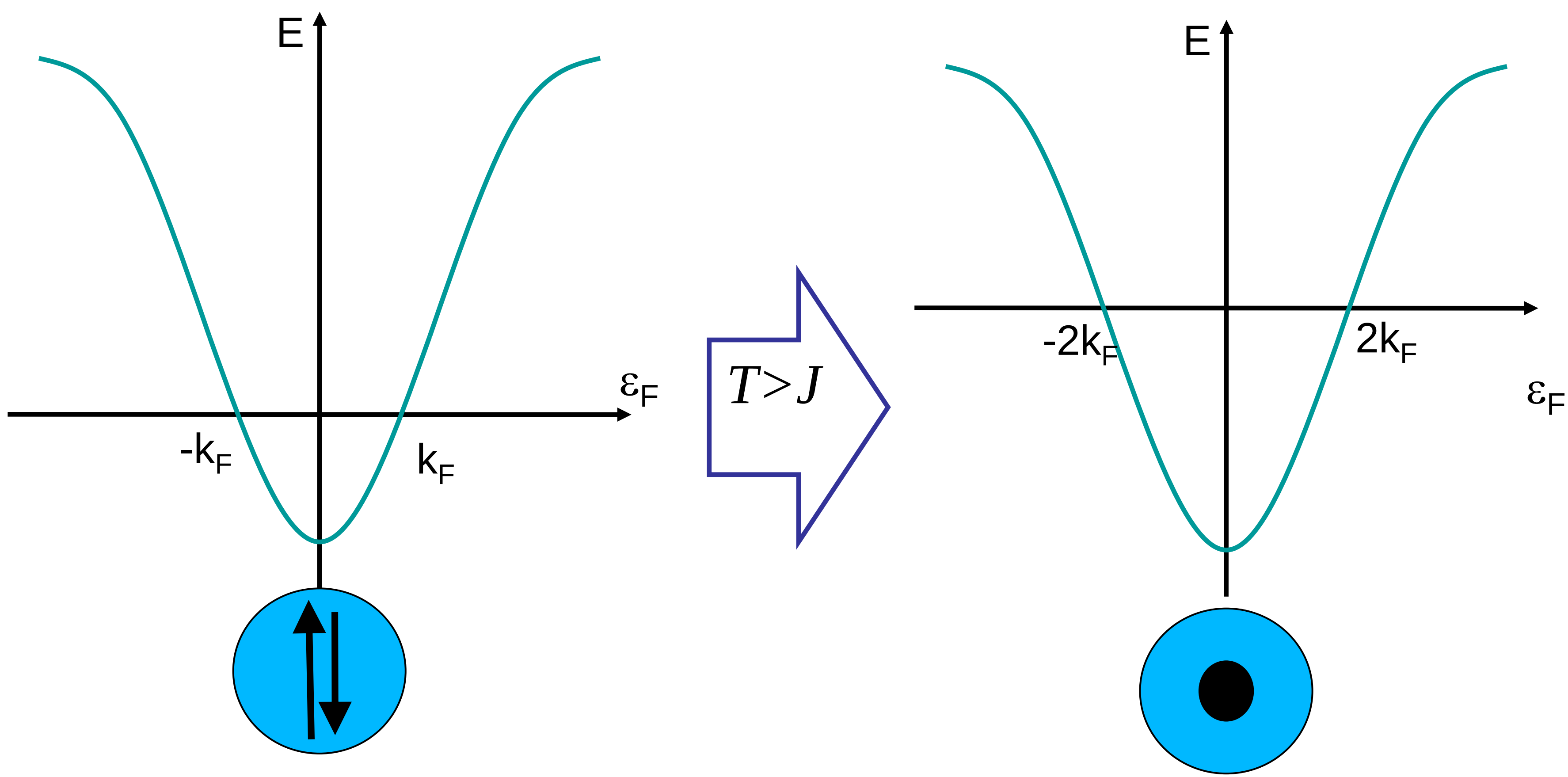
J=0.05; L=32, N=24; n=0.75



From spin-full to spin-less fermions

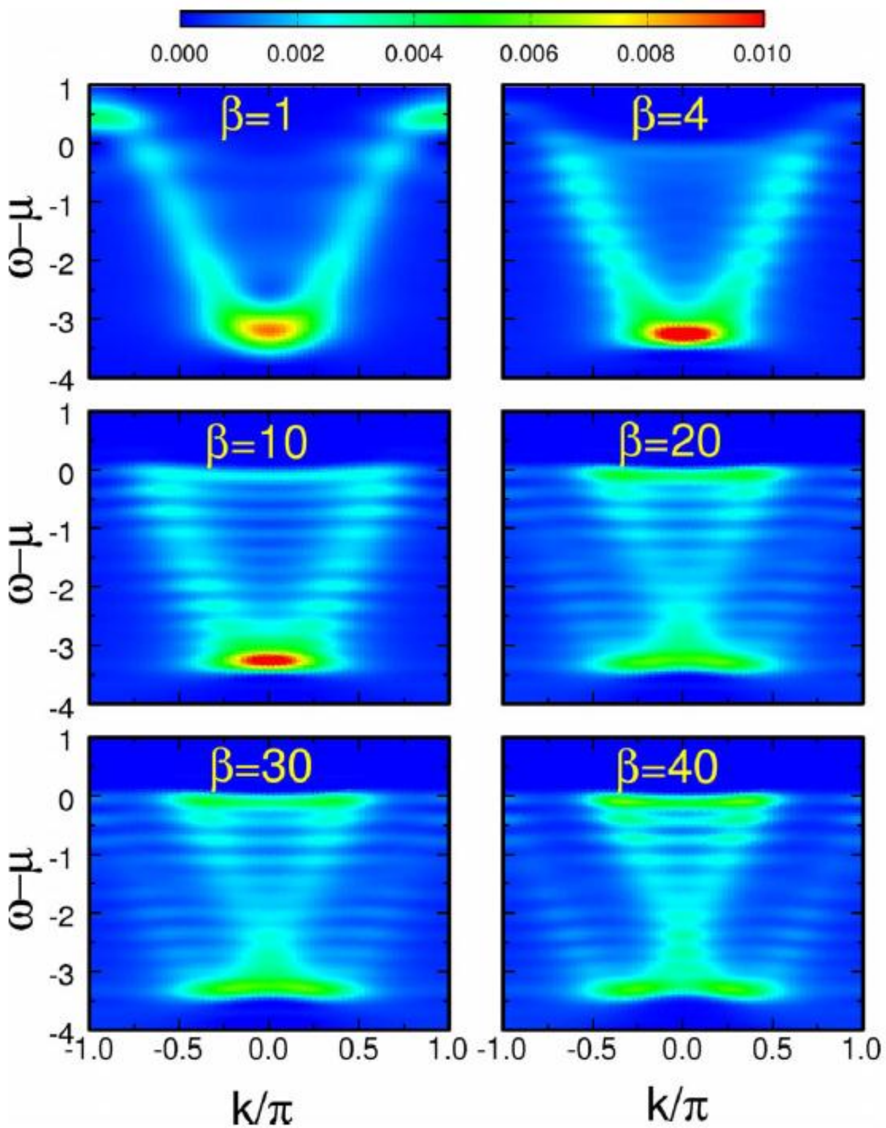
Spin-full fermions: we can put two fermion per state (one up, one down)

Spin-less fermions: we can put only one fermion per state



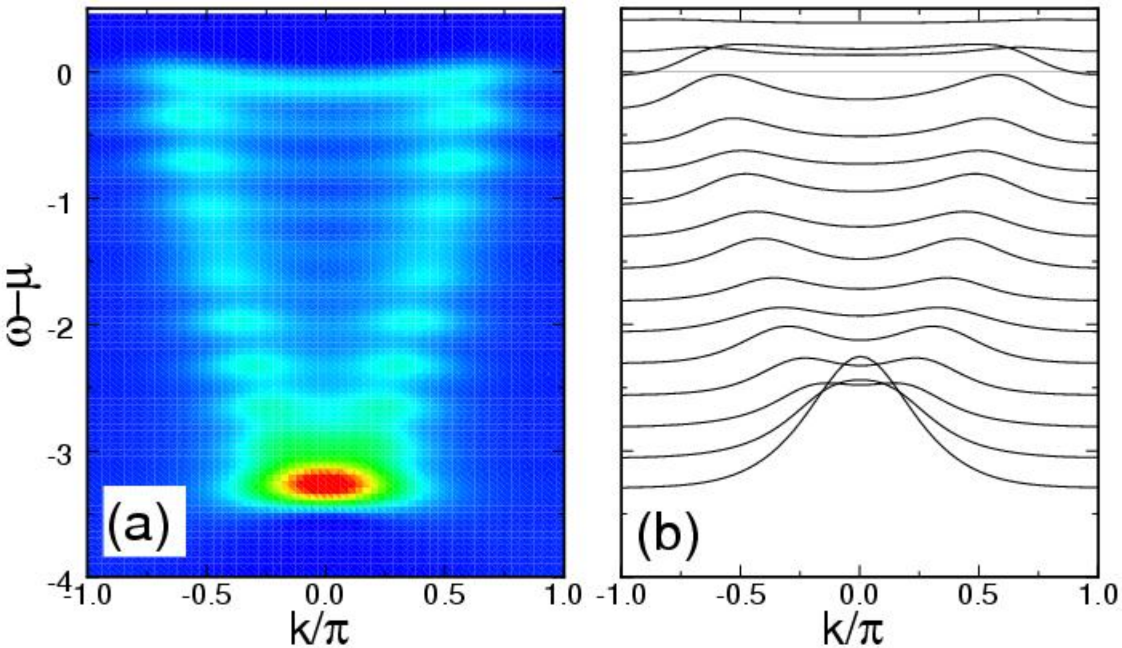
ARPES at finite T

L=32, N=24, J=0.05

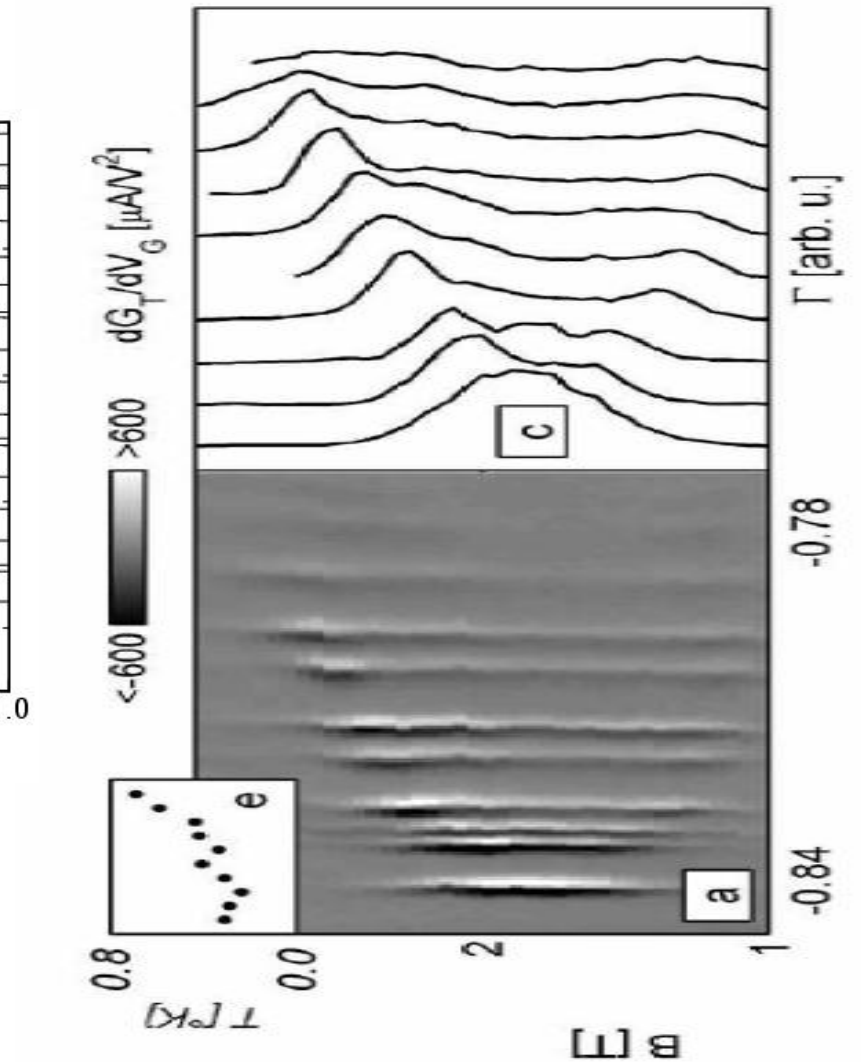


SILL regime

DMRG, $\beta=10$



Experiment



AEF and G. Fiete

H. Steinberg et al., PRB (06)

Infinite "spin temperature"

We introduce and auxiliary spin (ancilla)

$$|I_0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle \right)$$

$\uparrow$: "physical" spin

$\downarrow$: "ancilla"

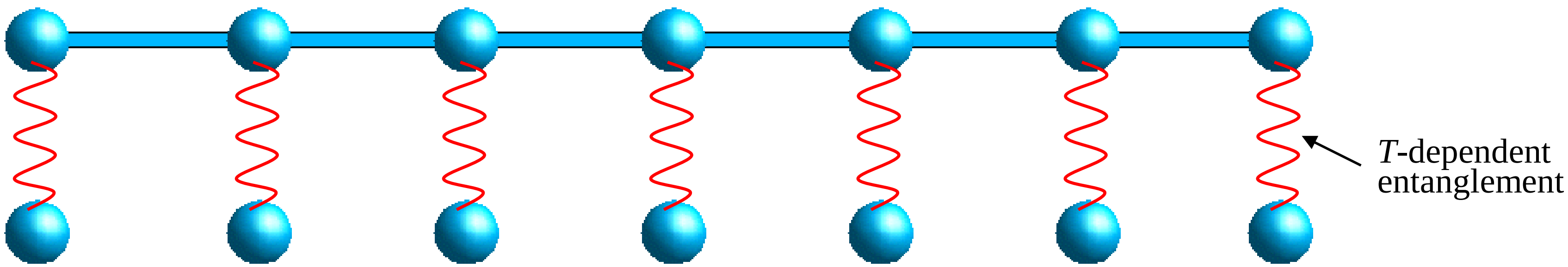
We trace over ancilla:

$$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The density matrix corresponds to the physical spin at infinite temperature!

Takahashi and Umezawa, Collect Phenom. 2, 55 (1975), Verstraete PRL 2004, Zwolak PRL 2004

Many spins



The thermal state is equivalent to evolving the maximally mixed state in imaginary time:

$$|\psi(\beta)\rangle = e^{-\beta H/2}\,|I\,\rangle$$

- The ancillas and the real sites do not interact!
- The **global** state is modified by the action of the Hamiltonian on the real sites, that are entangled with the ancillas.
- The mixed state can be written as a pure state in an enlarged Hilbert space (ladder-like).

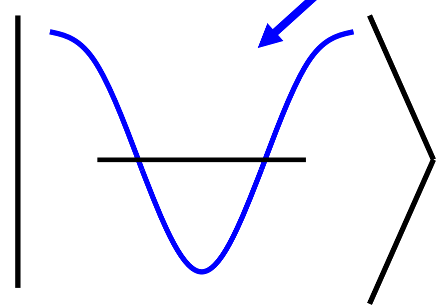
AEF and S. R. White, PRB, Rapid (05)

The factorized wave function

(Ogata and Shiba)

In the limit $U \to \infty, J \to 0$

$$|\mathrm{g.s.}\rangle = |\phi\rangle \otimes |\chi\rangle$$



$$\otimes \; |\sigma_1 \sigma_2 \sigma_3 \ldots \sigma_N\rangle$$

spin

charge

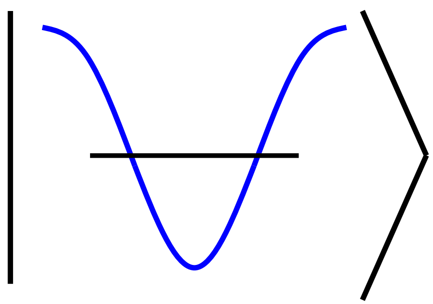
$$\epsilon(k) = -2t\cos(k)$$

All configurations are degenerate

This is not true with periodic boundary conditions: the spin introduces a twist in the fermion wave-function when a fermion hops across a boundary.

The factorized wave function (infinite *spin* Temperature)

$$\left| O(\beta) \right\rangle = \left| \phi \right\rangle \otimes \left| \chi \right\rangle$$



$$\otimes \left| S_1 S_2 S_3 \ldots S_N \right\rangle$$

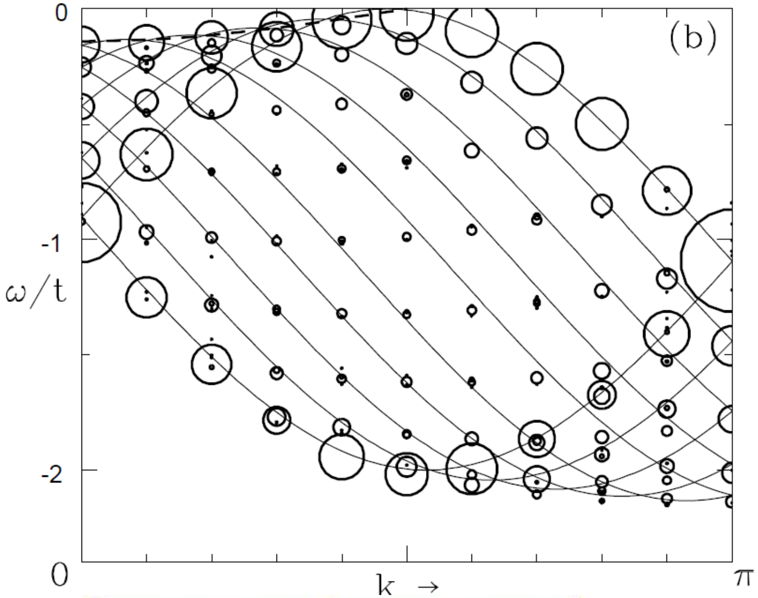
charge

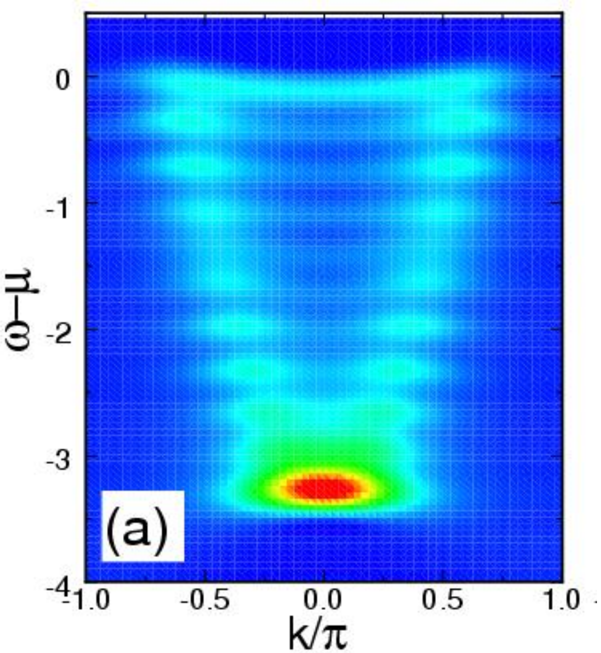
$$\epsilon(k) = -2t\cos(k)$$

Spin-ancilla **singlets**

The intepretation of the spectrum

R. Eder and Y. Ohta, ‘97

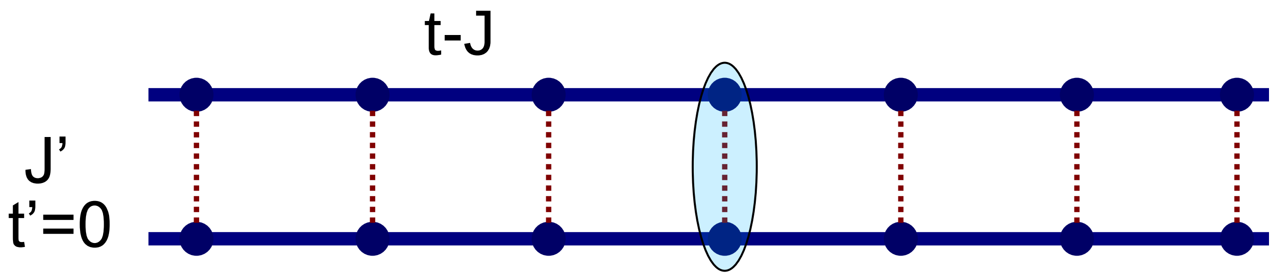




The spectrum of the does not change with temperature!
The spectral function is a convolution of the one from the spinless fermions and the spins. The spectral weight of the spins gets redistributed (in momentum k!), and changes the behavior of the spectral function.

SI behavior in the ground state of strongly interacting models

(I) t-J ladders



J=0,J'=0)

$$\left|\mathrm{g.s.}\right\rangle = \left|\varphi_1\right\rangle \otimes \left|\varphi_2\right\rangle \otimes \left|\chi_1\right\rangle \otimes \left|\chi_2\right\rangle$$

J=0,J' $\to\infty$)

$$\left|\mathrm{g.s.}\right\rangle = \left|\varphi^*\right\rangle \otimes \left|S\right\rangle$$

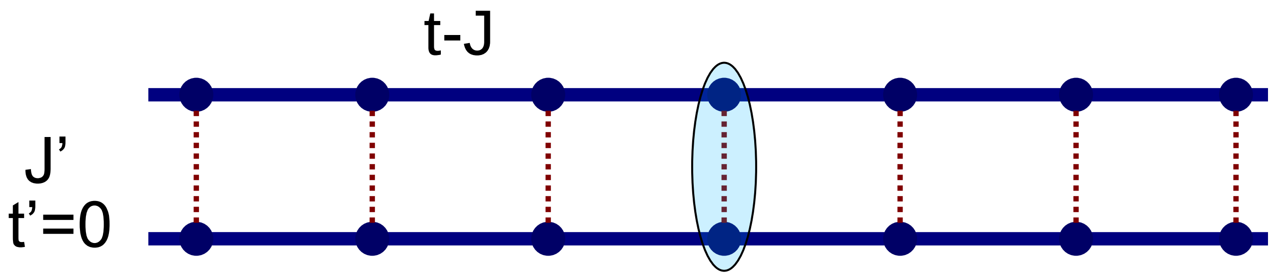
singlets

"heavy" charge

$$\varepsilon(k) = -t\cos(k)$$

AEF and G. Fiete

(I) t-J ladders



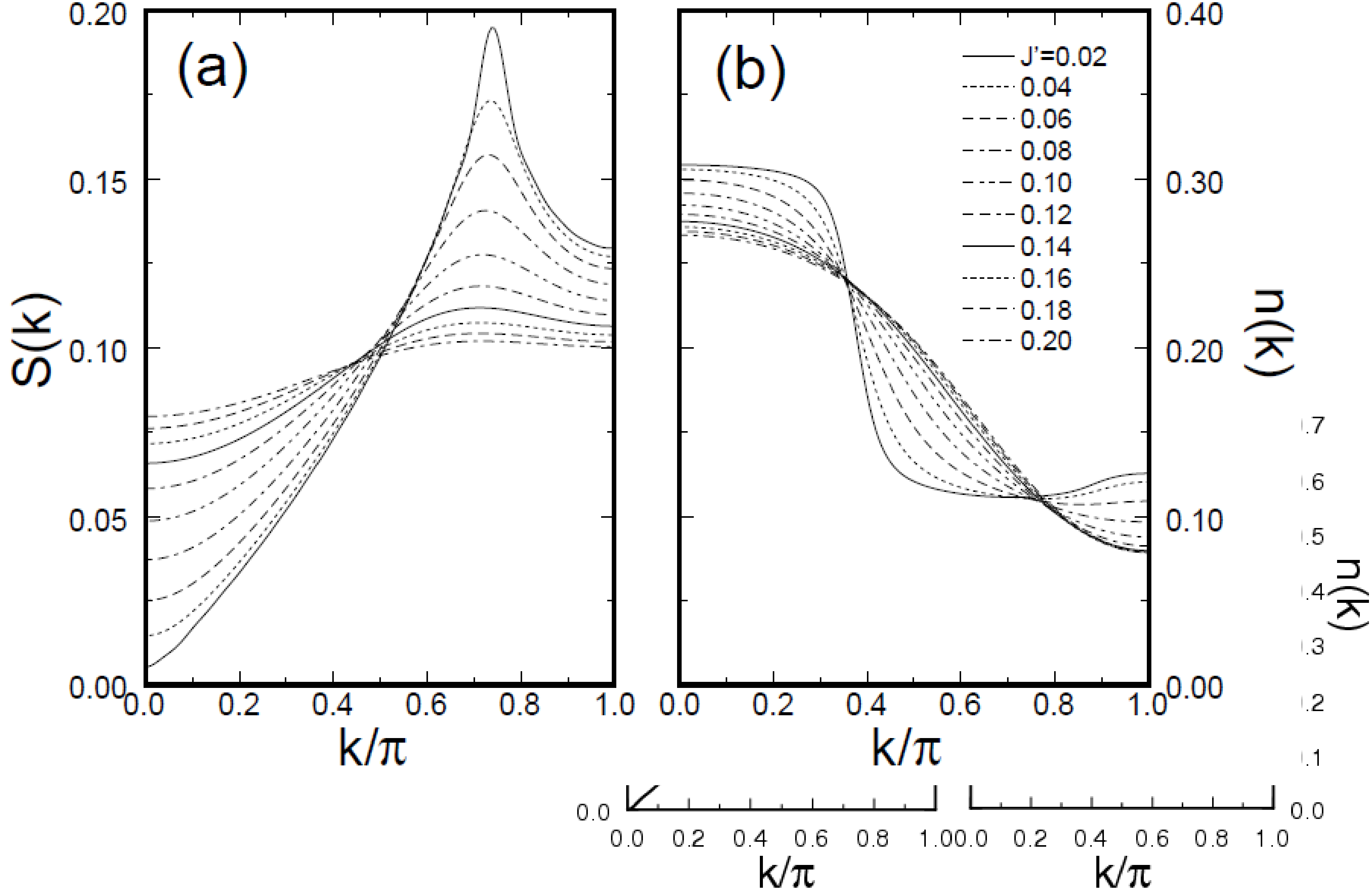
J=0,J'=0) $\left|\mathrm{g.s.}\right\rangle = \left|\varphi_1\right\rangle \otimes \left|\varphi_2\right\rangle \otimes \left|\chi_1\right\rangle \otimes \left|\chi_2\right\rangle$

In the intermediate regime, the spin will get entangled first, before the charges get entangled to form heavy pairs:

$$\left|\mathrm{g.s.}\right\rangle = \left|\varphi_1\right\rangle \otimes \left|\varphi_2\right\rangle \otimes \left|S\right\rangle$$

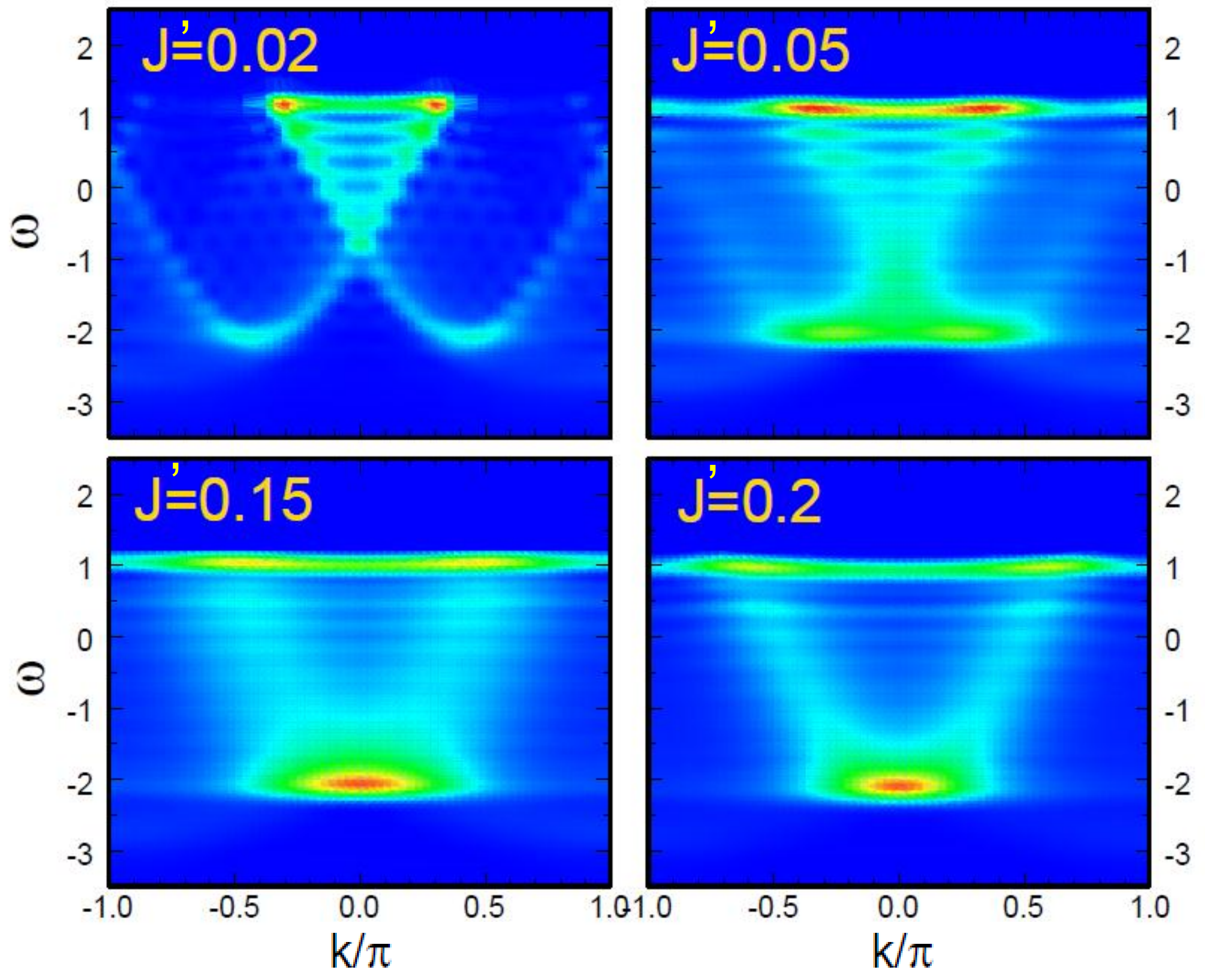
similar to Ogata and Shiba wave function at infinite spin T!!!

Correlation functions (J=0.05)

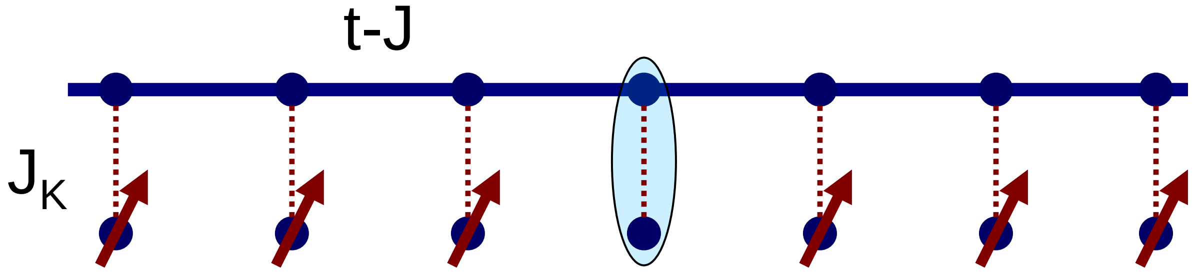


t-J ladder lattice at T=0

L=32,N=24,J=0.05

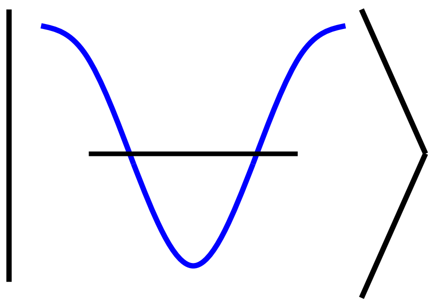


(II) Kondo lattice



The factorized wave function in the limit $J\to 0$, $J_K=0$

$$|\text{g.s.}\rangle = |\varphi\rangle \otimes |\chi\rangle \otimes |\sigma\rangle$$



$$\otimes\ |\sigma_1\sigma_2\sigma_3\ldots\sigma_N\rangle \otimes |\sigma_1\sigma_2\sigma_3\ldots\sigma_L\rangle$$

charge

$\epsilon(k) = -2t\cos(k)$

spin

impurities

All spin configurations are degenerate.

When we turn on the interactions with the impurities J_K:

(i) The system becomes ferromagnetic,

(ii) The conduction spins and the impurities get entangled

(iii) An exponentially small charge gap opens (to break a pair)

The factorized wave function in the limit $J \to 0$

$$|\text{g.s.}\rangle = |\varphi\rangle \otimes |\chi\rangle \otimes |\sigma\rangle$$

These get entangled first

$$|\text{g.s.}\rangle = |\varphi\rangle \otimes |\text{spin m-b state}\rangle$$

$J_K \to \infty$

$$|\text{g.s.}\rangle = |\varphi^*\rangle \otimes |\text{S}\rangle \otimes |\uparrow \ldots \uparrow\rangle$$

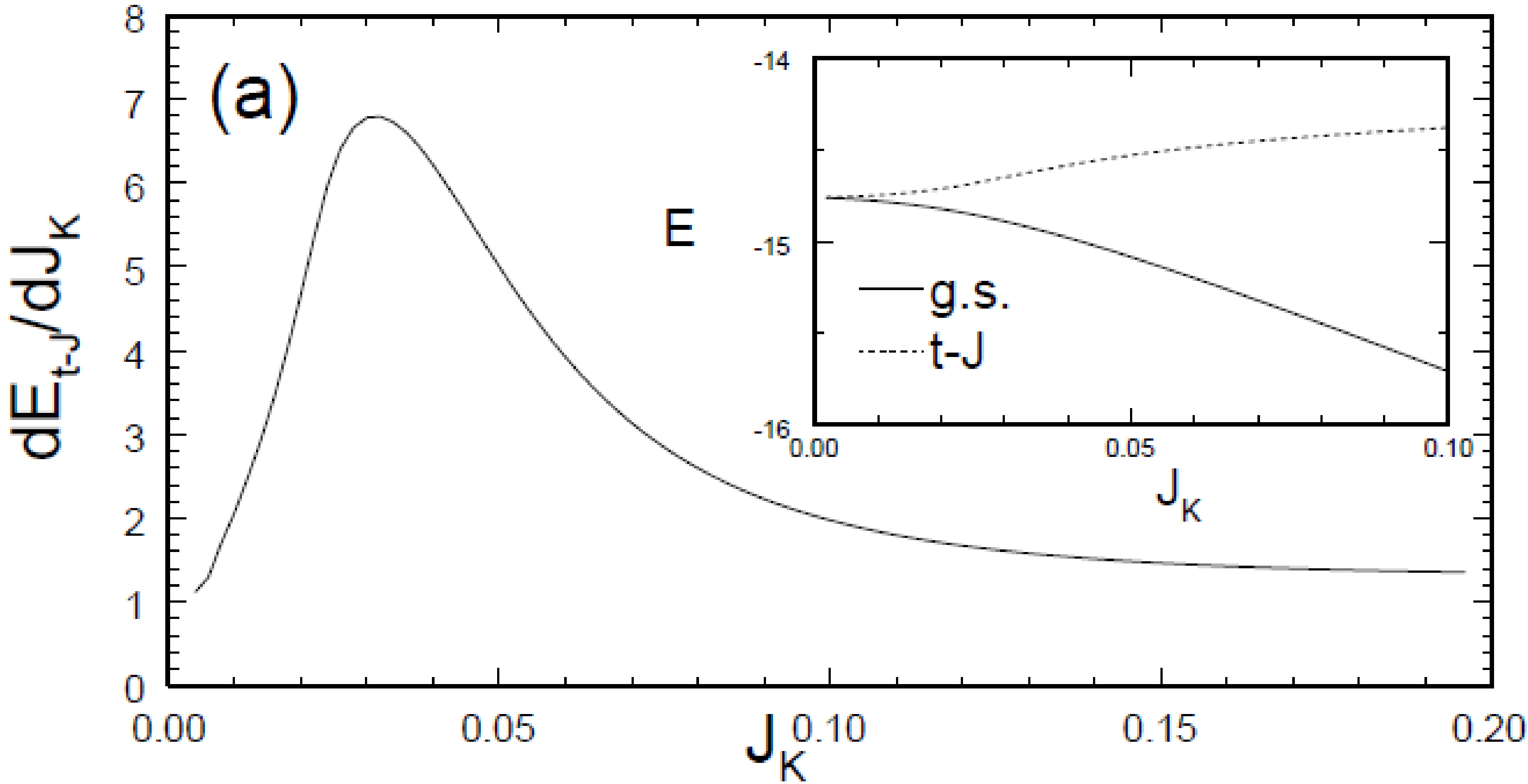
"heavy" charge

$$\varepsilon(k) = -t\cos(k)$$

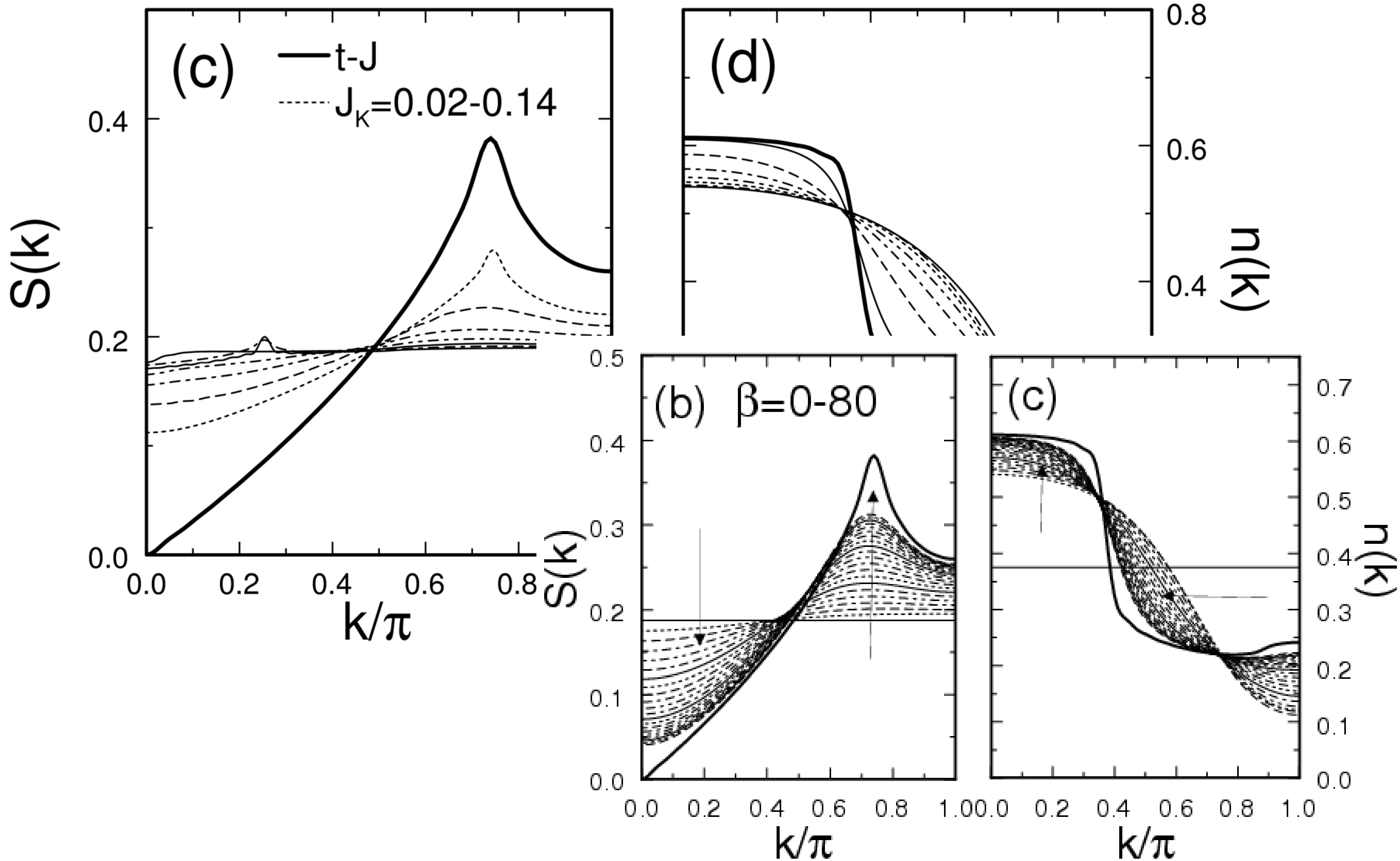
singlets

FM Unpaired impurities

Ground state energy and effective "specific heat" (J=0.05)

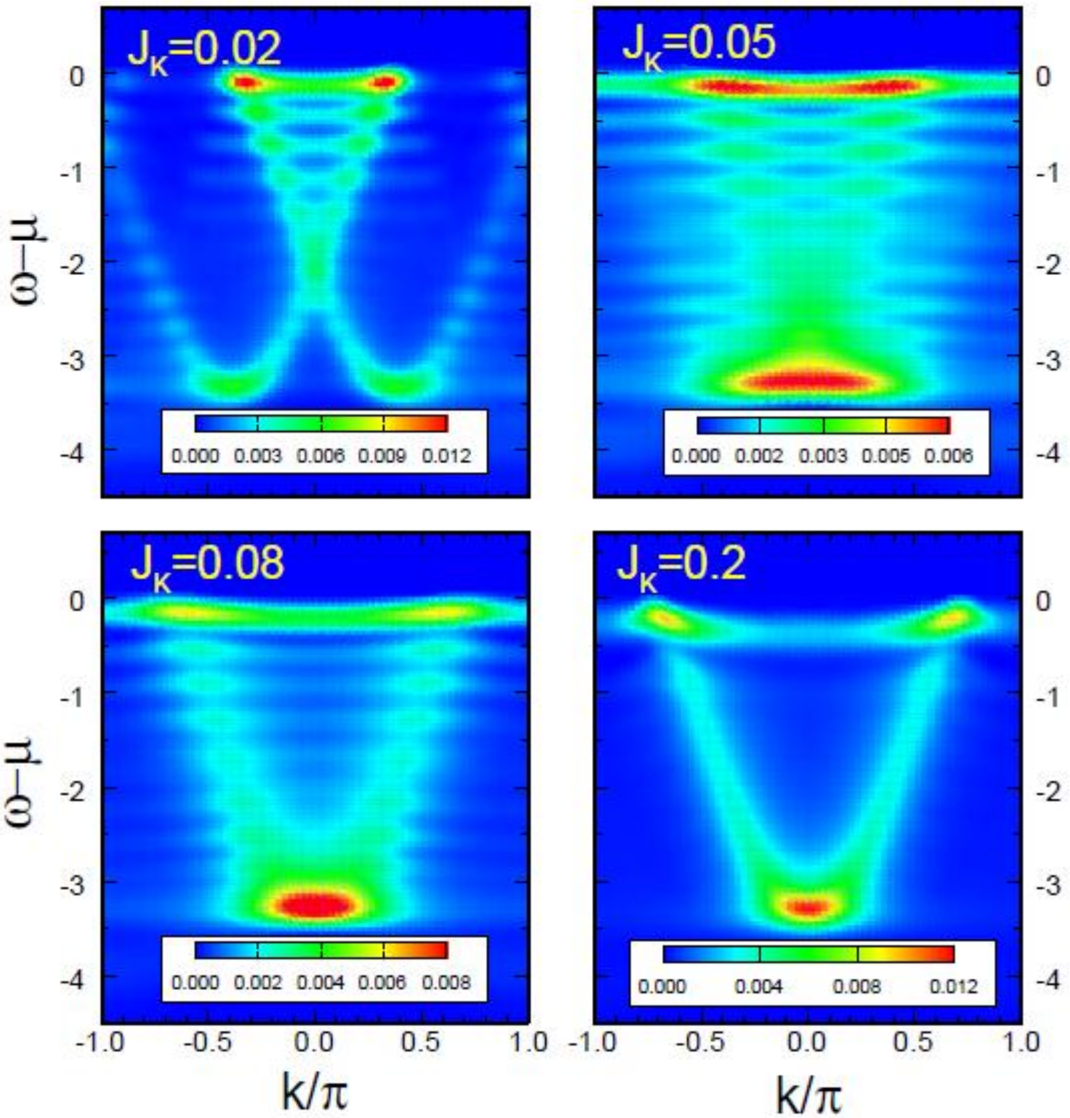


Correlation functions



Kondo lattice at T=0

L=32,N=24,J=0.05



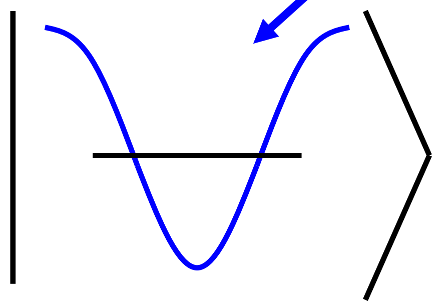
Toward a unified formalism

The factorized wave function

(Ogata and Shiba)

In the limit U→∞,J→0

$$|\mathrm{g.s.}\rangle = |\phi\rangle \otimes |\chi\rangle$$



$$\otimes\, |\sigma_1\sigma_2\sigma_3\ldots\sigma_N\rangle$$

charge

$\epsilon(k) = -2t\cos(k)$

spin

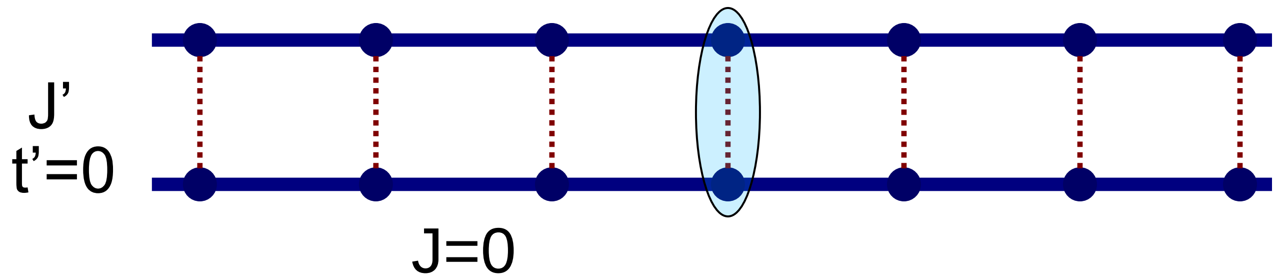
All configurations are degenerate

$$c_{i\sigma} \rightarrow \boxed{f_i}\,\boxed{Z_{i\sigma}} \qquad H = H_c + H_s$$

charge

spin

Variational formulation for the t-J ladder

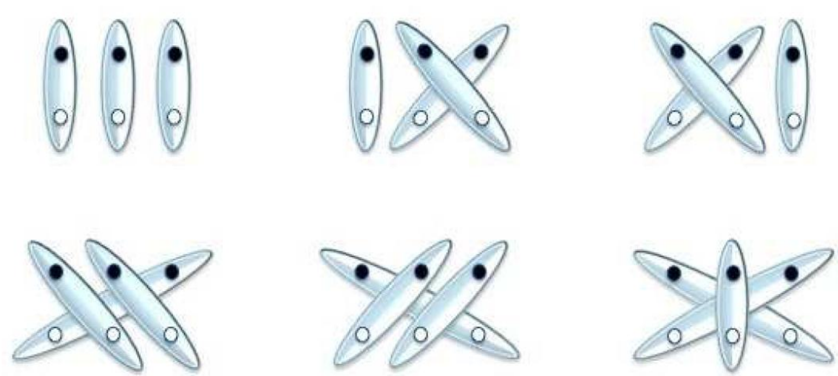


Intuitive argument (we assume periodic boundary conditions):

- All spins see a partner on the opposite leg with equal probability.
- When this happens, they become maximally entangled (form a singlet).
- Entanglement persists when they move apart since there are no competing interactions along the leg.

$$|\mathrm{g.s.}\rangle = |\varphi^*\rangle \otimes |S\rangle; \quad |S\rangle = \sum |x\rangle$$

The sum is over all possible valence bond coverings between the spins of opposite legs

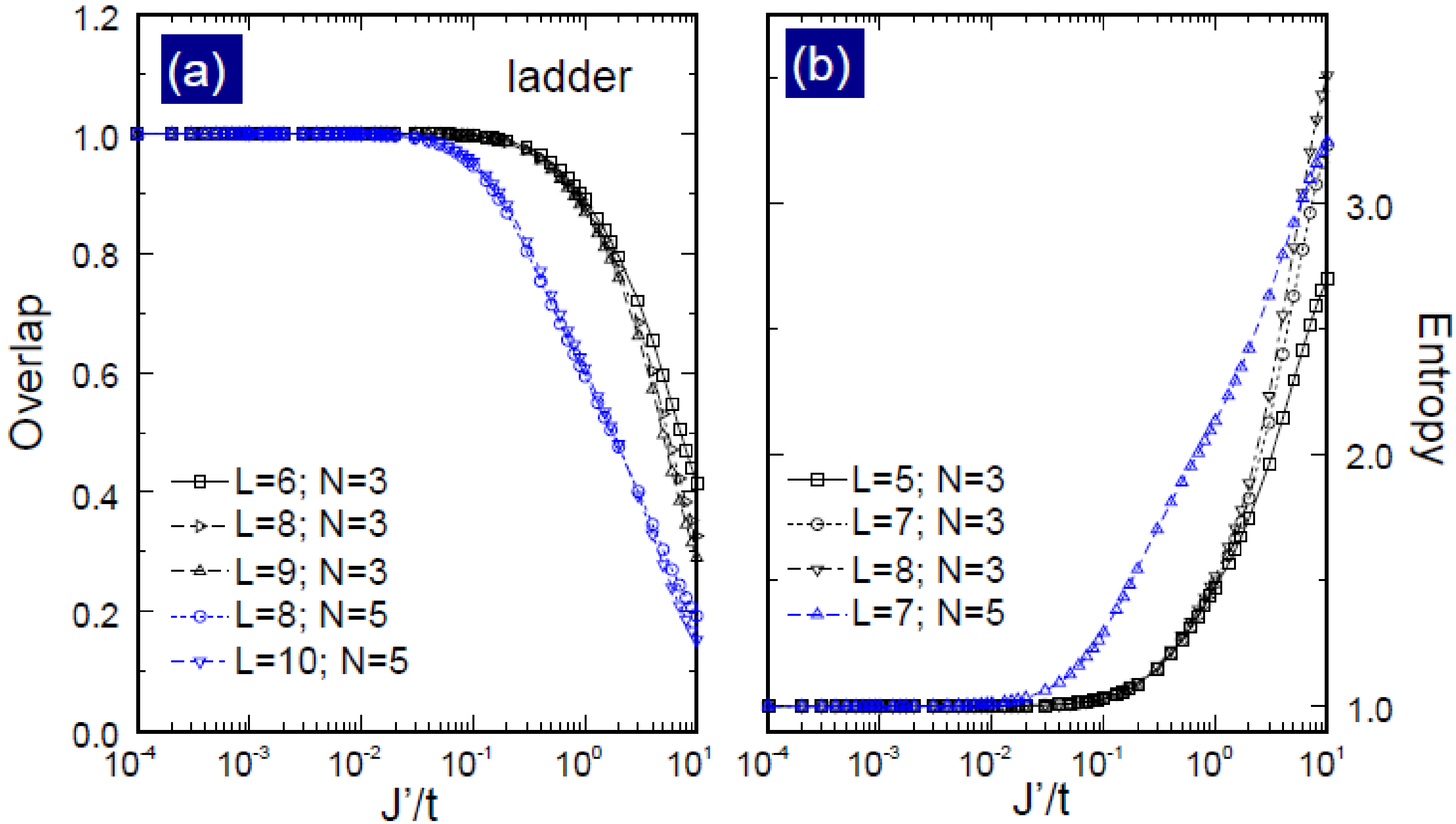


Results for t-J ladders

$$H_{\rm AB} = \sum_{i,j} \vec{s}_{i,{\rm A}} \cdot \vec{s}_{j,{\rm B}} = \vec{S}_{\rm A} \cdot \vec{S}_{\rm B} \longrightarrow \; S_{\rm A} = \log\left(N+1\right)$$

$$\langle \vec{s}_{i,{\rm A}} \cdot \vec{s}_{j,{\rm B}} \rangle = \frac{1}{N^2} \langle H_{\rm AB} \rangle = -\frac{1}{4} - \frac{1}{2N}$$

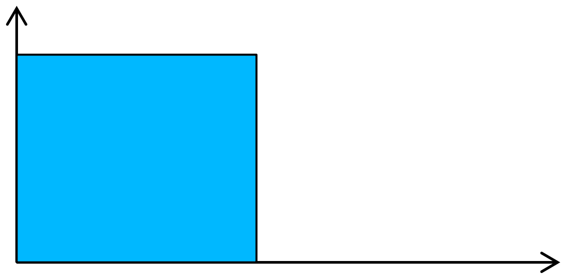
$$\langle \vec{s}_{i,1} \cdot \vec{s}_{j,2} \rangle = (-\frac{1}{4} - \frac{1}{2N}) \langle n_{i,1} n_{j,2} \rangle = (-\frac{1}{4} - \frac{1}{2N}) \left(\frac{N}{L}\right)^2$$



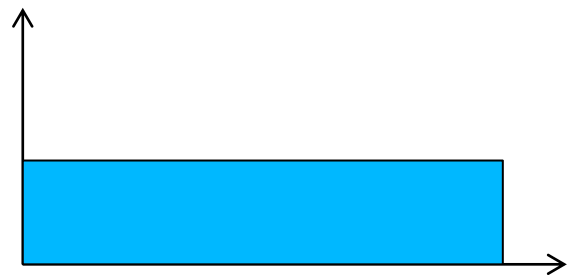
Momentum distribution function

(for a single chain)

$$n(k) = (1/L)\sum_{l,\sigma}\exp(ikl)\langle c^\dagger_{1,\sigma} c_{l,\sigma}\rangle \xrightarrow[\substack{c^\dagger_{1,\sigma} = Z^\dagger_{1\sigma} f^\dagger_1 \\ \langle Z^+ Z\rangle = 1}]{} n(k) = (1/L)\sum_{l,\sigma}\exp(ikl)\langle f_1^\dagger f_l\rangle$$

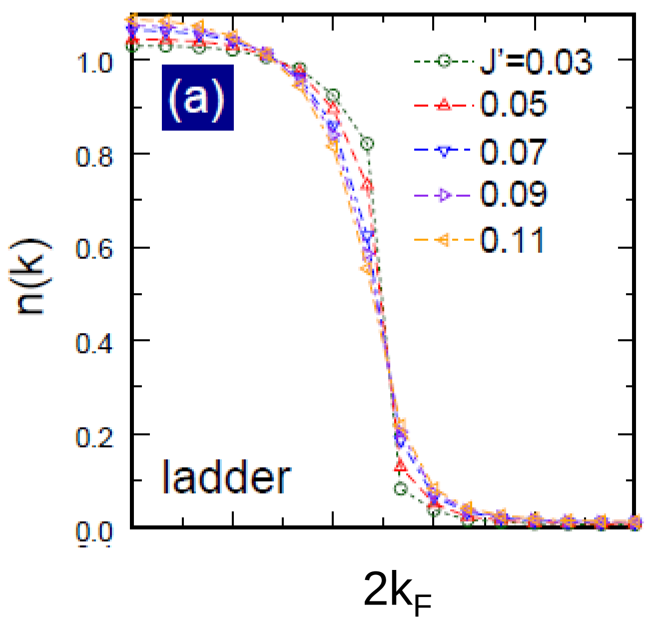


k_F

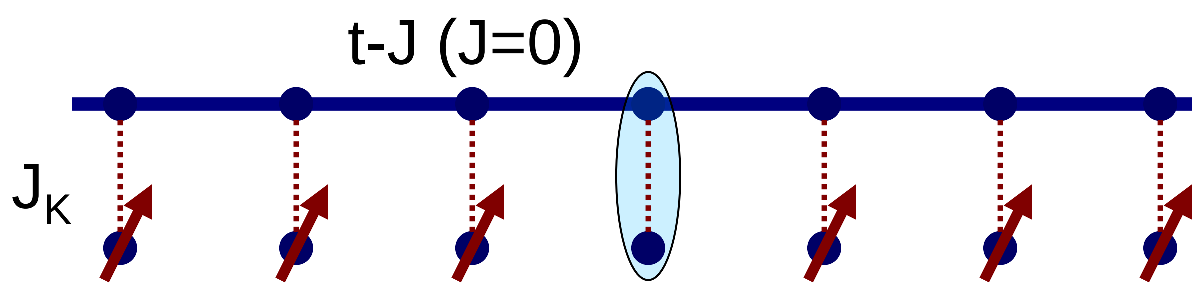


$2k_F$

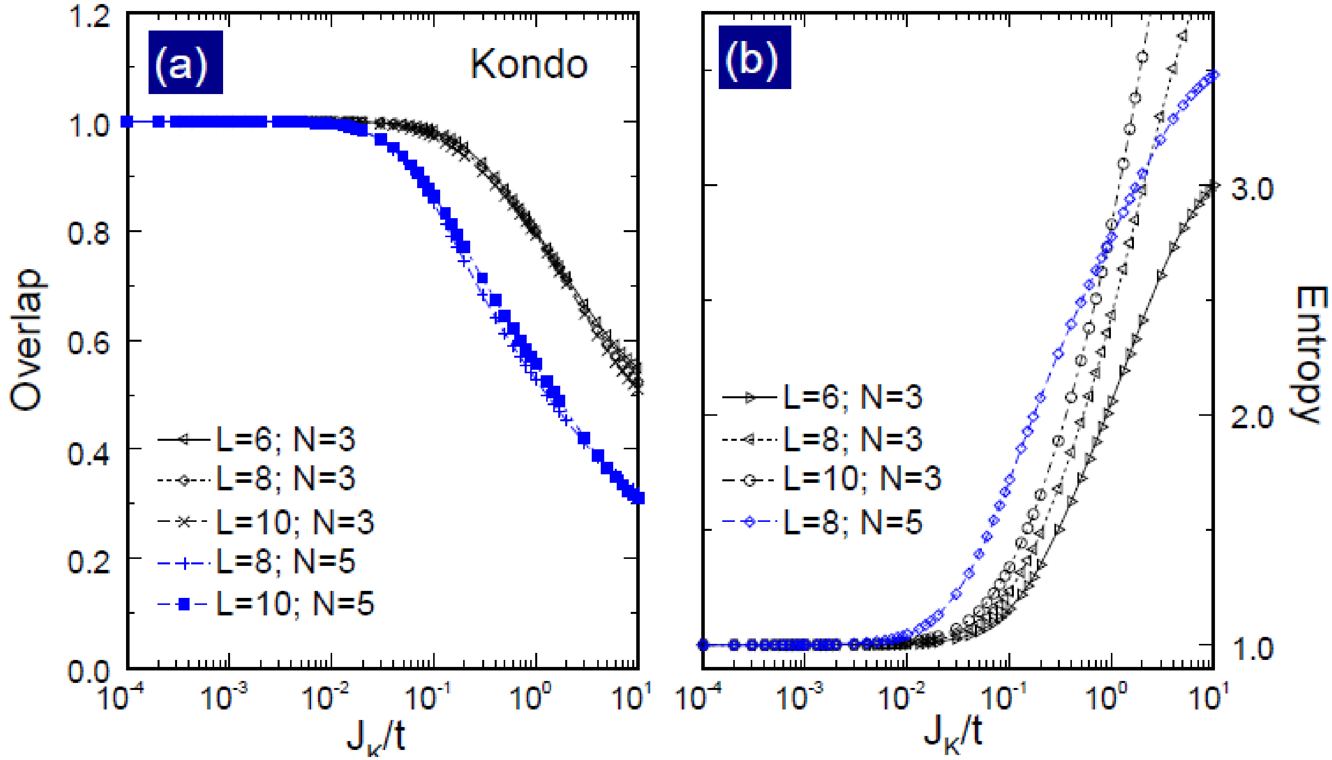
DMRG (L=30)



Results for the Kondo lattice

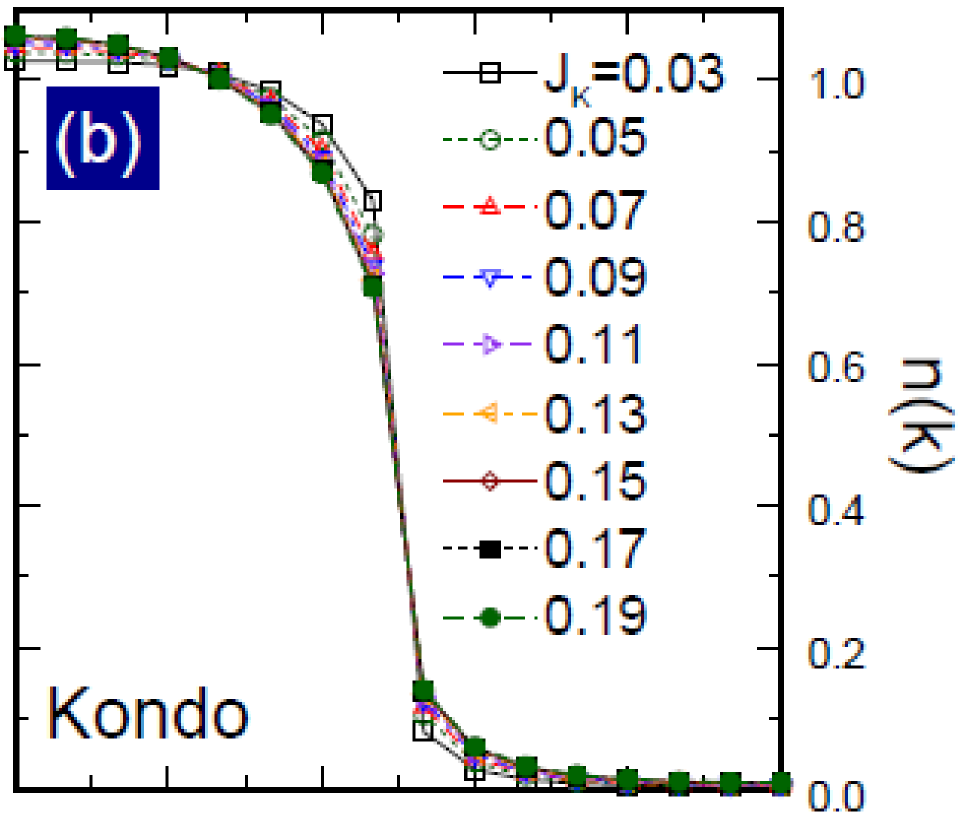


$$|g.s.\rangle = |\varphi^*\rangle \otimes |S\uparrow \ldots \uparrow\rangle$$

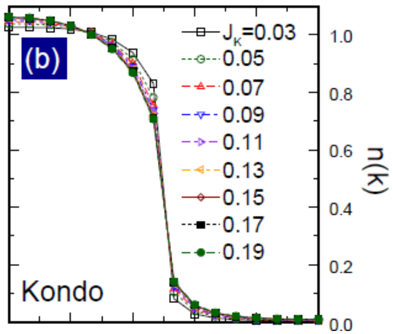


Momentum distribution function

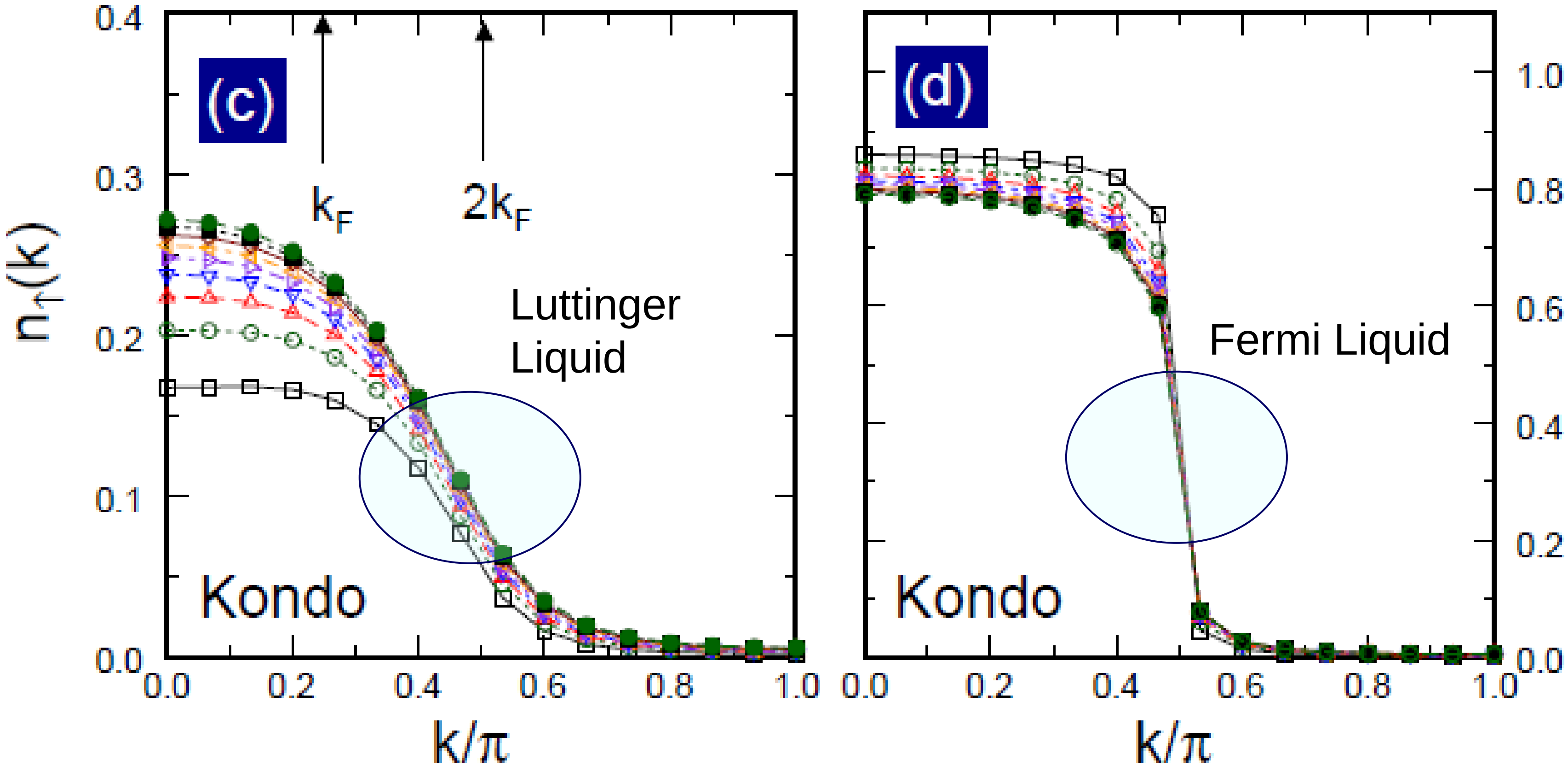
DMRG (L=30)



MDF per spin

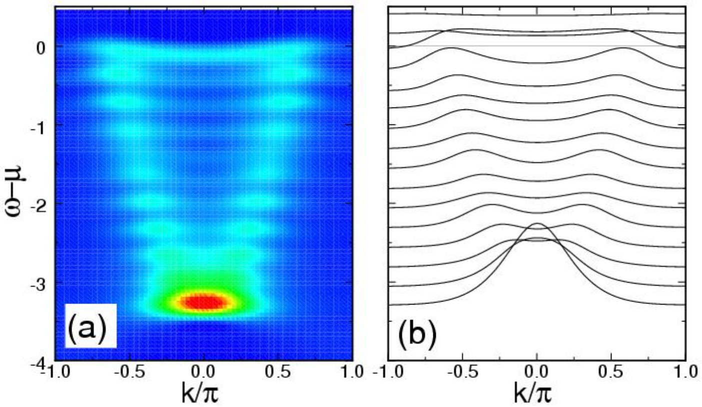


DMRG (L=30)



Conclusions

- We showed an application of the time dependent DMRG combining evolution in real-time and imaginary time.
- We studied the crossover from spin incoherent to spin coherent behavior
- We generalized the Ogata and Shiba's factorized wave function to finite *spin* temperatures
- We found that the t-J ladder in some regime of parameters and the Kondo lattice exhibit SI behavior in the *ground-state*.
- This SI behavior is not exactly SILL, but results indicate that it might be possible to describe it within the same framework, and may present some universal features.
- Is a "half-Luttinger liquid" a new kind of physics?



THANK YOU!

Evolution in imaginary time: single spin

We introduce and auxiliary spin (ancilla)

$$|I_0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle \right)$$

$\uparrow$: "physical" spin

$\downarrow$: "ancilla"

We trace over ancilla:

$$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

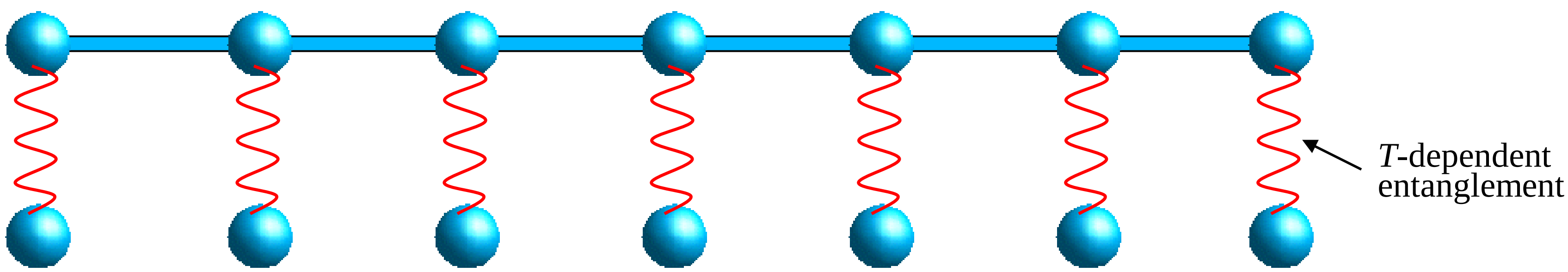
The density matrix corresponds to the physical spin at infinite temperature!

Takahashi and Umezawa, Collect Phenom. 2, 55 (1975), Verstraete PRL 2004, Zwolak PRL 2004

Evolution in imaginary time

The thermal state is equivalent to evolving the maximally mixed state in imaginary time:

$$|\psi(\beta)\rangle = e^{-\beta H/2}\, |I\rangle$$



•The ancillas and the real sites do not interact!

•The **global** state is modified by the action of the Hamiltonian on the real sites, that are entangled with the ancillas.

•The mixed state can be written as a pure state in an enlarged Hilbert space (ladder-like).

Evolution in imaginary time: Thermal averages

A thermal average :

$$\langle A\rangle = Z^{-1}(\beta)\mathrm{Tr}\{Ae^{-\beta H}\}, \qquad Z(\beta) = \mathrm{Tr}\{e^{-\beta H}\}.$$

Can be obtained using a wave function instead of density matrices!!!

$$\langle A\rangle = \frac{\langle\psi(\beta)|A|\psi(\beta)\rangle}{\langle\psi(\beta)|\psi(\beta)\rangle} = Z^{-1}(\beta)\sum_n \langle n|A|n\rangle e^{-\beta E_n}$$

with $Z(\beta)=\langle\psi(\beta)|\psi(\beta)\rangle$

AEF and S. R. White, PRB, Rapid (05)

Green's functions

The finite temperature Green's function can be obtained as:

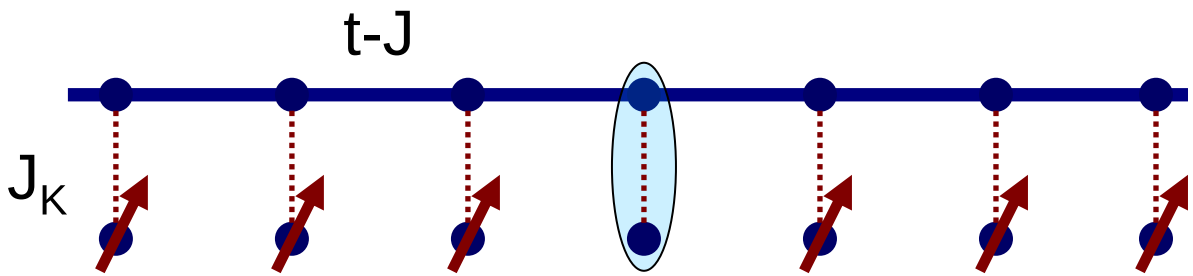
$$G(x-x_0,t,\beta)=\langle\psi(\beta)|e^{iH_{t\text{-}J}t}\hat{O}^{\dagger}(x)e^{-iH_{t\text{-}J}t}\hat{O}(x_0)|\psi(\beta)\rangle$$

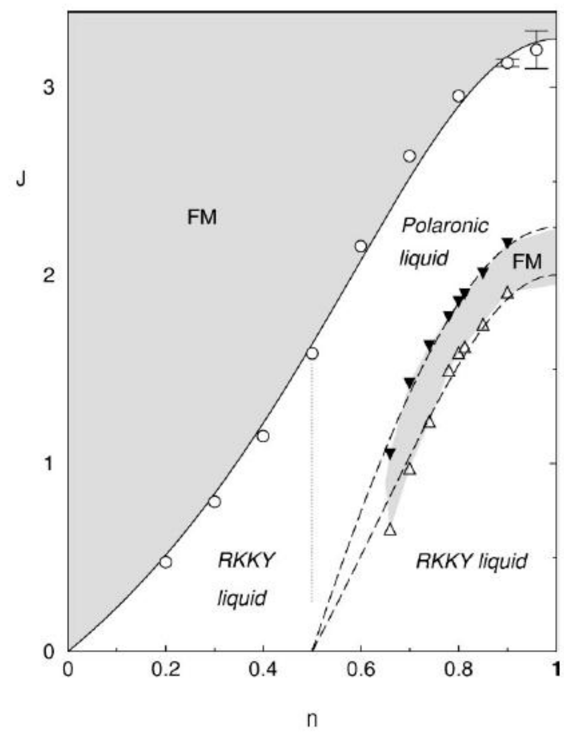
Since the thermal state is not an eigenstate, we need to evolve in time both:

$$e^{-iH_{t\text{-}J}t}|\psi(\beta)\rangle$$

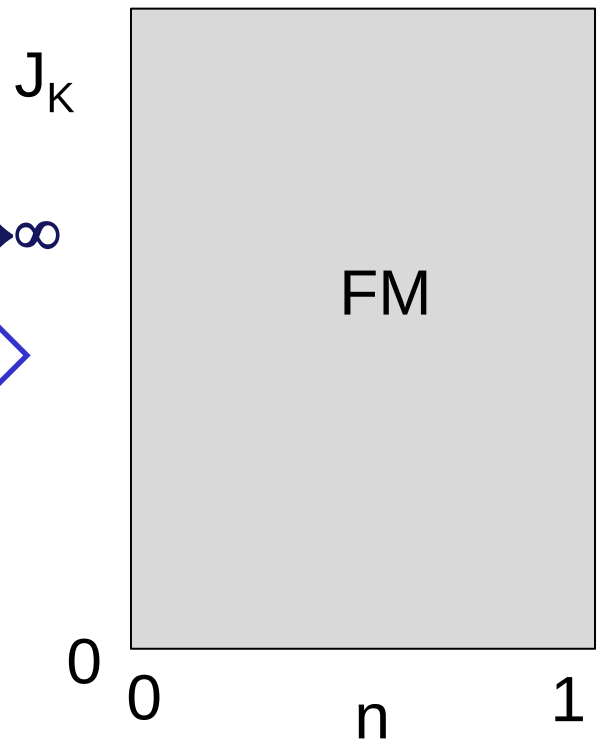
$$e^{-iH_{t\text{-}J}t}\hat{O}(x_0)|\psi(\beta)\rangle$$

(II) Kondo lattice





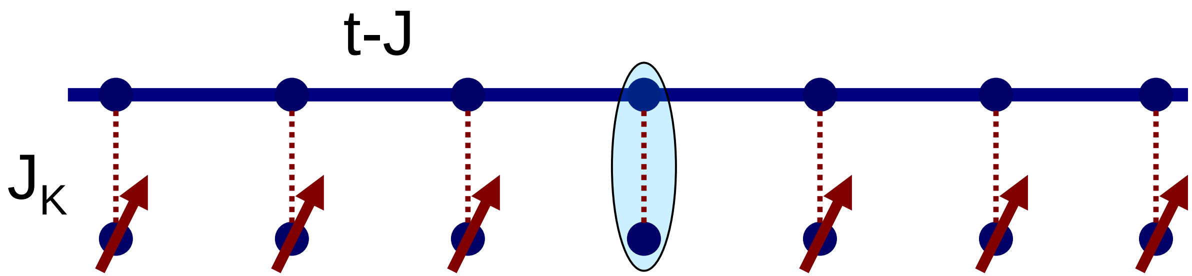
$J\rightarrow 0,\ U\rightarrow\infty$

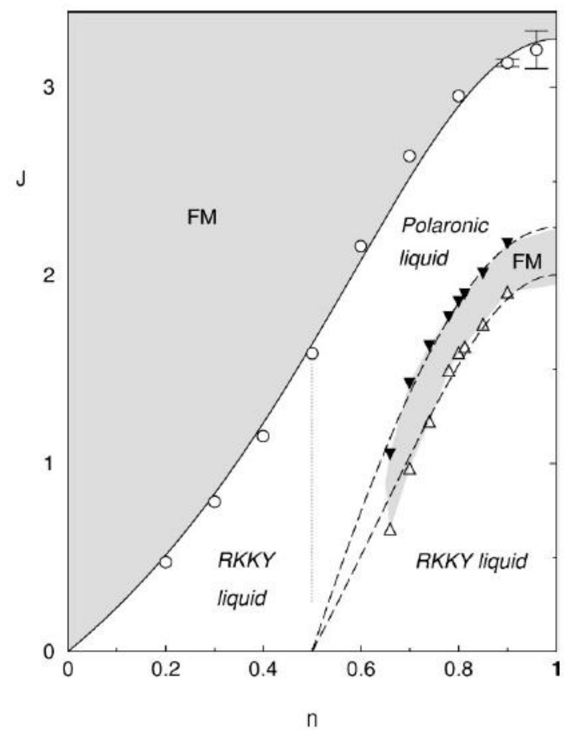


McCulloch et al, PRB ’02, K. Hallberg et al, PRL ‘04

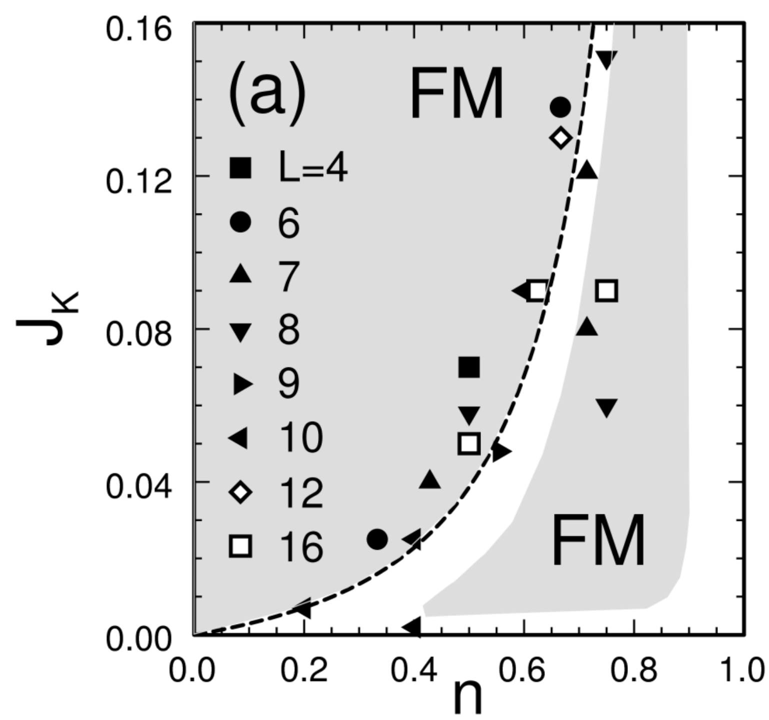
Tsunetsugu, Sigrist, Ueda, RMP ‘97

(I) Kondo lattice





***J*=0.05**



McCulloch et al, PRB ’02, K. Hallberg et al, PRL ‘04

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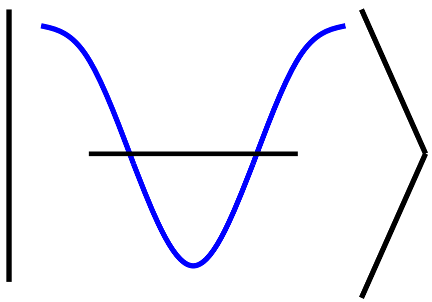
The factorized wave function in the limit $J\to 0$, $J_K=0$

$$\left|\text{g.s.}\right\rangle = \left|\varphi\right\rangle \otimes \left|\chi\right\rangle \otimes \left|\sigma\right\rangle$$



$$\otimes \left|\sigma_1\sigma_2\sigma_3\ldots\sigma_N\right\rangle \otimes \left|\sigma_1\sigma_2\sigma_3\ldots\sigma_L\right\rangle$$

charge

$\epsilon(k) = -2t\cos(k)$

spin

impurities

All spin configurations are degenerate.

When we turn on the interactions with the impurities J_K:

(i) The system becomes ferromagnetic,

(ii) The conduction spins and the impurities get entangled

(iii) An exponentially small charge gap opens (to break a pair)

The factorized wave function in the limit $J \to 0$, $J_K \to \infty$

$$|\text{g.s.}\rangle = |\varphi\rangle \otimes |\chi\rangle \otimes |\sigma\rangle$$

$J_K \to \infty$

$$|\text{g.s.}\rangle = |\varphi^*\rangle \otimes |S\rangle \otimes |\uparrow \ldots \uparrow\rangle$$

“heavy” charge

$$\varepsilon(k) = -t\cos(k)$$

singlets

FM Unpaired impurities

Ogata and Shiba wave function at infinite spin T!!!