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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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SMR. 767 - 8

MINIWORKSHOP ON STRONG CORRELATIONS AND QUANTUM CRITICAL PHENOMENA
(4 - 22 July 1994)

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DOPED SPIN-GAP INSULATORS

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Doped Spin-gap Insulators:

Pairing and Excitation Spectrum in doped t - J Ladders

Hirokazu Tsunetsugu (ETH)

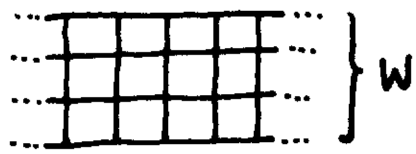
collaboration with Matthias Troyer (ETH)
T. Maurice Rice (ETH)
D. Würtz (ETH)
D. Poilblanc (Toulouse)

QESTION

What happens if holes are doped into a spin-gap insulator ?

Nice example :

- Heisenberg Spin Ladder



W : even $\Rightarrow$ $\Delta_{spin} > 0$

W : odd $\Rightarrow$ $\Delta_{spin} = 0$

OUTLINE

(1) 2-chain Spin Ladder Compounds

$(VO)_2P_2O_7$ } insulators ($S=1/2$)
$Sr_2Cu_4O_6$

(2) Heisenberg Ladders

excitations, thermodynamics
strong coupling fixed point
spin liquid ($\Delta_s>0$, $\xi<\infty$) — short range RVB

(3) Doped t-J Ladders

exact diagonalization (Lanczos, up to 2x10 sites)
strong coupling limit ← simple limit

a) hole binding
b) spin excitations
c) 1-particle excitations

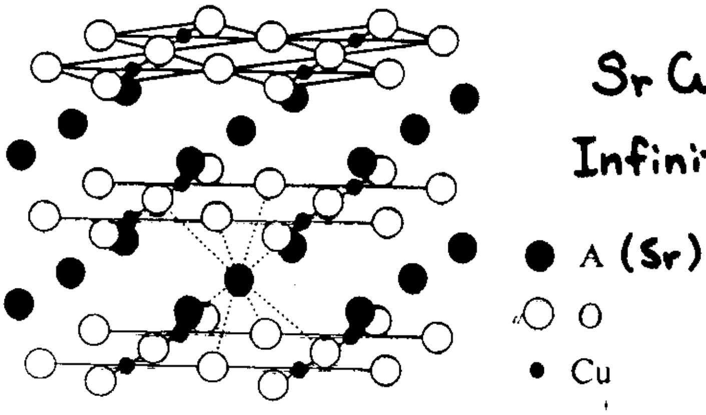
(4) Application to a 2D system

a possible alternative scenario
—— singlet stripe phases

$Sr_{2n-2}Cu_{2n}O_{4n-2}$

Kyoto Univ.

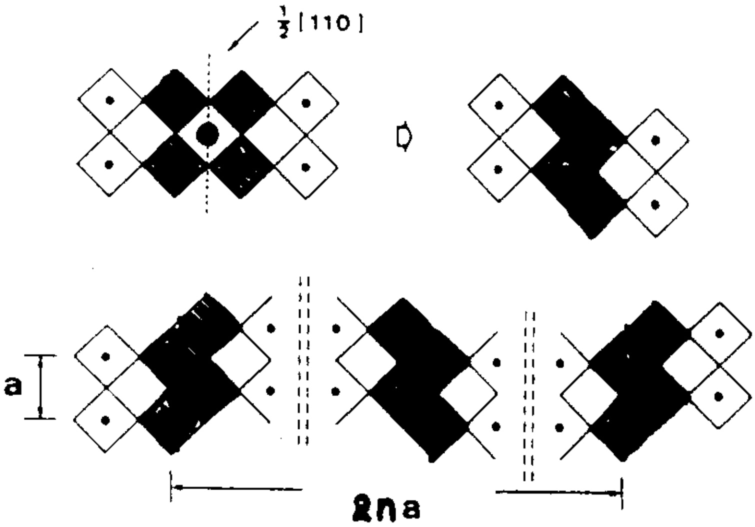
Parent Compound



$SrCuO_2$

Infinite Layer System

Shear Process



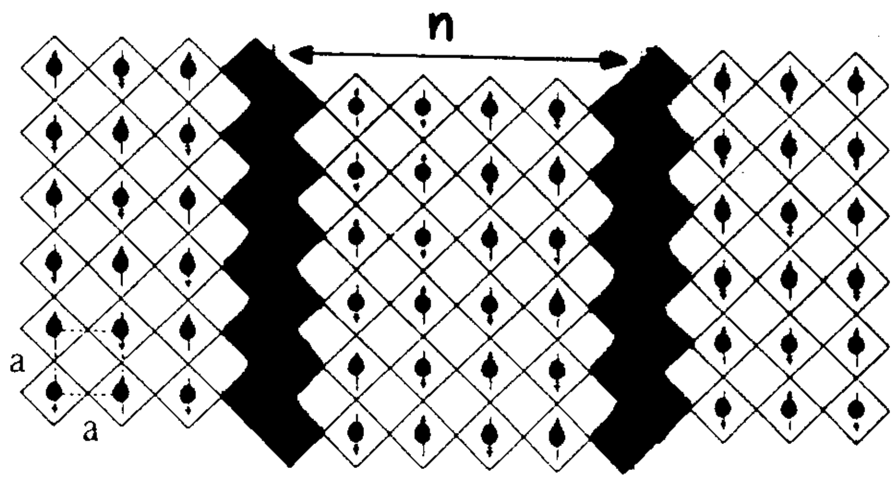
$(2n)\,SrCuO_2$

$-\ 2\,SrO$

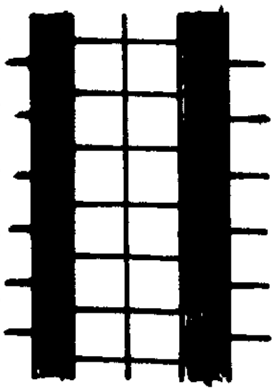
$\Downarrow$

$Sr_{2n-2}Cu_{2n}O_{4n-2}$

$Sr_2Cu_4O_6$	:	2 chain ladder	$\Delta_s = 420K$
$Sr_4Cu_6O_{10}$	:	3	$\Delta_s = 0$
$Sr_6Cu_8O_{14}$	:	4	



Cu-Network

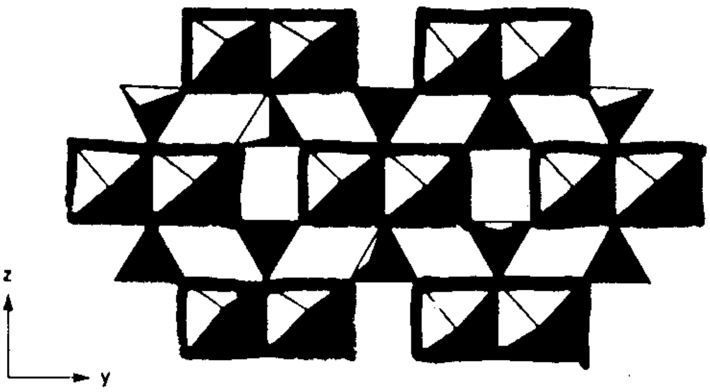


·····: Ferro bond

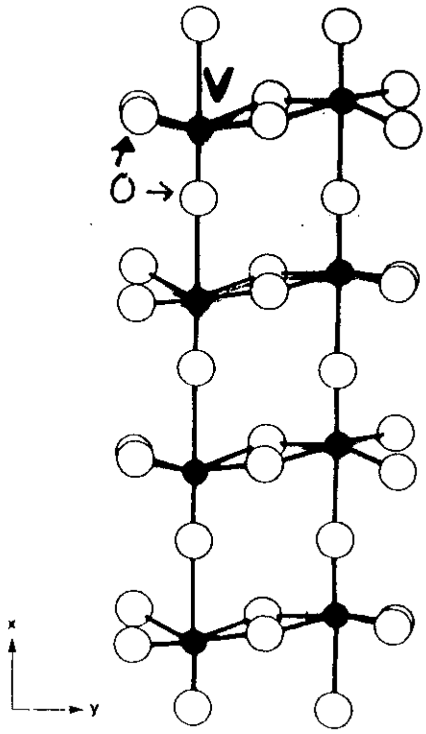
$(VO)_2P_2O_7$

D. C. Johnston et al. (PRB, '87)

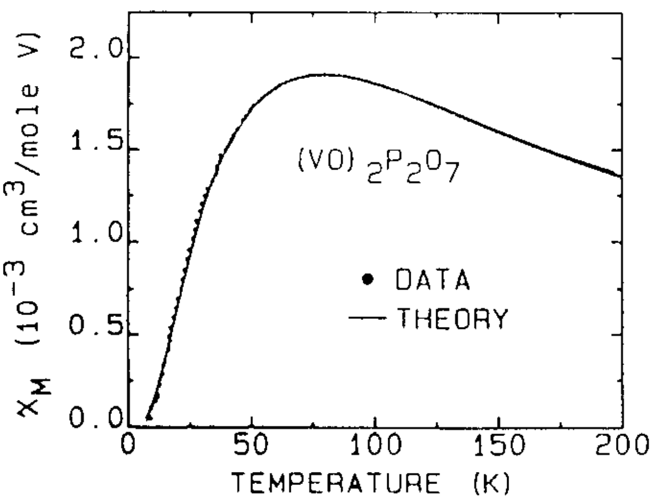
V^{4+} : $(3d)^1$ $\quad S = 1/2$

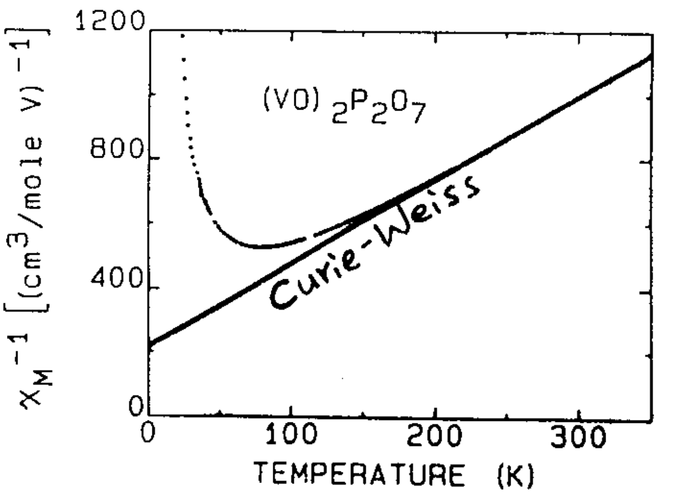


octahedra : V
tetrahedra : P
vertices : O



SUSCEPTIBILITY

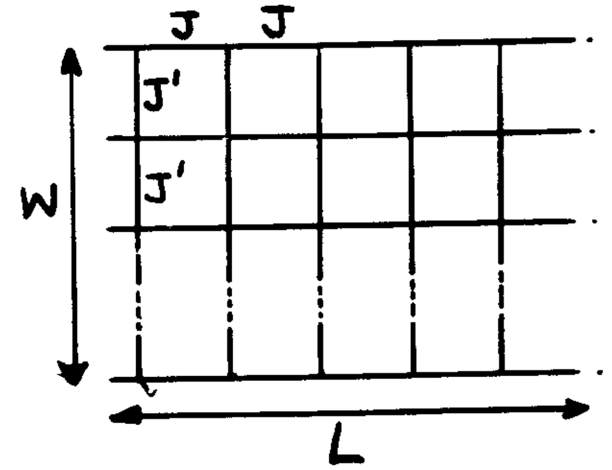




$\chi \sim C/(T - \Theta)$ (high T)

$$\begin{cases} C = 0.386 \text{ cm}^3\cdot\text{K/mole} \\ \quad \sim 0.375 \text{ (for } S = 1/2,\ g = 2) \\ \Theta = -84.1 \text{ K} \end{cases}$$

Heisenberg Ladder (= multi-chain)



$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij}\, \vec{S}_i \cdot \vec{S}_j \qquad (S = 1/2)$$

$$J_{ij} = \begin{cases} J & \text{(intra-chain)} \\ J' & \text{(inter-chain)} \end{cases}$$

$J, J' > 0$ (AF)

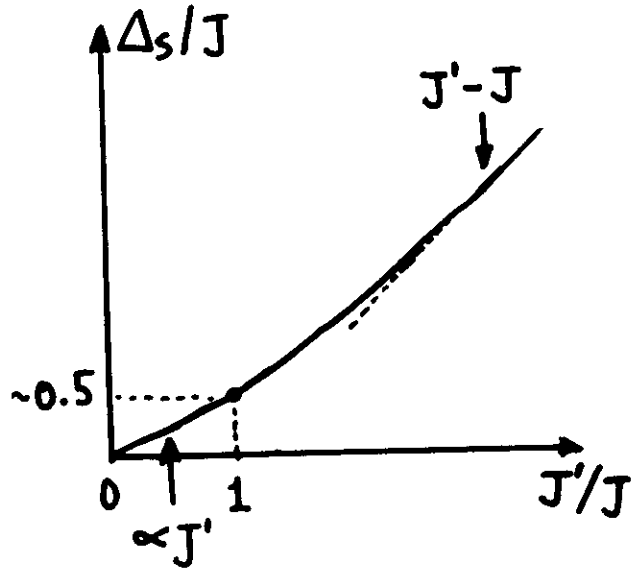
Spin gap : $\Delta_S \equiv \lim_{L \to \infty} \left[E_{GS}(S=1) - E_{GS}(S=0) \right]$

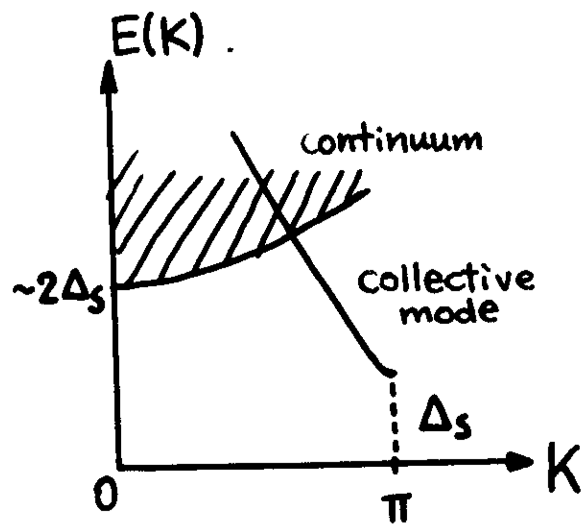
- W : odd $\Rightarrow$ $\Delta_S = 0$ for any J' Lieb-Shultz-Mattis
- W : even $\Rightarrow$ $\Delta_S > 0$ (at least for large J')

scales to the strong coupling limit $J'/J \to \infty$

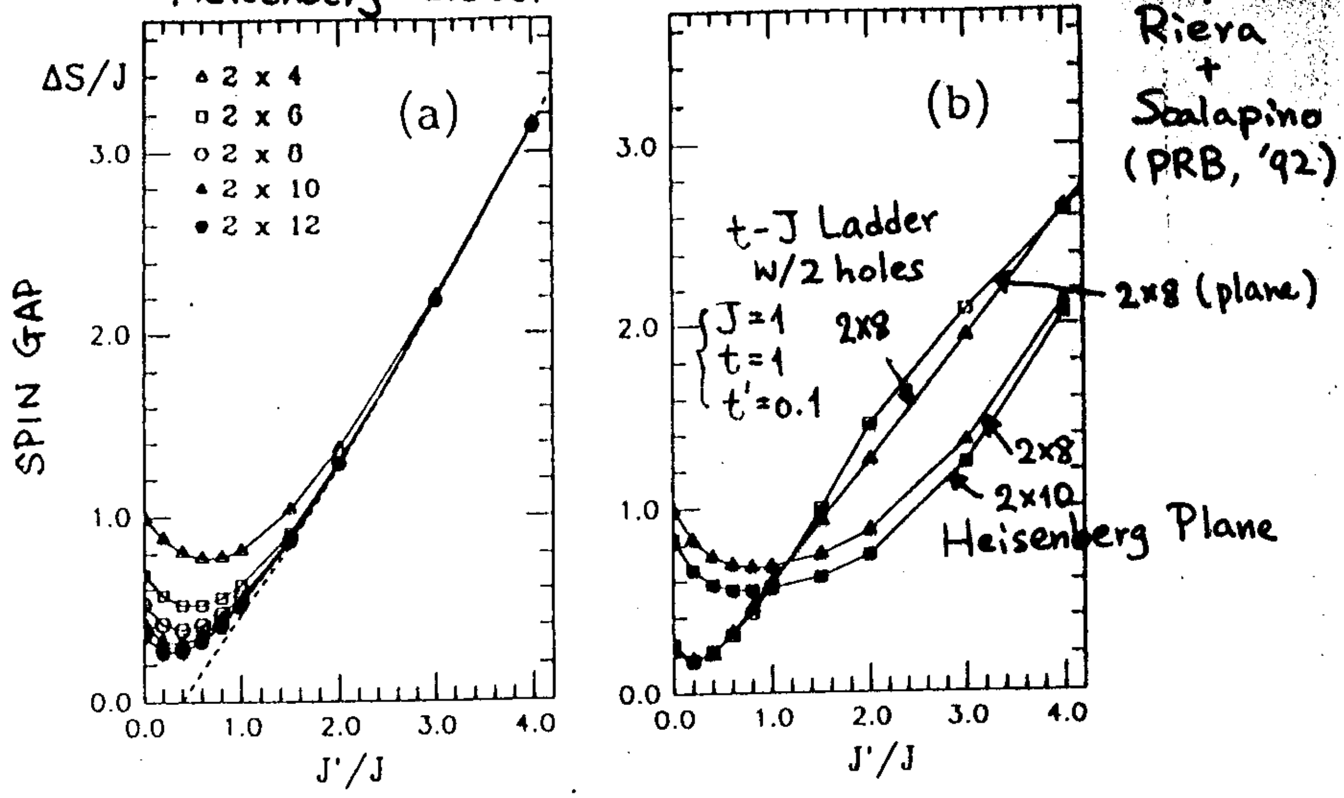
$\Rightarrow$ 1-rung G.S. $\begin{pmatrix} W: \text{odd} \to S = 1/2 \\ W: \text{even} \to S = 0 \end{pmatrix}$

$W = 2$ (double chain)



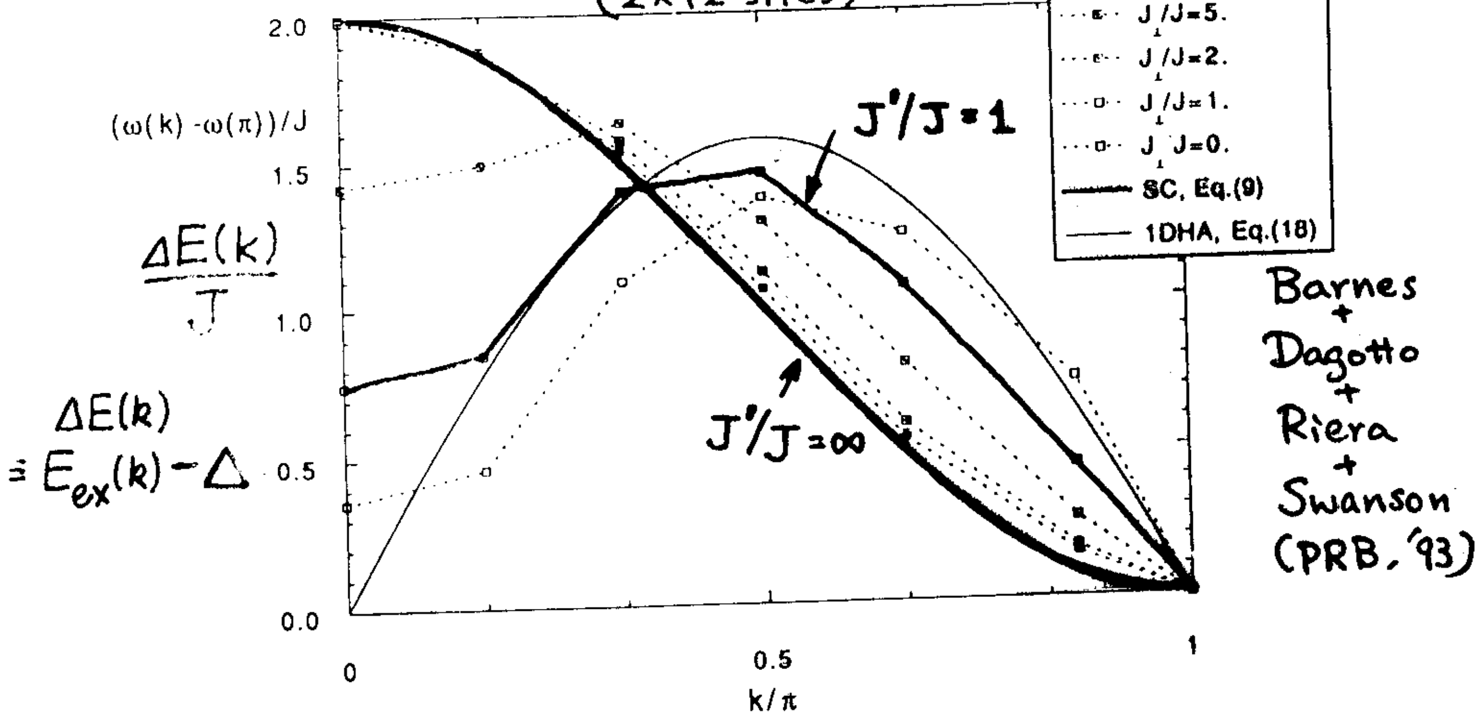


Heisenberg Ladder



(Heisenberg Ladder)

Excitation Spectrum
(2×12 sites)



[illegible], Würtz, '94

Simple Limit ($J' \gg t, J$)

easy to understand

⇒ trace back to the isotropic case $J' = J$
continuity argument

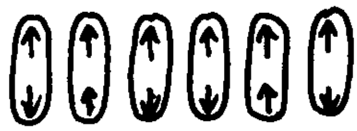
solve the single rung problem

⇒ make an effective model in the low energy sector

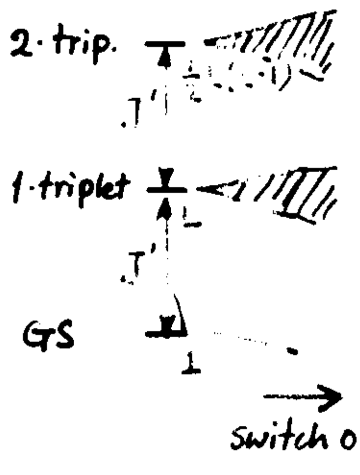
[A] Half Filling (= Heisenberg Ladder)

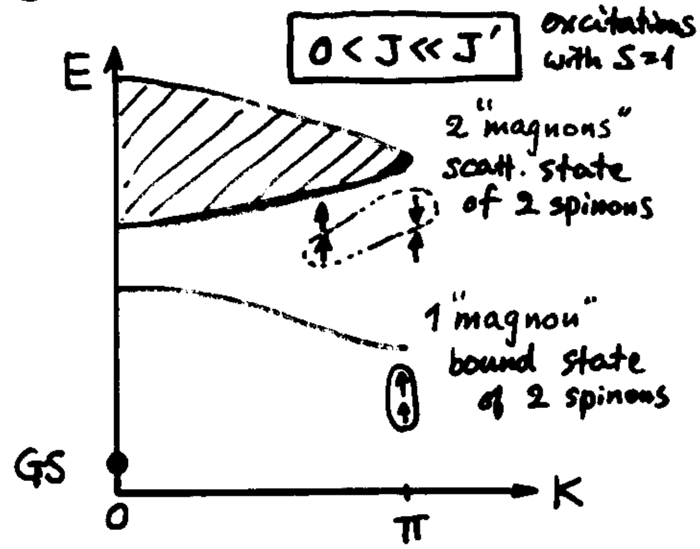
Ground State 

$$E_{GS} = L\left(-\underbrace{\tfrac{3}{4}J'}_{\text{spin}} - \underbrace{\tfrac{1}{4}J'}_{\text{charge}}\right) = -L\cdot J'$$

Excited States 

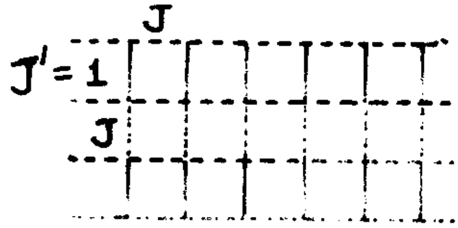
$$E_{exc} = J' \cdot (\#\text{ of triplets})$$

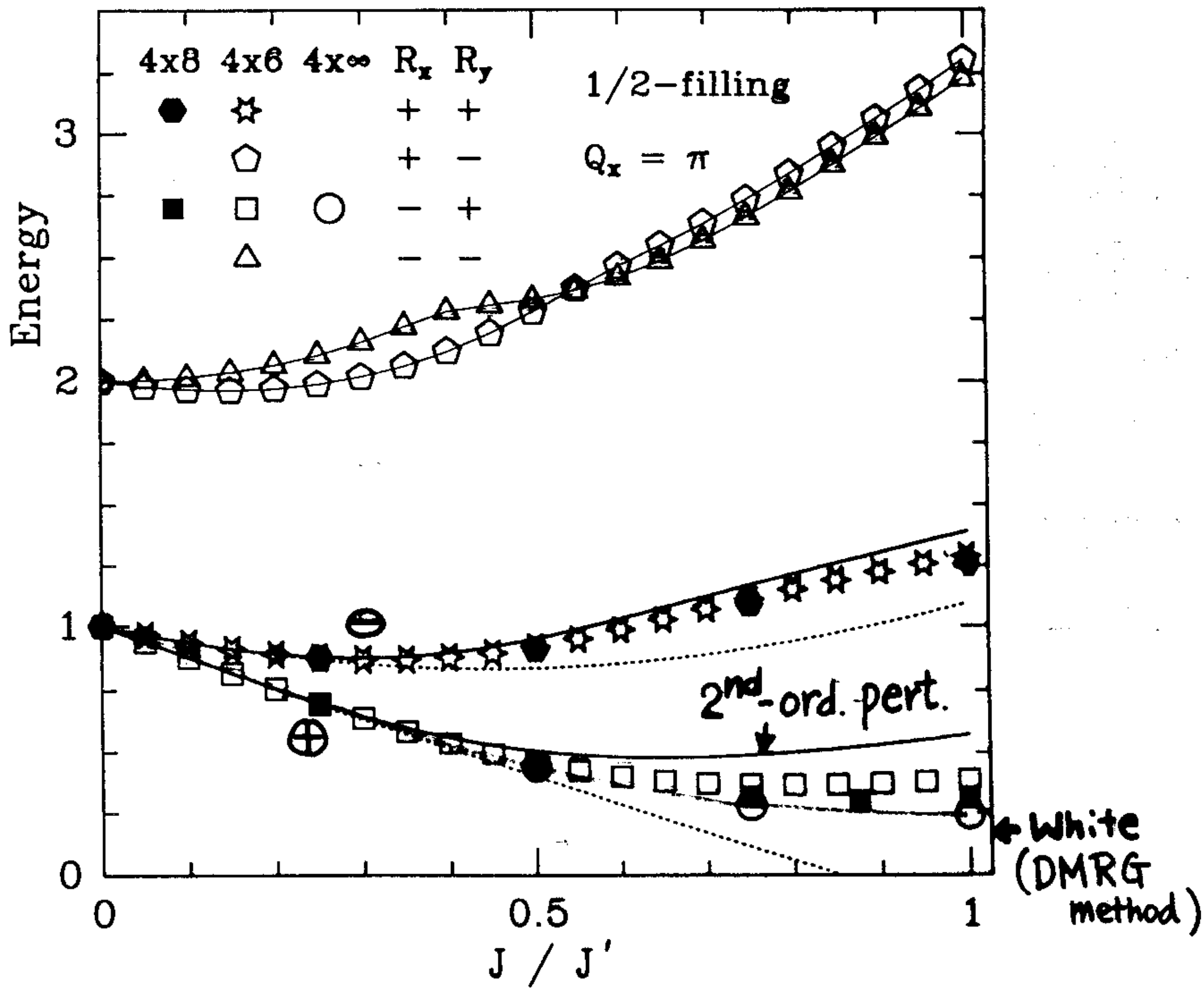


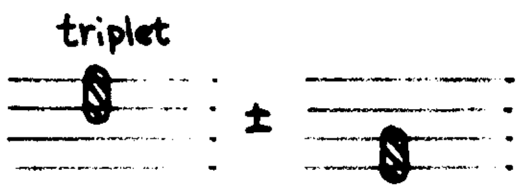


4-chain Heisenberg Ladder

Poilblanc + H.T. + Rice
(PRB, '94)







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Thermodynamics of 2-chain Heisenberg Ladders

[A] Quantum Transfer Matrix Method

map to (1+1)-dim classical system

Transfer matrix operating in the spatial direction : $\lambda_{Max} \Rightarrow F$

1st principle calculation

$L \to \infty$ limit is taken automatically

[B] A Simple Analytic Approximation

Basic Assumptions

- all the excitations are multi-"magnon" excitations
- neglect magnon-magnon interactions
- restrict # of magnons

simple reweighting of the Boltzman weights so as to give the correct entropy in $T \to \infty$ limit

$\Rightarrow$ Fits very well to the QTM results

free energy : $\tilde{f} = -\frac{1}{2\beta} \log\left[1 + (1 + 2\,\mathrm{ch}\,\beta h) Z(\beta)\right]$

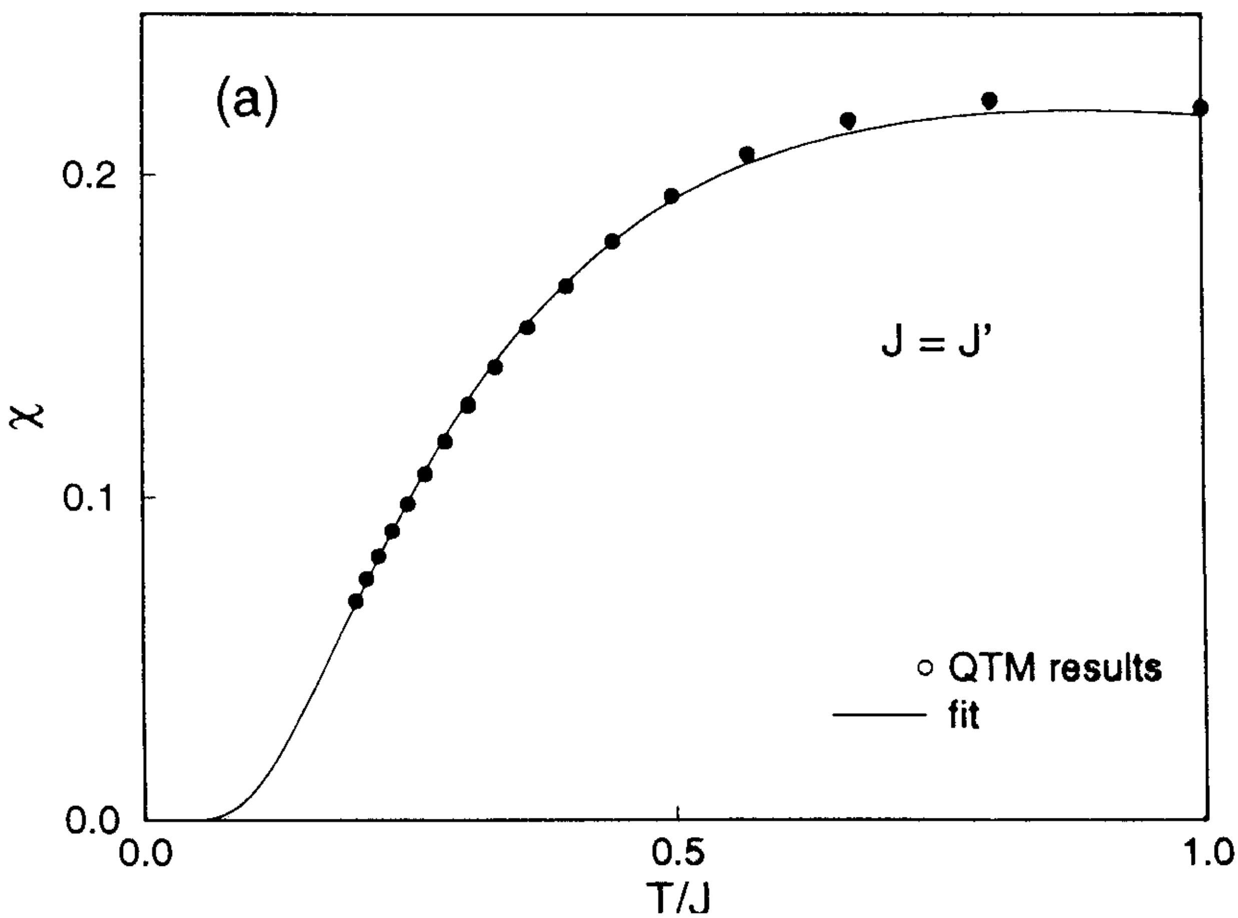
susceptibility : $\tilde{\chi} = \beta \cdot \frac{Z(\beta)}{1 + 3Z(\beta)}$

$$Z(\beta) \equiv \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \ \exp\left[-\beta\, \underbrace{\varepsilon_1(k)}_{\text{1-magnon energy}}\right]$$

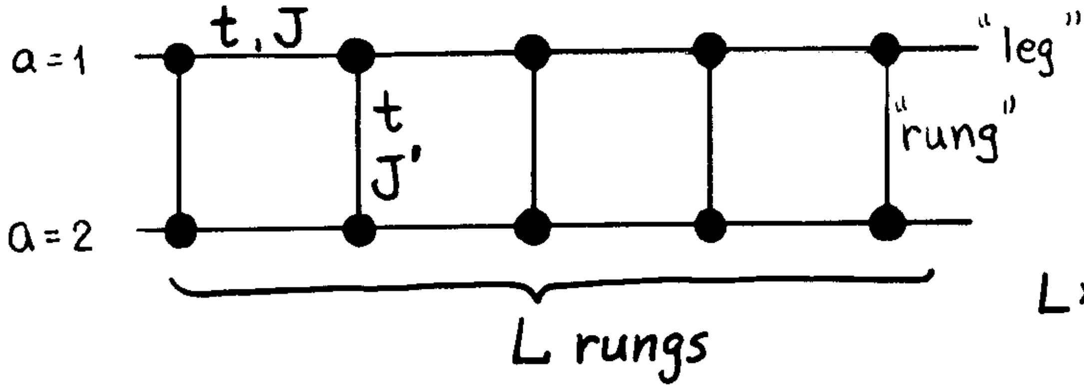
$$\left.\begin{aligned} \tilde{\chi} &\to \frac{1}{4T} \quad (T\to\infty) \\ &\to \beta^n e^{-\beta\Delta} \quad (T \to 0) \end{aligned}\right\} \text{correct in both limits}$$

$$n = \underset{\substack{\Uparrow \\ \text{dispersion}}}{\frac{-1}{\alpha}} + 1$$

(Troyer, Tsunetsugu
Würtz, '94



Model t – J Ladder (double chain)



L×2 sites

Hamiltonian

$$
\begin{aligned}
\mathcal{H} = & -t \sum_{j\sigma} \sum_{\underset{\leftarrow \text{chain index}}{a}} c^{\dagger}_{a\sigma}(j)\, c_{a\sigma}(j+1) + \mathrm{H.c.} \\
& -t \sum_{j\sigma} c^{\dagger}_{1\sigma}(j)\, c_{2\sigma}(j) + \mathrm{H.c.} \\
& + J \sum_{ja} \vec{S}_a(j)\cdot\vec{S}_a(j+1) - \tfrac{1}{4} n_a(j)\, n_a(j+1) \\
& + J' \sum_{j} \vec{S}_1(j)\cdot\vec{S}_2(j) - \tfrac{1}{4} n_1(j)\, n_2(j)
\end{aligned}
$$

cuprates
↑
$J/t = 0.3$
$(J'/t = 0.3)$

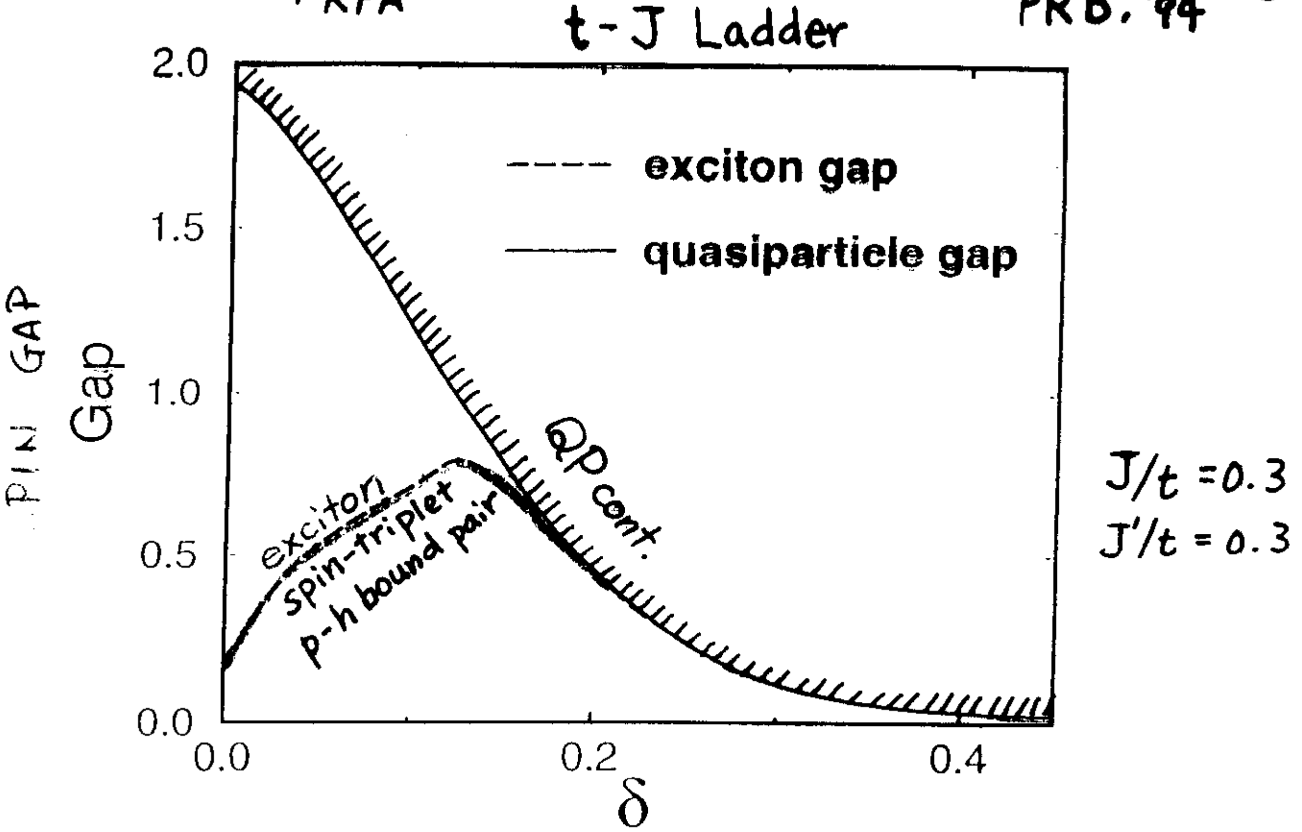
Local constraint : $n_{a\uparrow}(j)\, n_{a\downarrow}(j) = 0$ for $^{\forall} j, a$

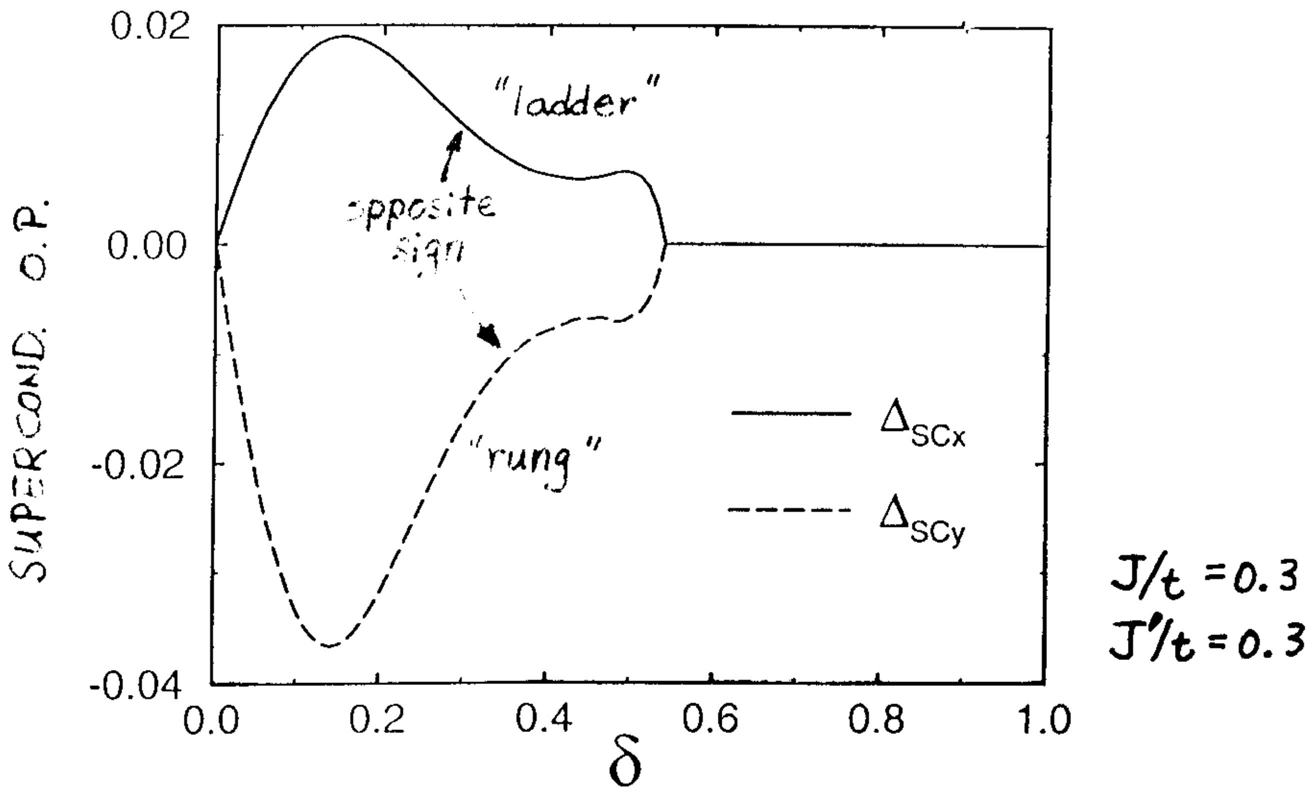
$J' \to \infty$ Simple Limit (decoupled rungs) ⇒ Good Starting Point

Def.
$$
\begin{cases}
n_{a\sigma}(j) \equiv c^{\dagger}_{a\sigma}(j)\, c_{a\sigma}(j) \\
n_a(j) \equiv \sum_{\sigma} n_{a\sigma}(j) \\
\vec{S}_a(j) \equiv \sum_{\alpha\beta} c^{\dagger}_{a\alpha}(j) \left(\tfrac{1}{2}\vec{\sigma}\right)_{\alpha\beta} c_{a\beta}(j)
\end{cases}
$$

d-wave RVB MF + Gutzwiller Renorm.
+ RPA

Sigrist + Rice + Zhang
PRB, '94





What we have done

Exact diagonalization (Lanczos)

8×2 sites with 0, 1, 2, 3, 4 holes
(10×2)

① Binding of 2 holes in Ground State

- E_B
- $\xi \quad \leftarrow \quad \langle n_h(r)\, n_h(0) \rangle$

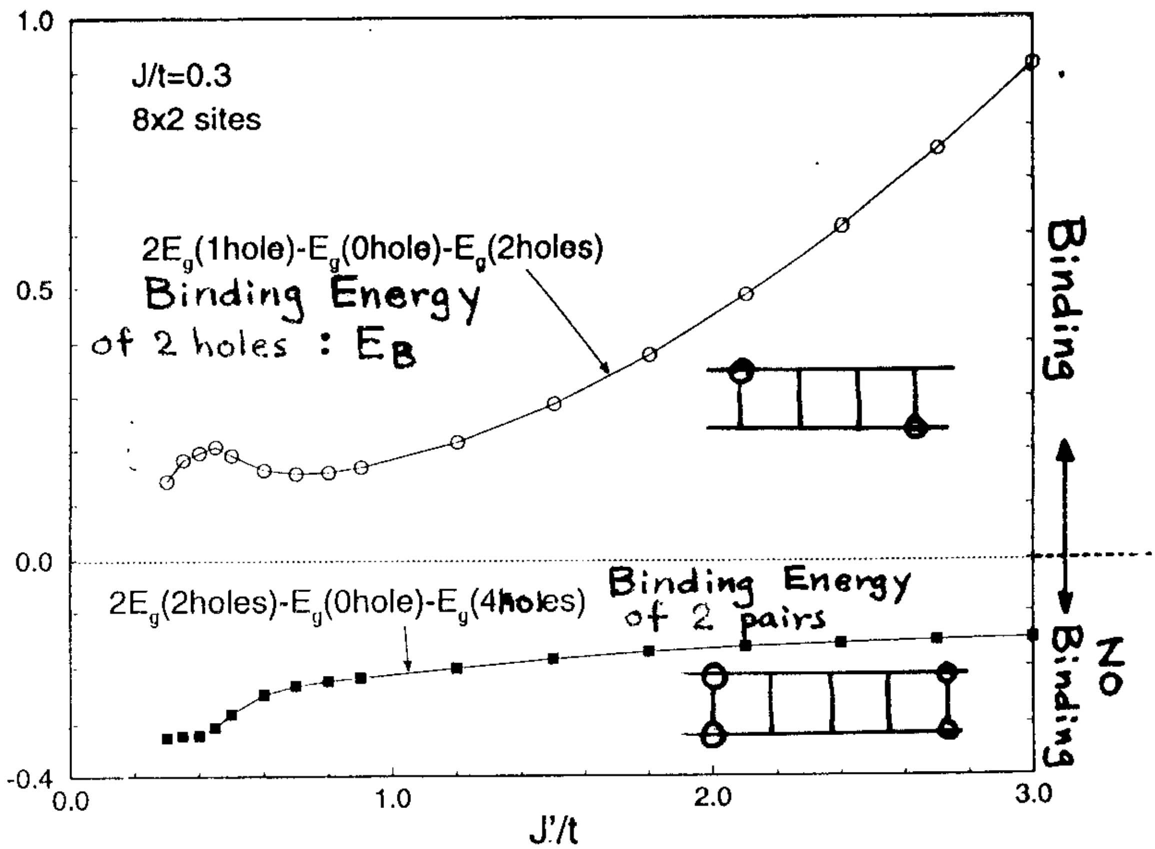
② Spin excitations

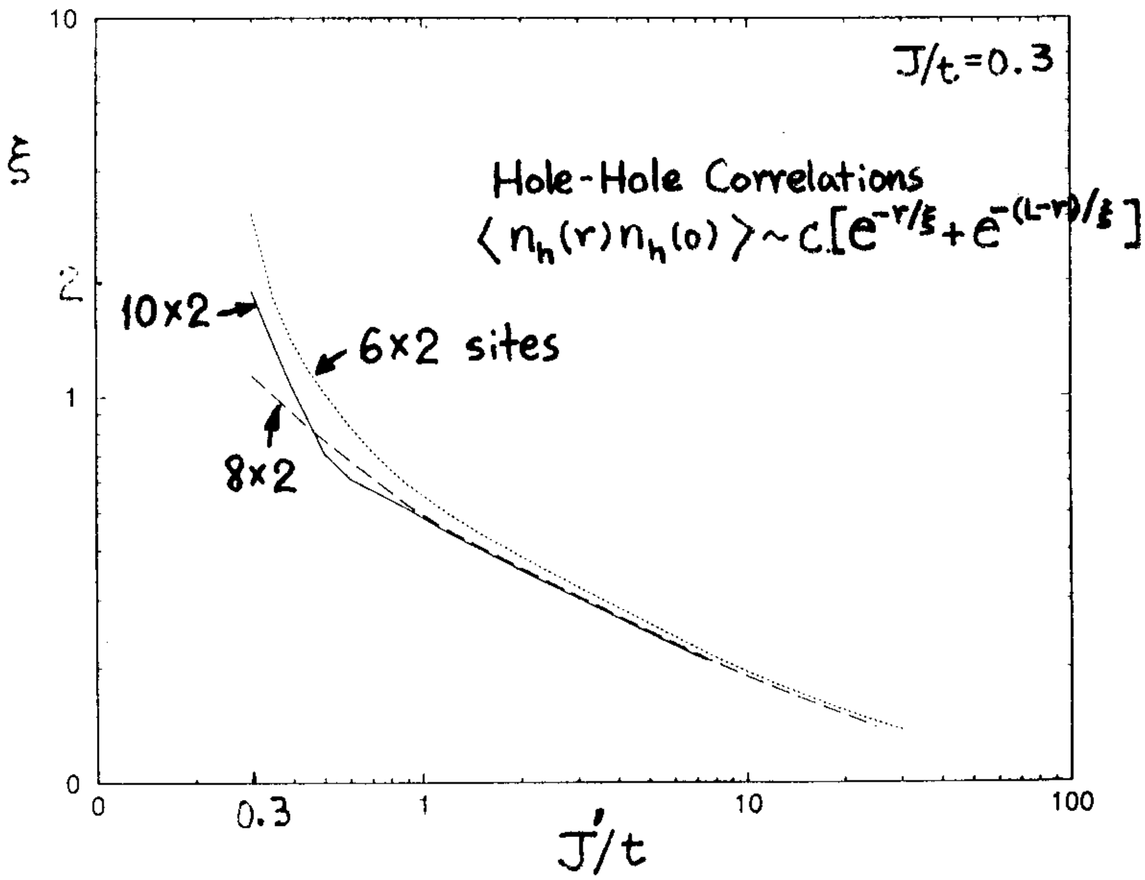
- Δ_S
- $\langle n_h(r)\, n_h(0) \rangle$, $\langle n_h(r)\, S^z(0) \rangle$
- $S(k, \omega)$

③ charge excitations / superconductivity

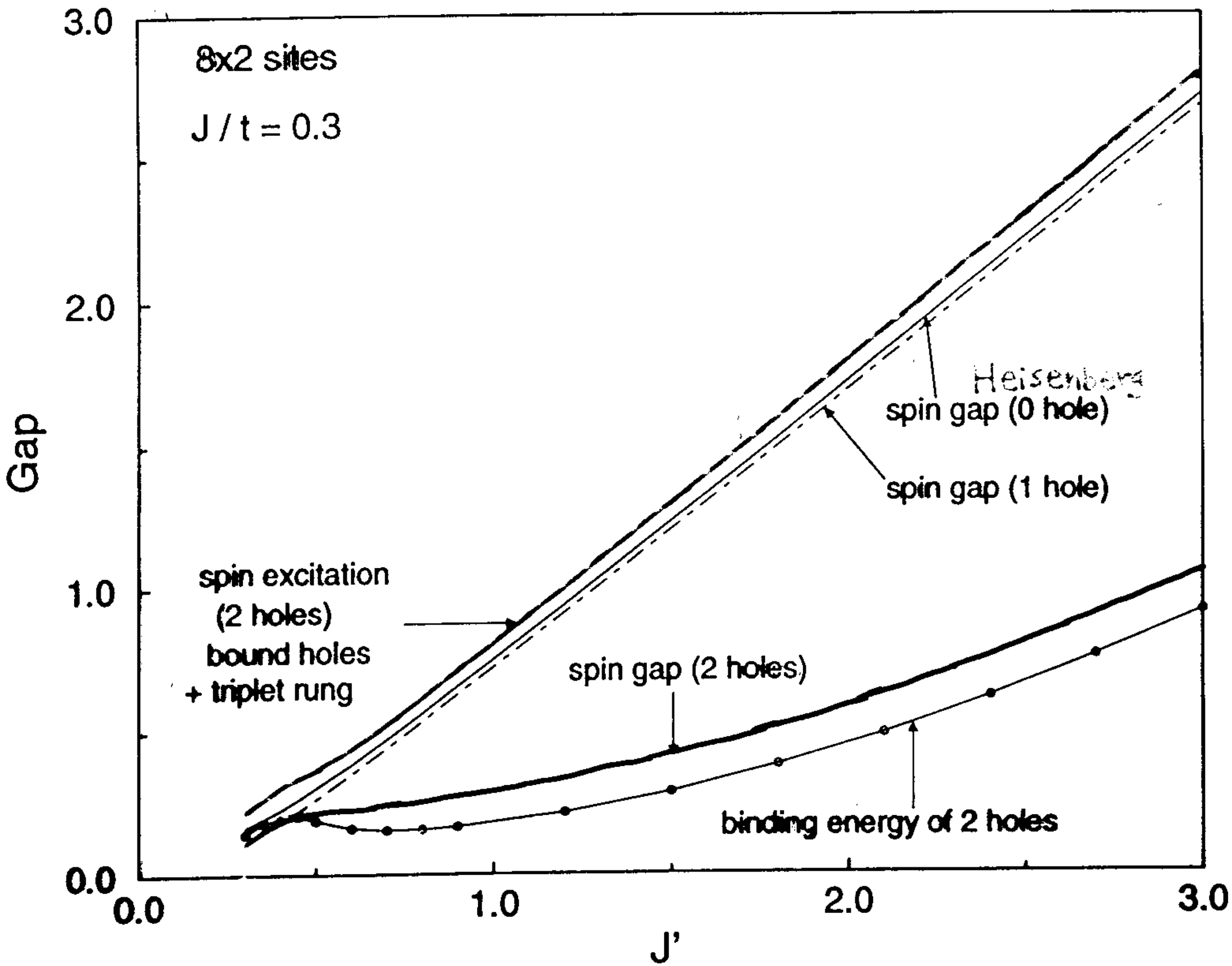
- energy spectrum (for 1, 2, 3 holes)
- spectral fn. of 1-particle Green's fn. (for. 2 holes)

Binding of 2 holes in the Ground State [t-J Ladder]



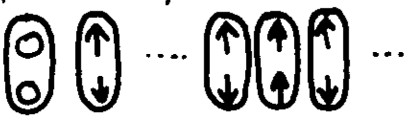


Spin Gap in [illegible] Ladder



2 Types of Spin Excitations upon doping ($J' \gg t, J$)

[1] Triplet away from the bound hole pair

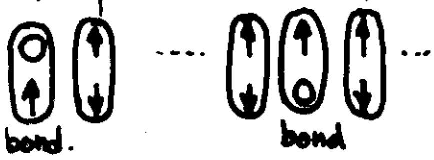


2 singlets are broken

$t_{eff}\begin{pmatrix}\circ\\ \circ\end{pmatrix} \sim \dfrac{t^2}{J' - \frac{4t^2}{J'}}$ kin. energy. (present in the G.S.)

$t_{eff}\begin{pmatrix}\uparrow\\ \uparrow\end{pmatrix} \sim \dfrac{J}{2}$ extra kin. energy gain

[2] Holon-Spinon Bound Pair



2 singlets are broken

$E\begin{pmatrix}\circ\\ \uparrow\end{pmatrix}_{bond} \sim -t$ chemical pot.

$t_{eff}\begin{pmatrix}\circ\\ \uparrow\end{pmatrix}_{bond} \sim \dfrac{t}{2}$ extra kin. energy gain

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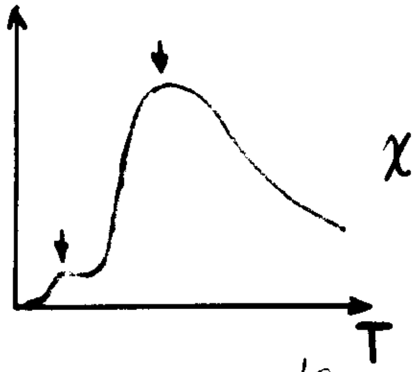
[ENRGY]

$$\left.\begin{aligned} E^{[1]}_{exc} &\sim J' - J \\ E^{[2]}_{exc.} &\sim J' - 2t - 2t + 2\frac{t^2}{J' - \frac{4t^2}{J'}} \end{aligned}\right\} \quad E^{[2]}_{exc} < E^{[1]}_{exc}$$

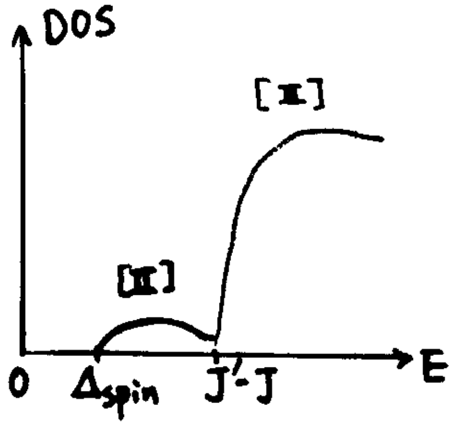
[# of allowed excitations]

$$\left.\begin{aligned} [1] &\propto 1-\delta \\ [2] &\propto \delta \end{aligned}\right\}$$

small doping
#[1] ≫ #[2]



$\chi(T) \Leftarrow$



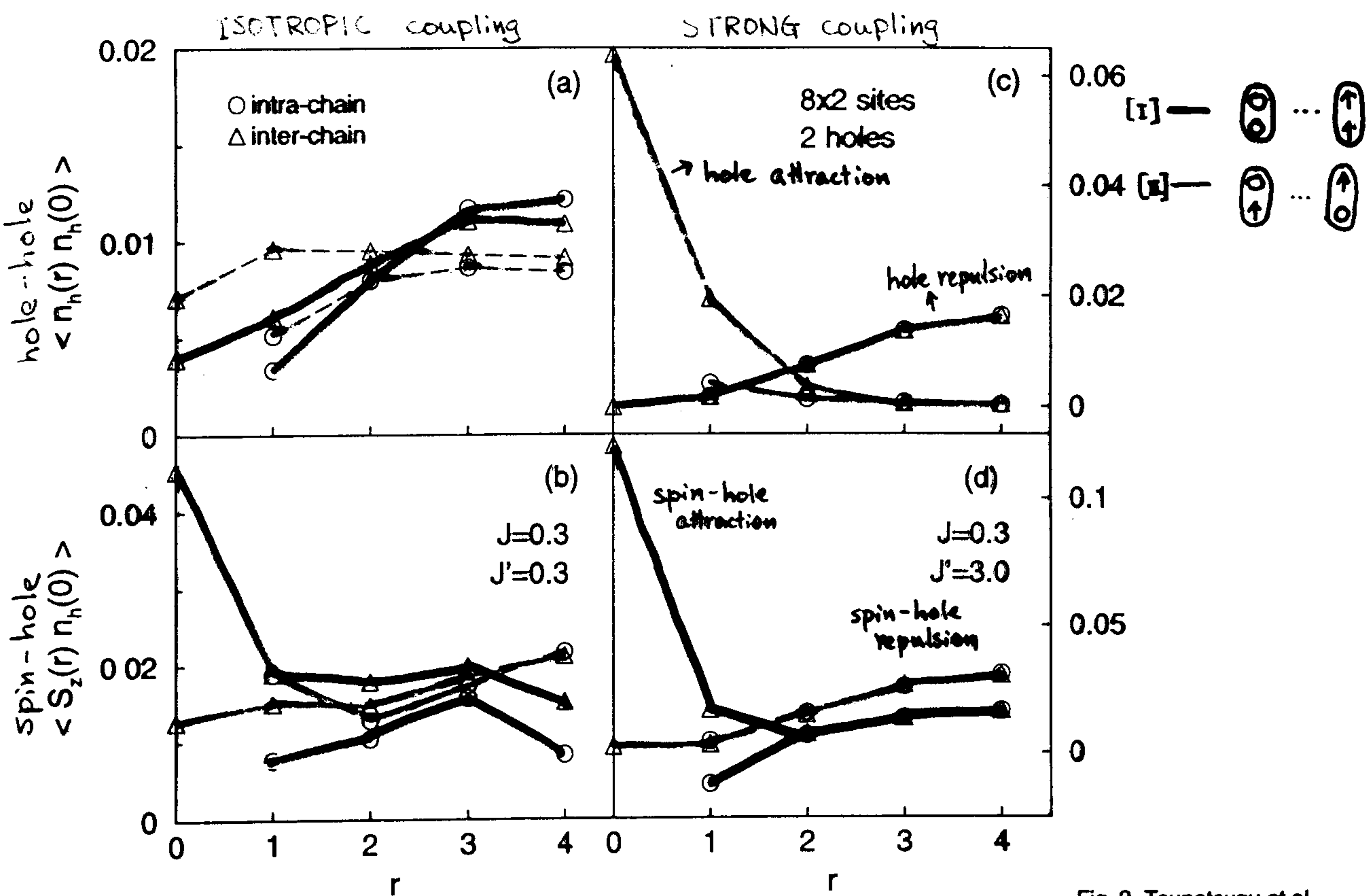
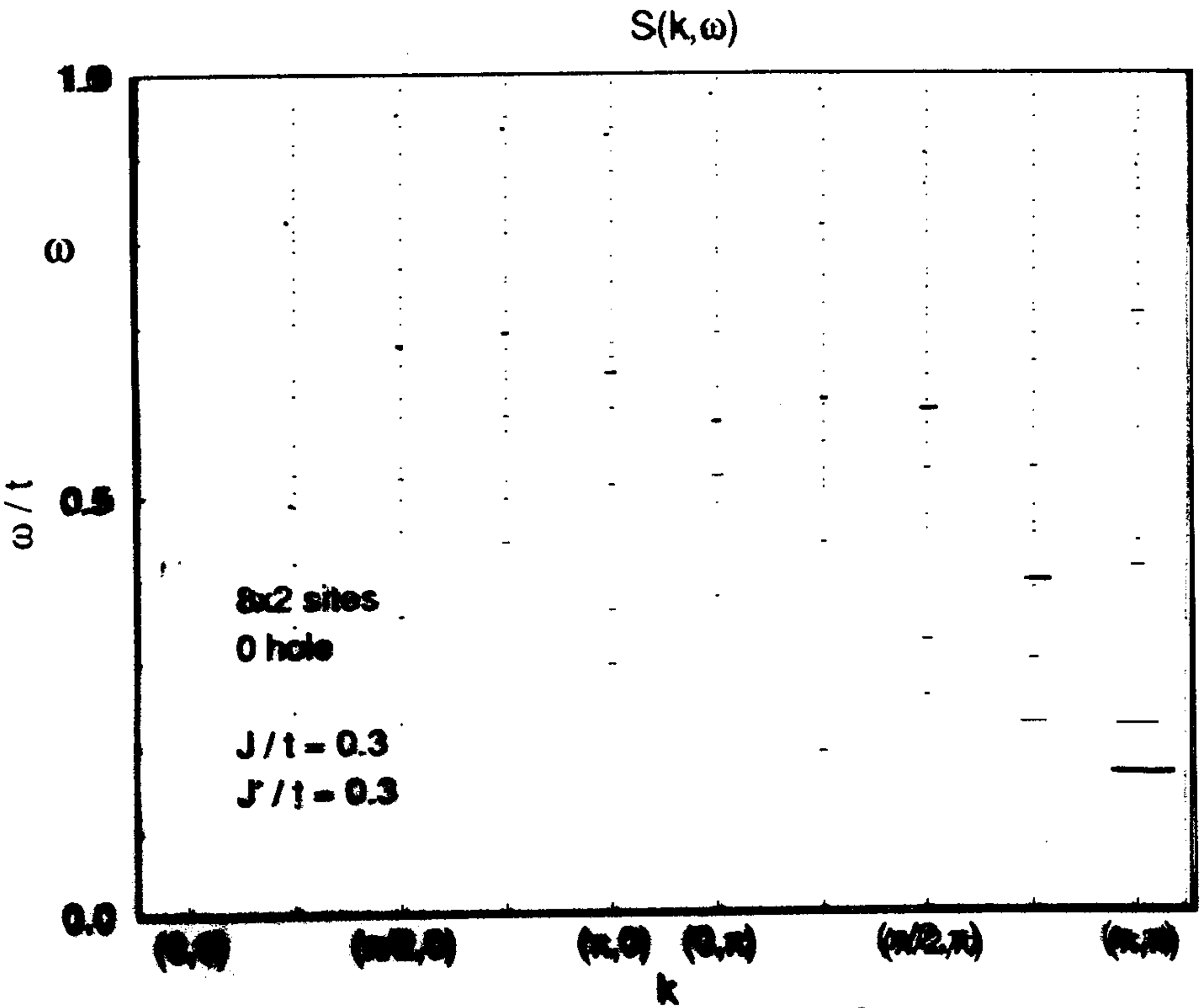


Fig. 2 Tsunetsugu et al.

Dynamical Spin Structure Factor

Fig. 3 Tsunetsugu et al.



2 holes/8×2 sites

APBC

$J/t = 0.3$

$J'/t = 0.3$

$$S(k,\omega) = \sum_n |\langle n| S_k^+ |GS\rangle|^2 \, \delta(E - E_n + E_{GS})$$

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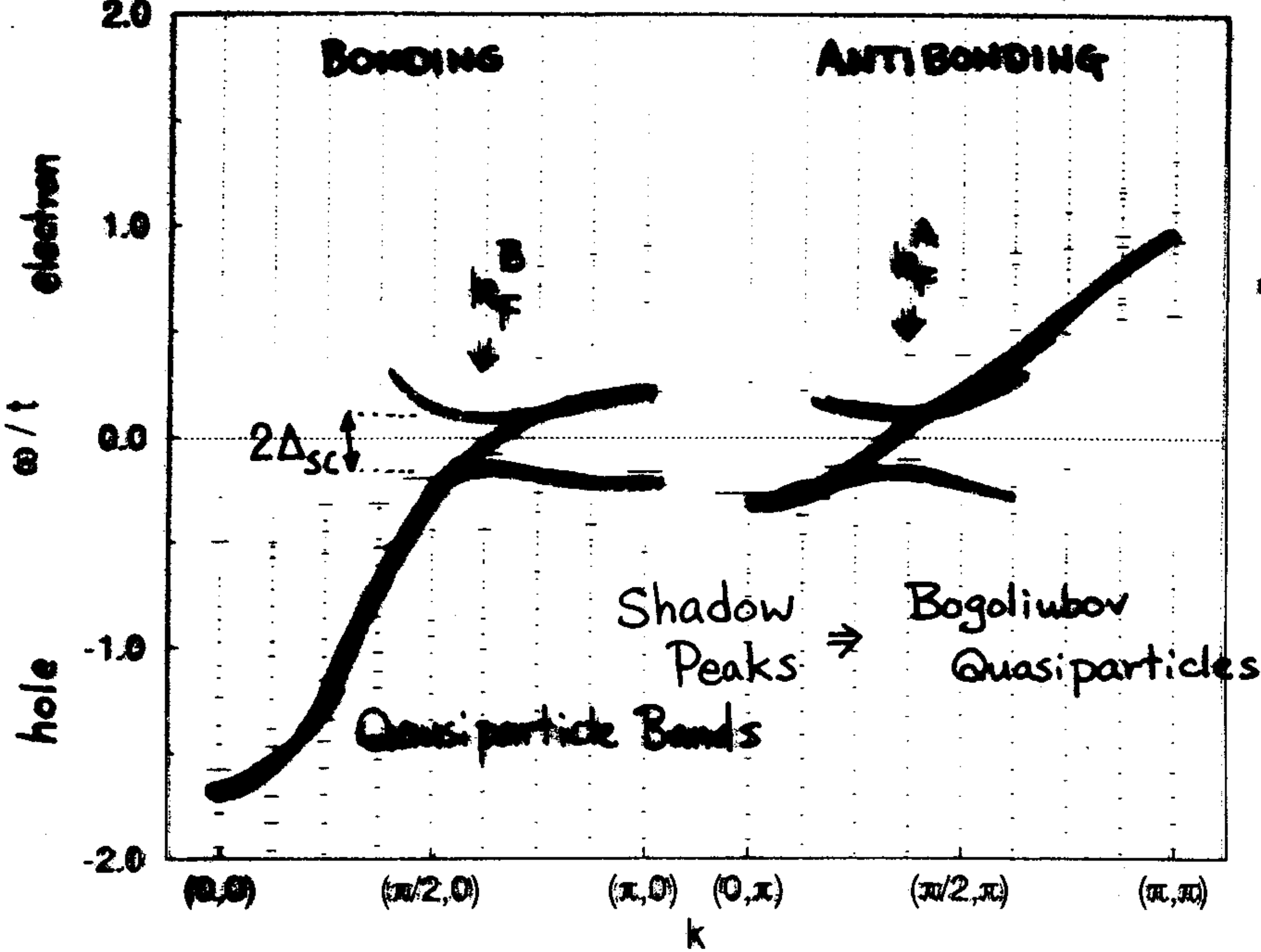
t-J Ladder

$A(k,\omega)$: Spectral fn. of the 1-particle Green fn.

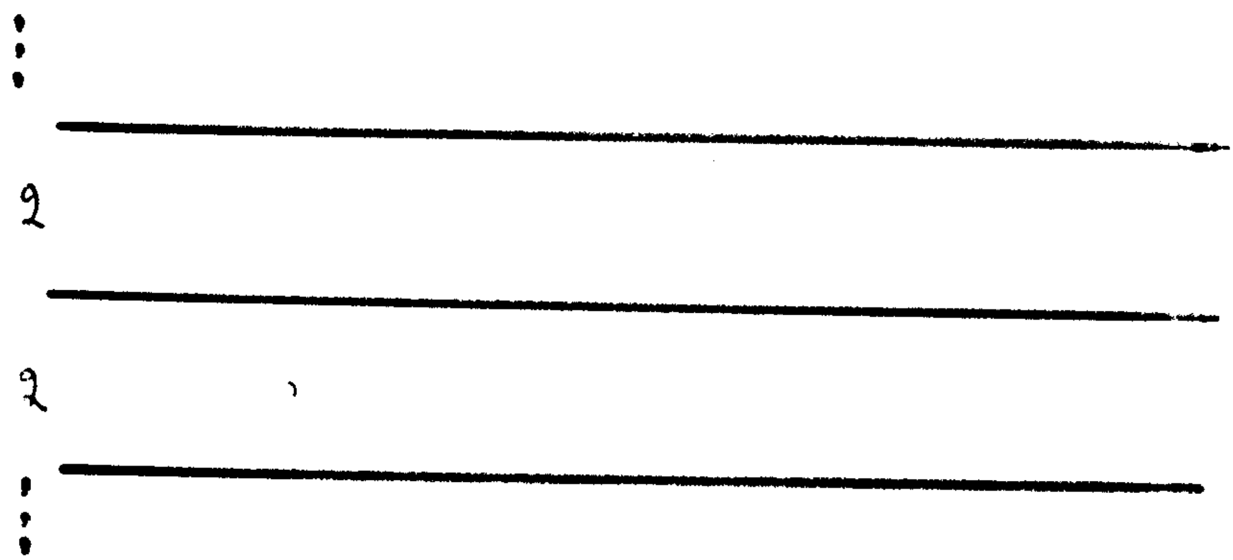
2 holes
8×2 sites
$J=J'=0.3t$



Split of the 2 bands
⇒ COHERENT interchain hopping

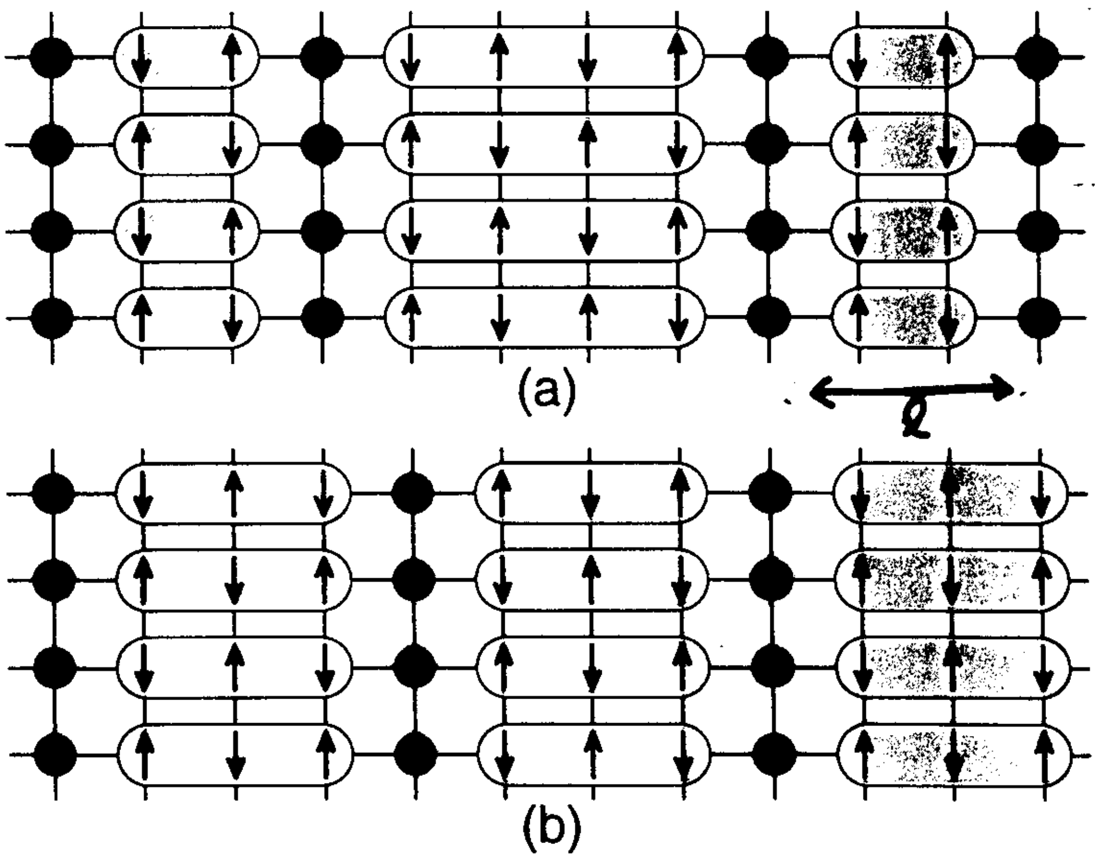
$k_F^B + k_F^A \simeq \pi(1-\delta)$
Luttinger's sum rule
⇒ LARGE Fermi surface

coupled ladders



mixture of 2- and 4-chain ladders

hole



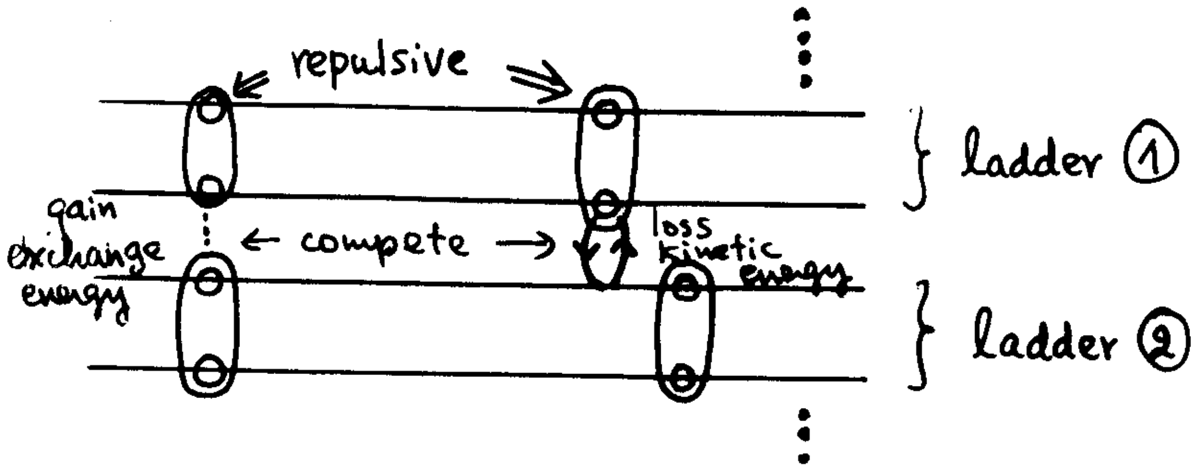
Singlet stripe phase

$\langle \ell \rangle_{av} = \delta^{-1}$

3-chain ladders

$$E_G(\text{3-chain}) > \left[\frac{1}{3} E_G(\text{2-chain}) + \frac{2}{3} E_G(\text{4-chain}) \right]$$

coupled ladders



singlet stripe phases may appear

if
① intra-ladder repulsion is so large that CDW correlations are dominant ($K_\rho < 1$)
② inter-ladder interaction is attractive

these conditions would be satisfied near the phase separation boundary

with decreasing J/t, inter-ladder interactions become repulsive

⇓

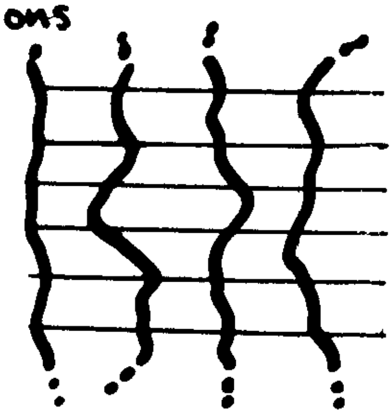
instability of singlet stripe phases

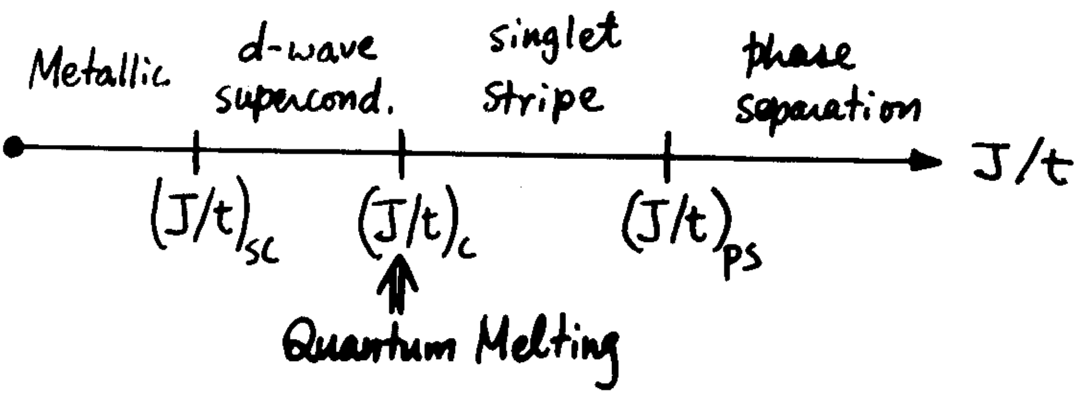
|||

Quantum Melting of hole lines

⇓

Bose condensation of hole pairs





CONCLUSIONS

(1) Heisenberg Ladders (2-chain)

"magnon" excitation = bound state of spinons

multi-"magnon" excitations ⇒ describe thermodynamics very well

(2) Doped t-J Ladders

≈ low density tightly bound pairs (cf. negative-U Hubbard)

But the Fermi surface is large $\propto n_e$

2 types of spin excitations

- HIGH energy part — continuos evolution from $\delta = 0$
  non-FL like
- LOW energy part — appear only upon doping
  QP like (charge +lel, spin ½)
  = spinon + holon bound pair

"Quasiparticle" spectra à la Bogoliubov

$$2\Delta_{QP} \approx \Delta_s \approx E_B$$

(3) 2D t-J model

singlet stripe phases — "CDW" stabilized by quantum spin fluctuations

⇓ Quantum Melting Transition

superconducting ($d_{x^2-y^2}$ symmetry)