Spin-1/2 frustrated antiferromagnet on a spatially anisotopic square lattice: contribution of exact diagonalizations. [PRB 69, 094418 (2004)]

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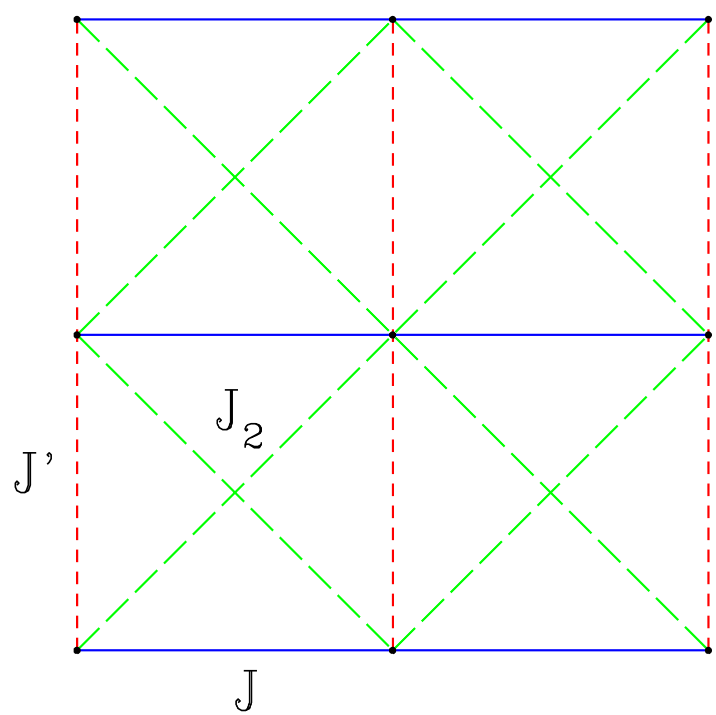
Extension of the $J_1 - J_2$ model on the square lattice $\rightsquigarrow$ $J - J' - J_2$ model:

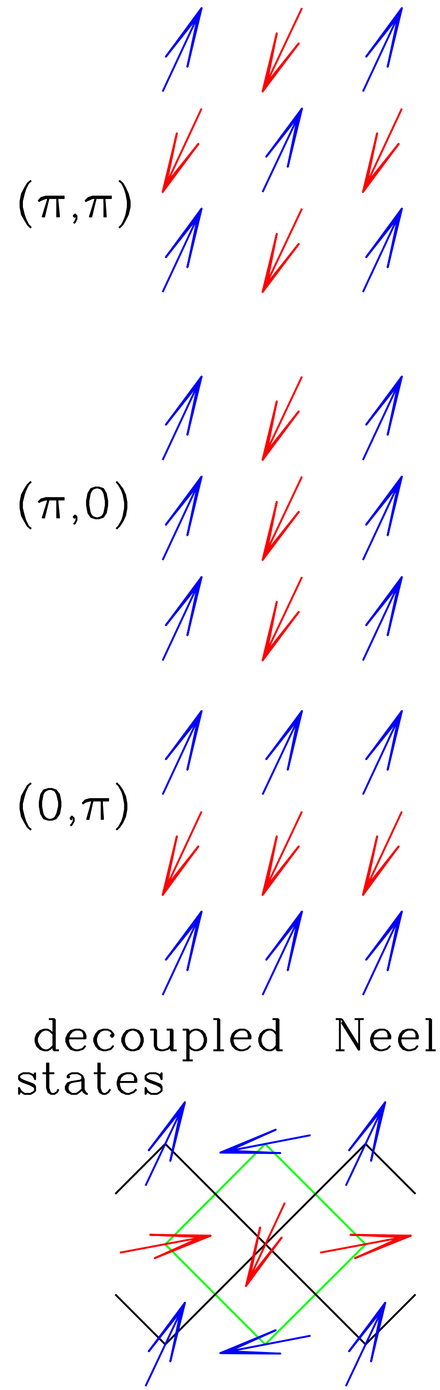
$$\mathcal{H} = \sum_{m=1}^{M} \sum_{l=1}^{L} [\, J\, \mathbf{S}_{l,m}.\mathbf{S}_{l+1,m} + J'\, \mathbf{S}_{l,m}.\mathbf{S}_{l,m+1} + J_2\, (\mathbf{S}_{l,m}.\mathbf{S}_{l+1,m+1} + \mathbf{S}_{l,m}.\mathbf{S}_{l+1,m-1}]$$



- AF interactions: $J, J', J_2 > 0$
- $\equiv$ Confederate Flag model (Nersesyan and Tsvelik)
- can be viewed (if $J' < J$) as an array of M chains of lenght L (with periodic boundary conditions in the horizontal and vertical directions).
- $J' = J \rightsquigarrow$ the $J_1 - J_2$ model.

The classical ground-state of the $J - J' - J_2$ model has:

- If $J' < J$:
  - if $J_2 < 0.5J'$: (π, π) Néel LRO
  - if $J_2 > 0.5J'$: $(\pi, 0)$ Néel LRO
  - if $J_2 = 0.5J'$: decoupled horizontal chains
- If $J < J'$:
  - if $J_2 < 0.5J$: (π, π) Néel LRO
  - if $J_2 > 0.5J$: $(0, \pi)$ Néel LRO
  - if $J_2 = 0.5J$: decoupled vertical chains
- If $J' = J$ ($J_1 - J_2$ model):
  - if $J_2 < 0.5J$: (π, π) Néel LRO
  - if $J_2 > 0.5J$: decoupled Néel states on interpenetrating square lattices.
  - if $J_2 = 0.5J$: decoupled horizontal and vertical chains



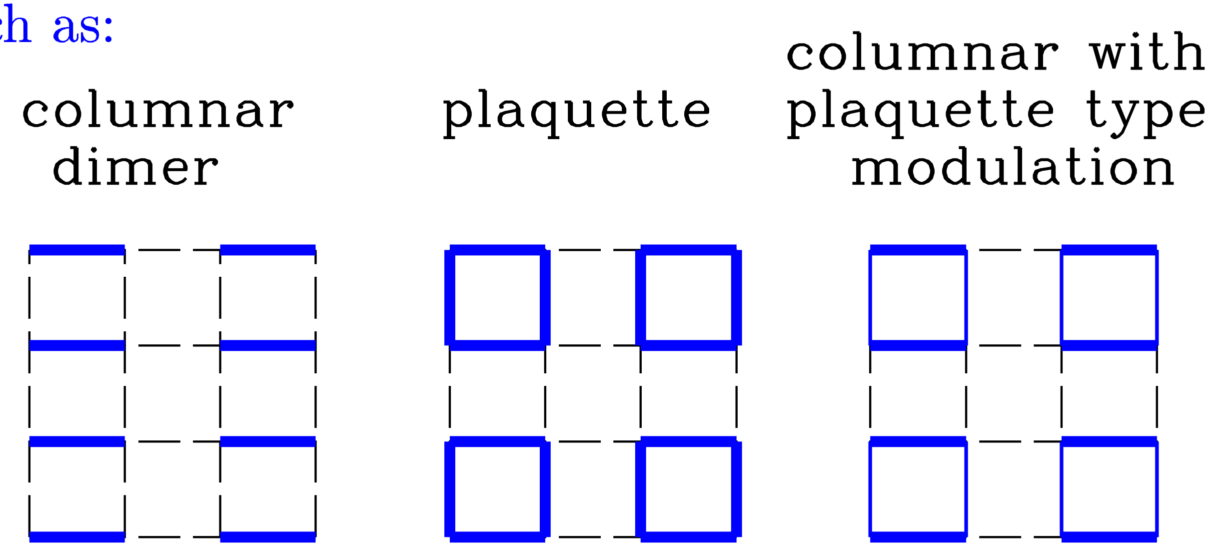
Much studied: the (2D) spin-1/2, $J' = J$, model ($J_1 - J_2$ model). Phases:

- (π, π) Néel LRO survives to quantum fluctuations (QF) up to $J_2 \lesssim 0.4J$,
- QF select a collinear Néel LRO $(\pi, 0)$ or $(0, \pi)$ if $J_2 \gtrsim 0.7J$,
- $0.4J \lesssim J_2 \lesssim 0.7J$, finite spin-gap, no Néel LRO

Néel states break $SU(2)$ symmetry and translational/rotational symmetries of the space group. No $SU(2)$ symmetry breaking for $0.4J \lesssim J_2 \lesssim 0.7J$.

Yet the nature of the ground-state for $0.4J \lesssim J_2 \lesssim 0.7J$ is still debated. Many have been proposed such as:

- a Valence Bond Crystal (VBC) ground-state such as: (translational/ rotational SB)
- a spin-liquid ground-state (no SB)



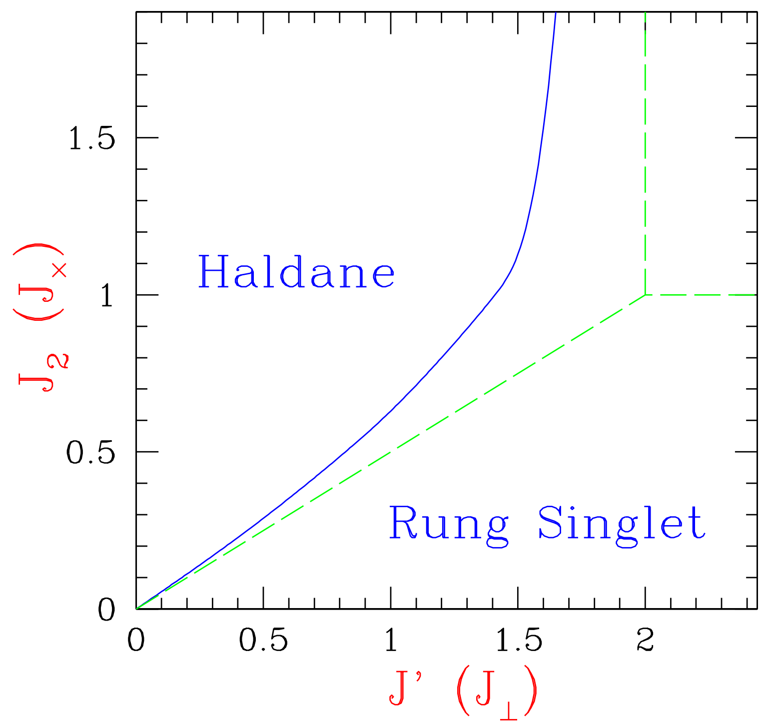
Also much studied: the (1D) spin-1/2 (M=2) ladder: $J' \to J_\perp$, $J_2 \to J_\times$

- Bosonization [Allen *et al* PRB 2000, Kim *et al* PRB 2000 ...]
- DRMG [Wang condmat/9803290, Hakobyan *et al* PRB 2001 ...]
  Series Expansions, Exact Diagonalization [Weihong *et al* PRB 98 ...]

▷ Two Gapped phases:

- "Rung Singlet"
- "Haldane"

▷ Gapped transition line



Less studied: M=3 ladder: Bosonization [Azaria *et al* PRB 1998], DRMG [Wang *et al* PRB 2002], two gapless phases, same location of transition line.

Crossover 1D ladder ($M = 2$) to 2D ($M \to \infty$)?

$\triangleright$ Studied for $J_2 = 0$ (no frustration), DRMG, QMC... [White *et al* PRL 1994, Greven *et al* PRL 1996, Frischmuth *et al* PRB 1996, Sandvik *et al* PRL 1999...]

$\Rightarrow$ Néel (π, π) for $M \to \infty$ if $J' > 0$

$\triangleright$ Studied with bosonization on the line $J_2 = 0.5J'$

(classical transition line $\to$ ground-state of disconected chains)

at $J_2, J' \ll J$, by: Nersesyan and Tsvelik PRB 2003,

Smirnov & Tsvelik PRB 03, Bhaseen & Tsvelik PRB 03.

$\Rightarrow$ novel RVB state, spin-liquid:

- ground-state has a 2^{M-1} degeneracy
- el. excitations: deconfined spinons propagating across the chains
- low lying singlet excitations below the spin-gap

Exact Diagonalizations of the $J - J' - J_2$ model

$J' \leq J$, samples of $M = 2, 4, 6$ chains of lenght L, $N \leq 36$ spins.

Suggest for both $L, M \to \infty$

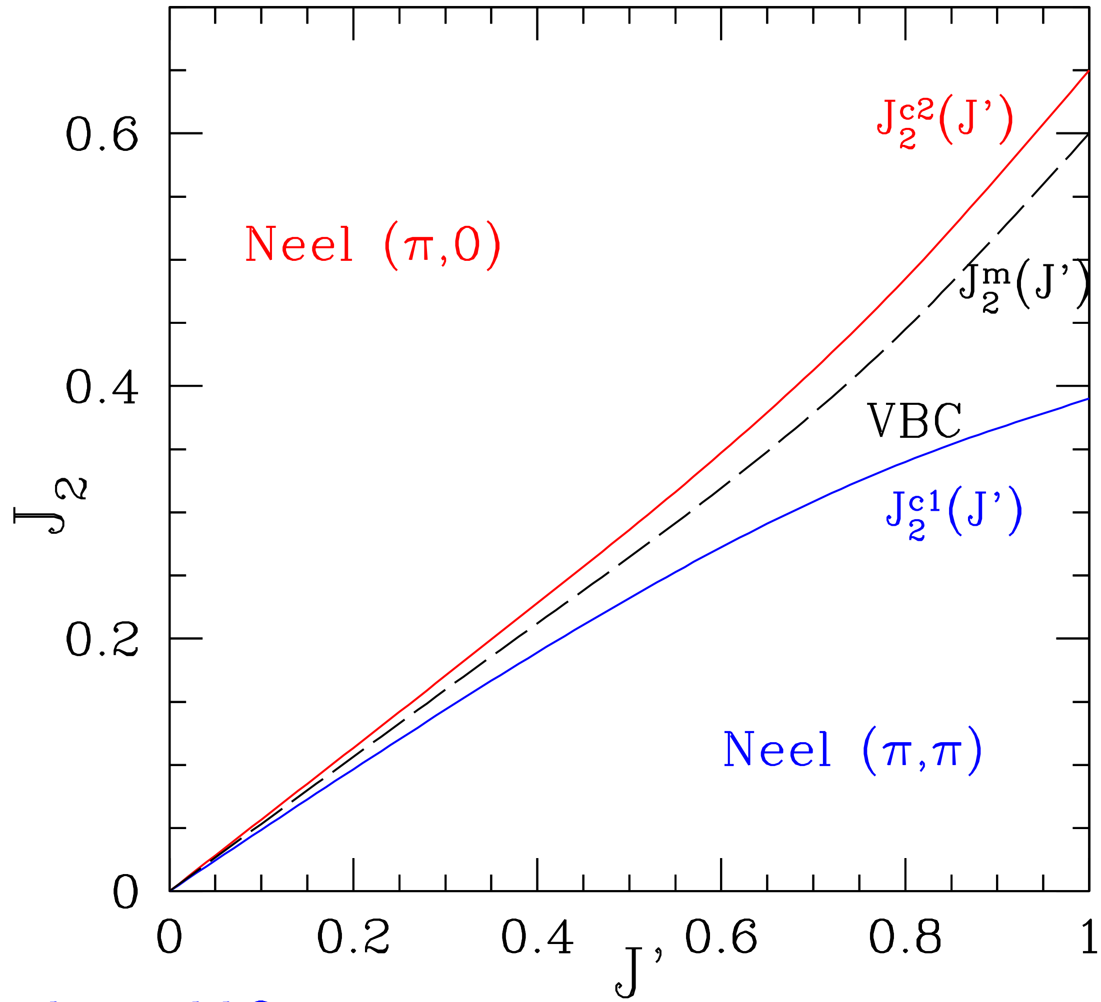
$\triangleright$ Two Néel phases (π, π), $(\pi, 0)$

$\triangleright$ No Néel LRO for $J_2^{c1}(J') \leq J_2 \leq J_2^{c2}(J')$

$\longrightarrow$ Valence Bond Crystal order of columnar dimers (could already appear for M even ≥ 2)

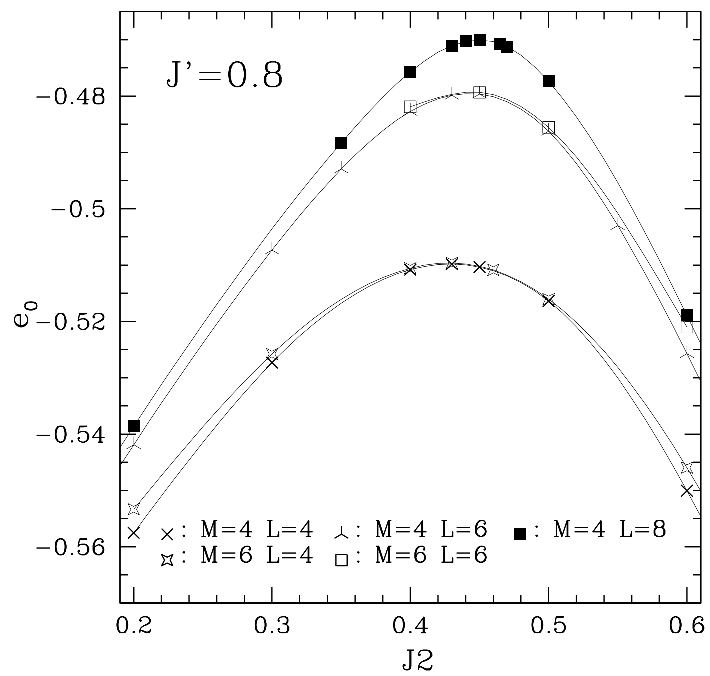
$\ominus$ except perhaps on the line of "maximum frustration" $J_2^m(J')$ (maxima of the energy/spin e_0)

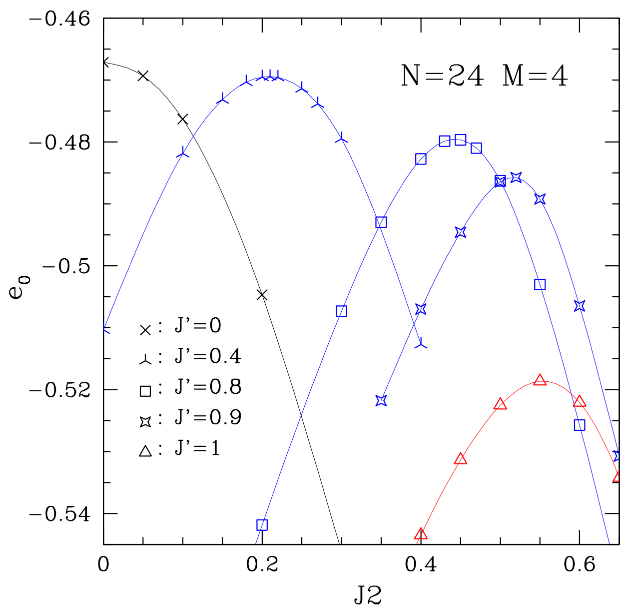
$\triangleright$ On $J_2^m(J')$ degeneracy corresponding to classical behavior of disconected chains is (partially) lifted $\rightarrow$ RVB state of Nersesyan and Tsvelik?

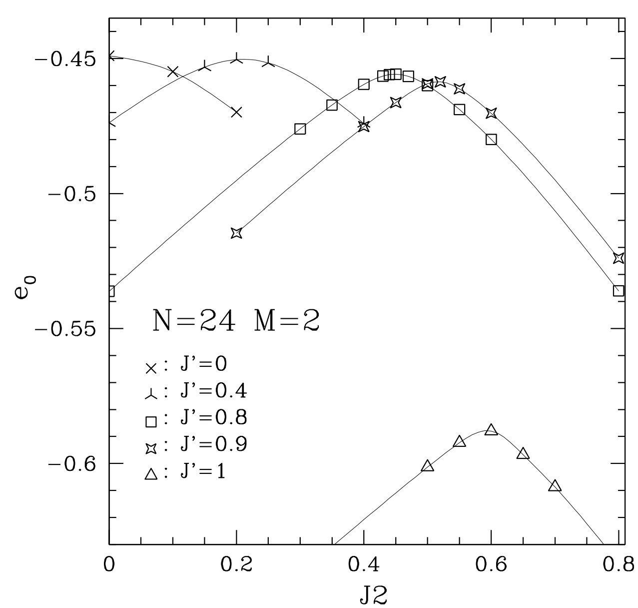


Energy per spin e_0:

- e_0 max for $J_2 \geq 0.5J'$. Line of maxima $J_2^m(J')$ deviates from the line $0.5J'$
- max. of e_0 quasi independent of M: the location of the line $J_2^m(J')$ is quasi independent of the number of chains.
- Drop of max. of e_0 for $M < L$ at large J': crossover J chains $\to$ J' chains







Néel states:

Their signature in the spectra:

A set of low lying states

- with energies that evolve as

$E(S) - E_0 \sim S(S+1)/N$

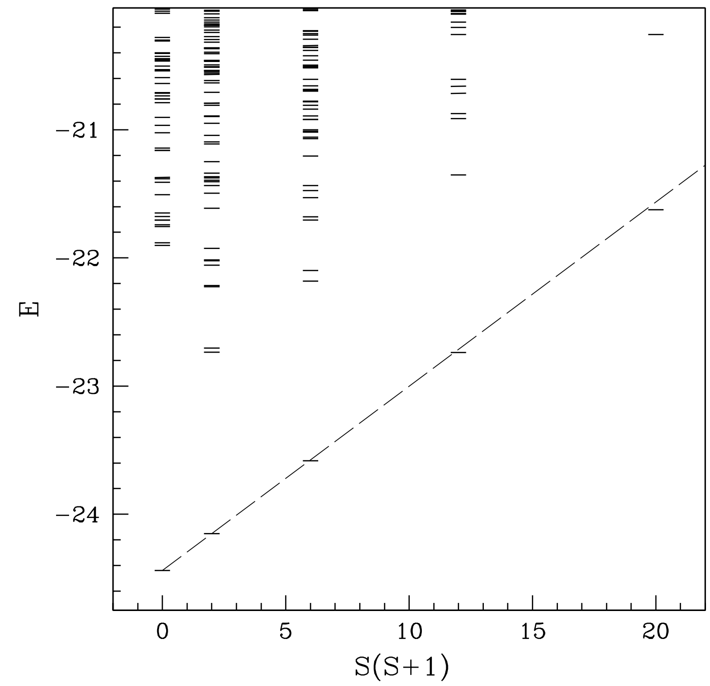
- which belong to IR specific of the magnetic order

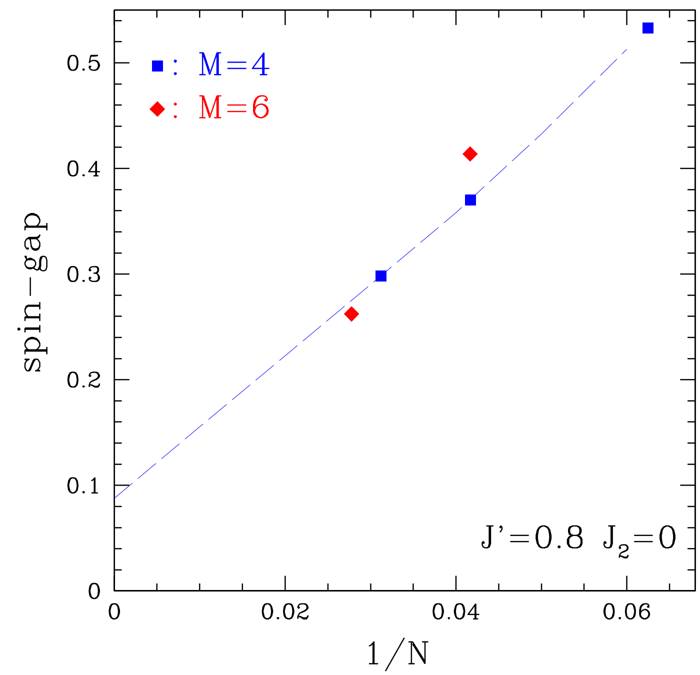
the so-called of "quasi degenerated joint states" (QDJS)

$*$ Néel LRO only for infinite number of chains.

Spin-gap finite for M finite (even)

$\rightsquigarrow$ "Haldane" phase





Intermediate region between Néel phases $J_2^{c1}(J') \leq J_2 \leq J_2^{c2}(J')$:

Disparition of the QDJS

▷ new low lying states, lowering of some singlet states:

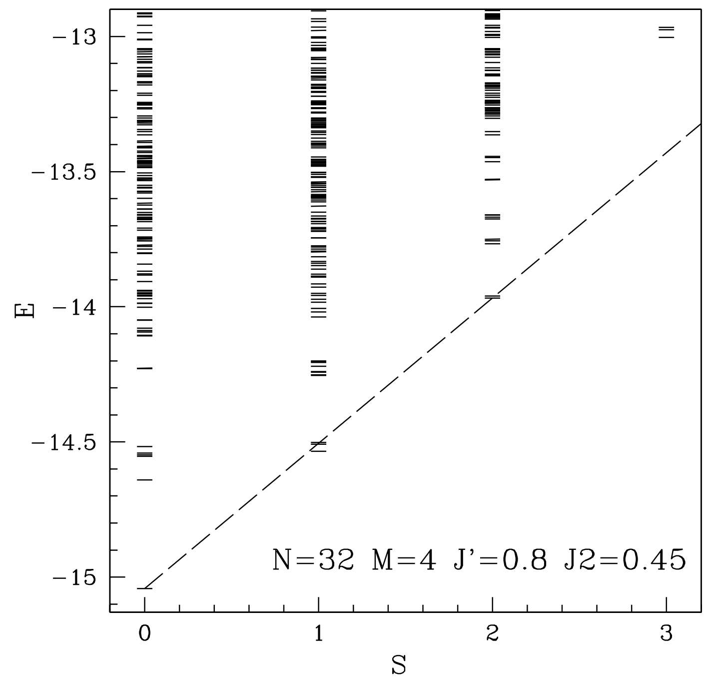
- few away $J_2^m \rightsquigarrow$ columnar dimer state
- many on J_2^m

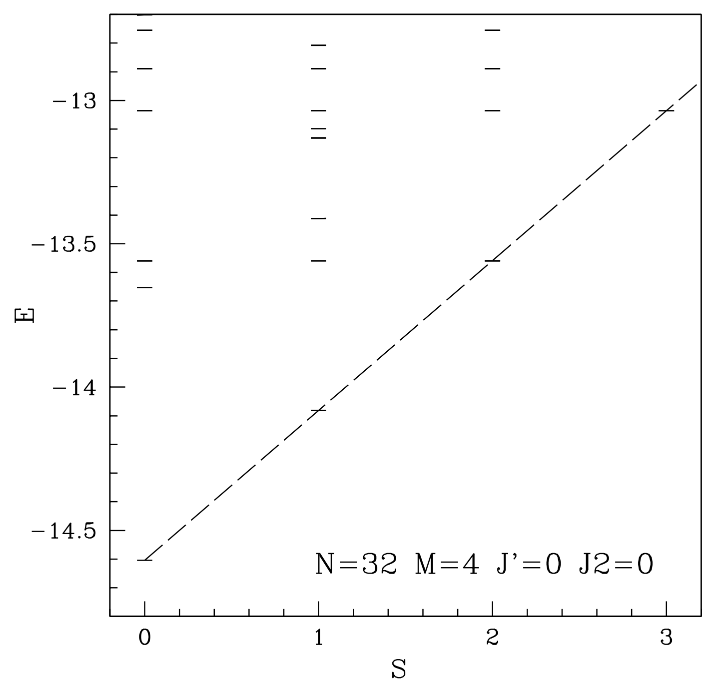
▷ $E(S) - E_0 \sim S$ turns linear in S on J_2^m

spectra looks $\sim$ disconected chains

but differences

$\rightsquigarrow$ RVB state of Nersesyan and Tsvelik?





Columnar dimer order adjacent to the (π, π) Néel phase $(J_2^{c1}(J') \le J_2 < J_2^m)$:

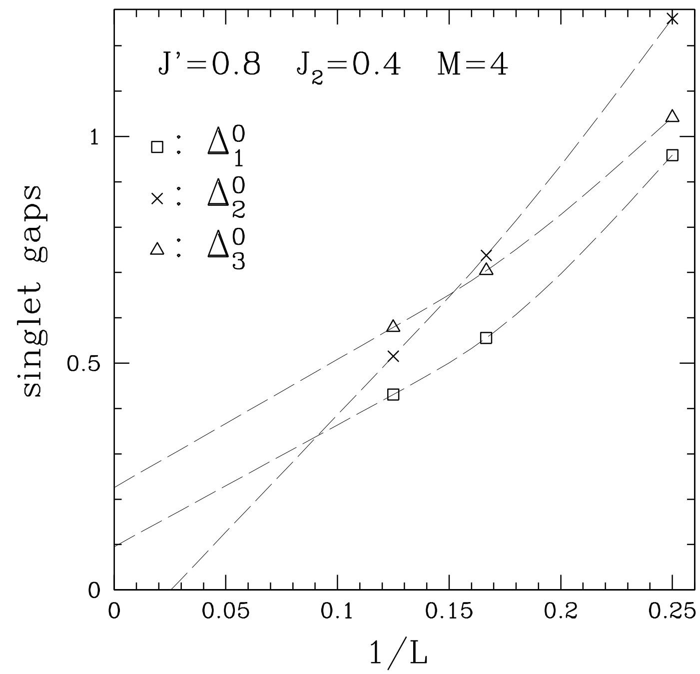
▷ Lowest singlet states:

- $|0>$: $[\mathbf{k} = 0, R(\pi) = 1, \sigma = 1])$ (trivial)
- $|1>$: $[\mathbf{k} = 0, R(\pi) = 1, \sigma = 1])$ (trivial)
- $|2>$: $[\mathbf{k} = (\pi, 0), R(\pi) = -1, \sigma = 1]$,
- $|3>$: $[\mathbf{k} = (0, \pi), R(\pi) = -1, \sigma = -1]$.

only gap Δ_2^0 to state $|2> \to 0$ as $L \to \infty$

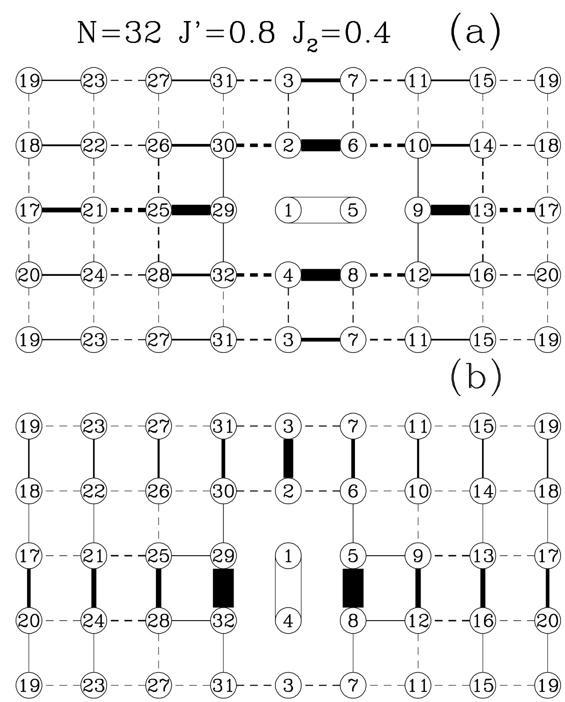
$\rightsquigarrow$ columnar $(\pi, 0)$ state

(ground-state twice degenerate)



▷ Dimer-dimer correlations:

- horizontal dimer-dimer correlations are consistent with the columnar $(\pi, 0)$ state
- yet, non negligible vertical dimer-dimer correlations, columnar $(0, \pi)$ state is close, selection of $(\pi, 0)$ state occurs at $L \to \infty$



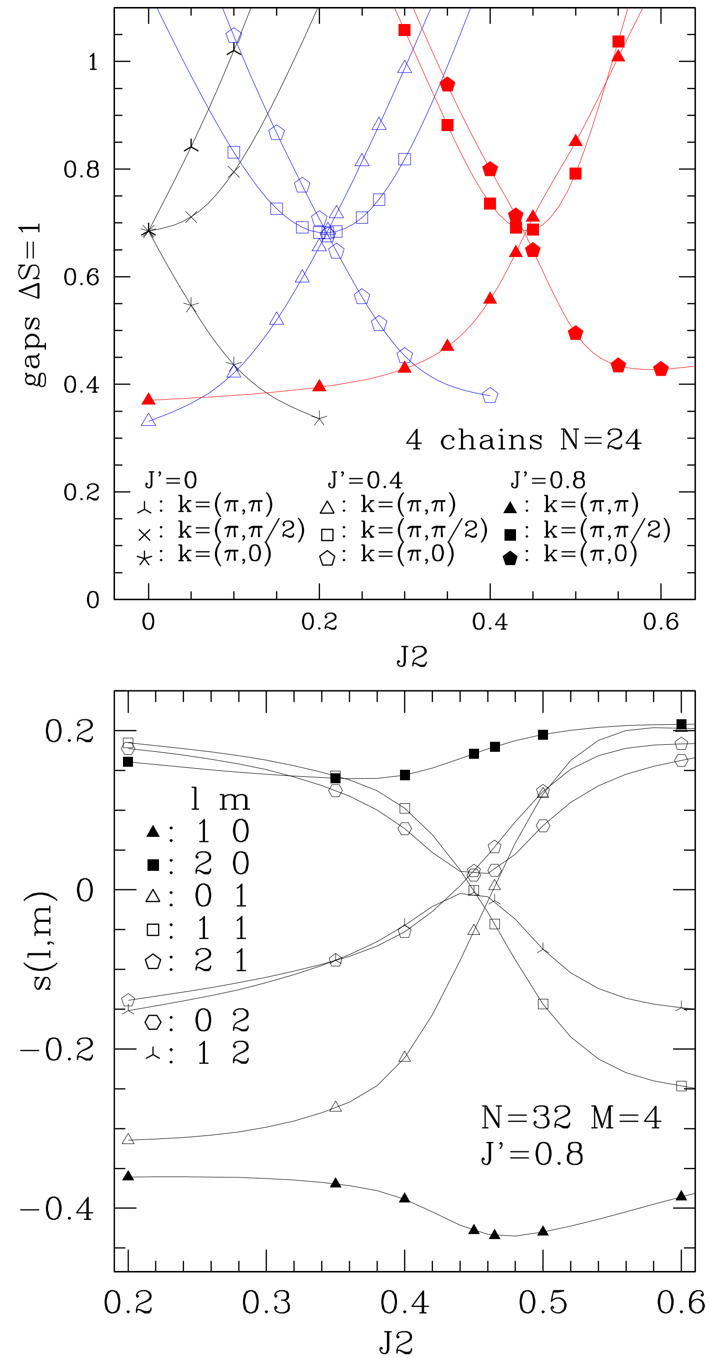
$J_2 = J_2^m(J')$, (on the line of maximum frustration):

▷ several features are similar to those expected for disconected chains:

- $E(S) - E_0 \sim S$
- same 1th $S = 1$ excitations:

M states at (π, k_y), quasi degenerates...

- quasi vanishing interchain spin-spin correlations



But the low-energy spectrum on J_2^m differs from the one of disconected chains:

▷ degenerate sets of lowest-lying $S = 0$ states for disconected chains are:

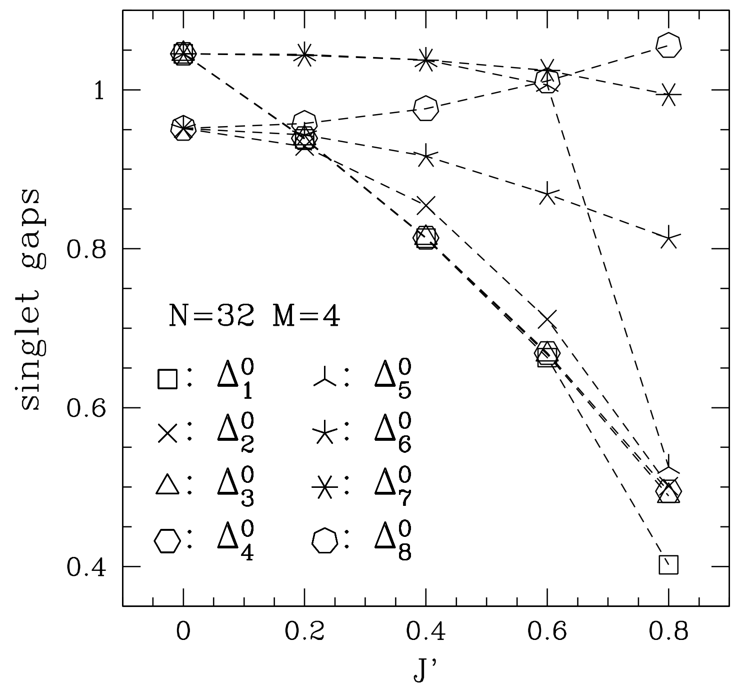
$$\begin{cases} |6>: & [\mathbf{k} = (\pi, \pm\pi/2), \sigma = -1] \\ |8>: & [\mathbf{k} = (\pi, \pi), R(\pi) = -1, \sigma = 1] \\ |2>: & [\mathbf{k} = (0, \pi), R(\pi) = -1, \sigma = -1] \end{cases}$$

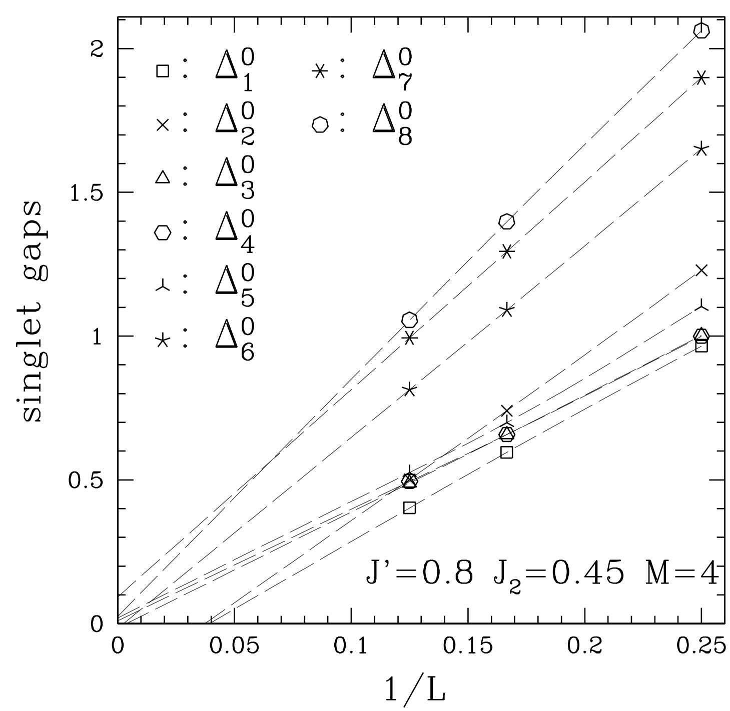
$$\begin{cases} |1>: & [\mathbf{k} = (0, 0), R(\pi) = 1, \sigma = 1] \\ |3>: & [\mathbf{k} = (0, \pi), R(\pi) = -1, \sigma = -1] \\ |4>: & [\mathbf{k} = (0, \pm\pi/2), \sigma = 1] \\ |5>: & [\mathbf{k} = (0, 0), R(\pi) = 1, \sigma = 1] \\ |7>: & [\mathbf{k} = (0, \pi), R(\pi) = 1, \sigma = 1] \end{cases}$$

⇝ degeneracies are lifted, 2D excited states

- ground-state degeneracy 2^{M-1}?

- gapless spectrum $M = 4$?

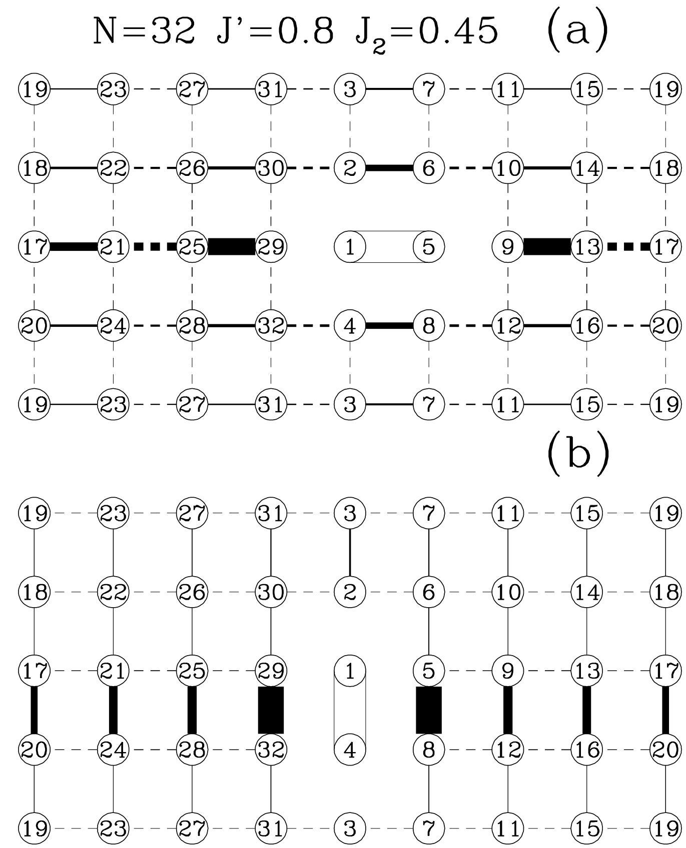




Pattern of dimer-dimer correlations at J_2^m:

▷ pictures strongly correlated pairs of adjacent chains, decorrelated from one pair to the next

$\sim$ RVB state of Nersesyan and Tsvelik.



$J_2^m < J_2 < (\pi, 0)$ Néel:

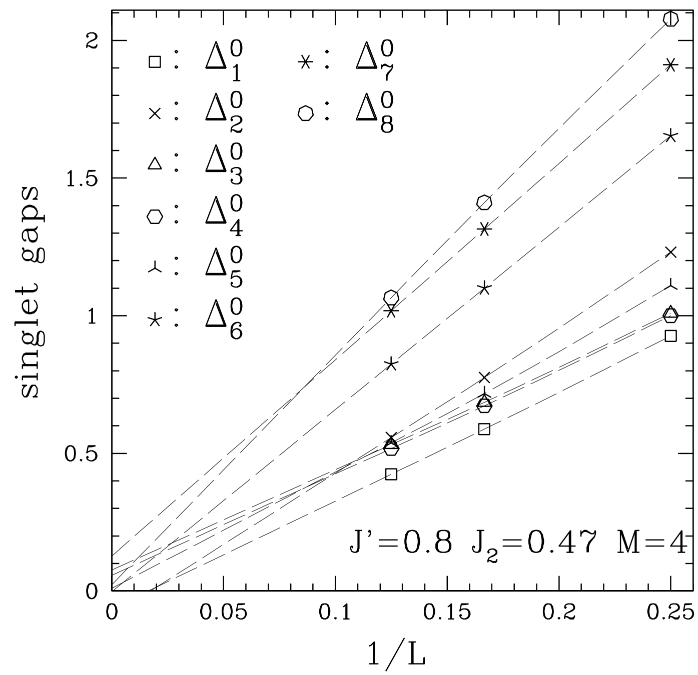
▷ very narrow region, uneasy to assess with present sizes

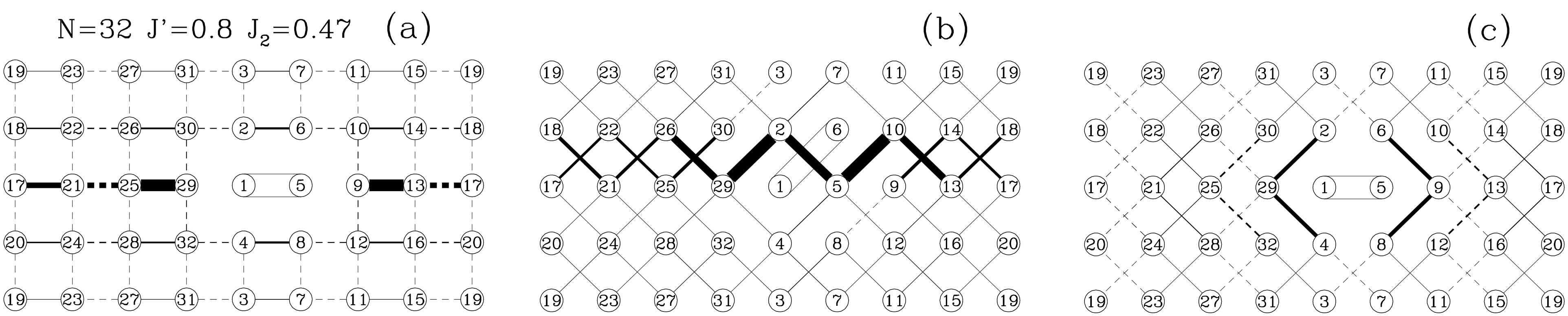
▷ $S = 0$ state(s) $|2>$, $(|1>?)$ could remain gapless

The patterns of dimer-dimer correlations could be compatible with a breaking of translational symmetry in the horizontal direction.

$\sim (\pi, 0)$ columnar dimer order?

- no plaquette order
- no staggered dimer order





Summary:

• ED results points to $(\pi, 0)$ columnar dimer order in the vicinity of the line of maximum frustration $J_2^m(J')$

▷ supported by recent bosonisation investigations:

-Starykh and Balents cond-mat/0402055
-Tsvelik, cond-mat/0404541

• suggest that dimer order extends up to $J' = J$ ($J_1 - J_2$ model)

• suggest that the novel RVB state of Nersesyan and Tsvelik occurs on $J_2^m(J')$ up to large values of interchain coupling

Open questions:

• nature of the phase on the $J_2 > J_2^m(J')$ side

• $J_1 - J_2$ model at the point of maximum frustration

• complete phase diagram of the ladders $M = 2, 4$ for $J' > 1$

• phase diagram in the vicinity of J_2^m for FM interchain couplings