Exact ground states with deconfined gapless excitations for the 3 leg spin-1/2 tube

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504. Wilhelm und Else Heraeus-Seminar

Quantum Magnetism in Low Spatial Dimensions

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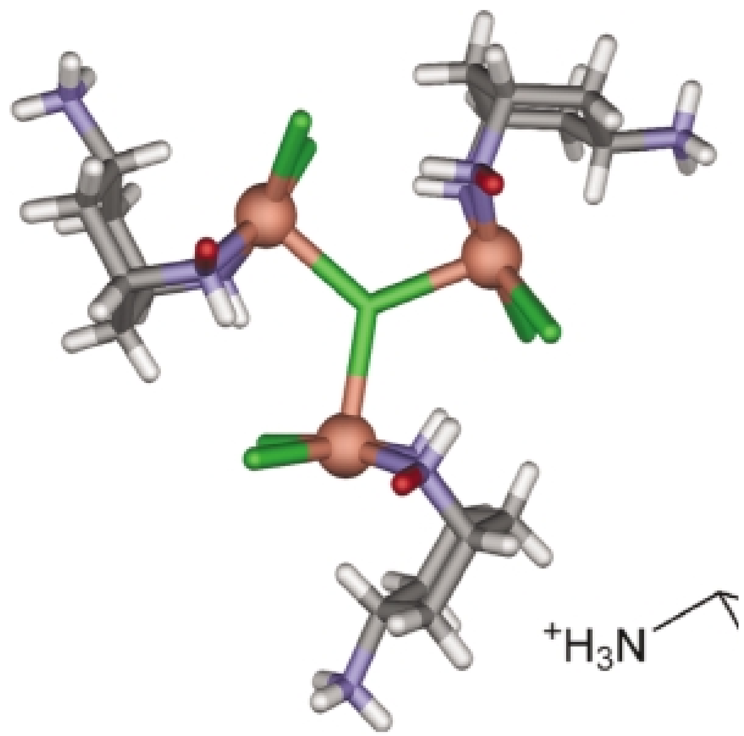
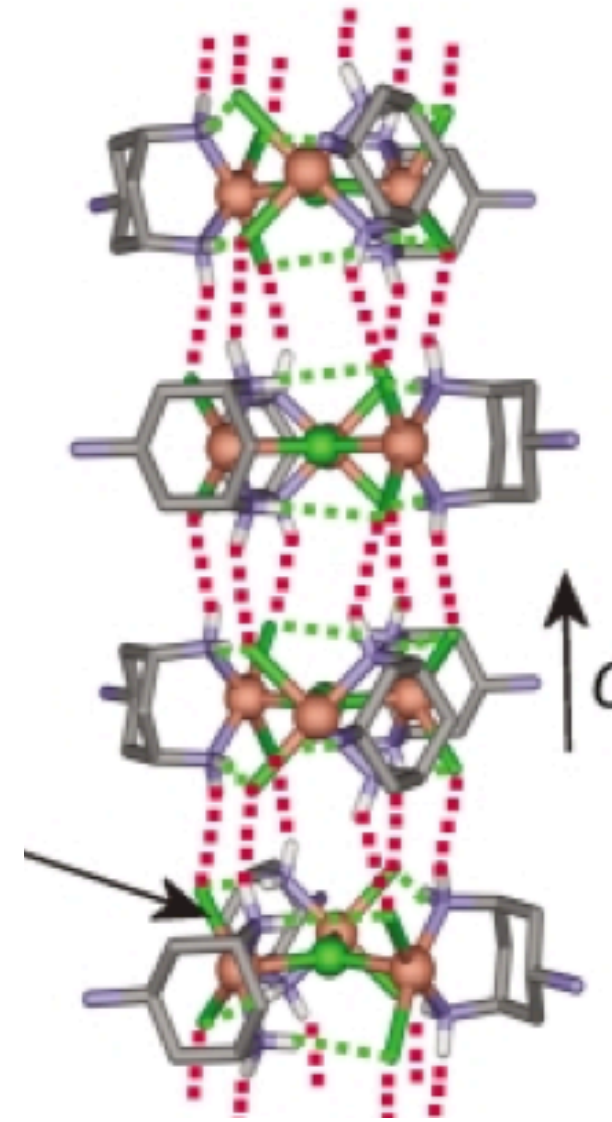
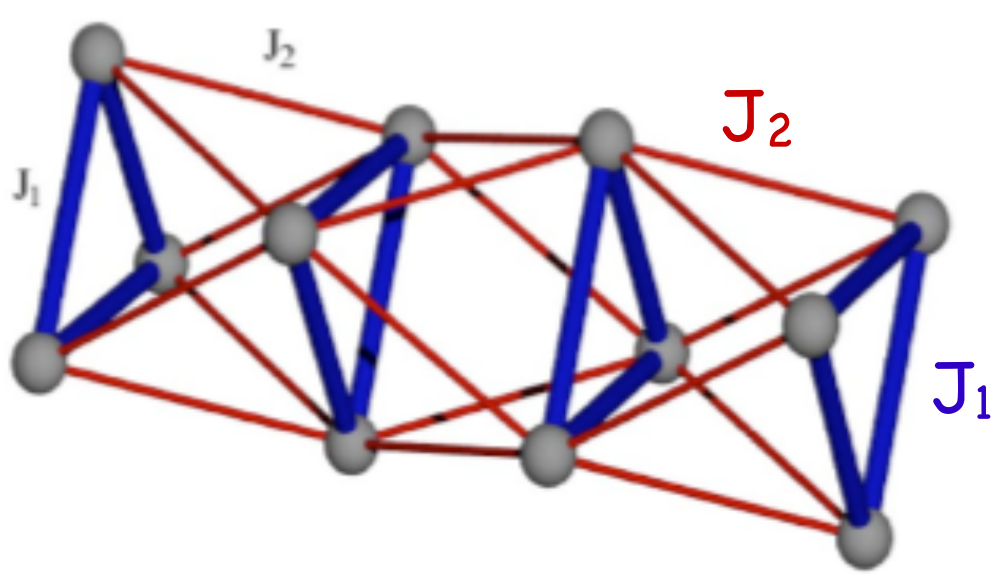
spin-1/2 tube

Three leg tubes

Cu_3Cl clusters in the $[(CuCl_2tachH)_3Cl]Cl_2$ organic molecule with 3 S=1/2 spins on the Cu ions.







(anti)columnar stacking with $J_1/J_2 \approx 3.4$

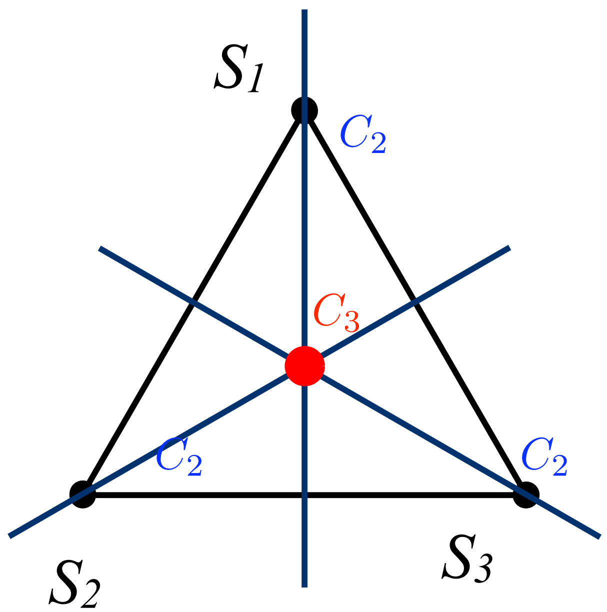
G. Seeber, P. Kögerler, B. M. Kariuki, and L. Cronin, Chem. Commun. (Cambridge) 2004, 1580 (2004)

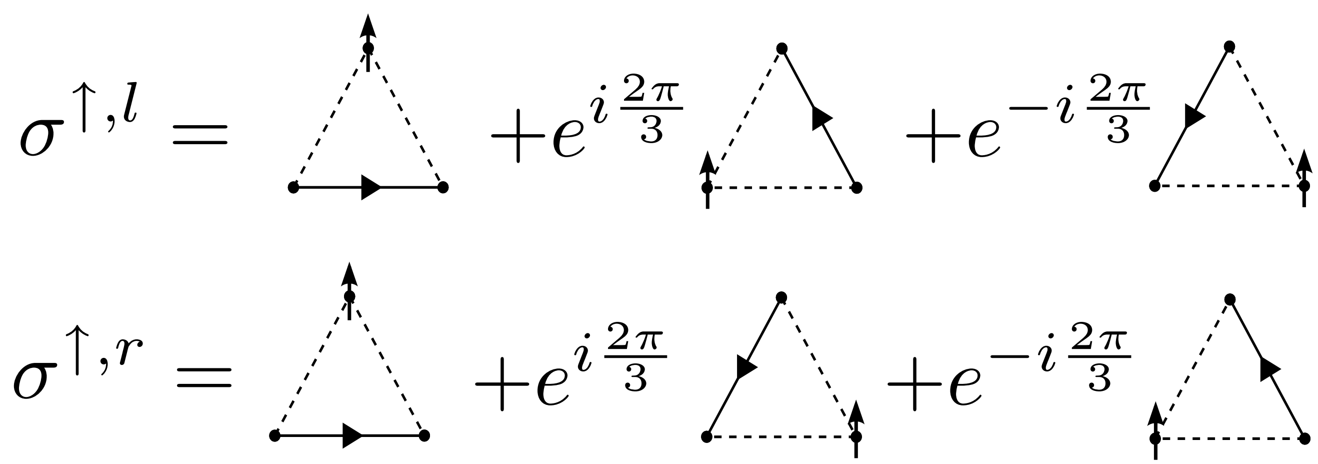
A single triangle

$$\mathbf{S}_1\cdot\mathbf{S}_2+\mathbf{S}_2\cdot\mathbf{S}_3+\mathbf{S}_3\cdot\mathbf{S}_1=\frac{1}{2}\left(\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3\right)^2+\text{const.}$$

4x $S^{TOT}=3/2$

4x $S^{TOT}=1/2$





D_3	E	$2C_3$	$3C_2'$
A_1	1	1	1
A_2	1	1	−1
E	2	−1	0

$$\mathbf{C}_3\sigma^{\uparrow,l}=e^{i\frac{2\pi}{3}}\sigma^{\uparrow,l}\qquad \mathbf{C}_2\sigma^{\uparrow,l}=-\sigma^{\uparrow,r}$$

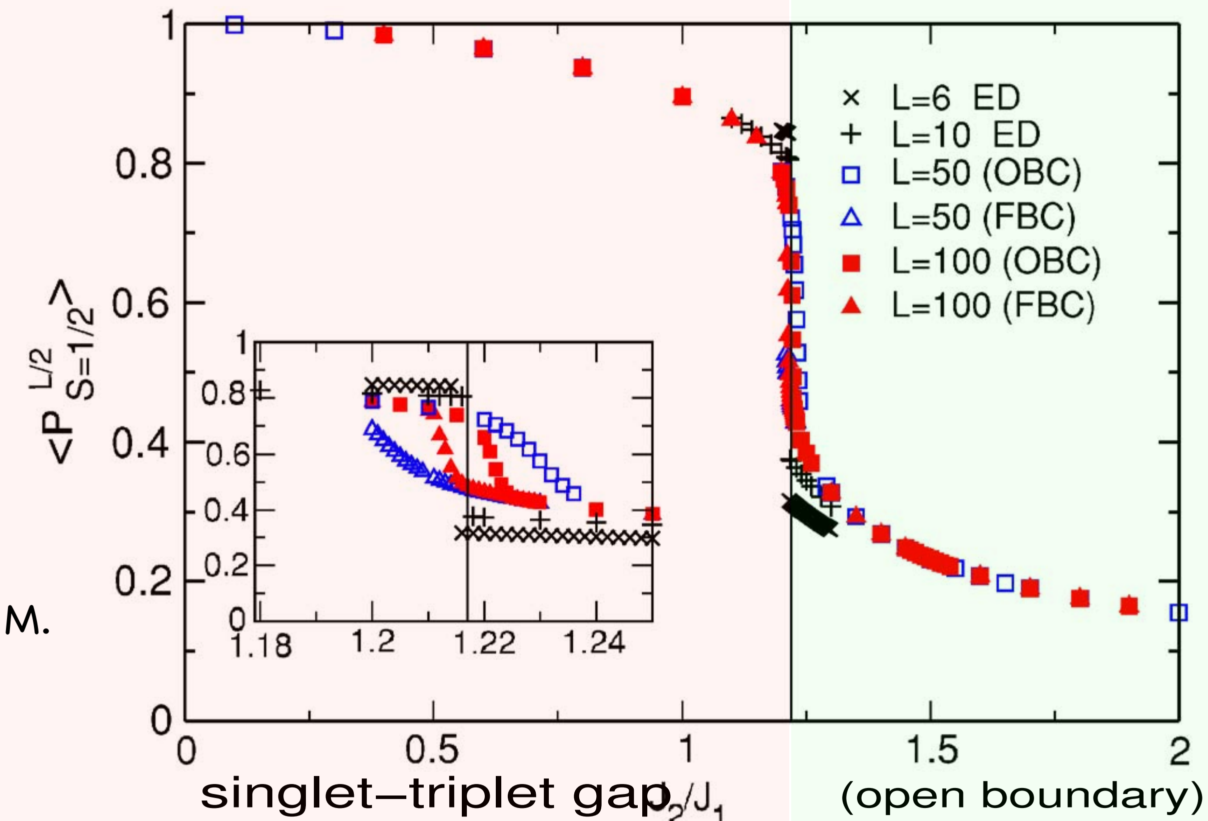
$$\mathbf{C}_3\sigma^{\uparrow,r}=e^{-i\frac{2\pi}{3}}\sigma^{\uparrow,r}\qquad \mathbf{C}_2\sigma^{\uparrow,r}=-\sigma^{\uparrow,l}$$

Three leg tubes

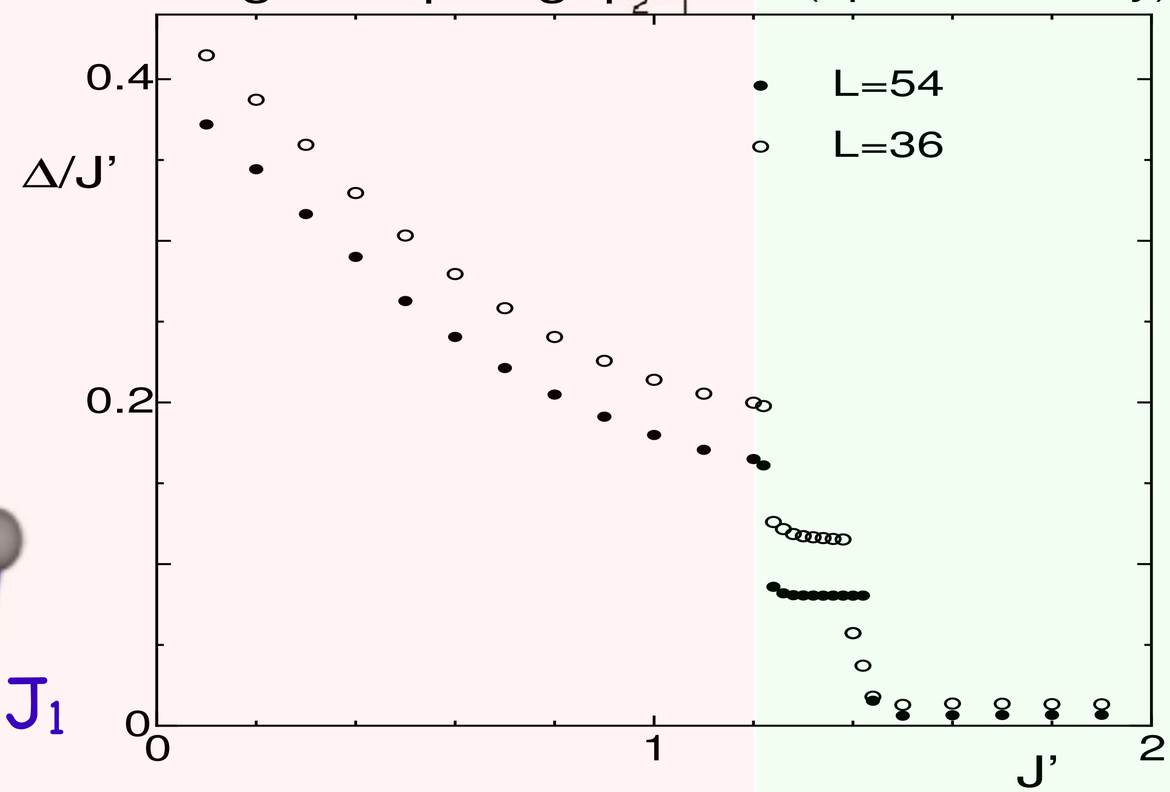
$J_1 >> J_2$ limit (decoupled triangles): effective S=1/2 model, degenerate ground state, gap

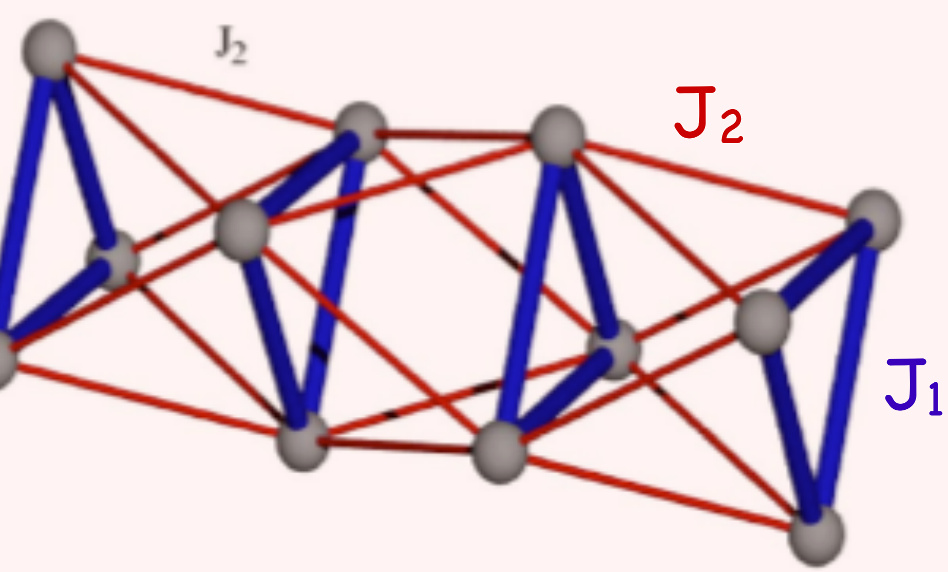
J.-B. Fouet, A. Läuchli, S. Pilgram, R. M. Noack, and F. Mila, PRB **73**, 014409 (2006)

K. Okunishi, S. Yoshikawa, T. Sakai and S. Miyashita, Progress of Theoretical Physics Supplement **159**, 297 (2005)



$J_1 << J_2$ limit: effective S=3/2 model, gapless





T. Sakai, M. Sato, K. Okamoto, K. Okunishi, and C. Itoi, J. Phys. Condens. Matter 22, 403201 (2010).

Heat Capacity Reveals the Physics of a Frustrated Spin Tube

Nedko B. Ivanov,[1,2,*] Jürgen Schnack,[2,†] Roman Schnalle,[2] Johannes Richter,[3] Paul Kögerler,[4] Graham N. Newton,[5] Leroy Cronin,[5] Yugo Oshima,[6] and Hiroyuki Nojiri[6,‡]

$J_1 \ll J_2$ limit: effective S=3/2 model, gapless

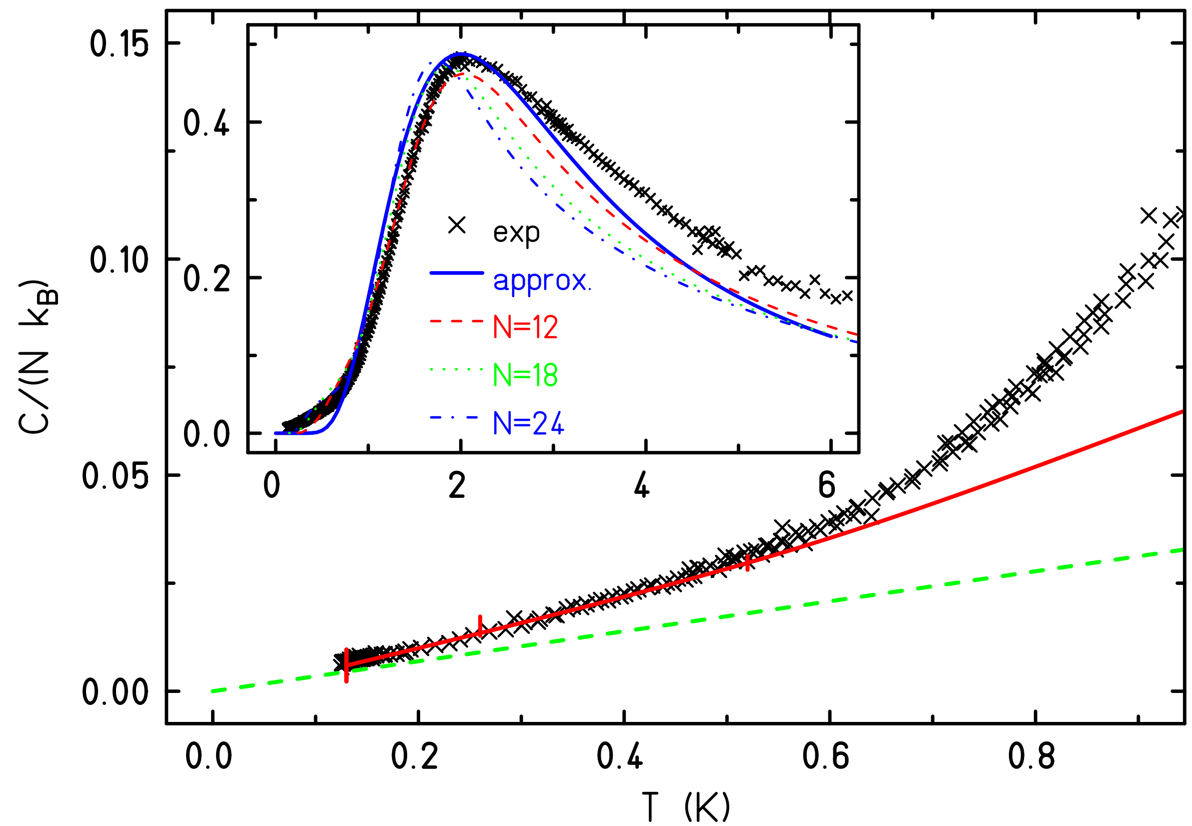
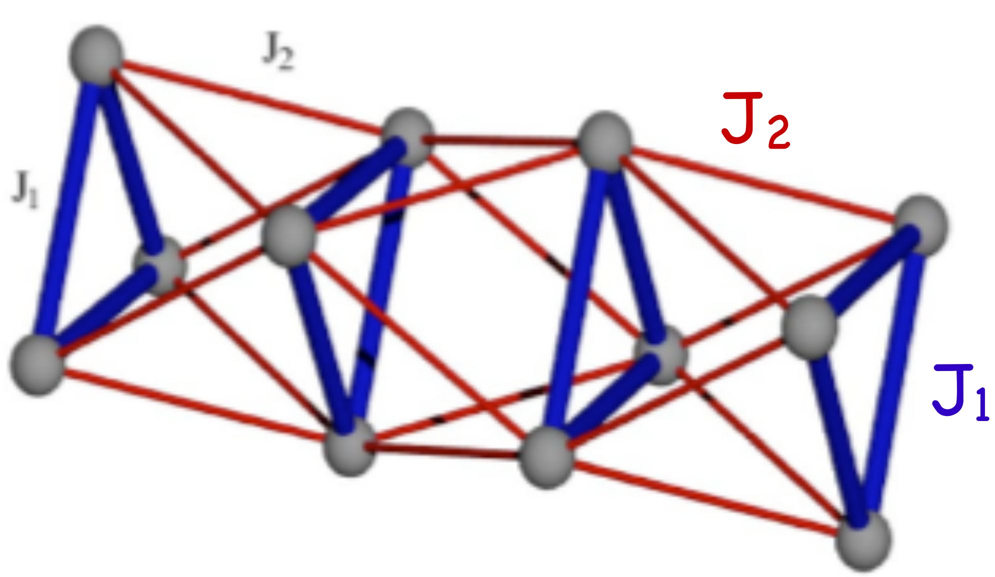
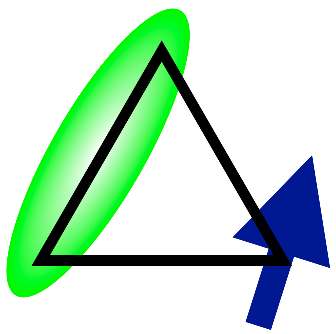


FIG. 4 (color online). Specific heat (per Cu spin) of $[(CuCl_2tachH)_3Cl]Cl_2$. The symbols always denote the experimental values. Main figure: The solid curve is the QMC result for a spin-3/2 chain of length $L = 100$. The dashed line provides the linear specific heat corresponding to the universal Tomonaga-Luttinger liquid form presented by Eq. (8), by using the extrapolation result $v_s = 10.06$ K. Inset: The solid curve depicts the two-level approximation (9). The broken curves denote the specific heat for three complete diagonalizations for finite sizes.

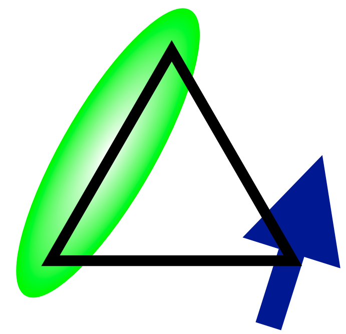
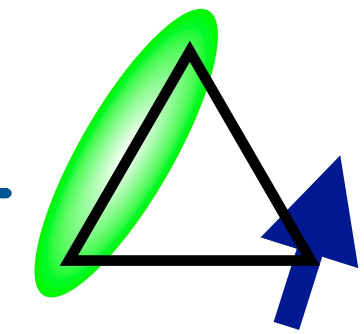


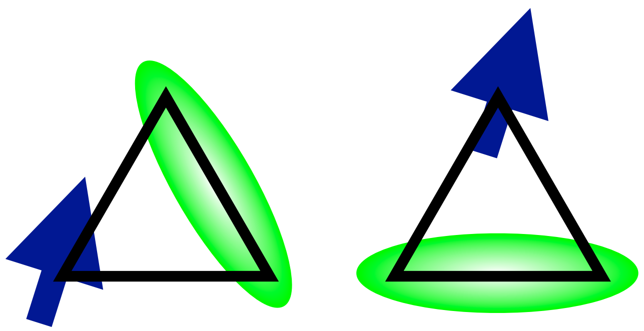
Models with projection operators

Majumdar-Ghosh model: ground state



is an eigenstate of the Heisenberg Hamiltonian on a triangle:

H  = −3/4 

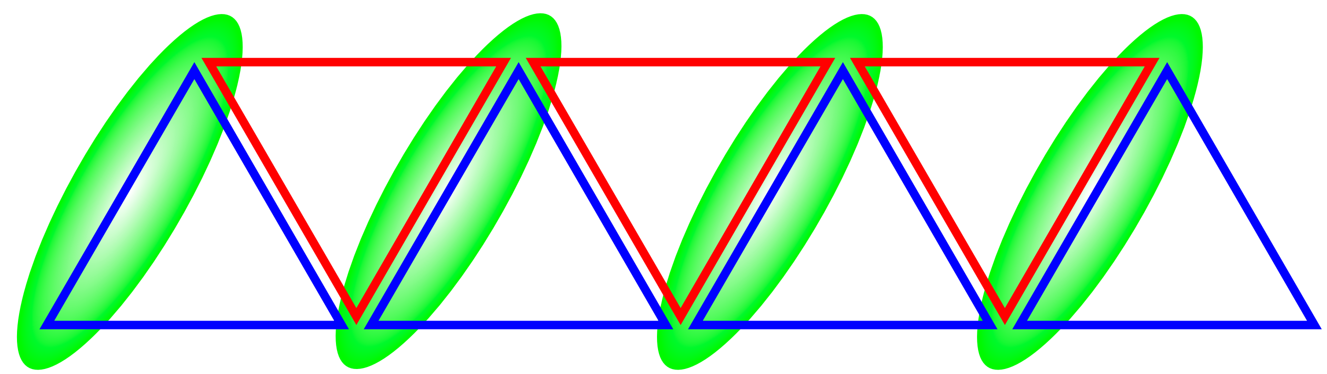


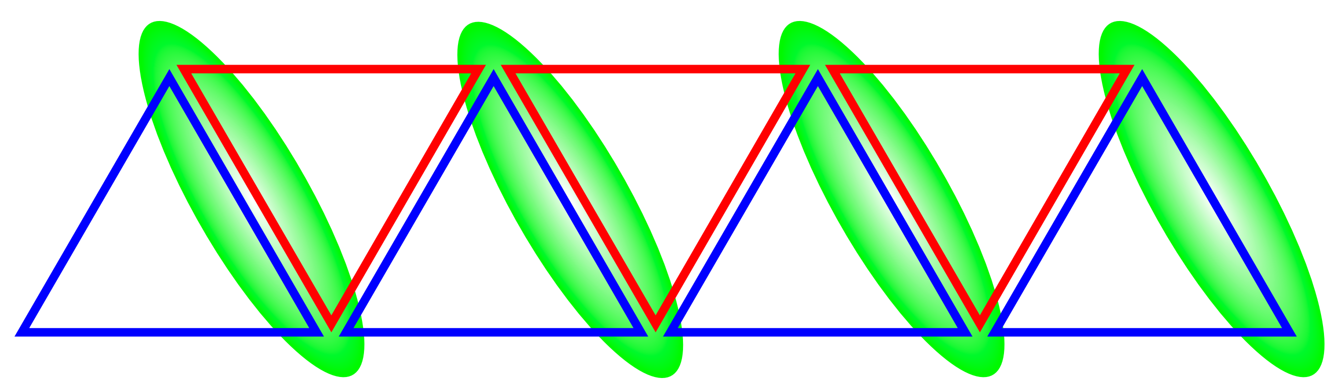
are also eigenstates

$$H_{MG} = \sum_i \mathrm{Proj}\left(|\mathbf{S}_{i-1} + \mathbf{S}_i + \mathbf{S}_{i+1}| = \frac{3}{2}\right)$$

$$H_{MG} = \sum_i \mathbf{S}_i \mathbf{S}_{i+1} + \frac{1}{2} \sum_i \mathbf{S}_i \mathbf{S}_{i+2}$$

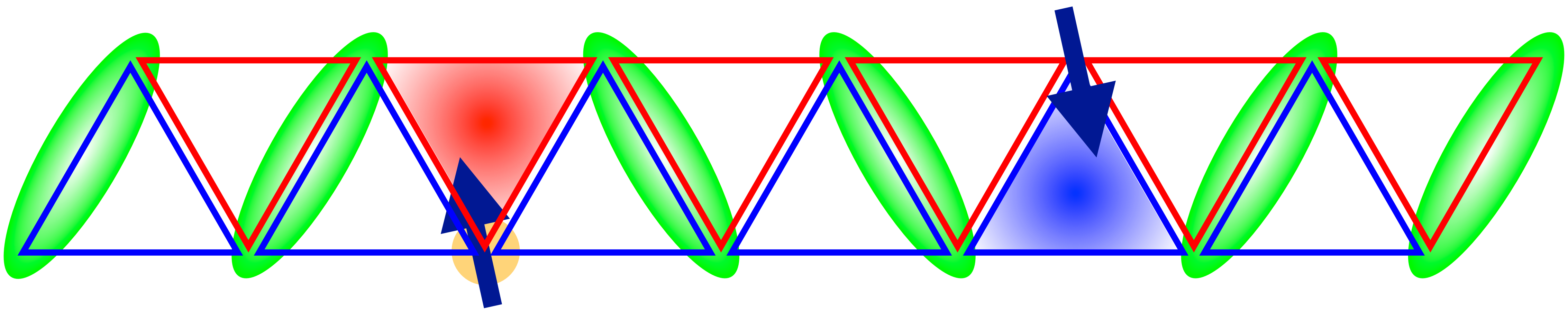
Two **exact** groundstates, with broken translational symmetry





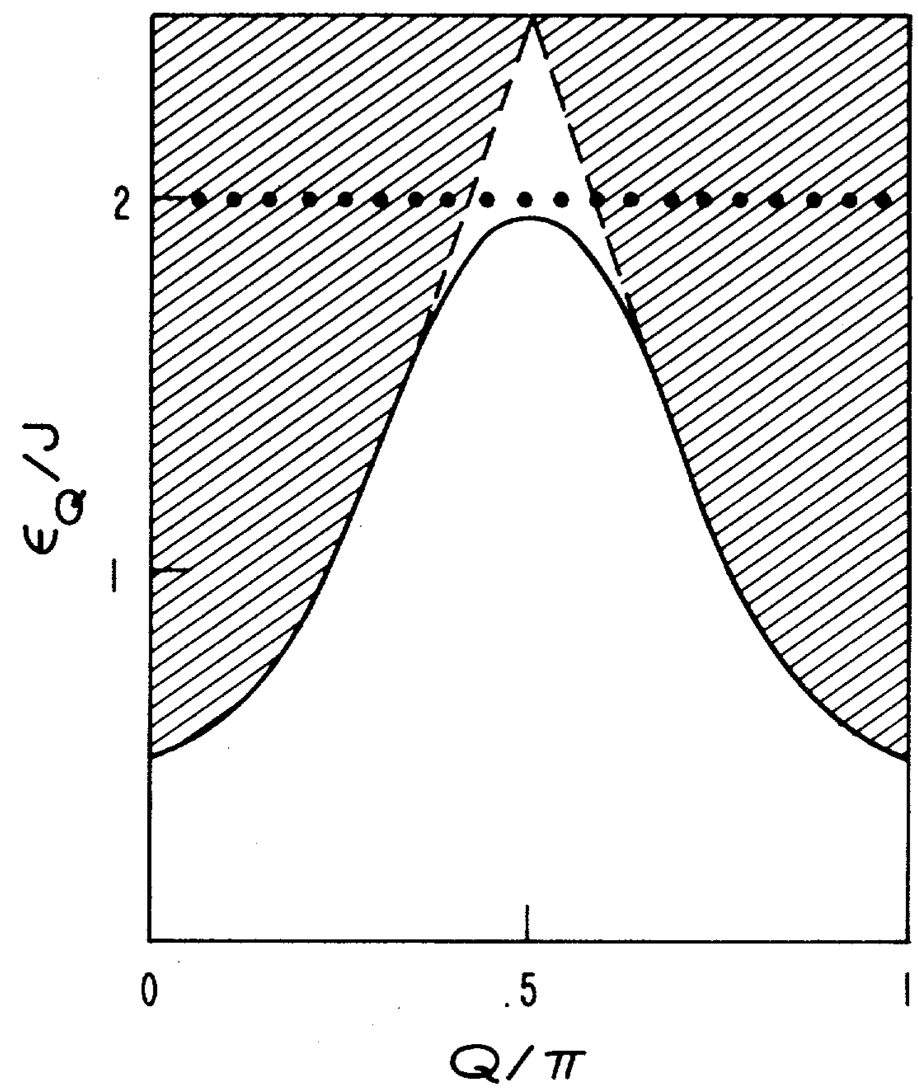
C K Majumdar and D Ghosh,
J. Math. Phys. 10, 1388 (1969).

Majumdar-Ghosh model: excitations



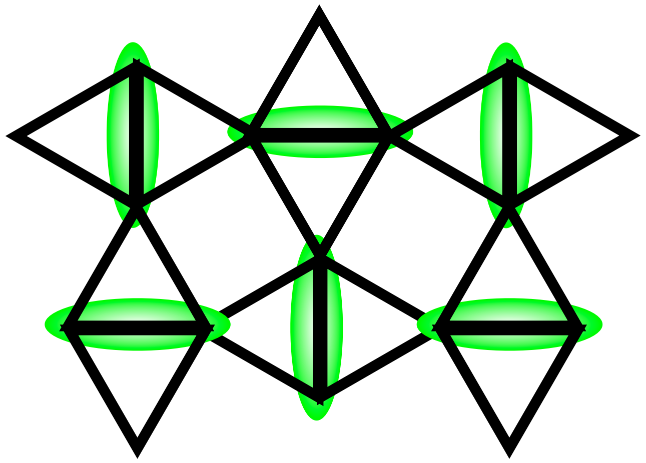
B. Sriram Shastry and Bill Sutherland,
Excitation Spectrum of a Dimerized Next-Neighbor Antiferromagnetic Chain,
Phys. Rev. Lett. **47**, 964-967 (1981)

- gapped spectrum
- bound state at higher energies

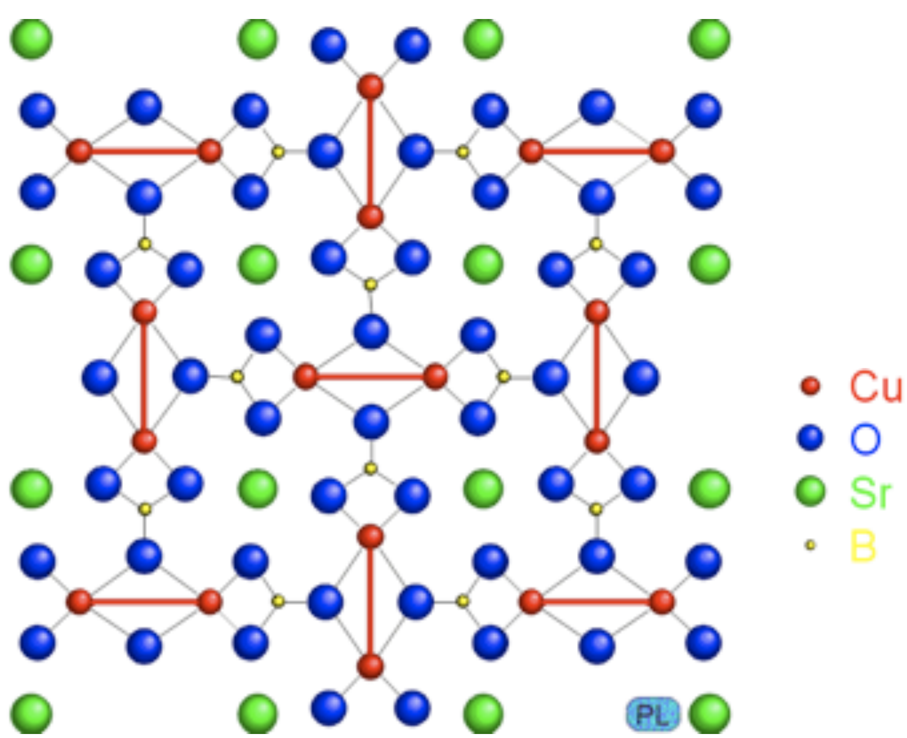


Projection operator approach continued...

The 2D Shastry-Sutherland model, with edge and corner sharing traingles

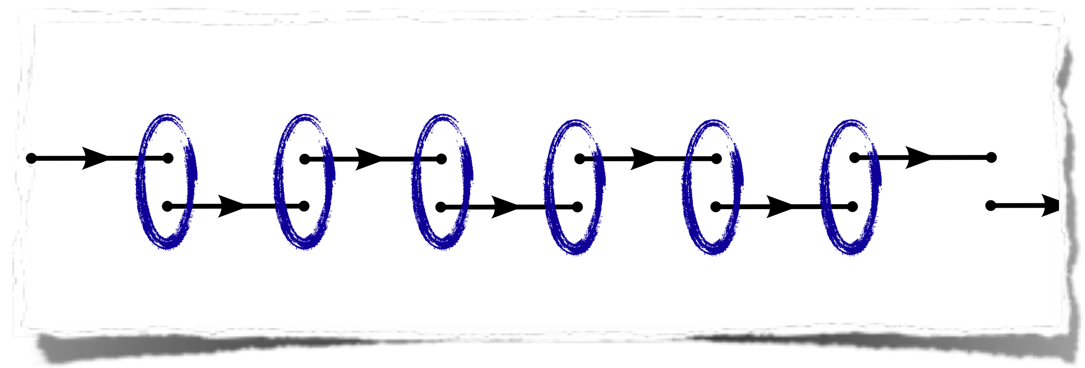


Experimental realization: SrCu2(BO3)2



Exact ground state for S=1 spin chain:

$$H_{AKLT} = \sum_i \text{Proj}\left(|\mathbf{S}_i + \mathbf{S}_{i+1}| = 2\right)$$



$$H_{AKLT} = \sum_i \frac{1}{3} + \frac{1}{2}\mathbf{S}_i\mathbf{S}_{i+1} + \frac{1}{6}\left(\mathbf{S}_i\mathbf{S}_{i+1}\right)^2$$

I Affleck, T Kennedy, E H Lieb, and H Tasaki, Comm. Math. Phys. 115, 477 (1988).

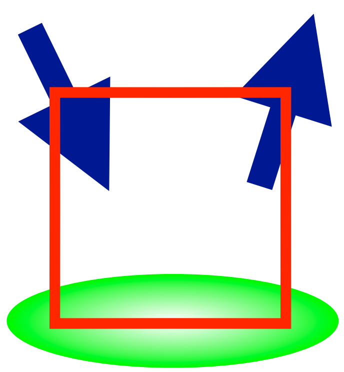
S=1/2, 2D square lattice

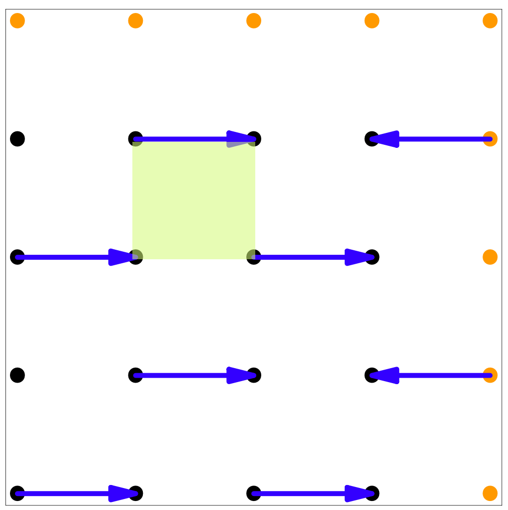
C D Batista, S. A. Trugman
Phys. Rev. Lett. **93**, 217202 (2004):

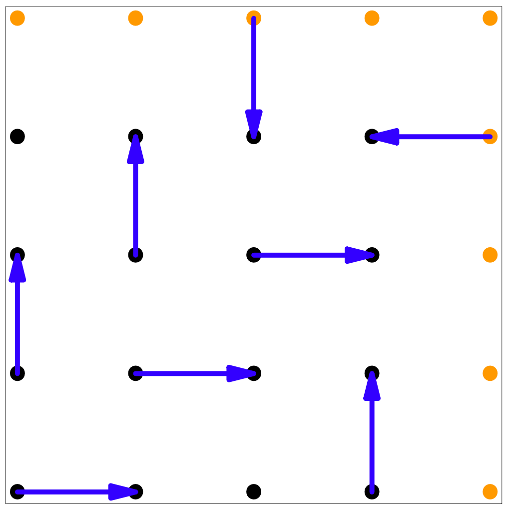
$$H = \sum_{\alpha\square} \mathcal{R}_\alpha$$

R projects out the spin 0 and 1 states of a square, S=2 cost energy

$$\mathcal{R}_\alpha = -\frac{1}{4} + \frac{1}{6}\sum_{i,j\in\alpha} P_{ij} + \frac{1}{12}\sum_{i,j,k,l\in\alpha} P_{ij}P_{kl}$$

$\mathcal{R}_\alpha$  =0



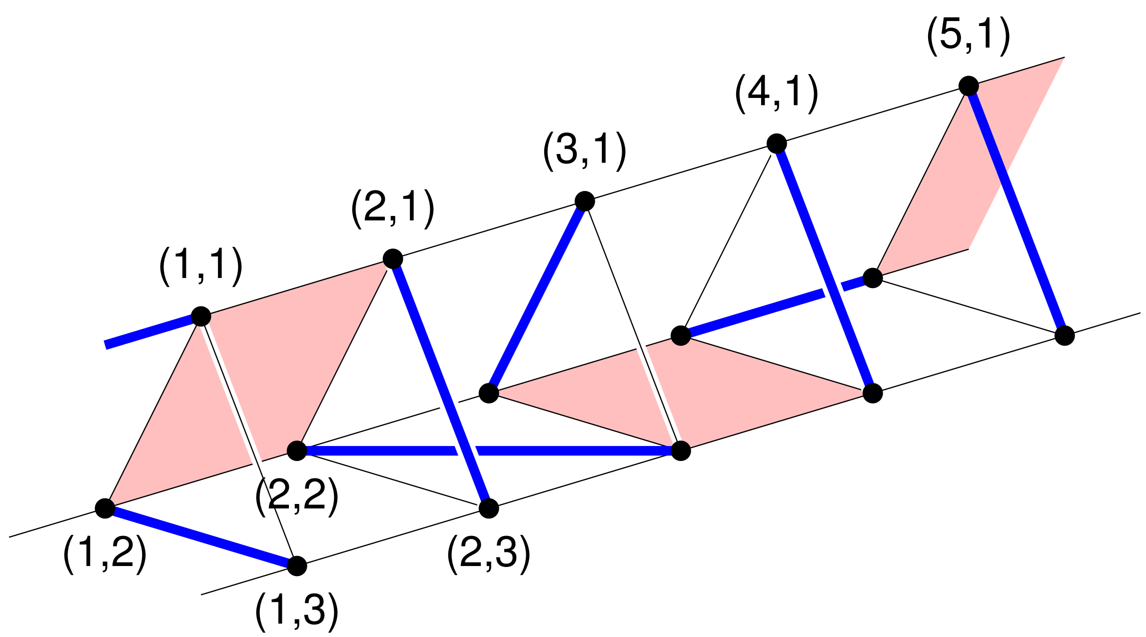


- N spins ->N/2 singlet bonds, N plaquettes: every plaquette should have a singlet
- Many nearest neighbour valence bond covering ground state
- From ED we find non-trivial singlet, even triplet ground states with 0 energy!

spin-1/2 tube with projection operators

Three leg tube with projection operators

$$\mathcal{H} = K_\triangle \sum_{i=1}^{L} P_i + K_\Box \sum_{i=1}^{L} \sum_{j=1}^{3} R_{(i,j)(i+1,j)(i+1,j+1)(i,j+1)}$$



$$R_\alpha = (\mathbf{S}_\alpha \cdot \mathbf{S}_\alpha)(\mathbf{S}_\alpha \cdot \mathbf{S}_\alpha - 2)/24$$

$$\mathbf{S}_\alpha = \sum_{(i,j)\in\alpha} \mathbf{S}_{(i,j)}$$

No nearest neighbour valence bond covering...

$$\tilde{\mathbf{S}}_i = \sum_{j=1}^{3} \mathbf{S}_{(i,j)}$$

$$P_i = (4\tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_i - 3)/12$$

Three leg tube with projection operators

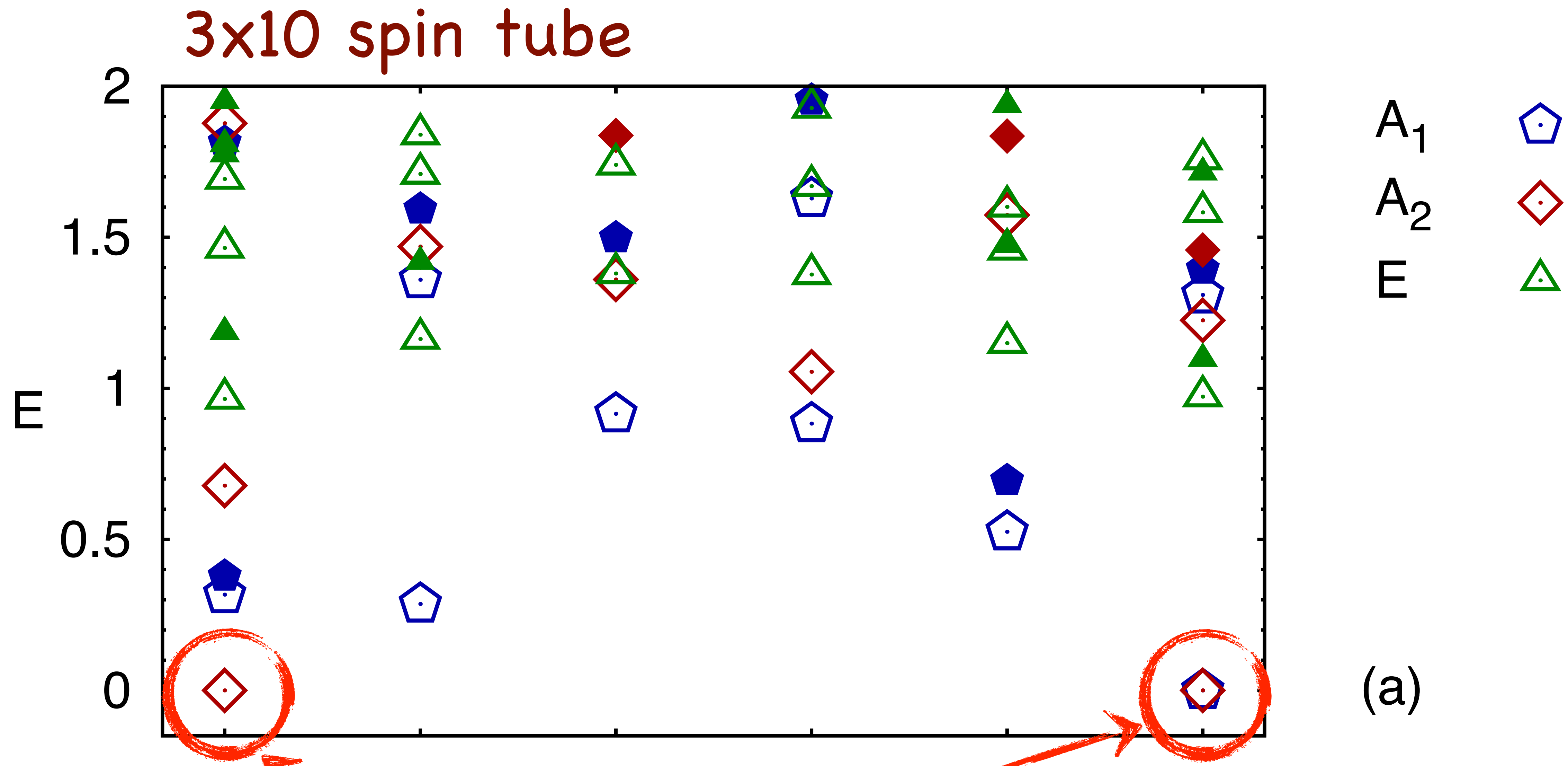
$$\mathcal{H} = K_{\triangle} \sum_{i=1}^{L} P_i + K_{\square} \sum_{i=1}^{L} \sum_{j=1}^{3} R_{(i,j)(i+1,j)(i+1,j+1)(i,j+1)}$$

The Hamiltonian with spin operators:

$$\begin{aligned}\mathcal{H} = \sum_{i=1}^{L} \sum_{j=1}^{3} \Big\{ & J_{\perp} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} + J_1 \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + J_2 \left(\mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j+1} + \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j-1} \right) \\ & + J_{\mathrm{RE}} \big[(\mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j})(\mathbf{S}_{i,j+1} \cdot \mathbf{S}_{i+1,j+1}) + (\mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1})(\mathbf{S}_{i+1,j} \cdot \mathbf{S}_{i+1,j+1}) \\ & + (\mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j+1})(\mathbf{S}_{i,j+1} \cdot \mathbf{S}_{i,j+1}) \big] \Big\}\end{aligned}$$

$$\begin{aligned} J_{\perp} &= 5K_{\square}/6 + 2K_{\triangle}/3 \\ J_1 &= 5K_{\square}/6 \\ J_2 &= 5K_{\square}/12 \\ J_{\mathrm{RE}} &= K_{\square}/3 \end{aligned}$$

Numerical results, $K_\triangle$=0



1 + 2 = 3 ground states, even though we cannot cover the tube with valence bonds. What are these states?

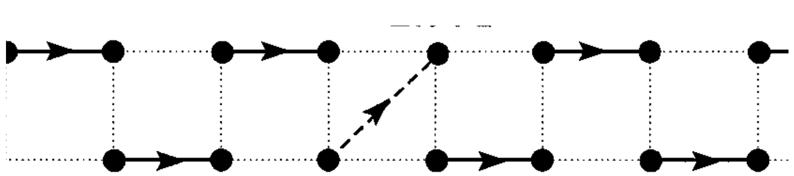
Effective model for large K△/K□

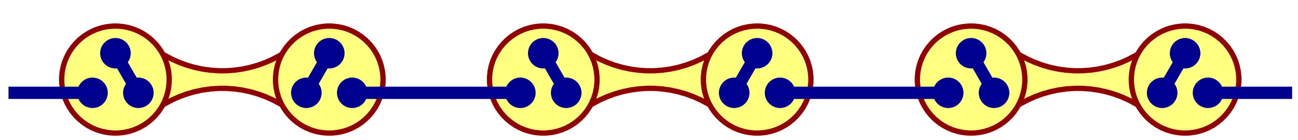
$$\mathcal{H} = K_\triangle \sum_{i=1}^{L} P_i + K_\square \sum_{i=1}^{L} \sum_{j=1}^{3} R_{(i,j)(i+1,j)(i+1,j+1)(i,j+1)}$$

triangles are in S=1/2 state,
degenerate perturbation theory in the spin-chirality sector:

$$\mathcal{H}' = \frac{5}{9} \sum_{i=1}^{L} \left(\frac{3}{4} + \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_{i+1} \right) \left(1 + \hat{\tau}_i^+ \hat{\tau}_{i+1}^- + \hat{\tau}_i^- \hat{\tau}_{i+1}^+ \right)$$

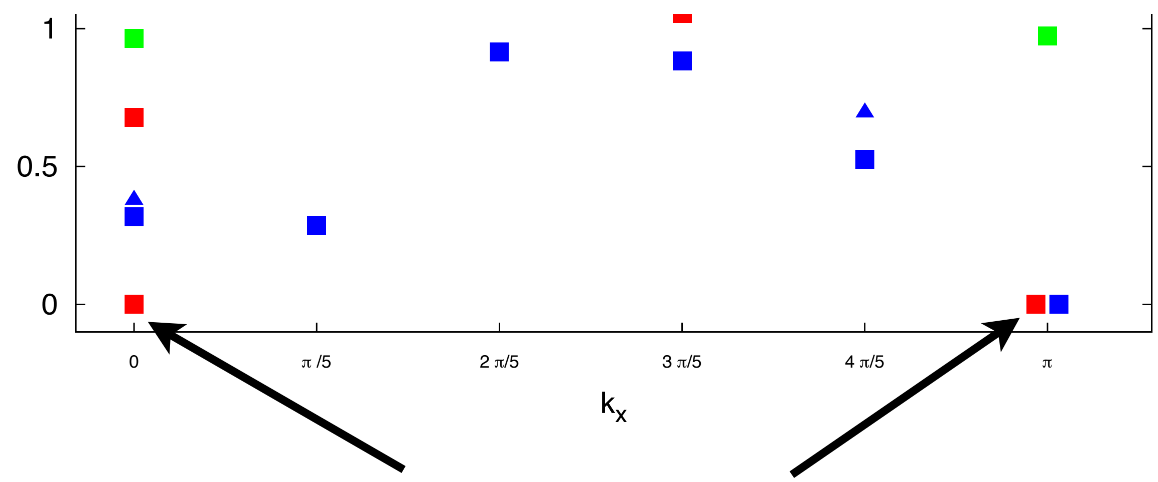
exact GS of H' given of as alternation of spin and chirality valence bonds (A. K. Kolezhuk, H.-J. Mikeska, PRL **80**, 2709 (1998))



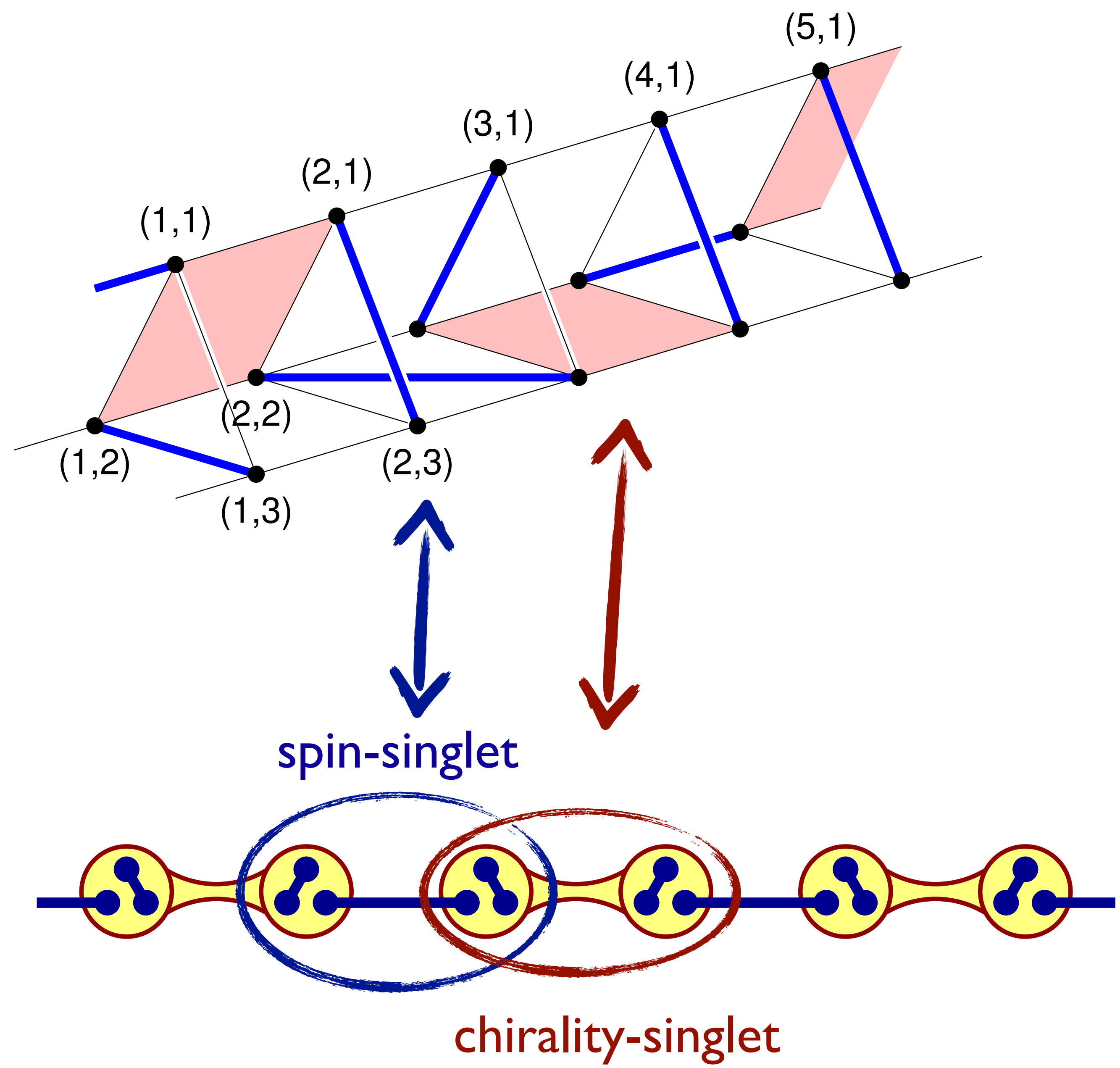


2 exact eigenstates

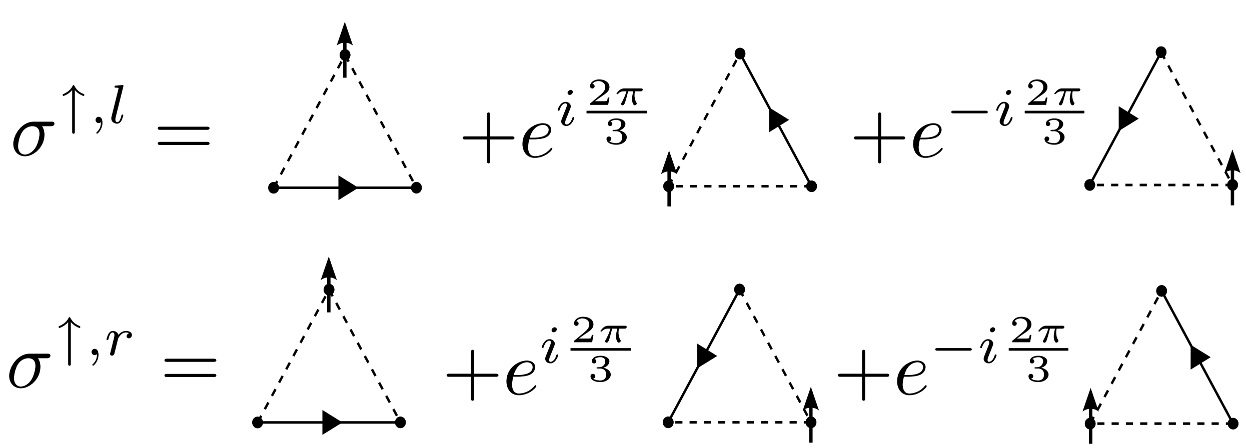
2 Exact eigenstates (GS) for arbitrary $K_\triangle/K_\square$



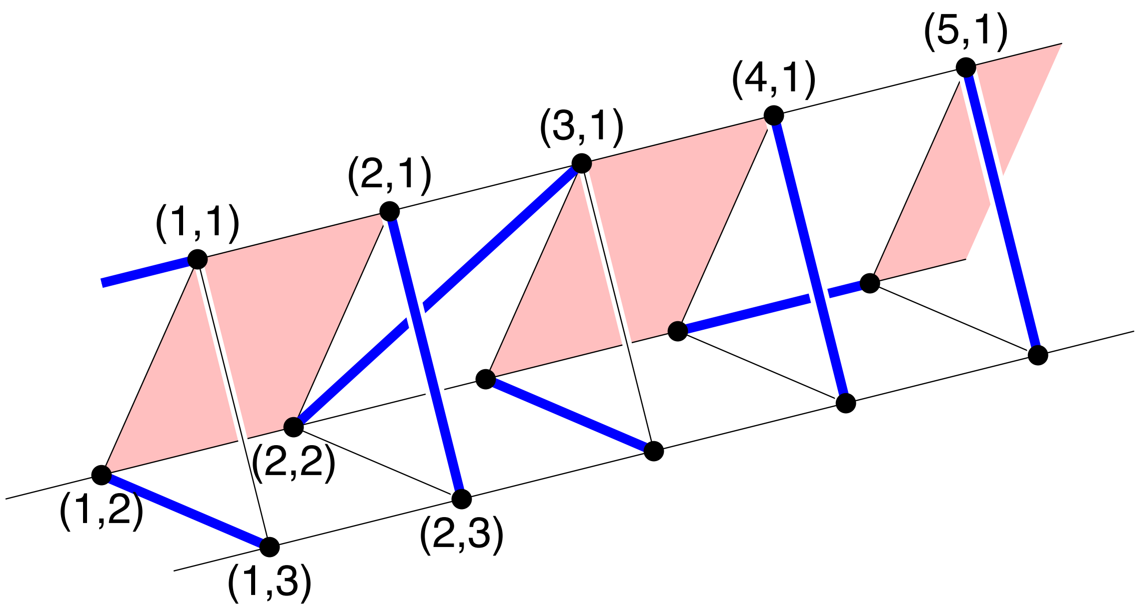
S=1/2 of each level

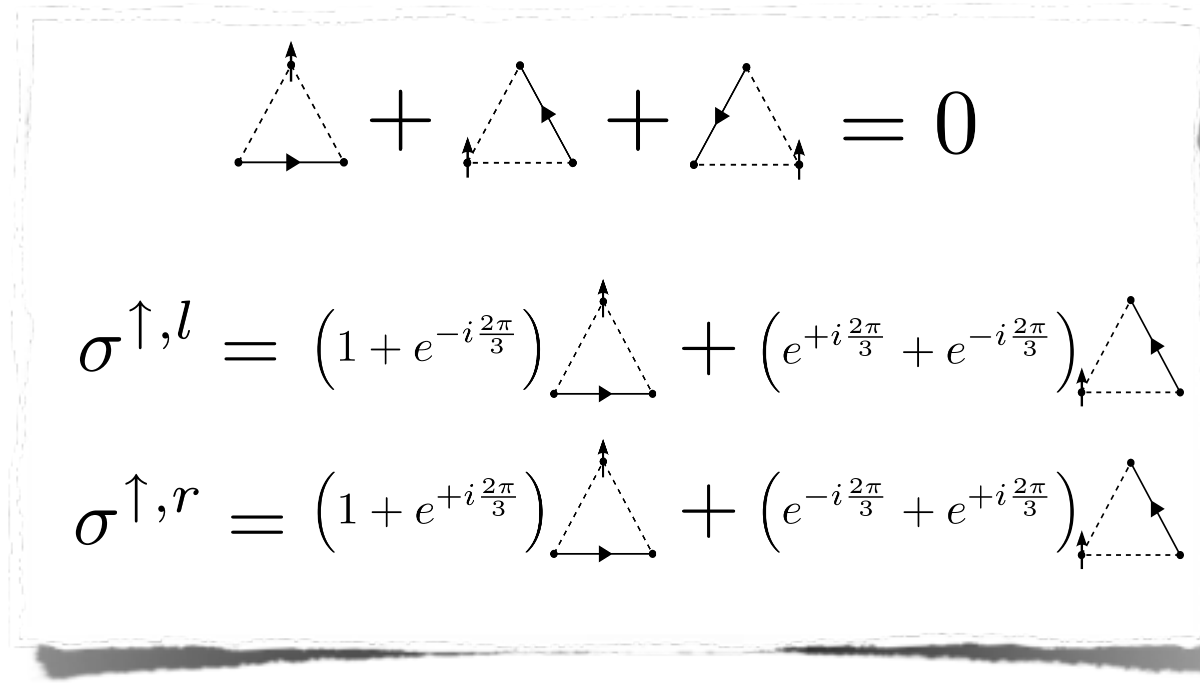


basis:

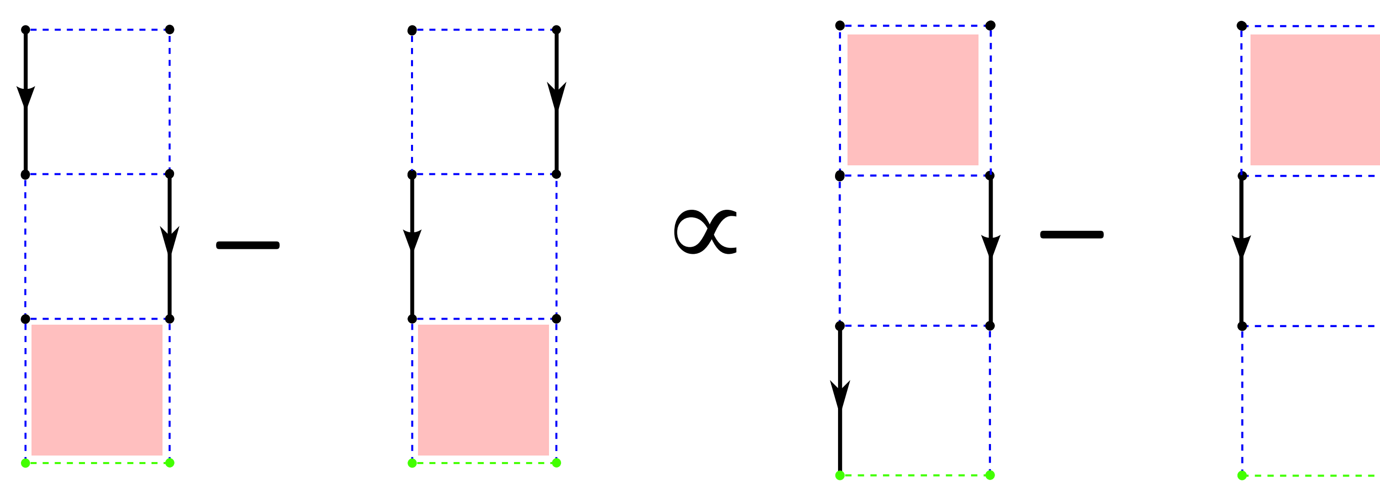


How does it work?





$$\sigma^{\uparrow,l} \otimes \sigma^{\uparrow,r} - \sigma^{\uparrow,r} \otimes \sigma^{\uparrow,l} \propto$$



It works because of linear dependence

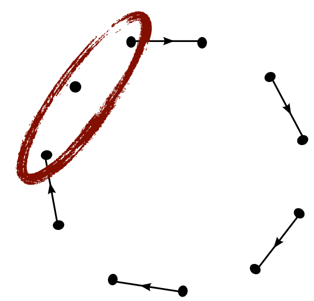
We found 2 out of 3 eigenstates.

Search for the 3rd GS: Tubes of odd length

Majumdar-Ghosh:

$$H_{MG} = \sum_i \mathrm{Proj}\left(|\mathbf{S}_{i-1}+\mathbf{S}_i+\mathbf{S}_{i+1}| = \frac{3}{2}\right)$$

for odd length: E>0



The effective model is gapped:

A. K. Kolezhuk, H.-J. Mikeska, PRL **80**, 2709 (1998)

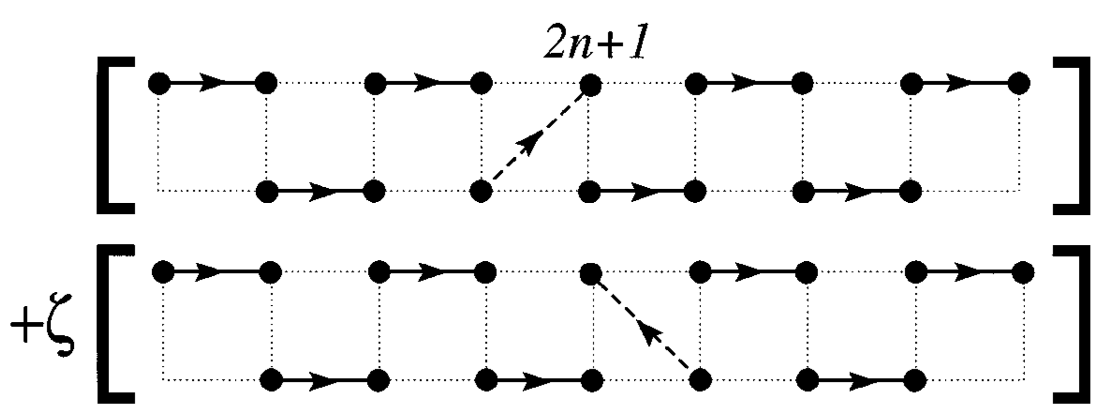


FIG. 1. The states $|n\rangle^{\zeta}_{t,s}$ used in Eq. (11), in a special case of the model (7). Thick solid lines indicate singlet bonds, and thick dashed lines can be either singlets or triplets. Arrows indicate the "direction" of the singlet bonds [i.e., $|s_{1\to2}\rangle = 2^{-1/2}(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)$].

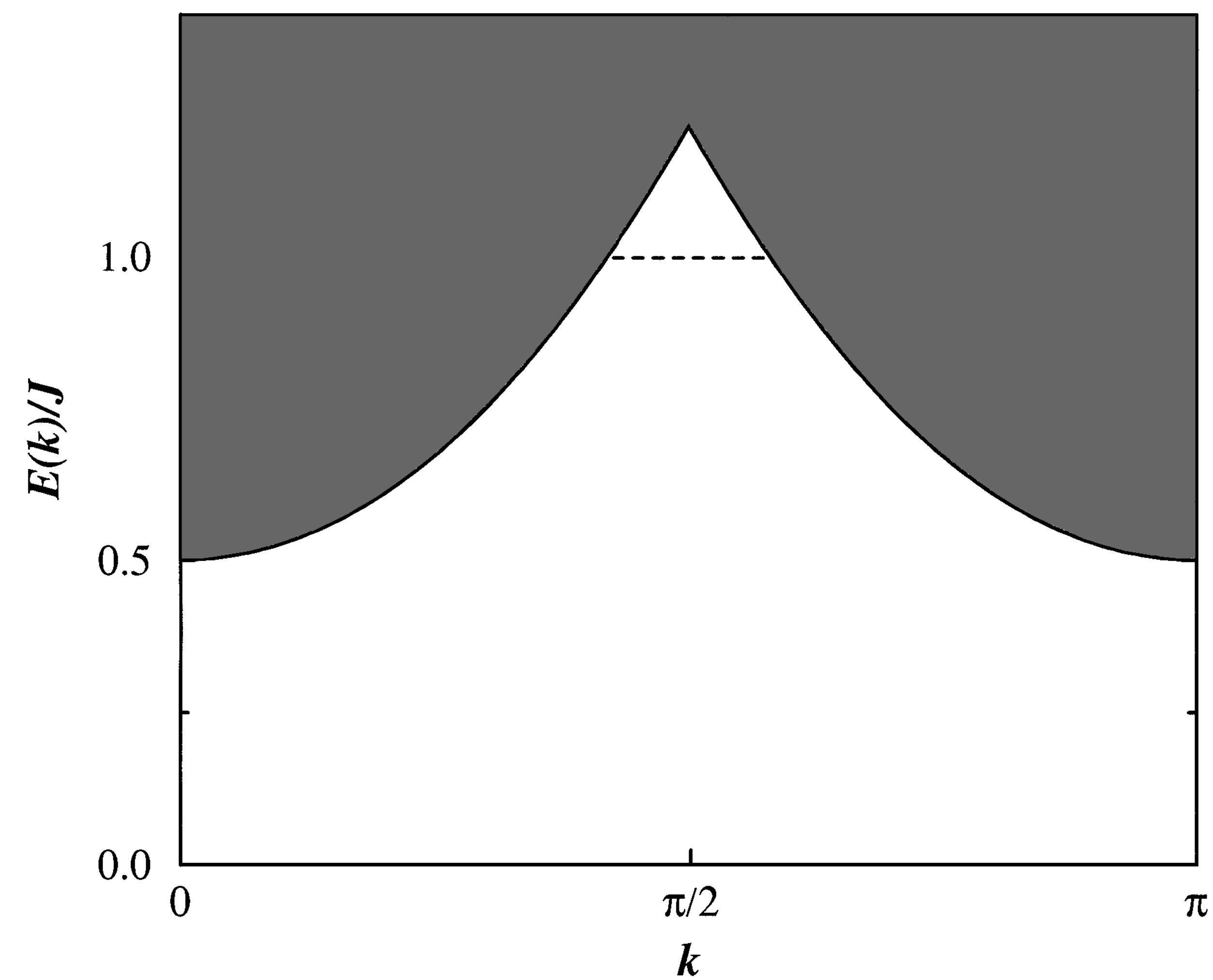
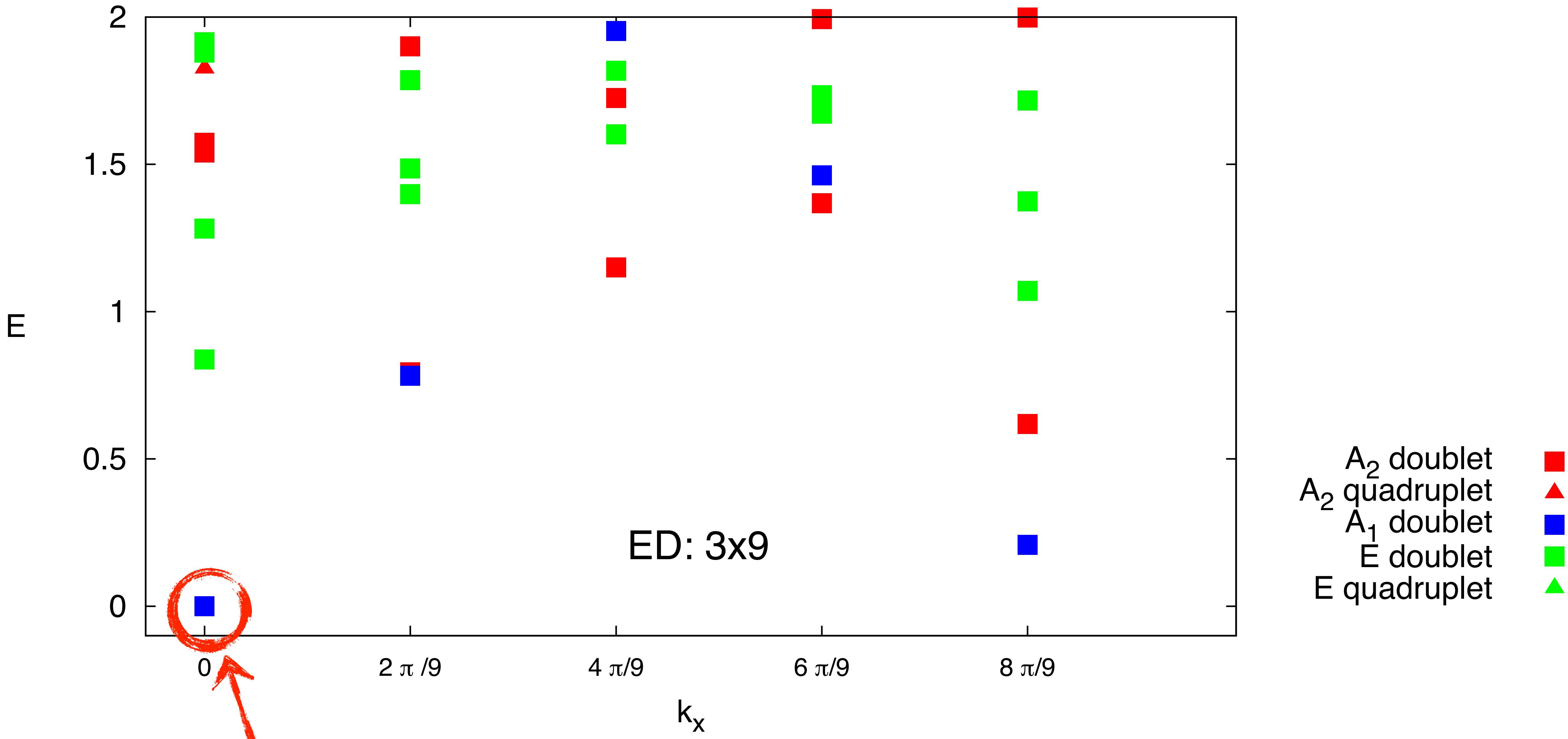


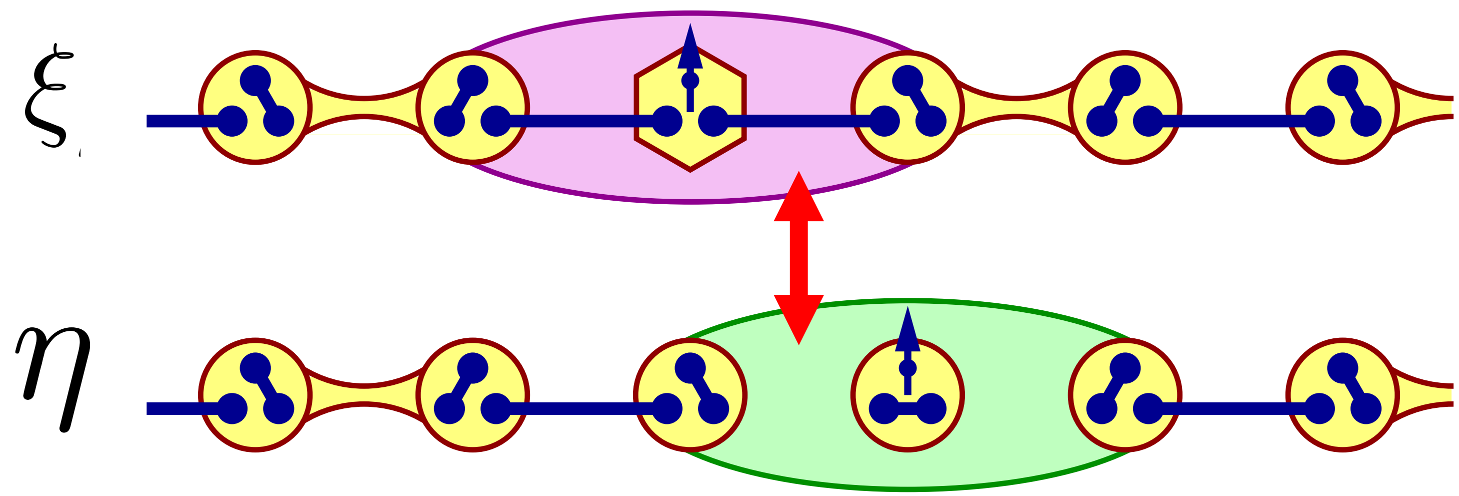
FIG. 2. The excitation spectrum of the model (7). The continuum is determined by free two-soliton states; its lowest boundary is 16-fold degenerate. The dashed line is determined by the Haldane triplet excitation (13) and indicates a variational estimate for bound soliton-antisoliton states.

Search for the 3rd GS:
Tubes of odd length, K△=0



exact ground state
with 0 energy

Variational approach - single domain wall, $K_\triangle$=0



$$\mathcal{H}_{1\mathrm{dw}}(k) = \begin{pmatrix} \frac{10}{3}\left(1 - a_L \cos k\right) & -\frac{10}{\sqrt{3}}\left(\cos k - a_L\right) \\ -\frac{10}{\sqrt{3}}\left(\cos k - a_L\right) & 10\left(1 - a_L \cos k\right) \end{pmatrix}$$

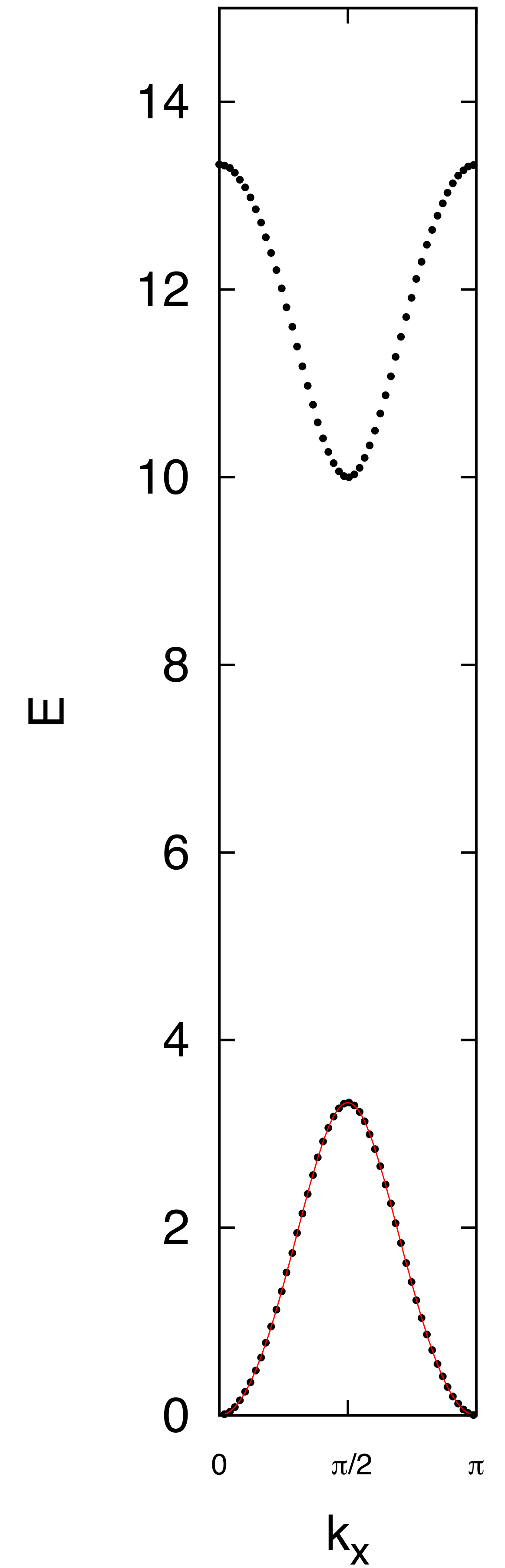
+ an overlap matrix

$$a_L = 2^{3-L}$$

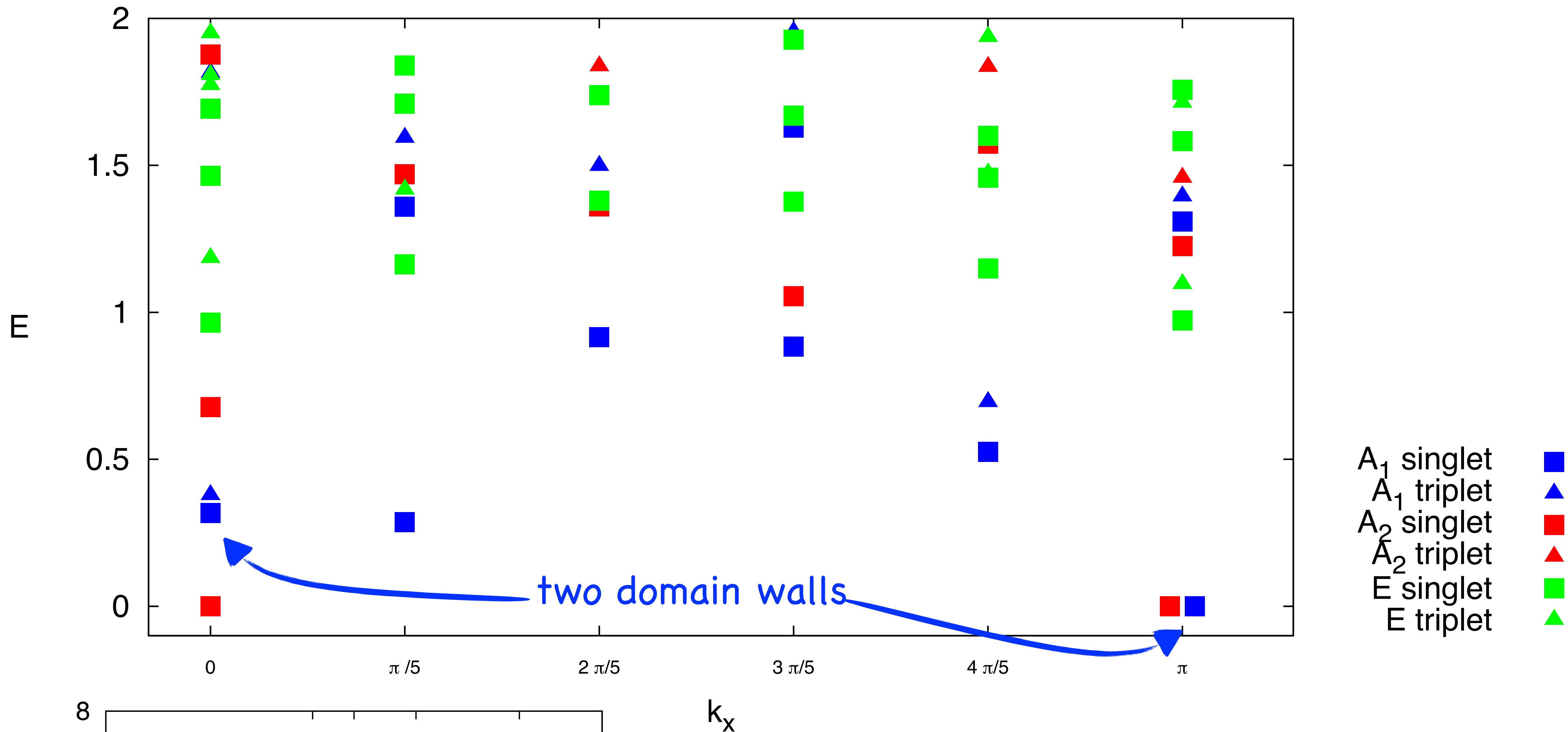
$$E_1^{\pm}(k) = \frac{5}{36}\left(4 \pm \sqrt{10 + 6\cos 2k}\right)$$

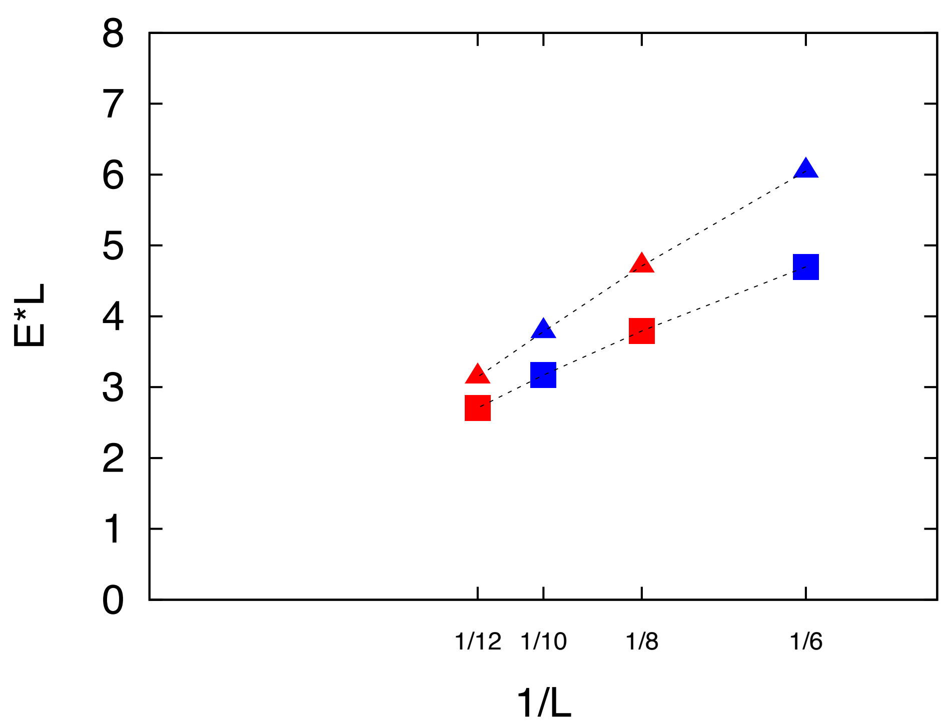
GS (with no gap):

$$|\psi_{1\mathrm{DW}}\rangle = \sqrt{3}|\xi^{\sigma}_{k=0}\rangle + |\eta^{\sigma}_{k=0}\rangle$$



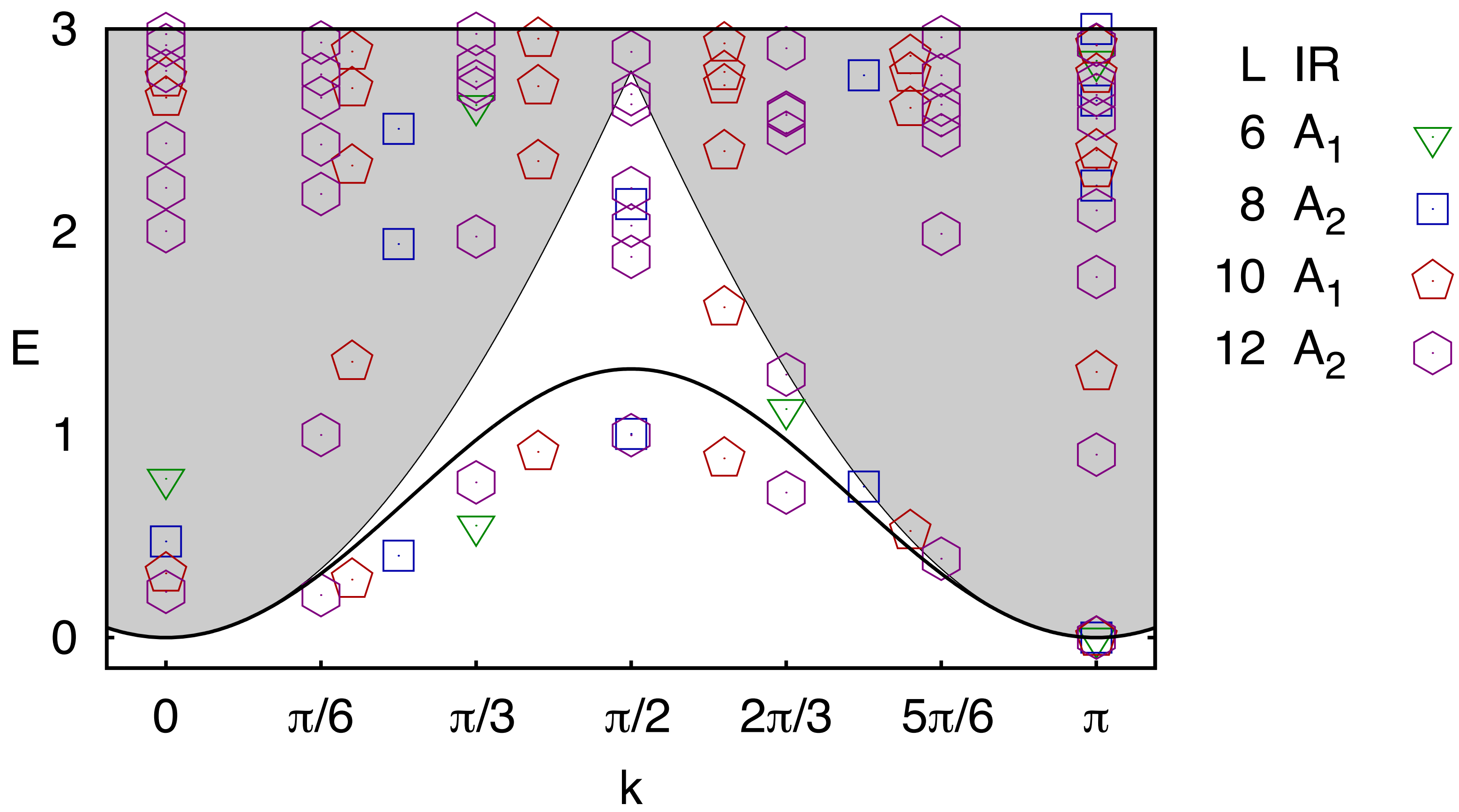
Tubes of even length: third ground state, $K_\triangle=0$

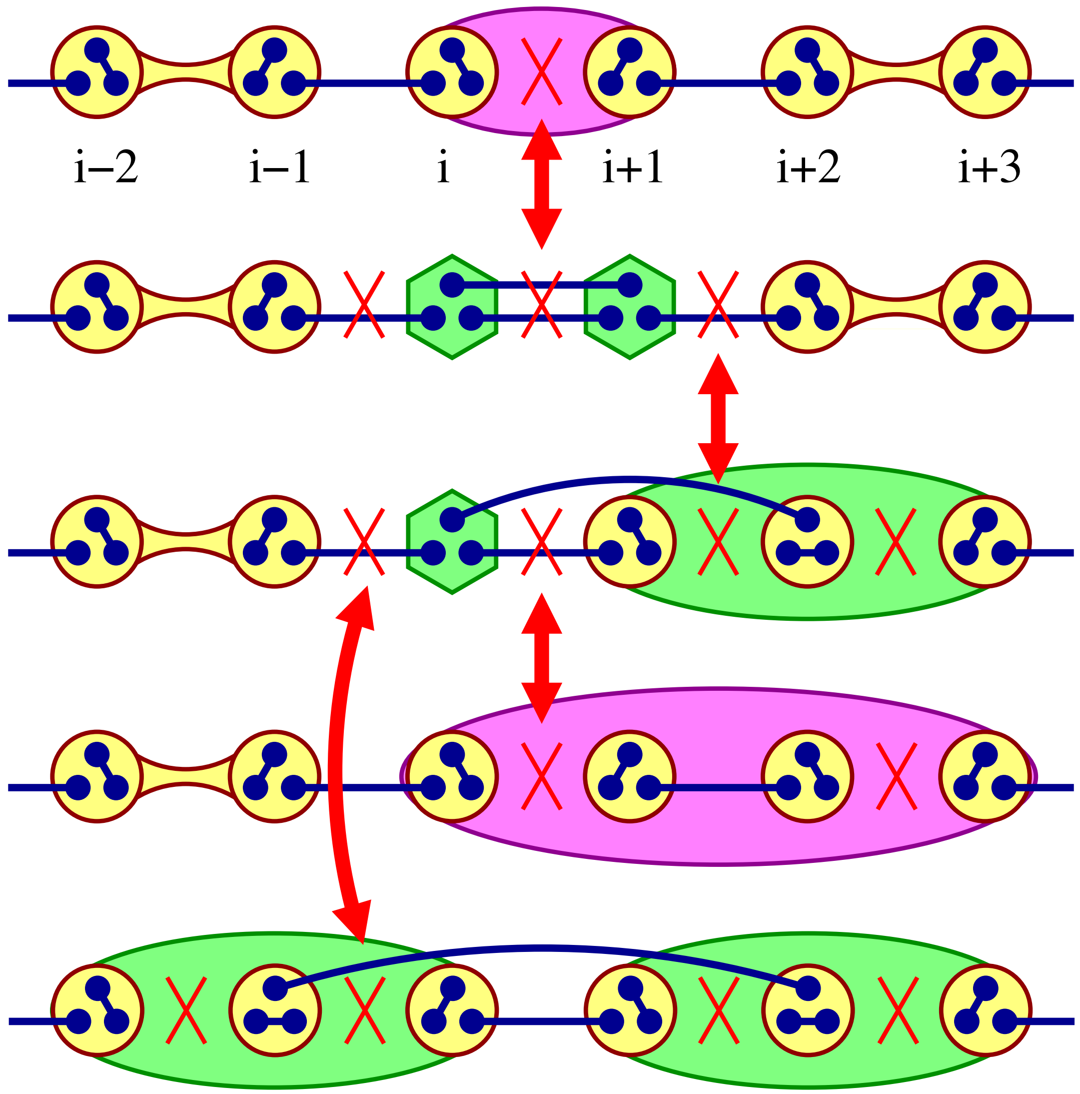




large L: the gap at k=0 is a finite size effect

Variational approach of even length, $K_\triangle=0$





bound state for all k,
closing as k^4

$$\Psi_{2dw} = \sqrt{2}\zeta(\pi) + 2\sqrt{3}\,|\xi\xi\,(\pi,1)\rangle + 3\sum_{l=4,\mathrm{odd}}^{L/2}(-1)^{\frac{l-1}{2}}\,|\xi\xi\,(\pi,l)\rangle - \sqrt{3}i\sum_{l=2,\mathrm{even}}^{L-2}(-1)^{\frac{l}{2}}\,|\xi\eta\,(\pi,l)\rangle - \sum_{l=1,\mathrm{odd}}^{L/2}(-1)^{\frac{l-1}{2}}\,|\eta\eta\,(\pi,l)\rangle$$

The ground state is a “equal amplitude” superposition of distant domain walls

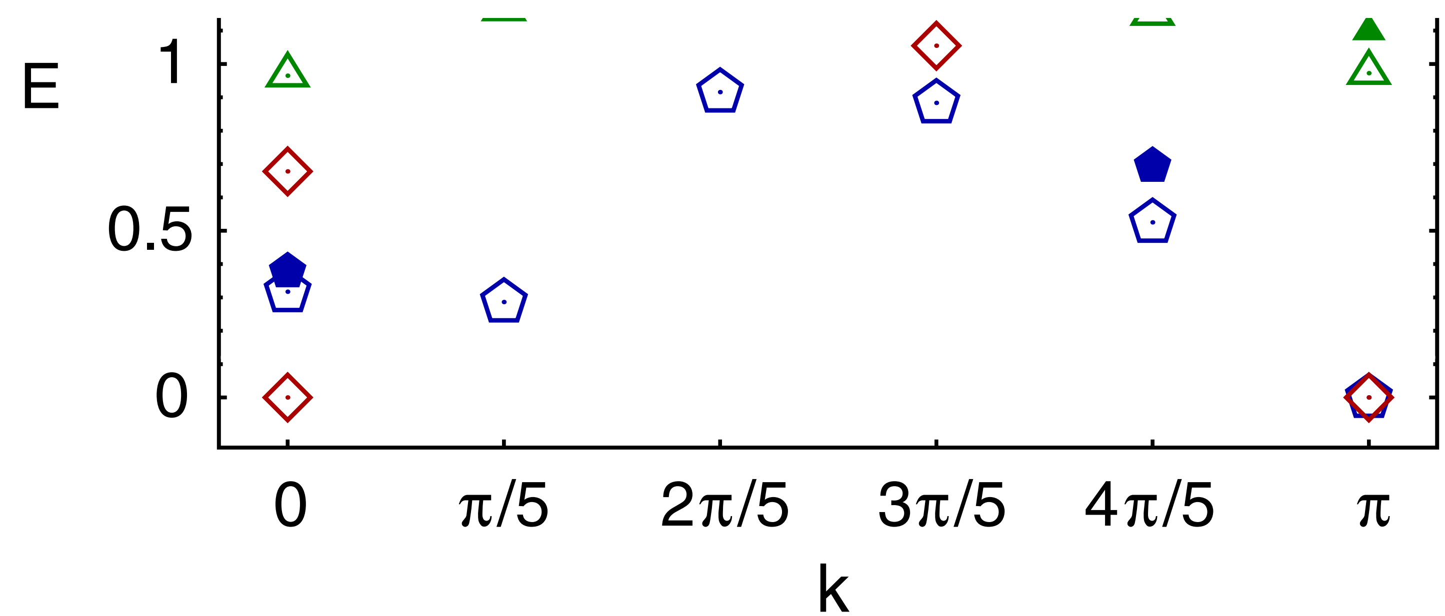
Lieb-Schultz-Mattis theorem

1D spin chains with SU(2) and translational invariant Hamiltonians and half-integer spins in the unit cell, either have gapless excitations or degenerate ground-states in the thermodynamic limit.

- 1D Heisenberg chain:
  unique ground state+ gapless excitations(spinwaves)

- Majumdar Ghosh:
  2 degenerate ground states +gap

we have 3 ground states...



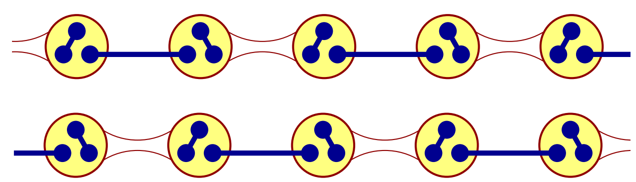
E. H. Lieb, T. D. Schultz, and D. C. Mattis., Ann. Phys.(N.Y) 16, 407 (1961).

Lieb-Schultz-Mattis theorem and the three ground states.

third ground state

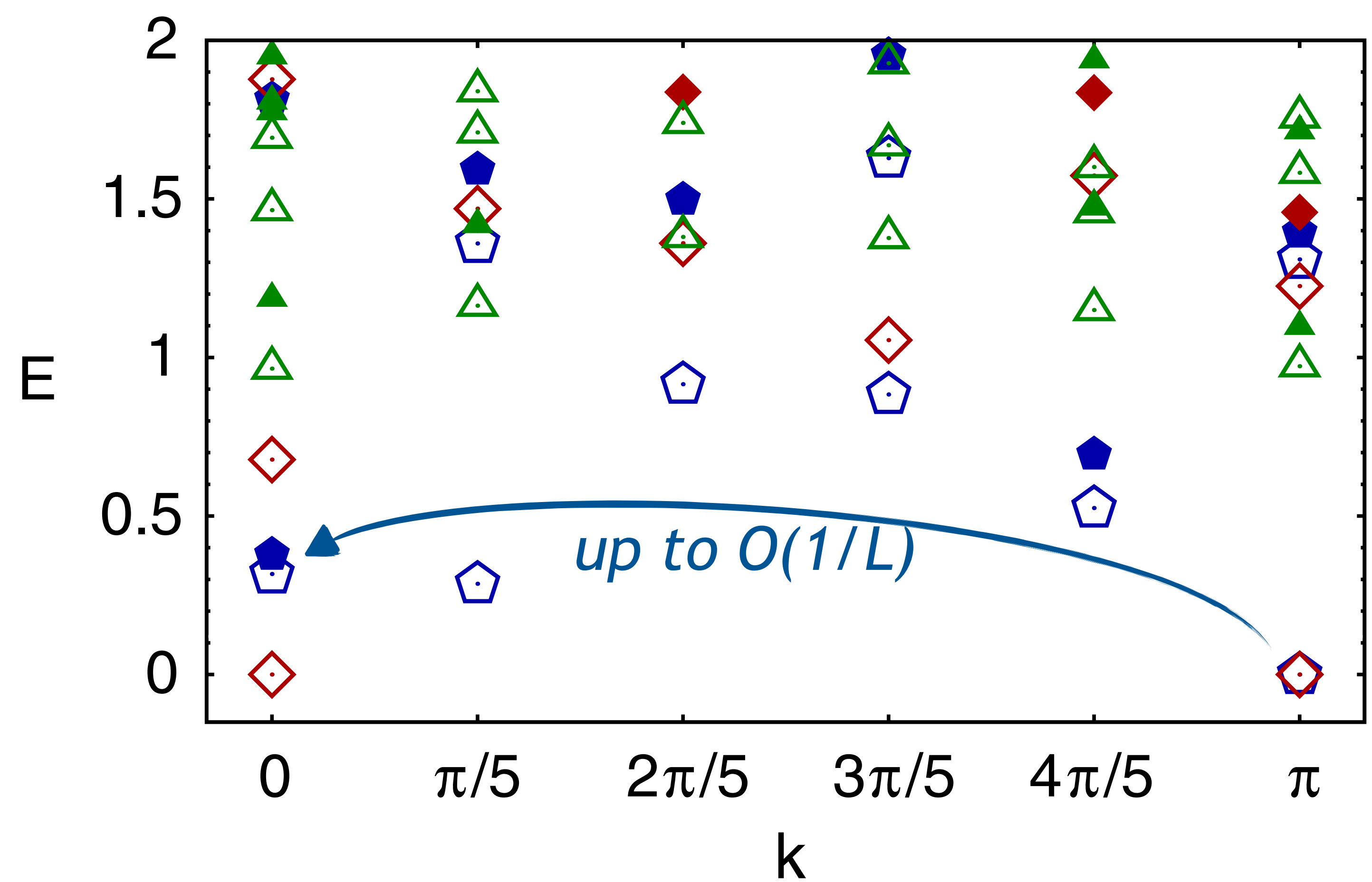
$\Psi_{\sigma,1} =$

$\Psi_{\sigma,2} =$

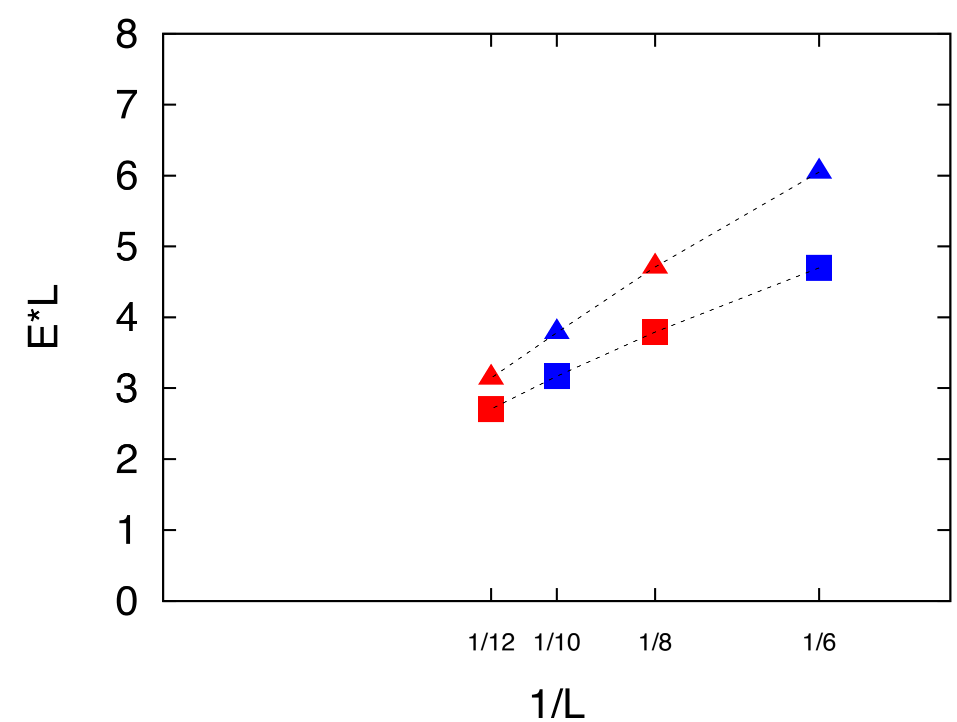


$$\Psi_{\sigma,1} + \Psi_{\sigma,2} \quad \underset{U_{2\pi}}{\overset{U_{2\pi}}{\rightleftarrows}} \quad \Psi_{\sigma,1} - \Psi_{\sigma,2}$$

up to O(1/L)



the ‘gap’ is closing



Varying K△ away from 0

$$\mathcal{H} = K_{\triangle} \sum_{i=1}^{L} P_i + K_{\square} \sum_{i=1}^{L} \sum_{j=1}^{3} R_{(i,j)(i+1,j)(i+1,j+1)(i,j+1)}$$

$$\tilde{\mathbf{S}}_i = \sum_{j=1}^{3} \mathbf{S}_{(i,j)}$$

$$P_i = (4\tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_i - 3)/12$$

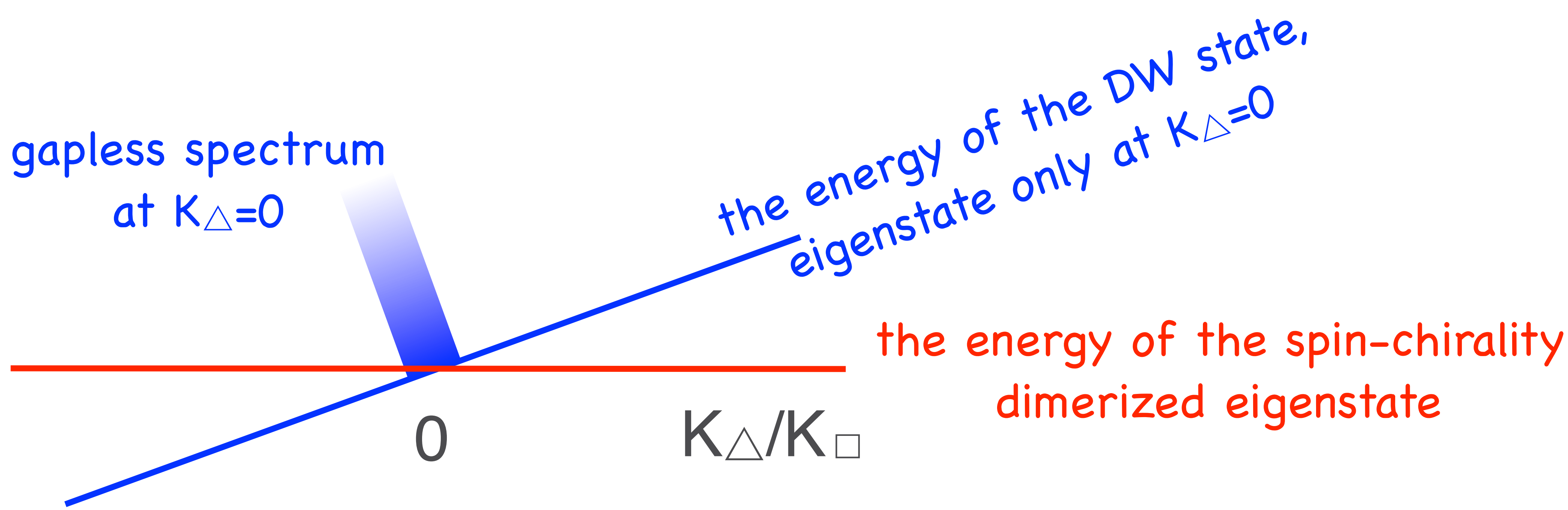
the K△ acts like chemical potential on

the density of the S=3/2 △ states

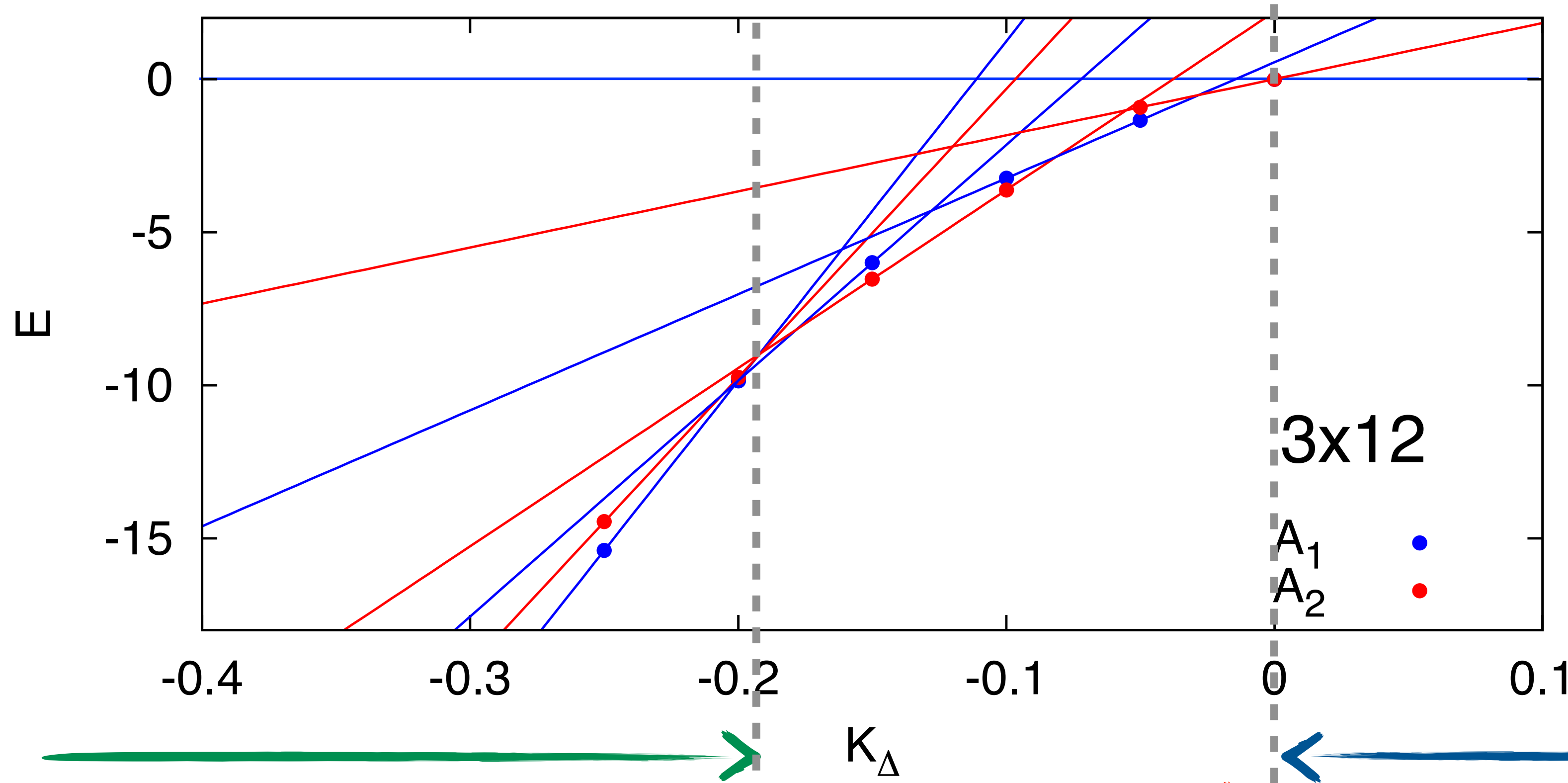
From the Hellman-Feynman theorem:

$$\frac{\partial E_{\mathrm{GS}}}{\partial K_{\triangle}} = \langle \psi_{1\mathrm{DW}} | \sum_i P_i | \psi_{1\mathrm{DW}} \rangle = \frac{3}{4}$$

$$|\psi_{1\mathrm{DW}}\rangle = \sqrt{3} |\xi^{\sigma}_{k=0}\rangle + |\eta^{\sigma}_{k=0}\rangle$$



Tuning the interactions...

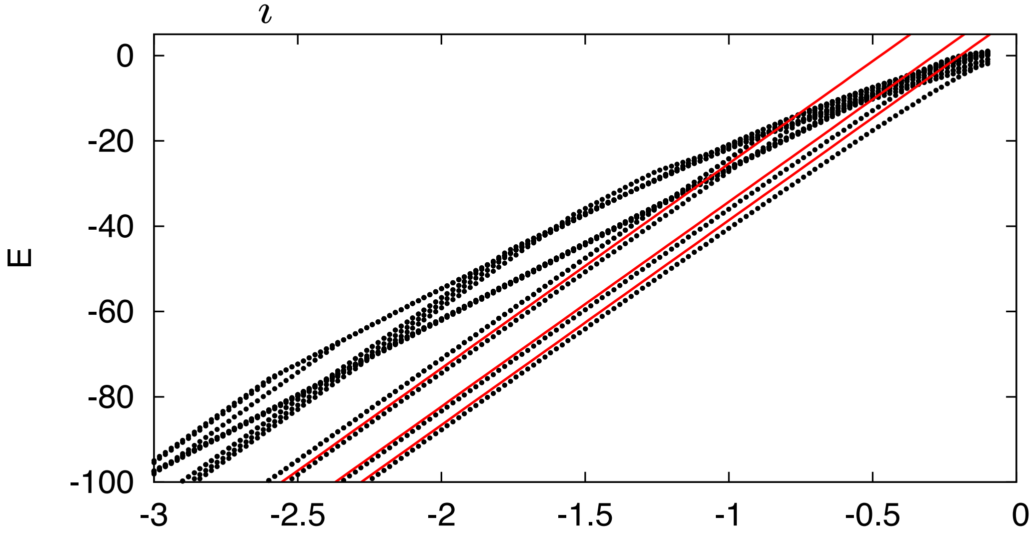


S=3/2 model

?

dimer-product GS

$$\mathcal{H} = \sum_i \frac{7}{12}\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{18}\left(\mathbf{S}_i \cdot \mathbf{S}_{i+1}\right)^2$$

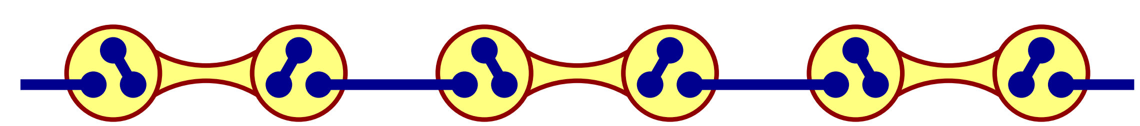


no exact ground state,
gapless excitations

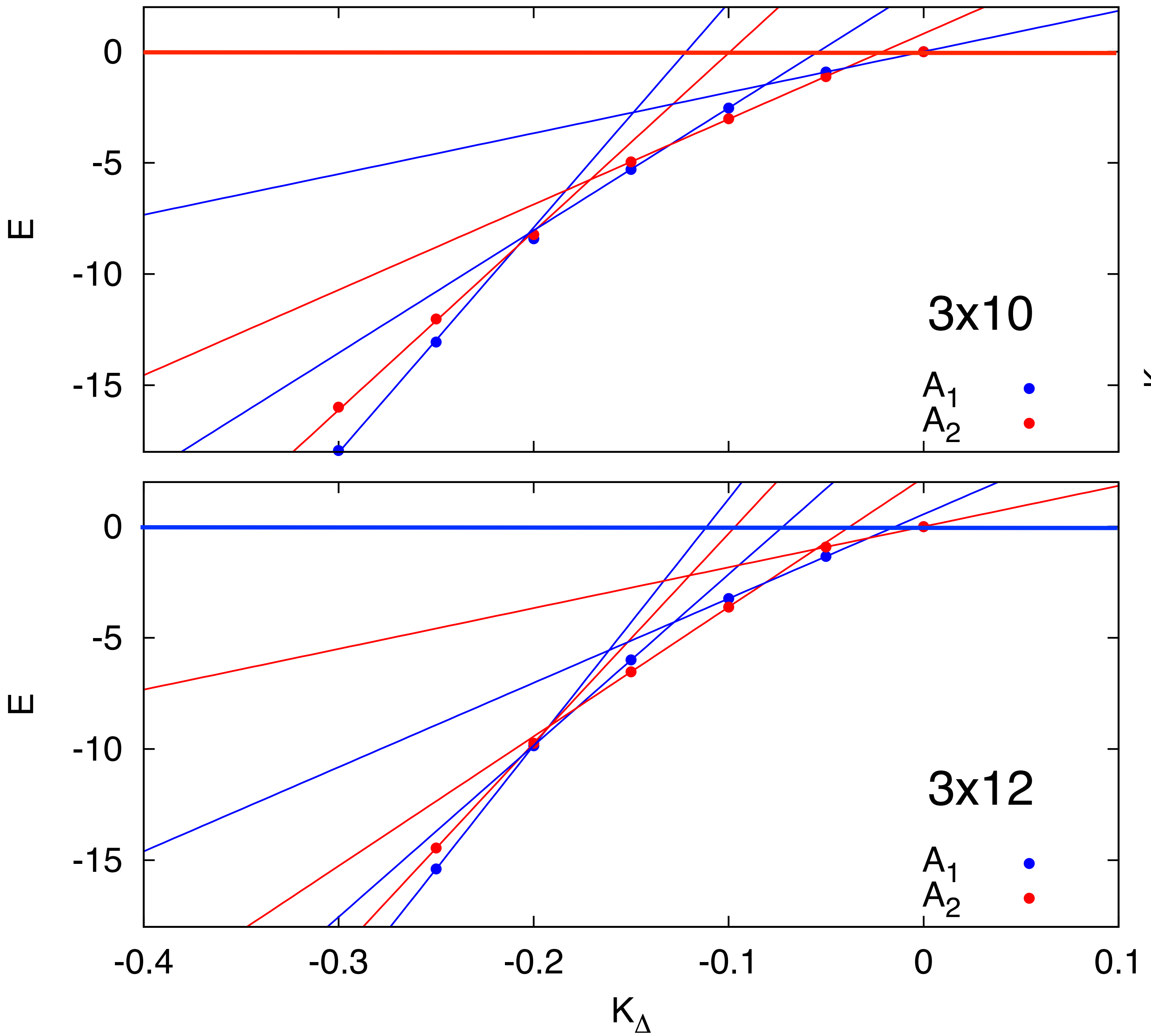
$$\mathcal{H}' = \frac{5}{9}\sum_{i=1}^{L}\left(\frac{3}{4} + \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_{i+1}\right)\left(1 + \hat{\tau}_i^+ \hat{\tau}_{i+1}^- + \hat{\tau}_i^- \hat{\tau}_{i+1}^+\right)$$

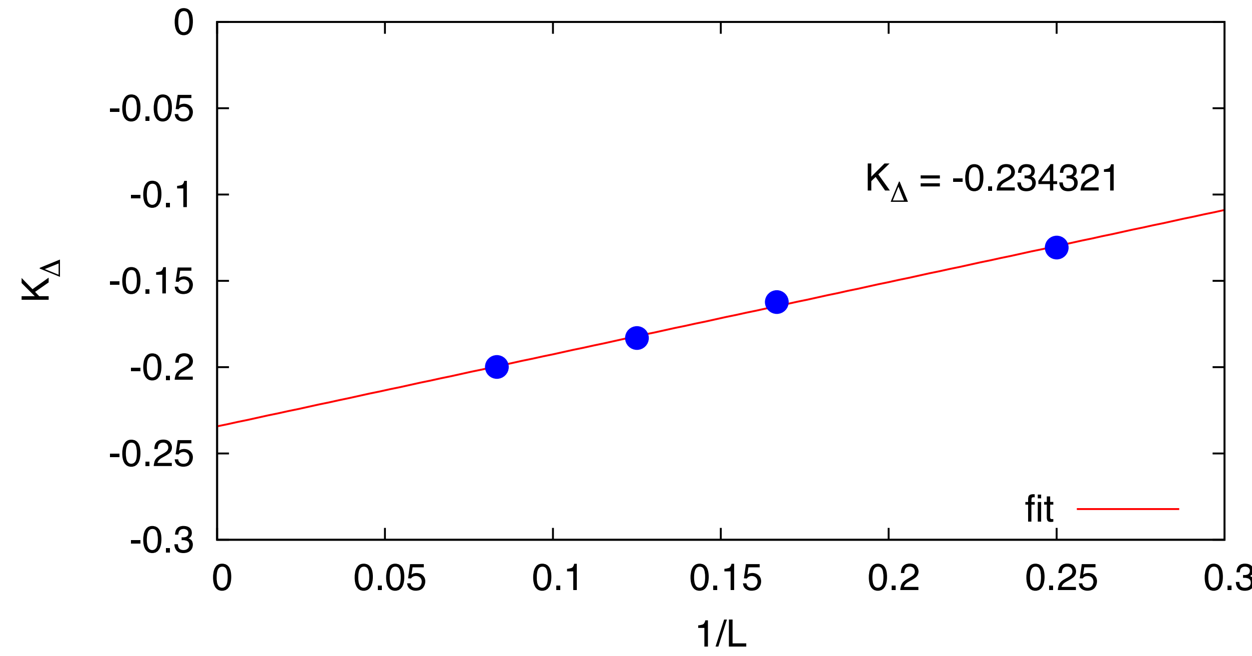
0 for singlet
1 for triplet

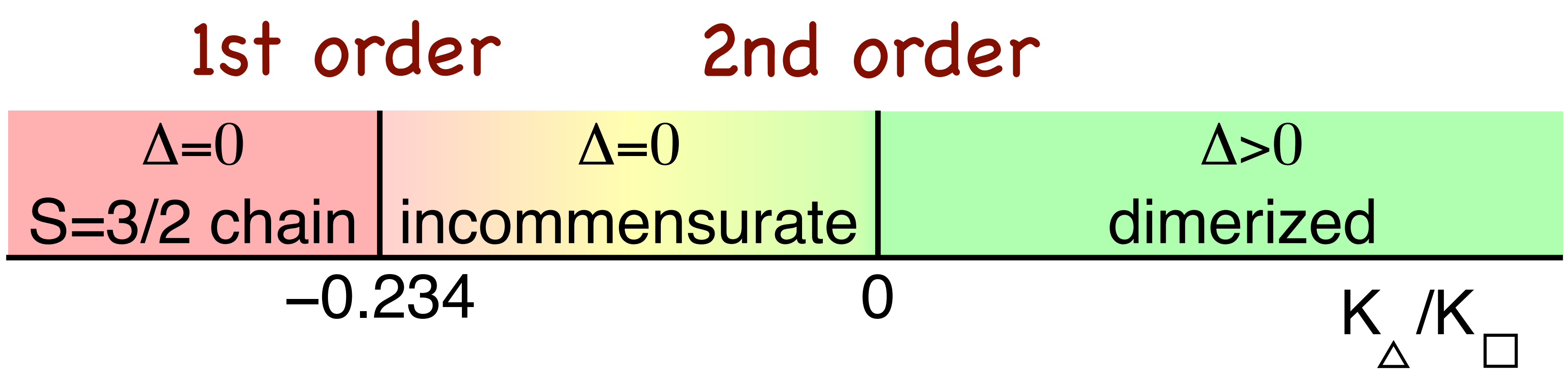
0 for singlet,
1 for |ll> or |rr>
2 for |lr>+|rl>



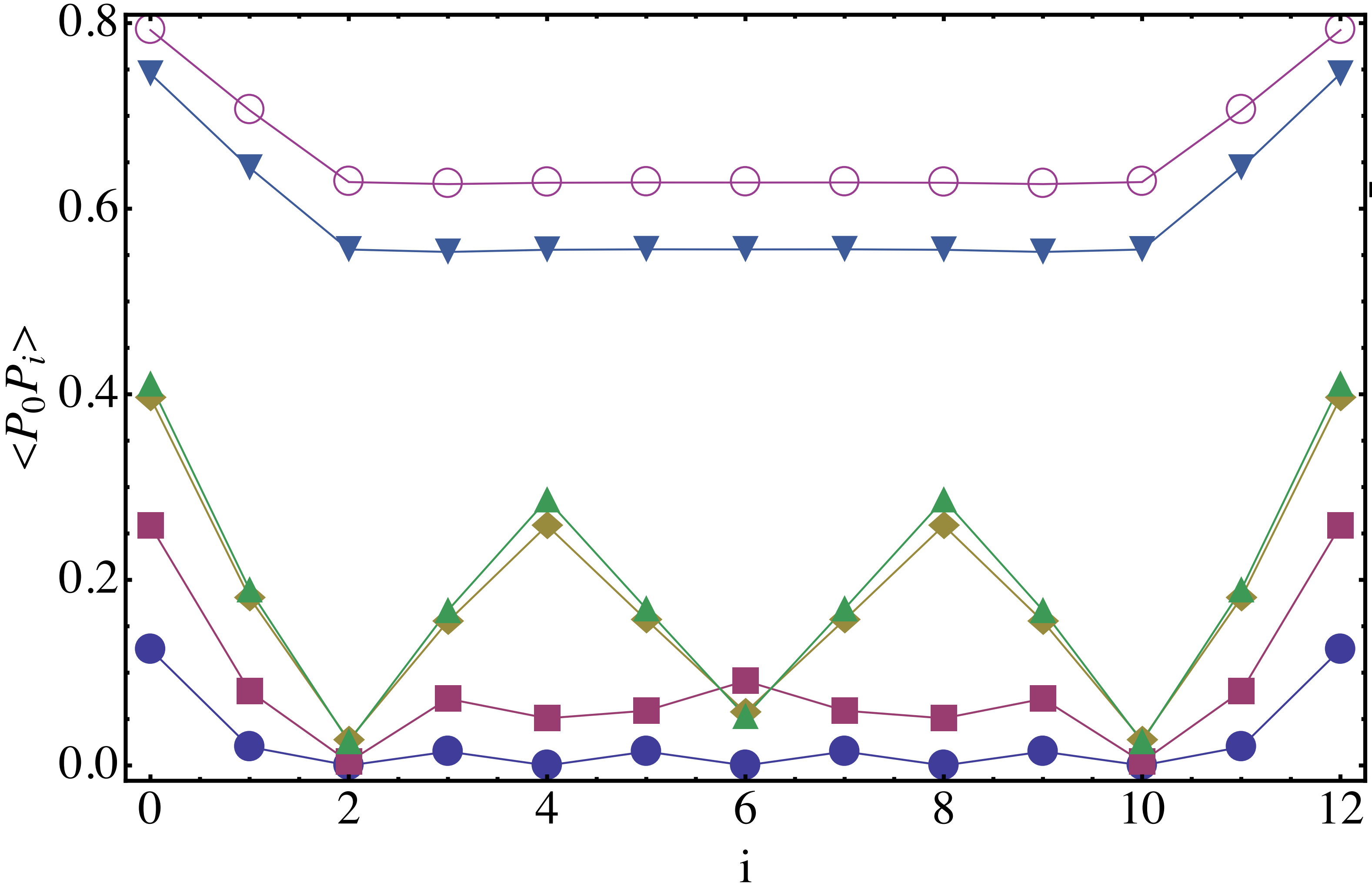
Tuning the interactions

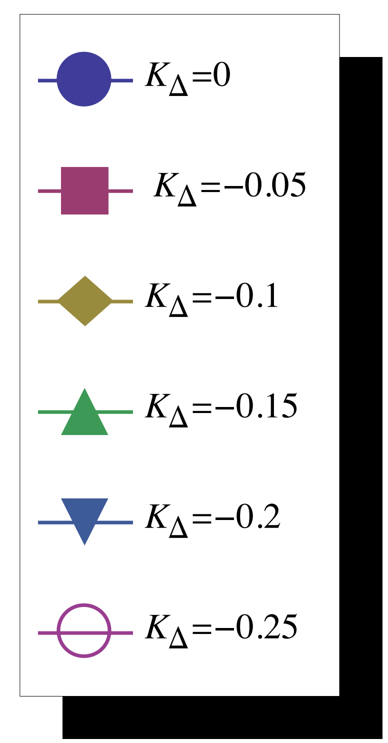


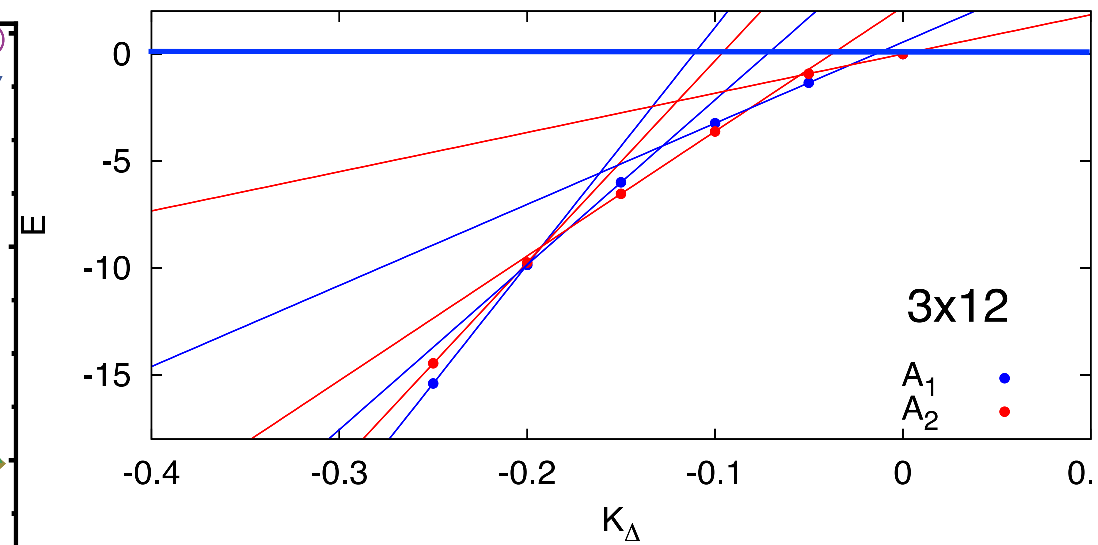


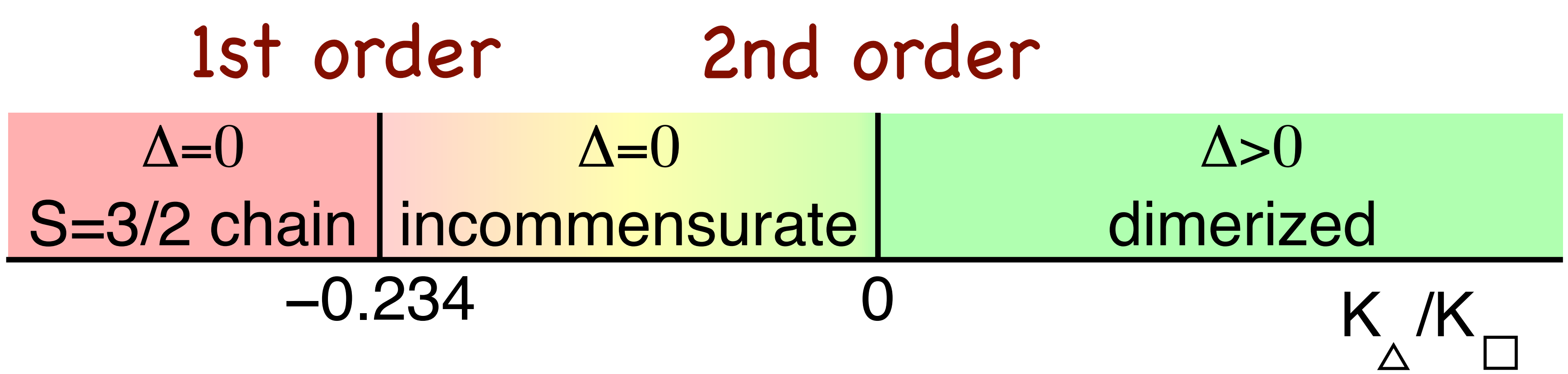


Spin-3/2 correlation functions - real space

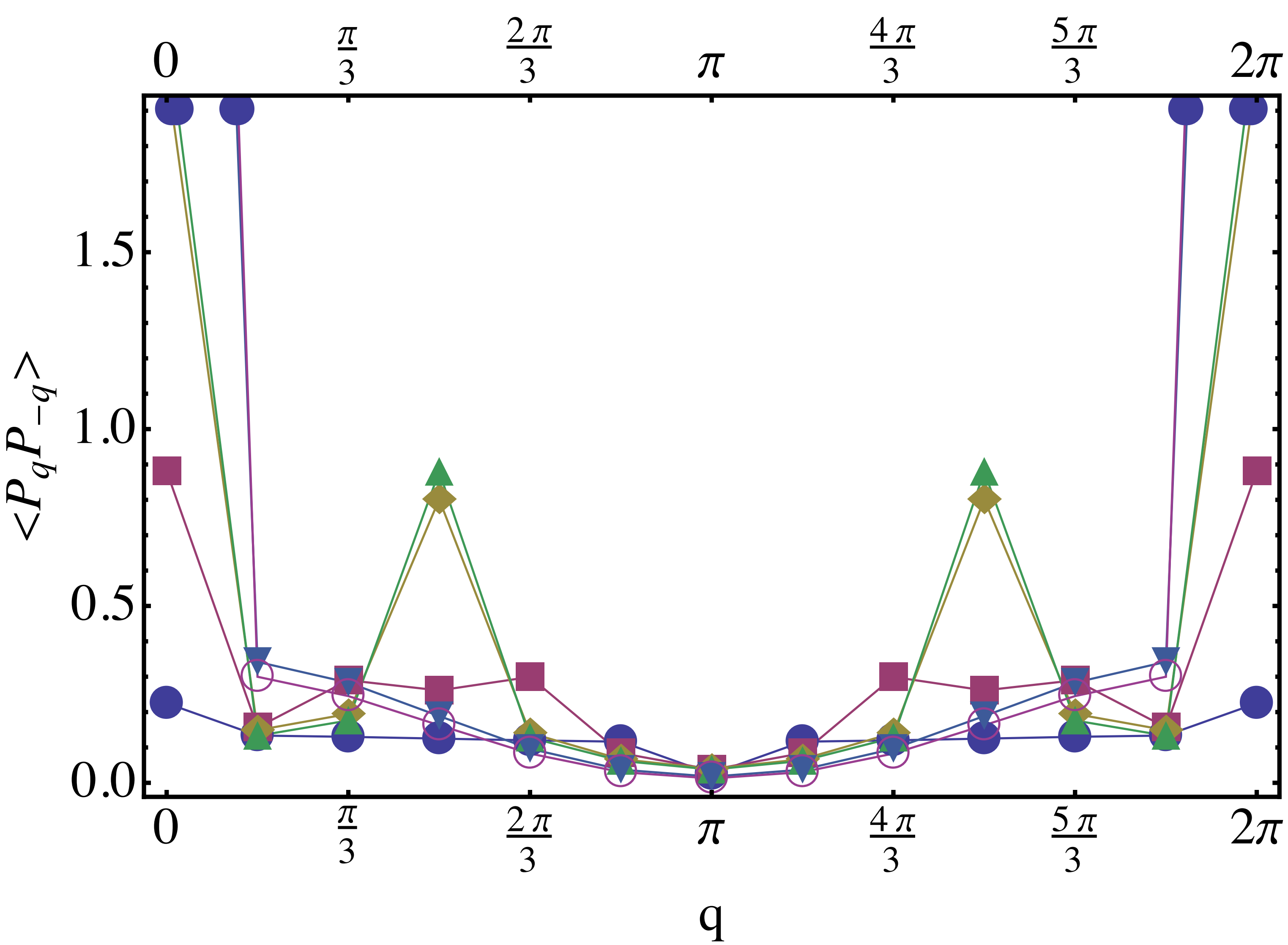


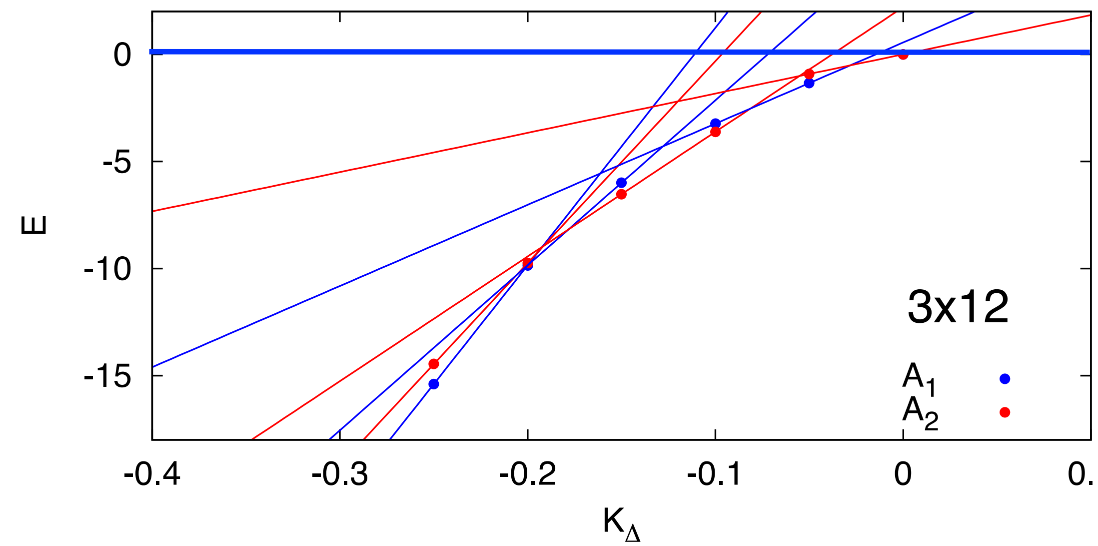


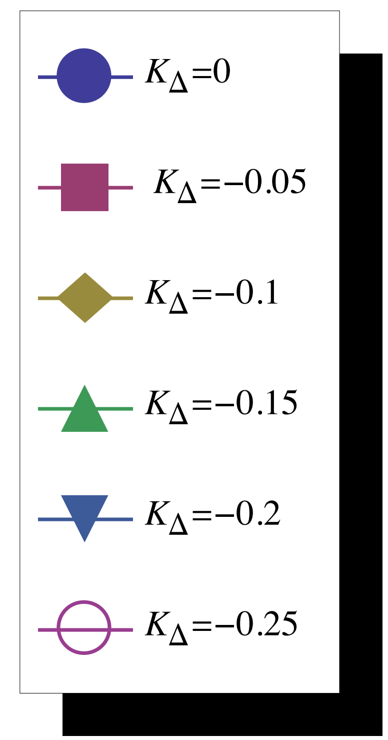


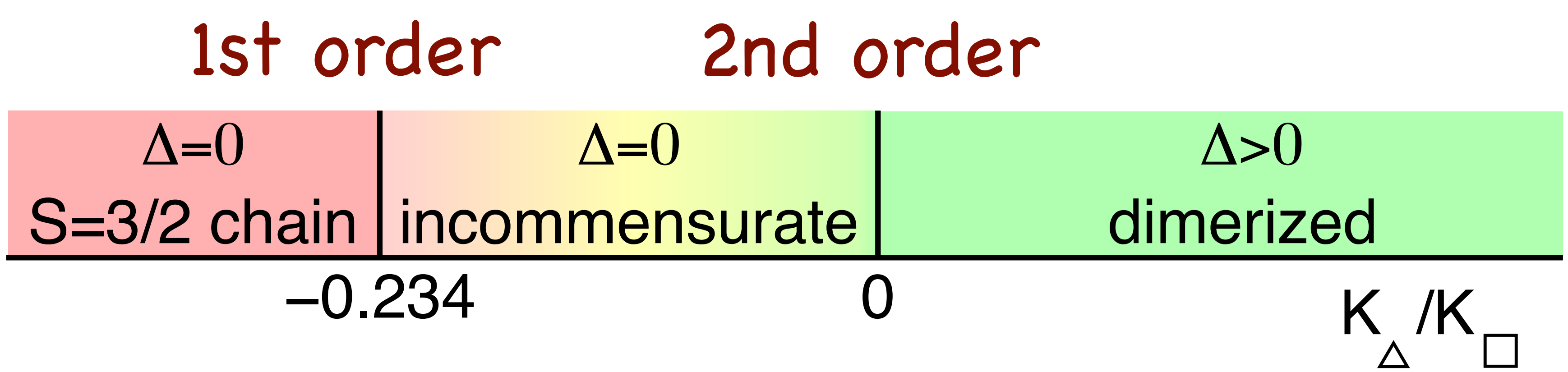


Spin-3/2 correlation functions - momentum space

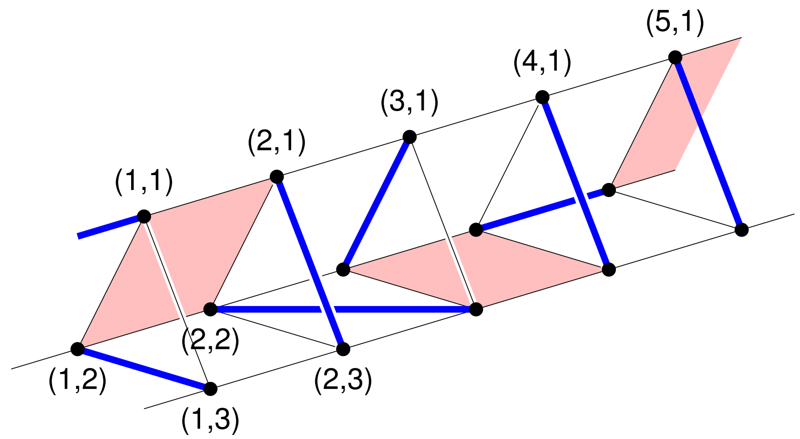




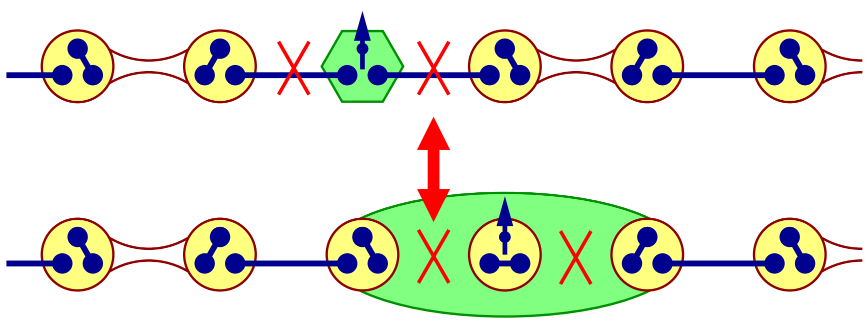


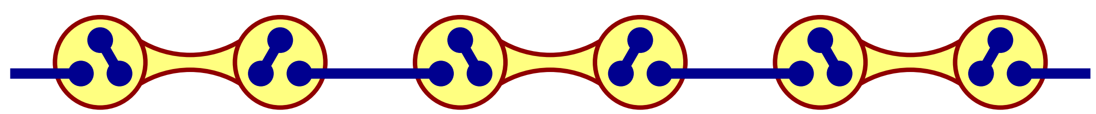


Conclusions

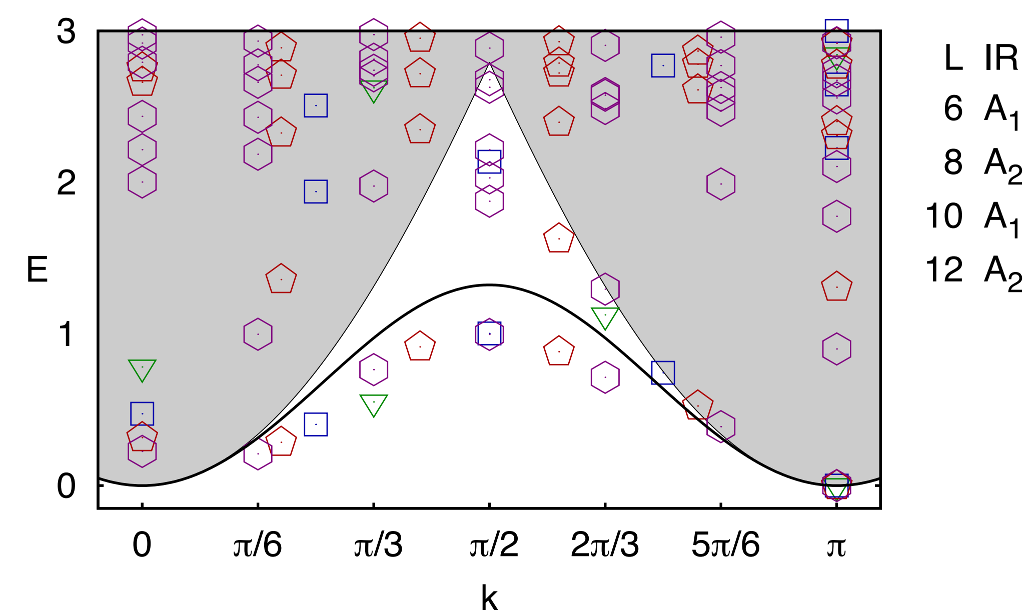


1 exact ground state with gapless spectrum at a quantum phase transition point

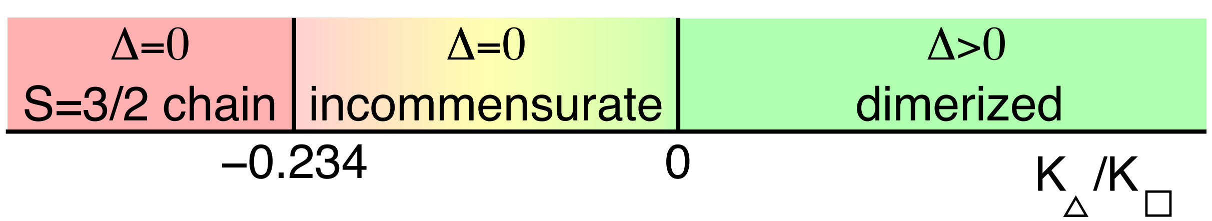




2 exact ground states



phase diagram with a new phase



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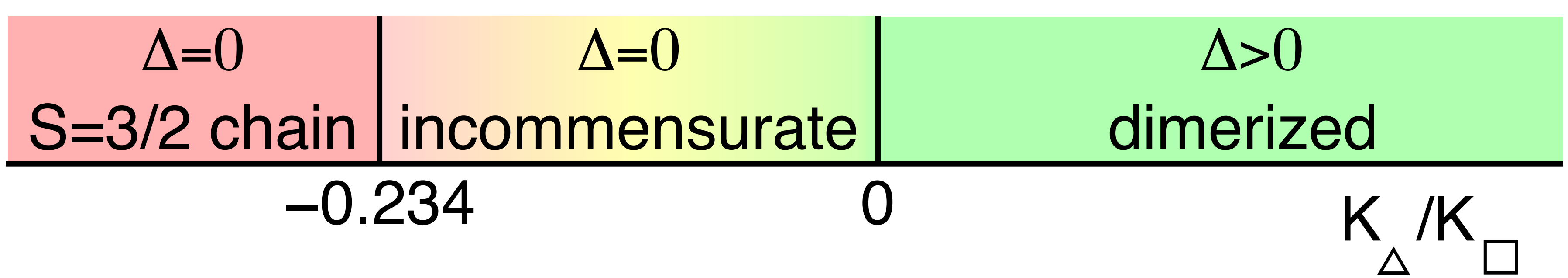
Open questions

5-leg tubes ... N-leg tubes ... two-dimensional system ?

Is it quantum critical?

Effect of magnetic field...

How relevant is the incommensurate phase for the spin tube with Heisenberg interactions only?



How good is the variational wave function for the purely Heisenberg spin-tube?

Thank you for your attention