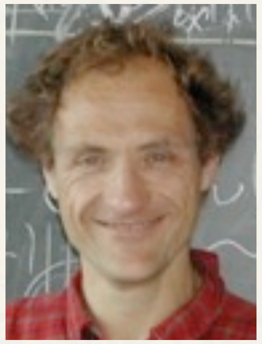
Exact ground states in three-leg spin tubes

Miklós Lajkó
Wigner Research Centre for Physics
Institute for Solid State Physics and Optics
Budapest

Karlo Penc



Philippe Sindzingre

3th June, 2013

Emergent Quantum Phases in Condensed Matter Workshop

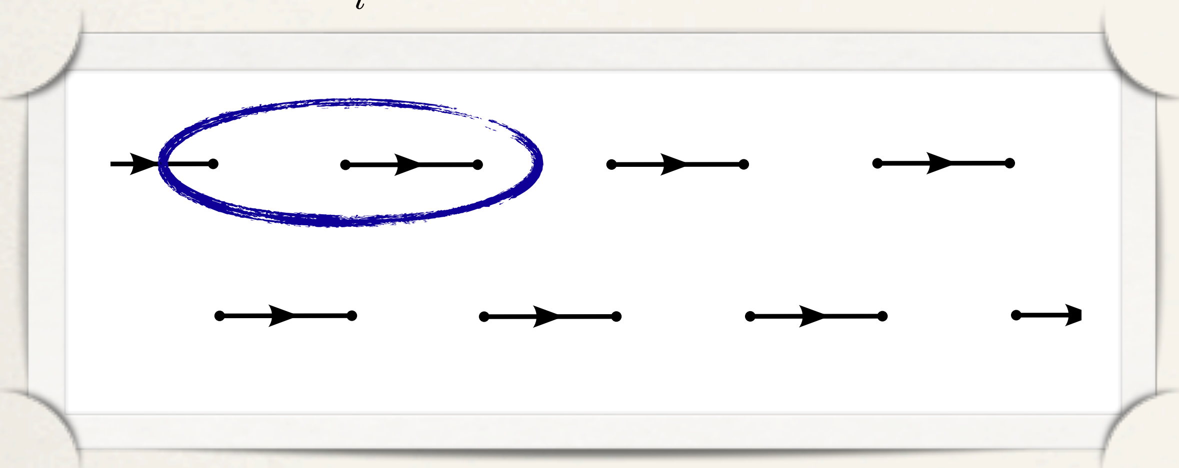
Outline

- Projection based Hamiltonians
- 2D S=1/2 lattice
- 3-leg spin tubes
- Projection based model on the spin tube
- Numerical results
  - Exact ground states
  - Variational estimates
  - Tuning the interactions

Projection operator approach

Exact ground state for S=1/2 spin chain

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

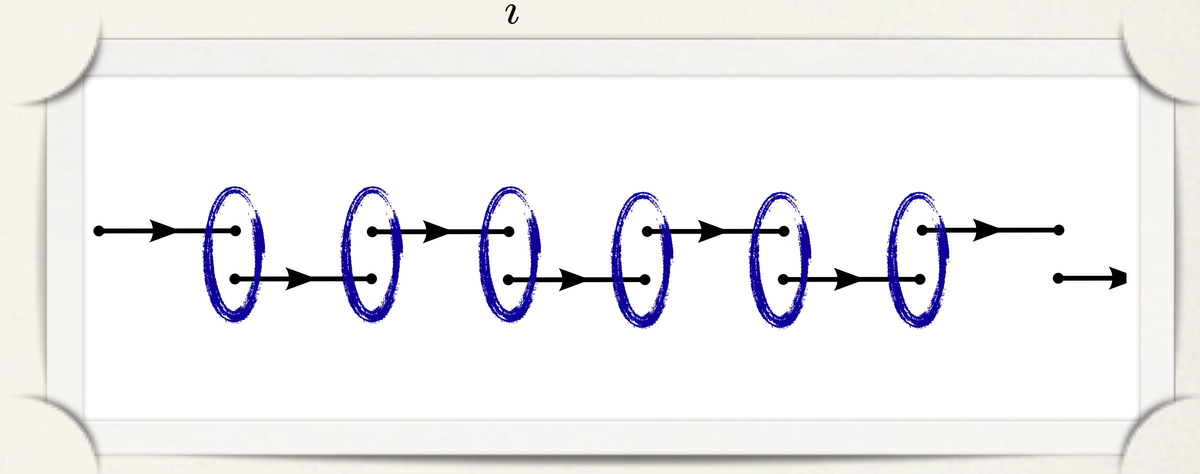


$$H_{MG} = \sum_i \mathbf{S}_i \mathbf{S}_{i+1} + \frac{1}{2} \sum_i \mathbf{S}_i \mathbf{S}_{i+2}$$

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

Exact ground state for S=1 spin chain

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



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

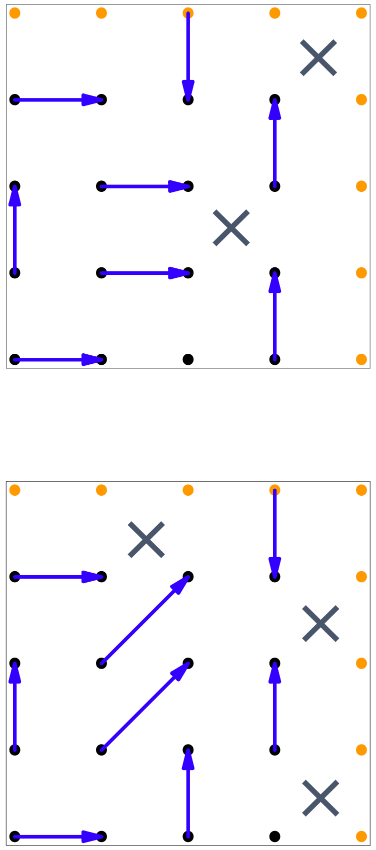
I Affleck, T Kennedy, E H Lieb, and H Tasaki,
Comm. Math. Phys. 115, 477 (1988).

S=1/2 square lattice

$$H = \sum_{\alpha:\Box} \mathrm{Proj}\left\{S^T_\alpha = 2\right\}$$

- $L_1 x L_2 = N$ spins ->N/2 singlet bonds, N plaquettes every plaquette should have a singlet
- Many nearest neighbour valence bond covering ground state if L_1 and L_2 are even

- Exact diagonalization: Non-trivial singlet, even triplet ground states, even when L_1 or L_2 are odd (or both!!)

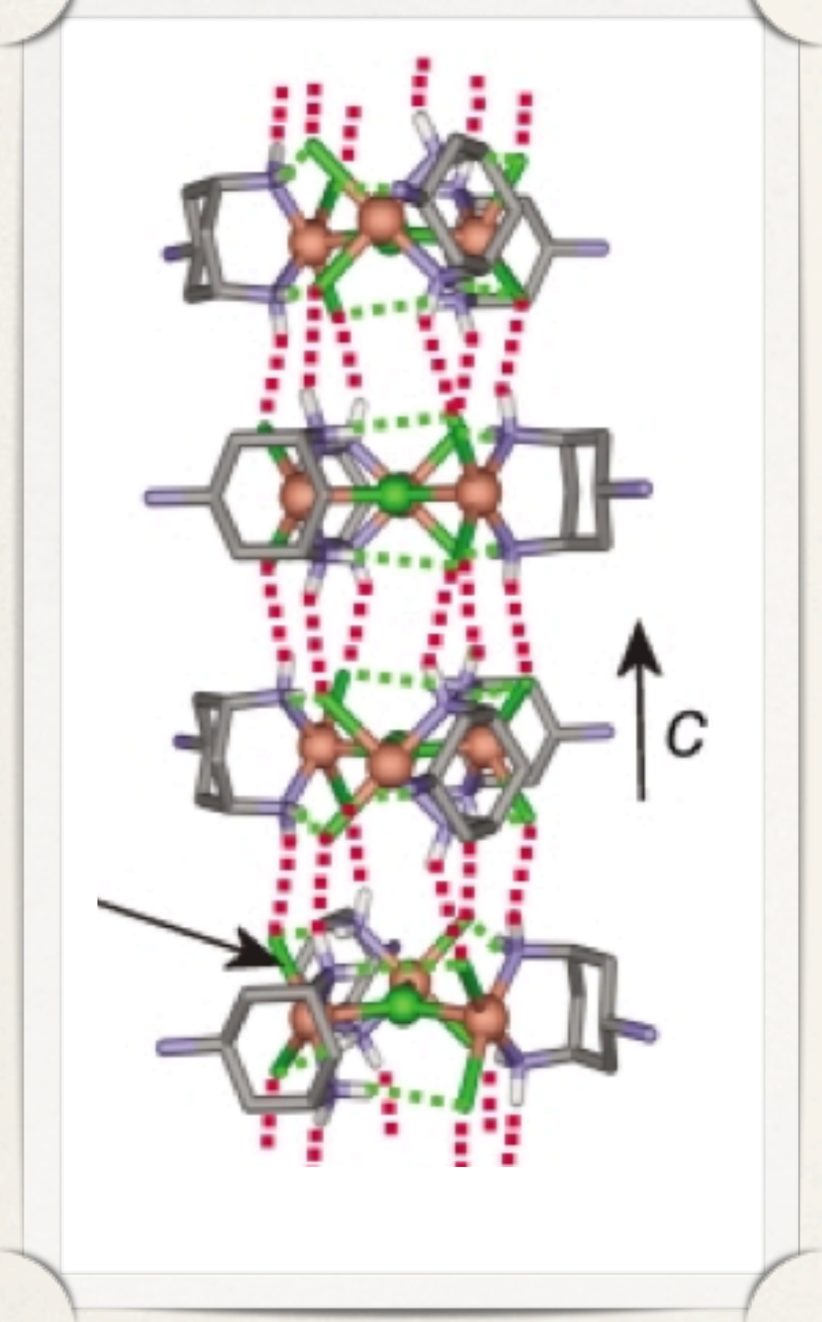


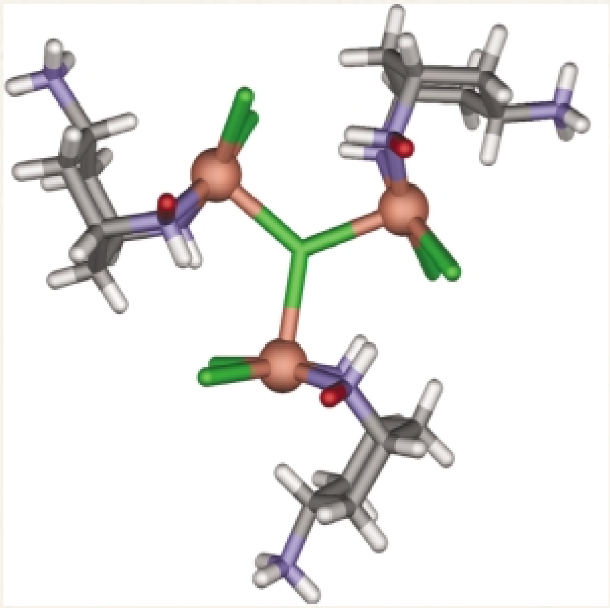
Simplest case: three-leg tube

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

Three-leg tubes

$[(CuCl_2tachH)_3Cl]Cl_2$

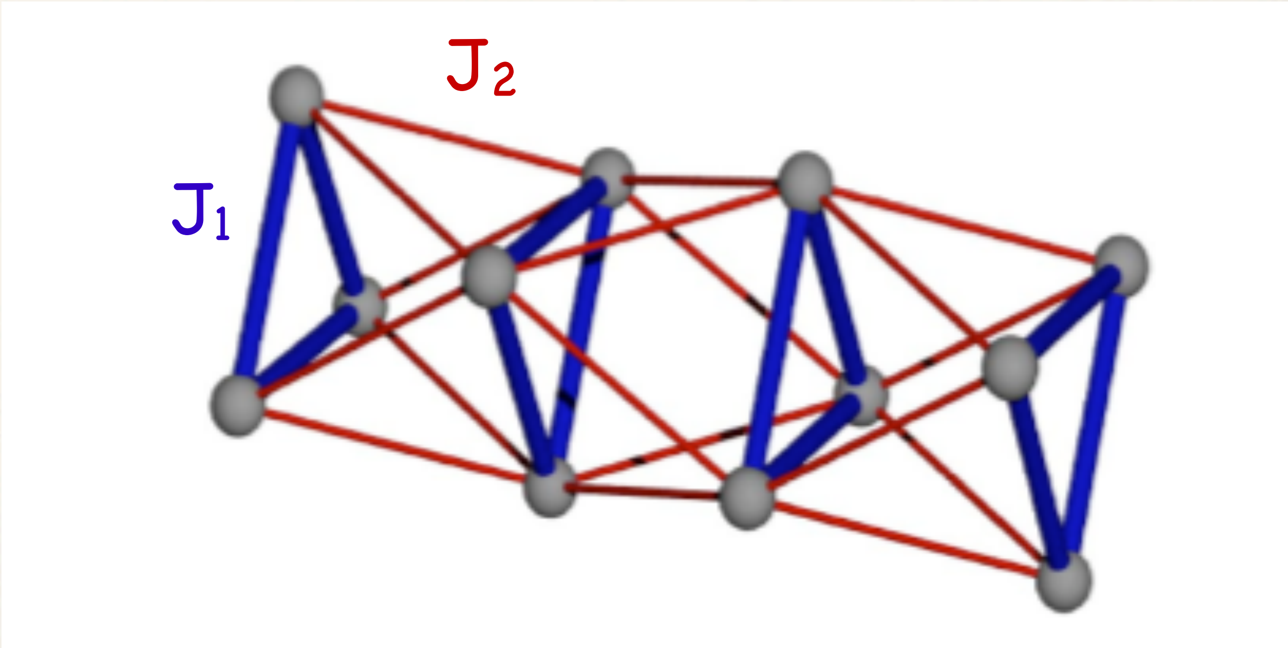




Cu$_3$Cl triangles

S=1/2

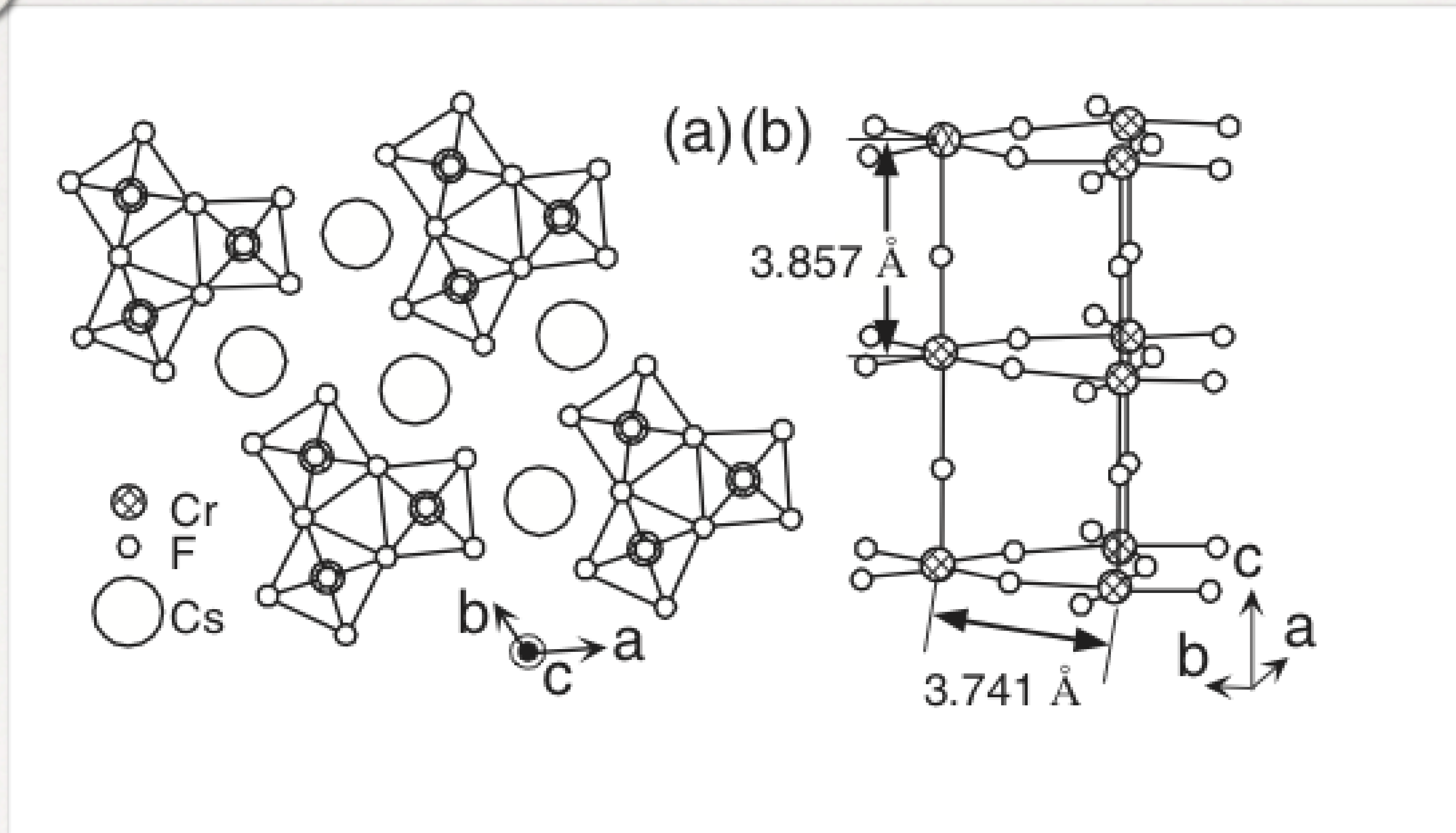
$J_1/J_2 \approx 3.4$



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

Three-leg tubes

$CsCrF_4$

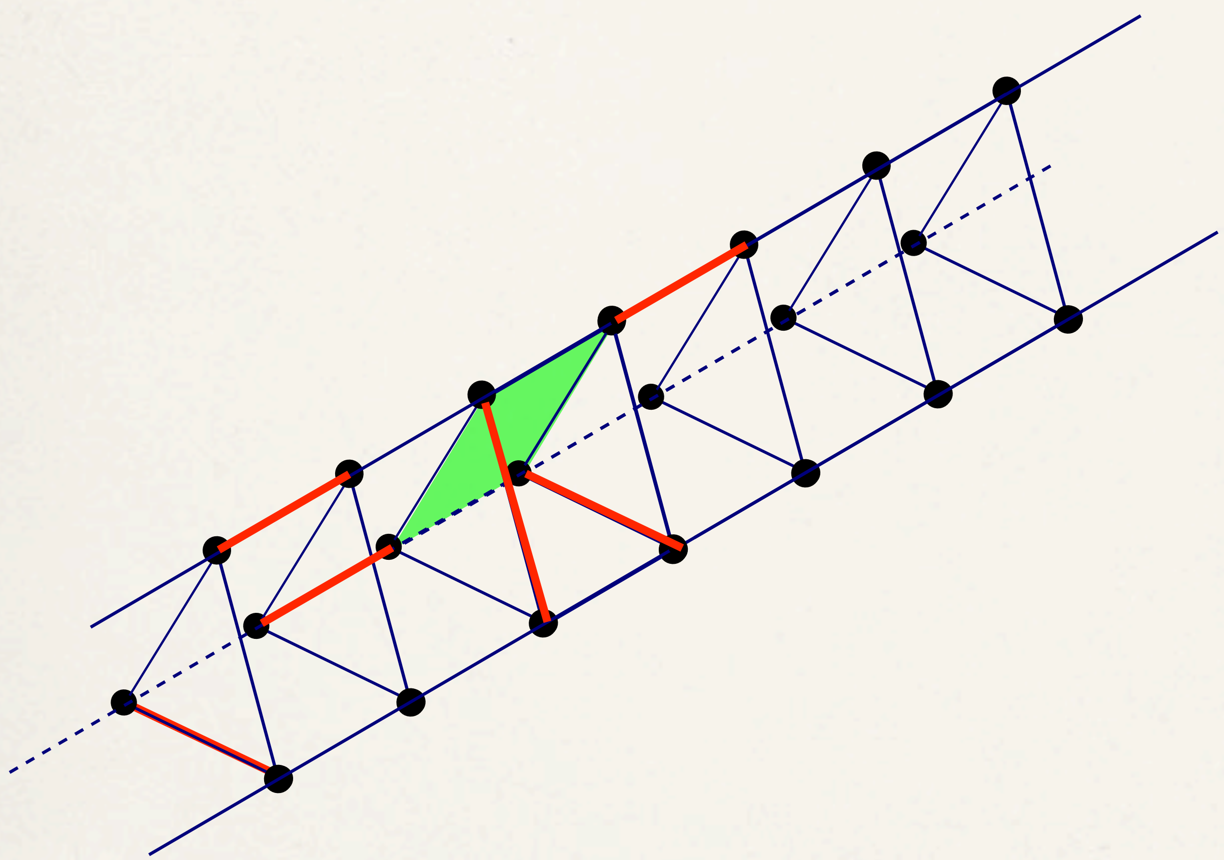


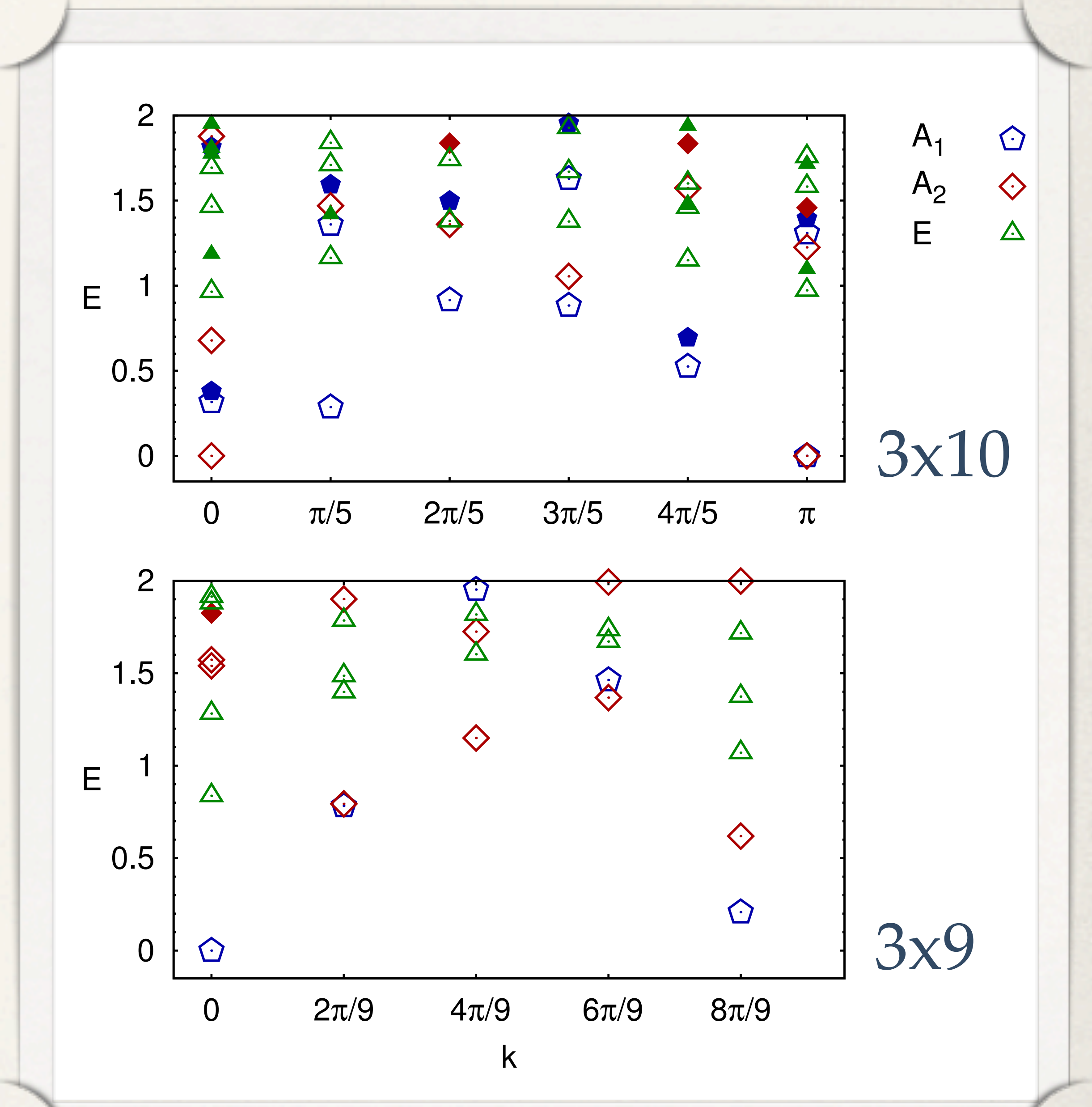
Cr^{3+} ions e_g^3 band: S=3/2

Hirotaka Manaka et al., Journal of the Physical Society of Japan, 78(9):093701, 2009.

Three-leg tube + projection operator

$$H = \sum_{\alpha:\square} \mathrm{Proj}\left\{S^T_\alpha = 2\right\}$$

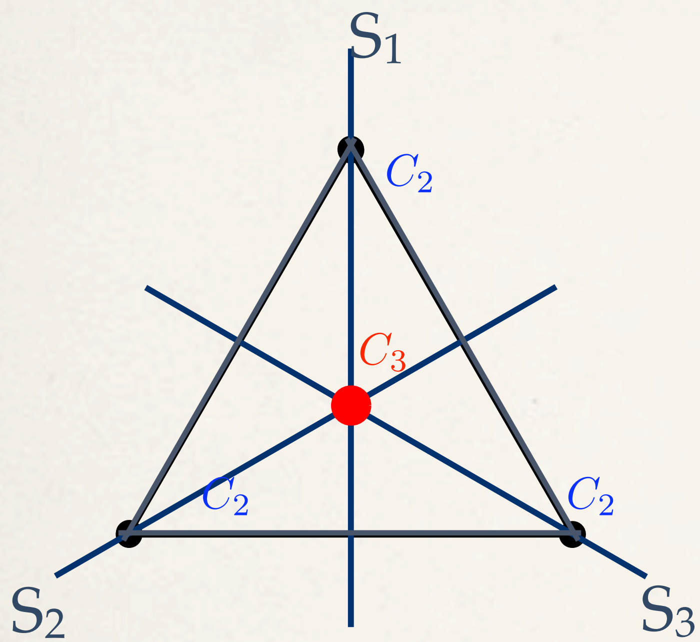




No nearest neighbour valence bond ground states

Exact diagonalization: 0 energy ground states

Single spin-triangle



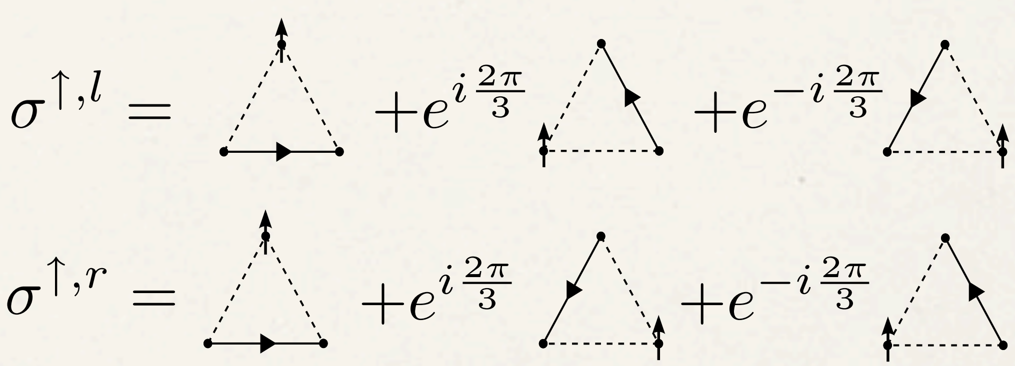
$$\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_1 = \frac{1}{2}\left(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3\right)^2 + \text{const.}$$

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

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



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

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

Three-leg tube + projection operator

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

$$P_i = \mathrm{Proj}\left\{ S_i^{\triangle} = 3/2 \right\} \qquad R_{\alpha} = \mathrm{Proj}\left\{ S_{\alpha}^{T} = 2 \right\}$$

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

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

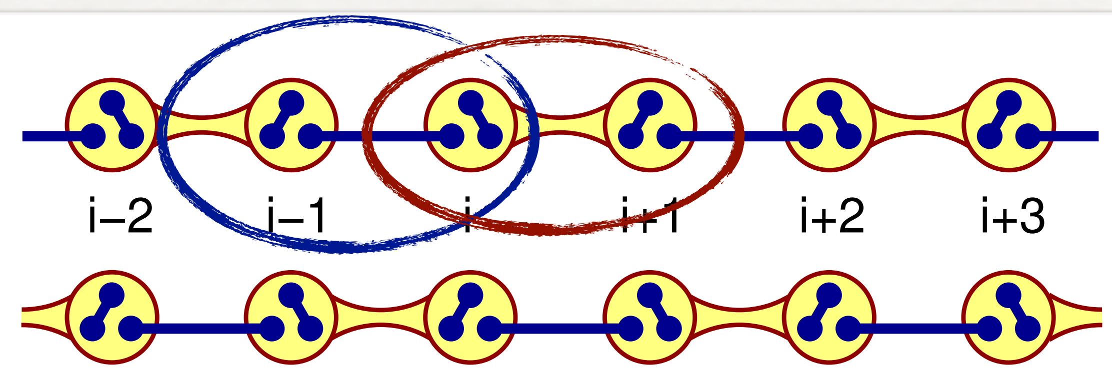
Weakly coupled triangles

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

$K_{\Delta} \gg 1$

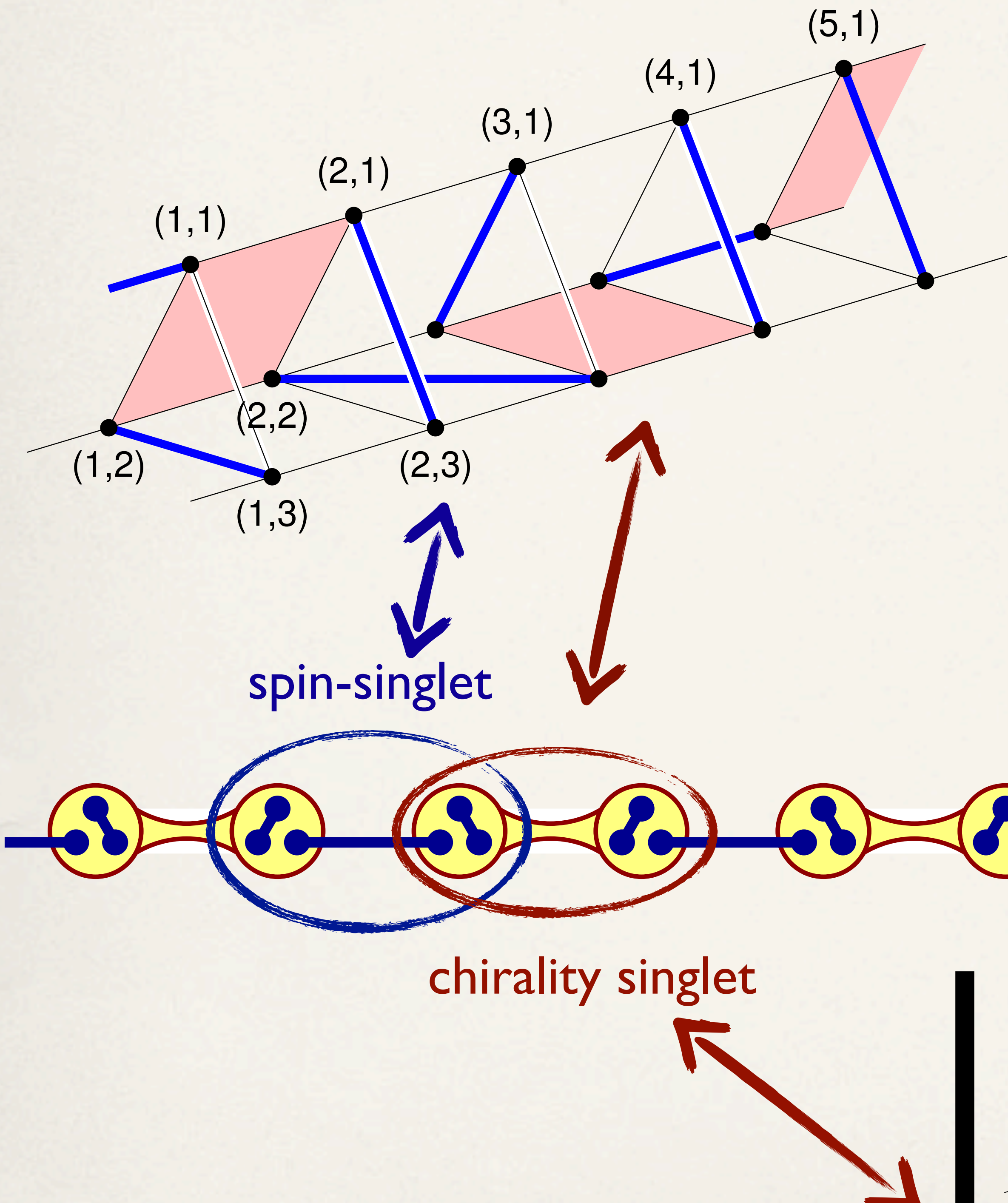
$$\mathcal{H}' = \frac{5}{9} \sum_{i=1}^{L} \left(\frac{3}{4} + \hat{\boldsymbol{\sigma}}_i \cdot \hat{\boldsymbol{\sigma}}_{i+1} \right) \left(1 + \hat{\tau}_i^+ \hat{\tau}_{i+1}^- + \hat{\tau}_i^- \hat{\tau}_{i+1}^+ \right),$$

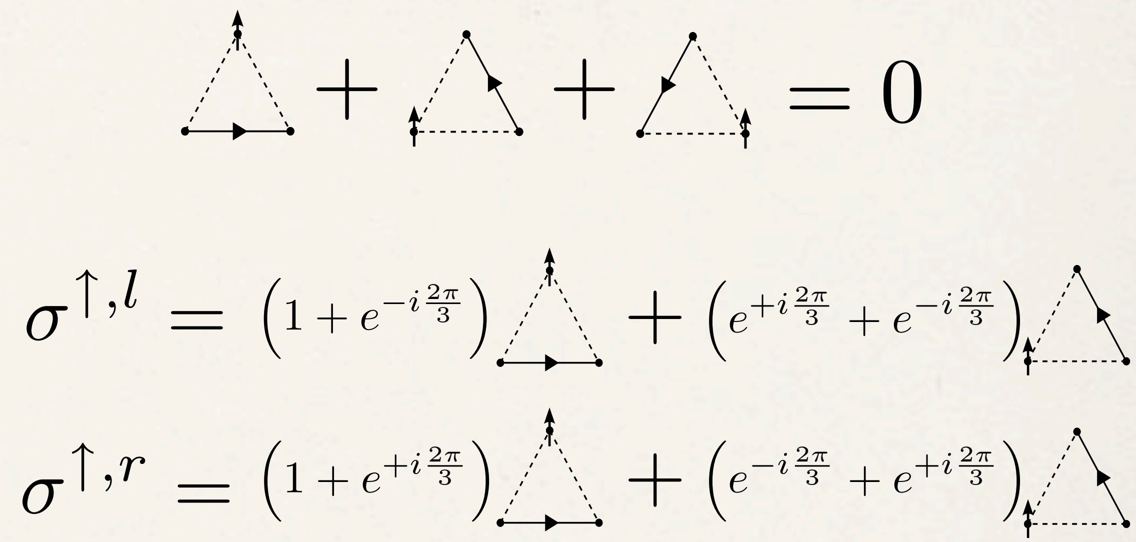
0 for spin singlet 0 for chirality singlet

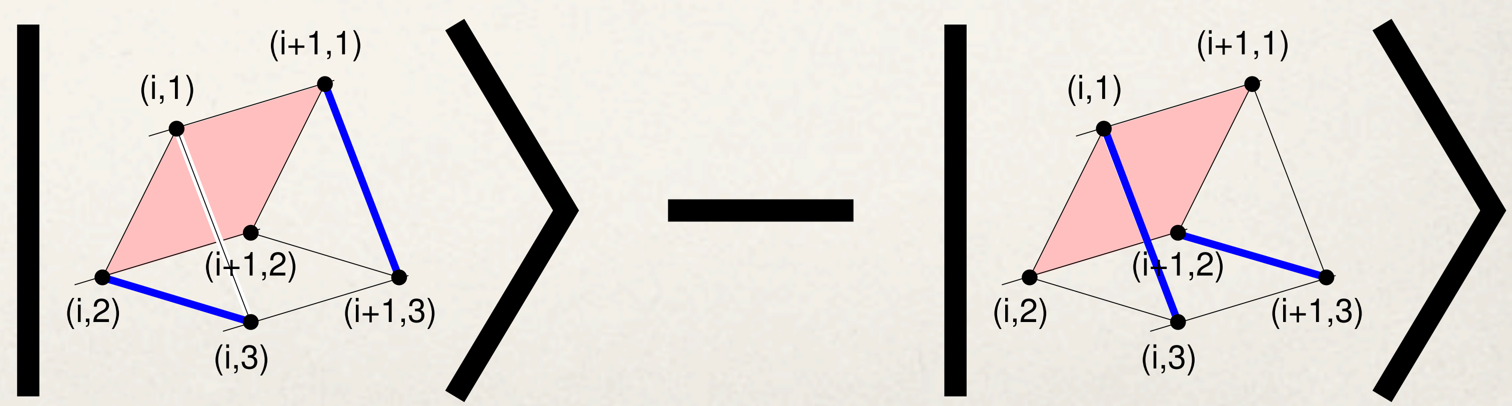


Ground states of $\mathcal{H}$ for all $K_{\Delta} \geq 0$

Dimerized ground states at $K_\Delta = 0$







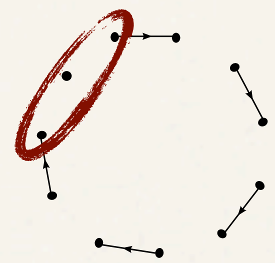
Tubes of odd length, $K_\Delta = 0$

Majumdar-Ghosh:

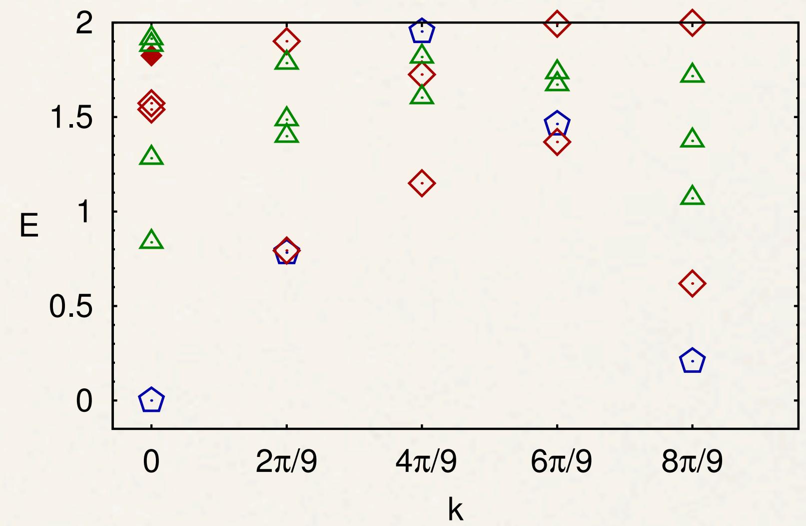
$$H_{MG} = \sum_i \mathrm{Proj}\left(|\mathbf{S}_{i-1} + \mathbf{S}_i + \mathbf{S}_{i+1}| = \frac{3}{2}\right)$$

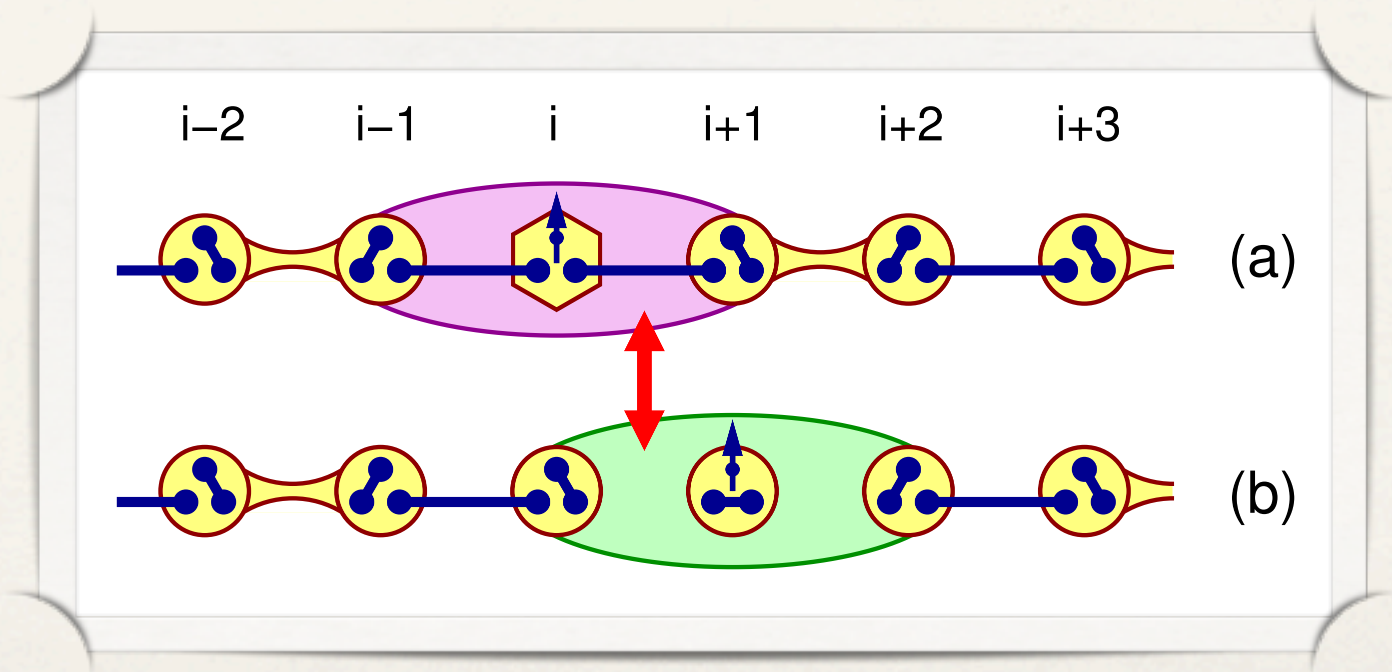
for odd length:

$E_g > 0$, gapless

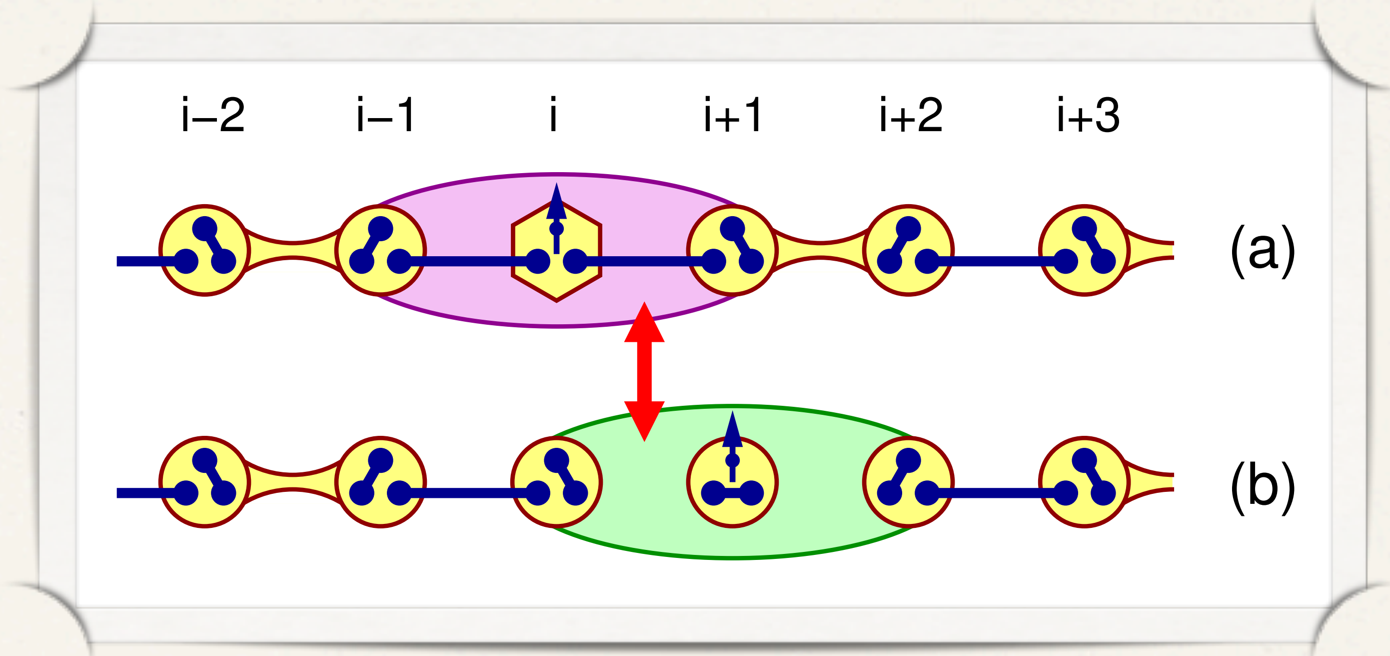


$$\mathcal{H} = K_\triangle \sum_{i=1}^{L} P_i + K_\square \sum_{i=1}^{L} \sum_{j=1}^{3} R_{(i,j)(i+1,j)(i+1,j+1)(i,j+1)}$$





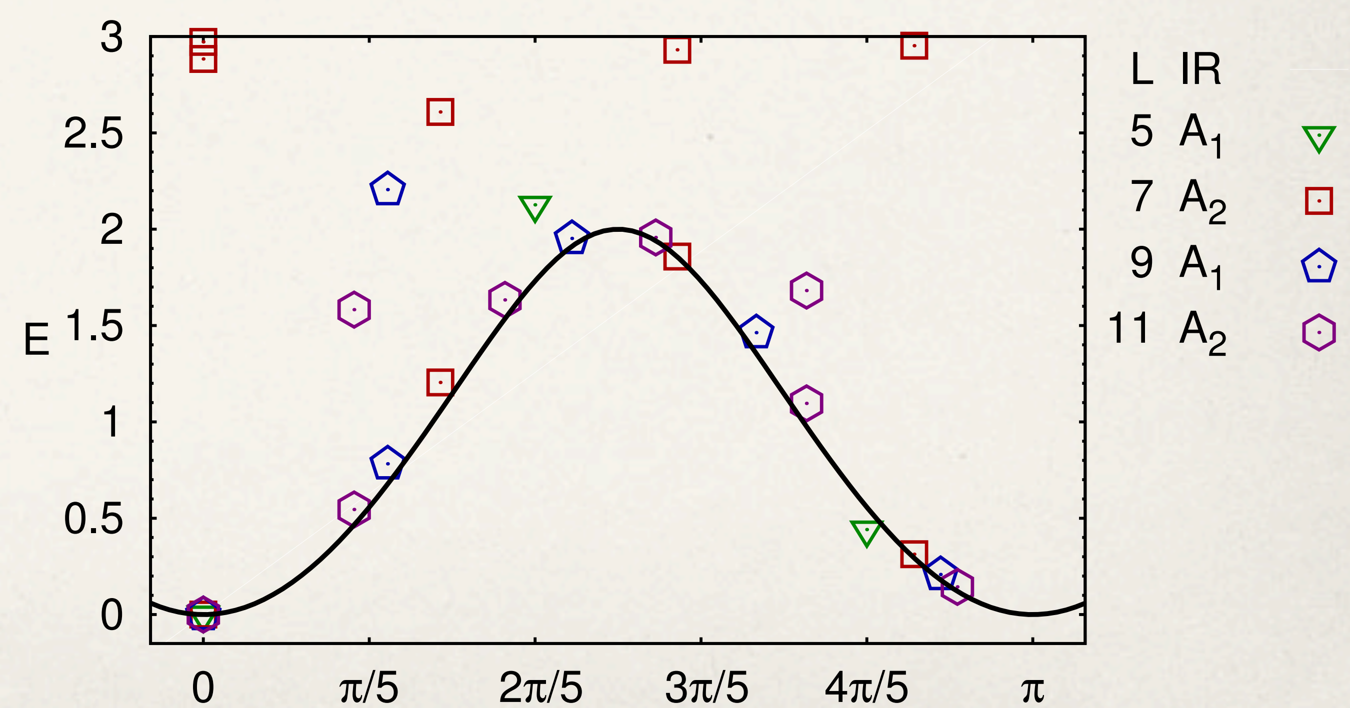
Tubes of odd length, $K_\Delta = 0$



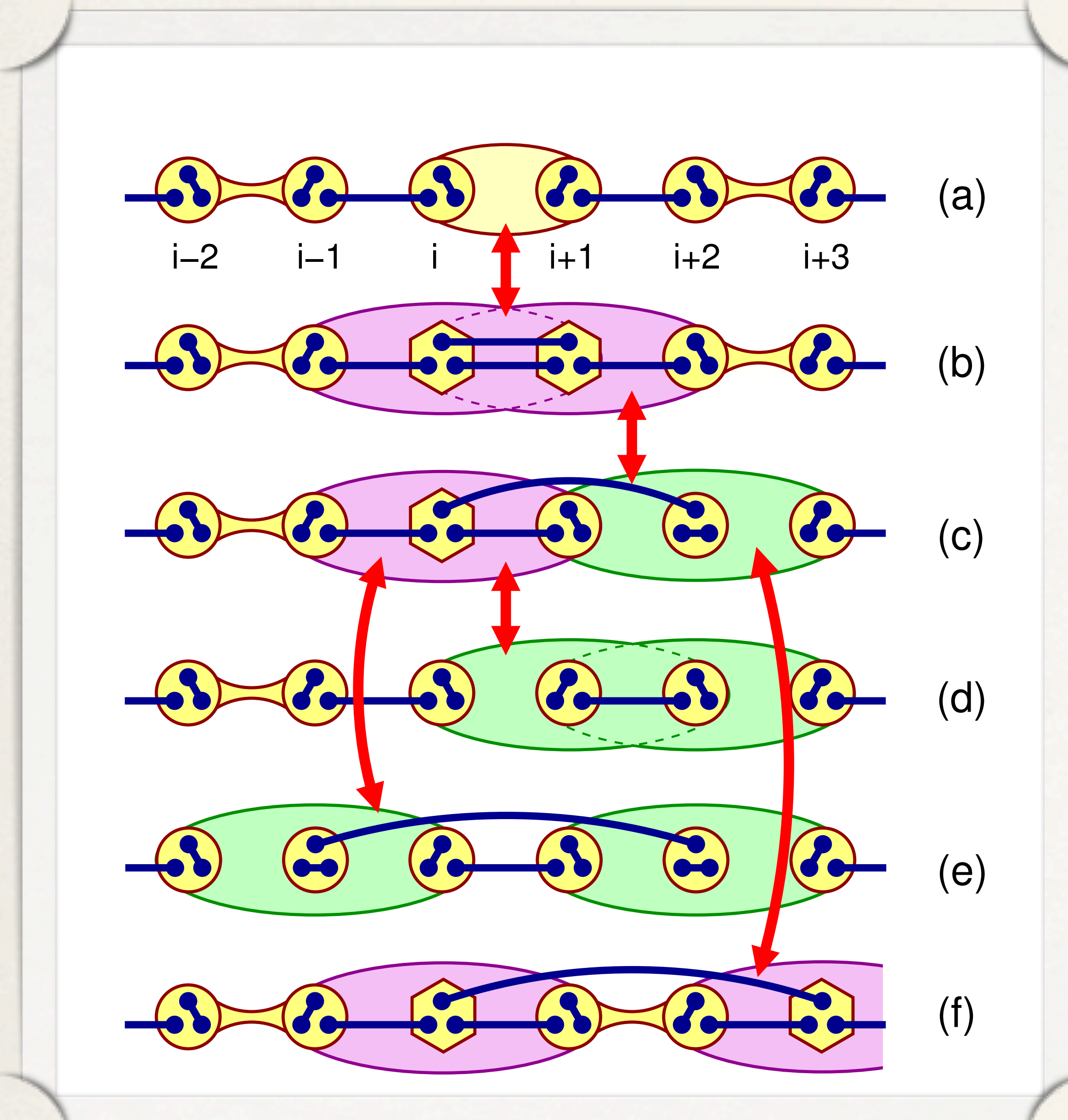
$$\mathcal{H}_{1\mathrm{dw}}(k) = \begin{pmatrix} \frac{10}{3}\left(1 - a_L \cos k\right) & -\frac{10}{\sqrt{3}}\left(\cos k - a_L\right) \\ -\frac{10}{\sqrt{3}}\left(\cos k - a_L\right) & 10\left(1 - a_L \cos k\right) \end{pmatrix}$$

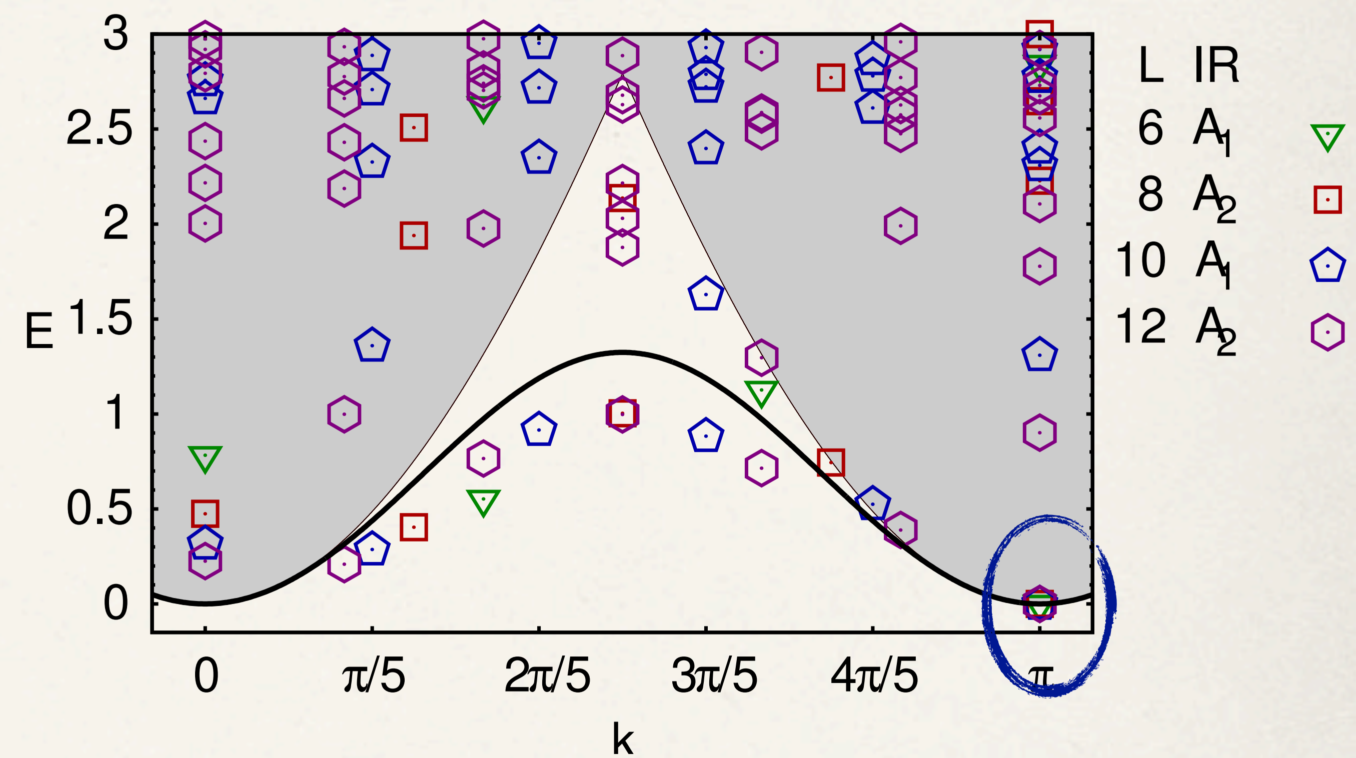
$$a_L = 2^{3-L}$$

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



Tubes of even length, $K_\Delta = 0$

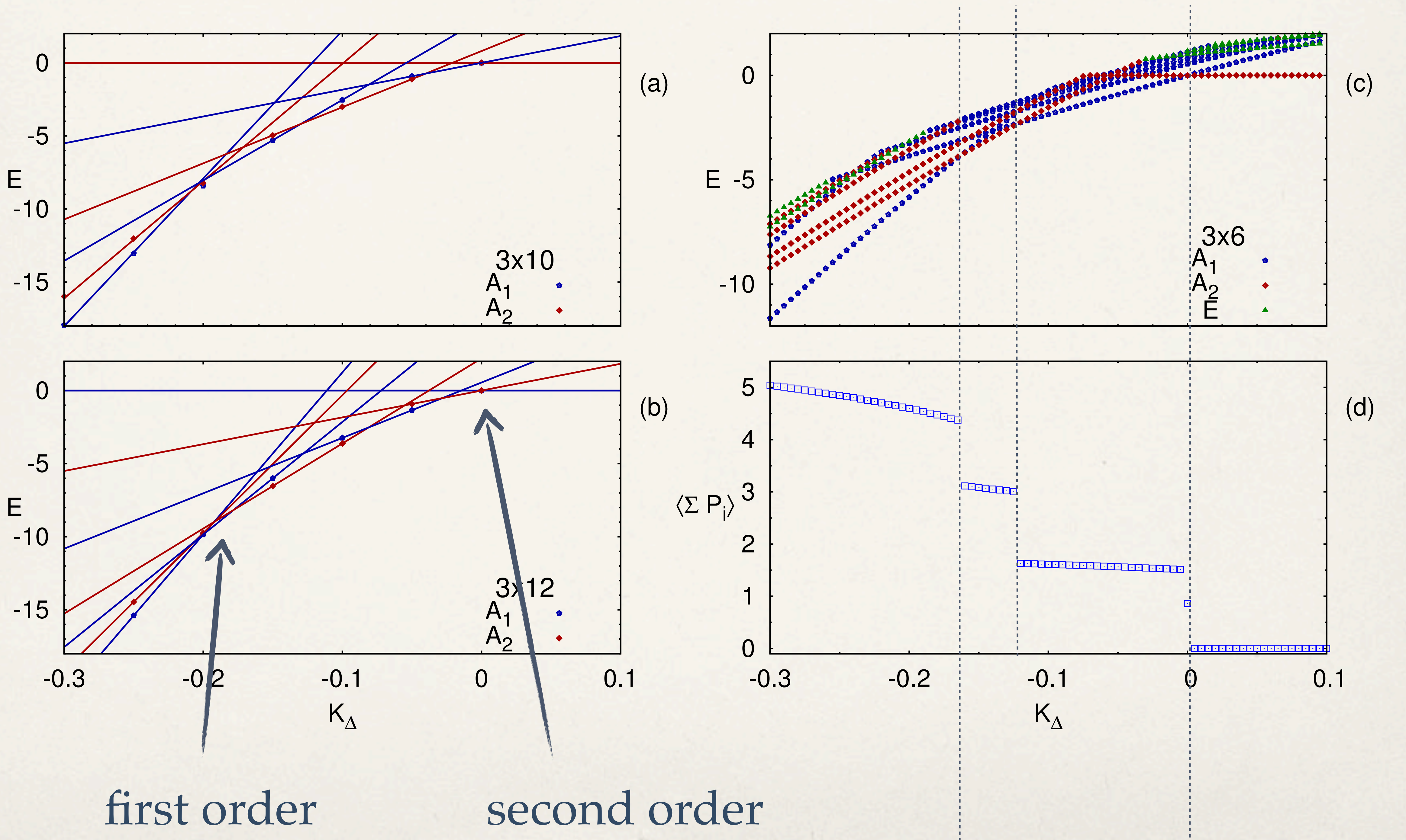




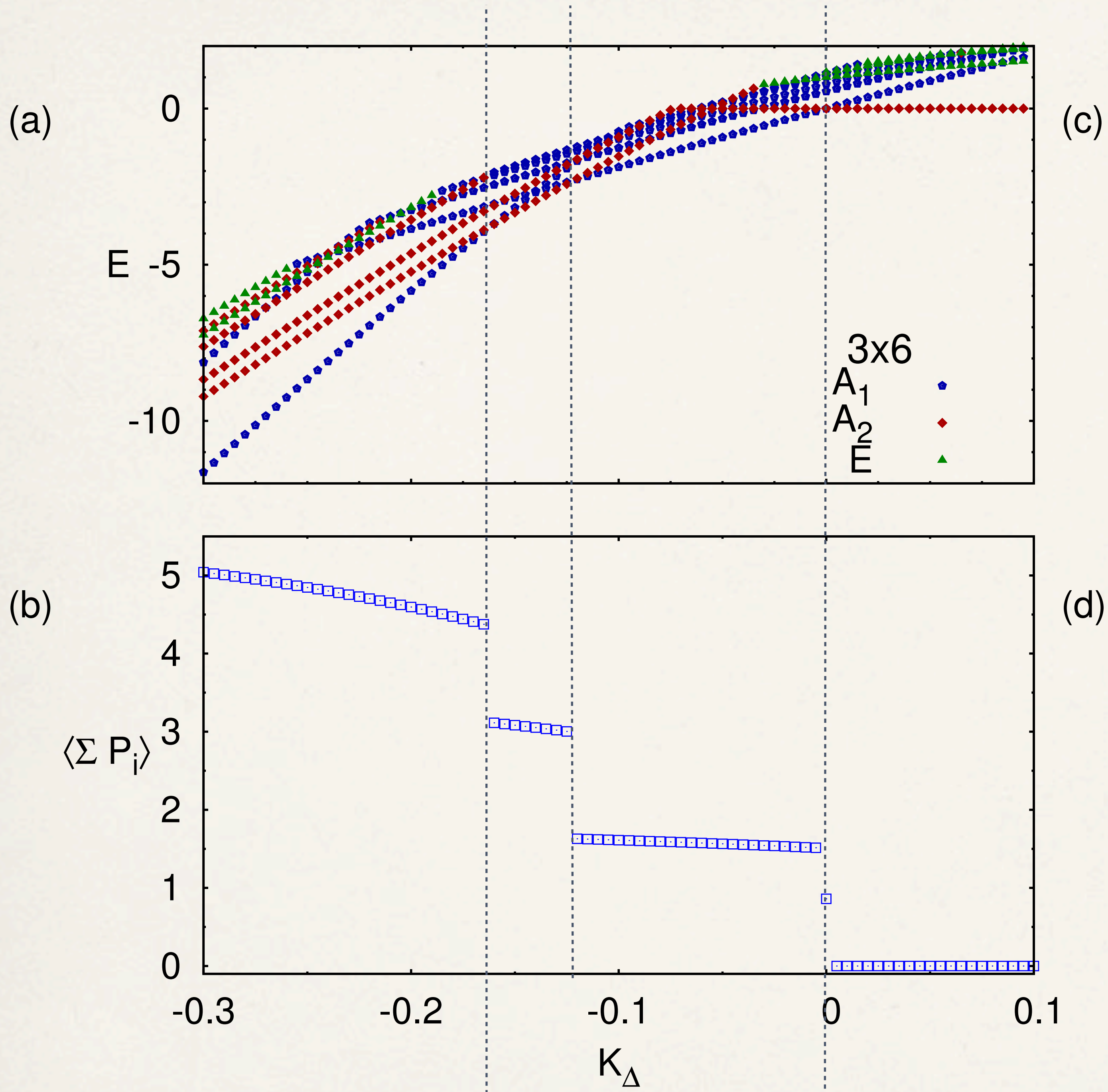
deconfined two domain wall ground state with 0 energy for finite L

Tuning away from $K_\Delta = 0$

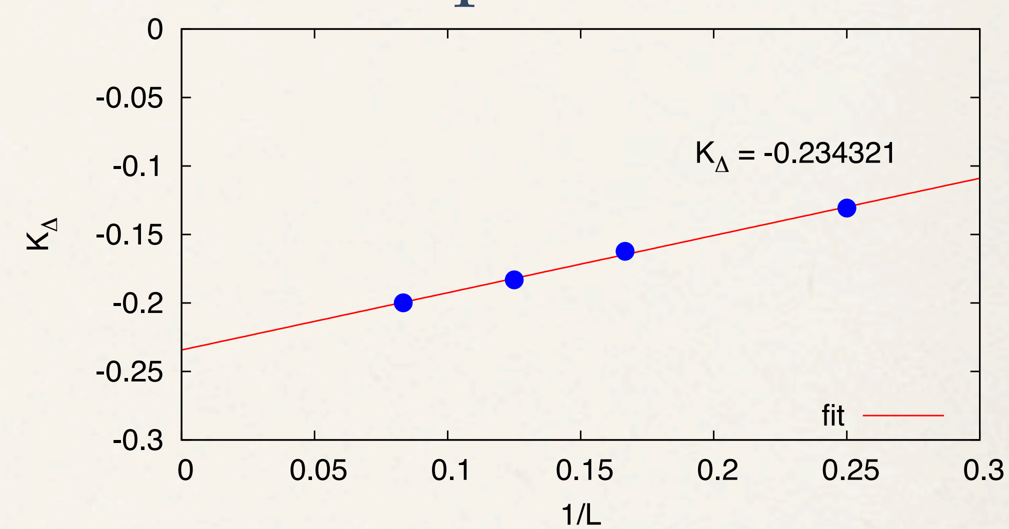
$$\mathcal{H} = K_\triangle \sum_{i=1}^{L} P_i + K_\square \sum_{i=1}^{L}\sum_{j=1}^{3} R_{(i,j)(i+1,j)(i+1,j+1)(i,j+1)} \qquad P_i = \mathrm{Proj}\left\{S_i^\triangle = 3/2\right\}$$



Tuning away from $K_\Delta = 0$

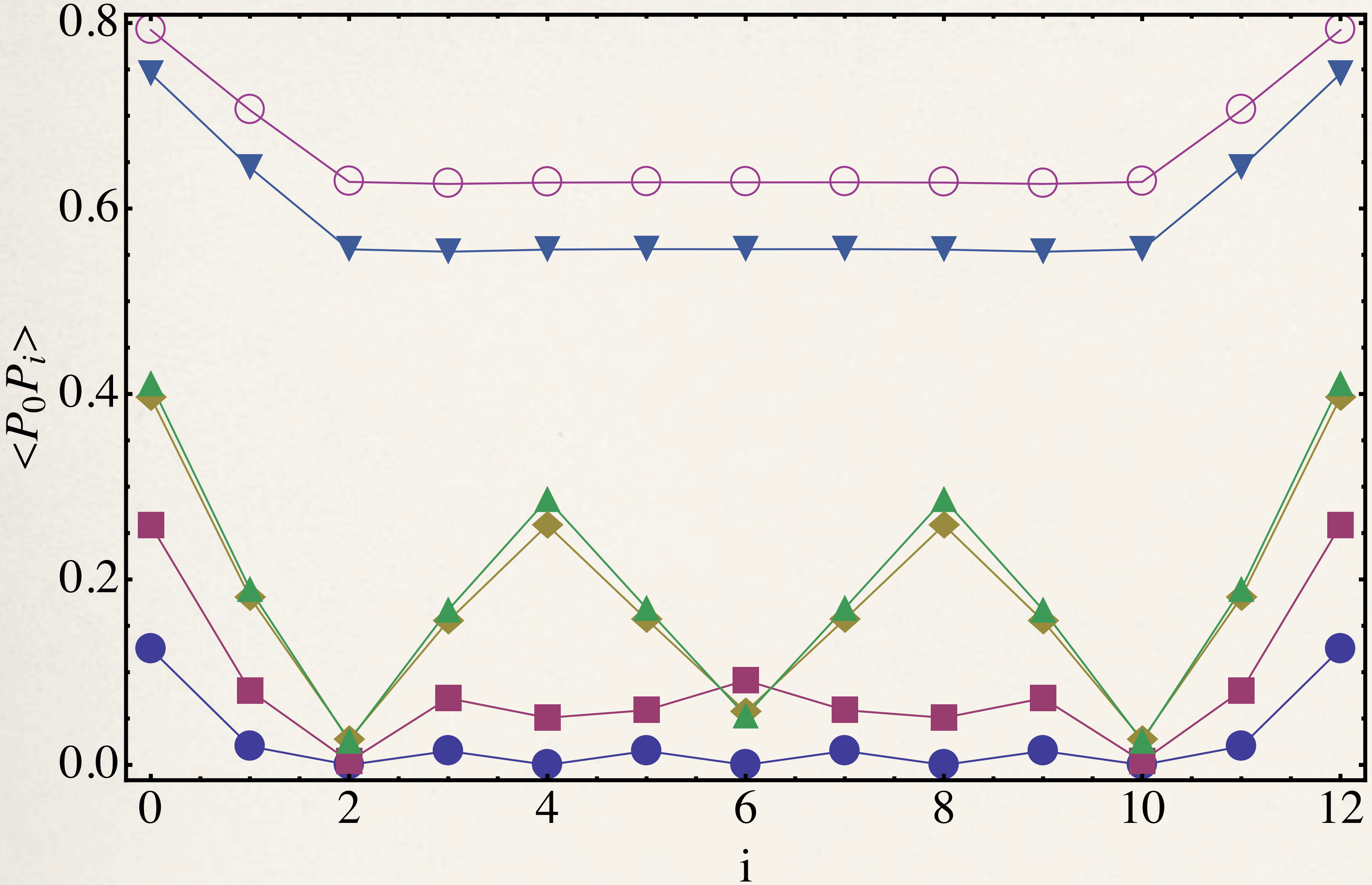


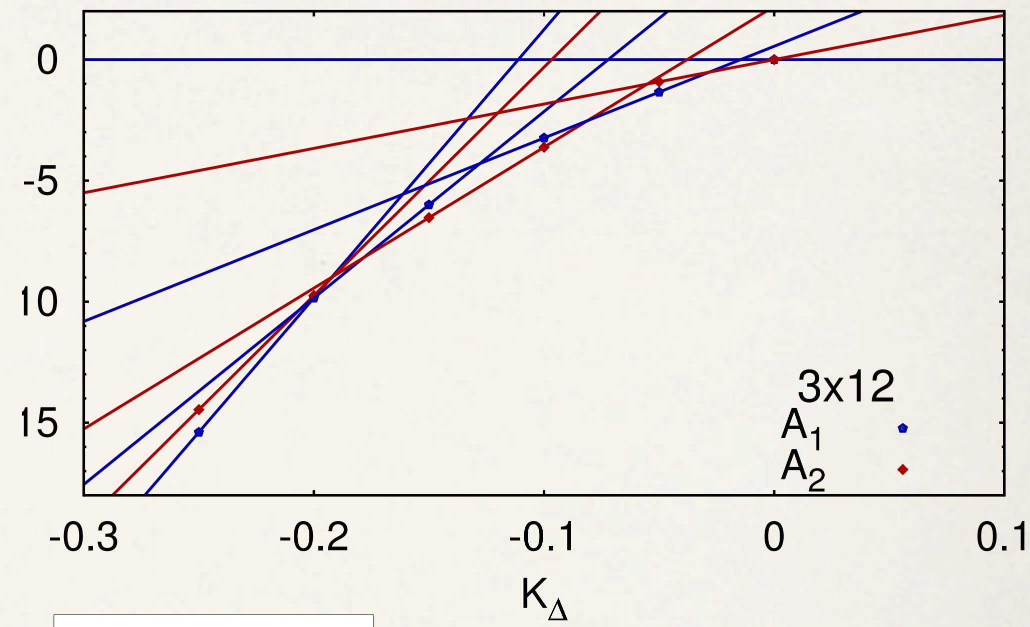
S=3/2 phase starts at

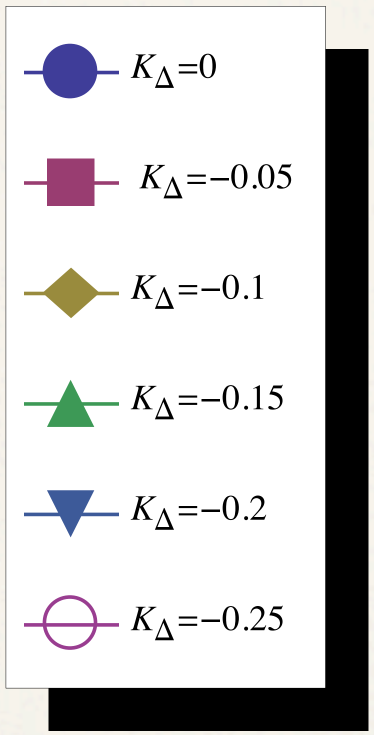


S=3/2 Heisenberg	domain walls	spin-chiral dimerized exact ground states
no exact ground state	gapless	gapped
gapless excitations	excitations	excitations

Spin-3/2 correlation functions



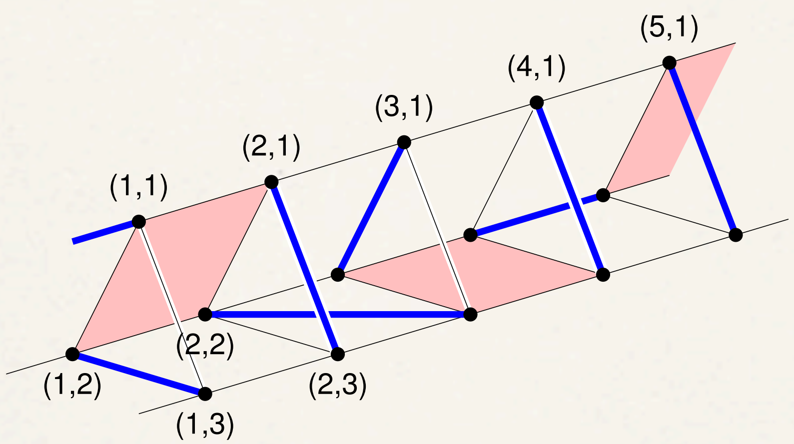


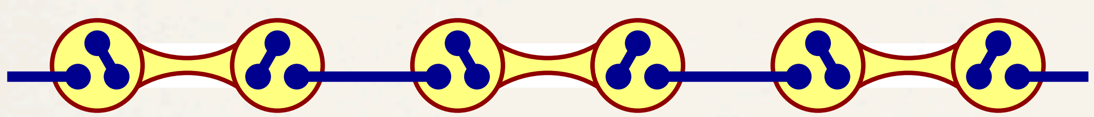


domain walls in pairs

Conclusions

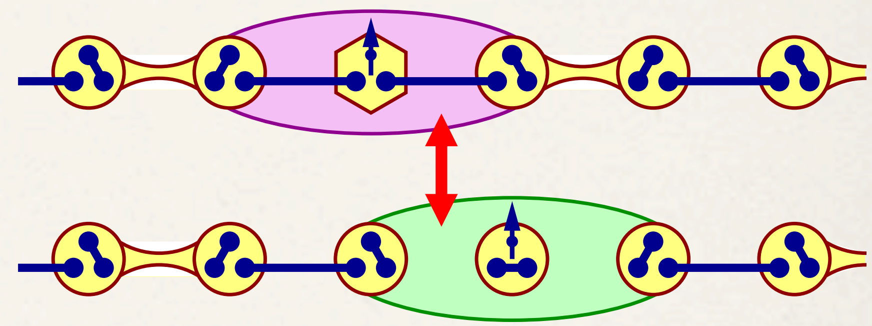
$$\mathcal{H} = K_{\triangle}\sum_{i=1}^{L} P_i + K_{\square}\sum_{i=1}^{L}\sum_{j=1}^{3} R_{(i,j)(i+1,j)(i+1,j+1)(i,j+1)}$$

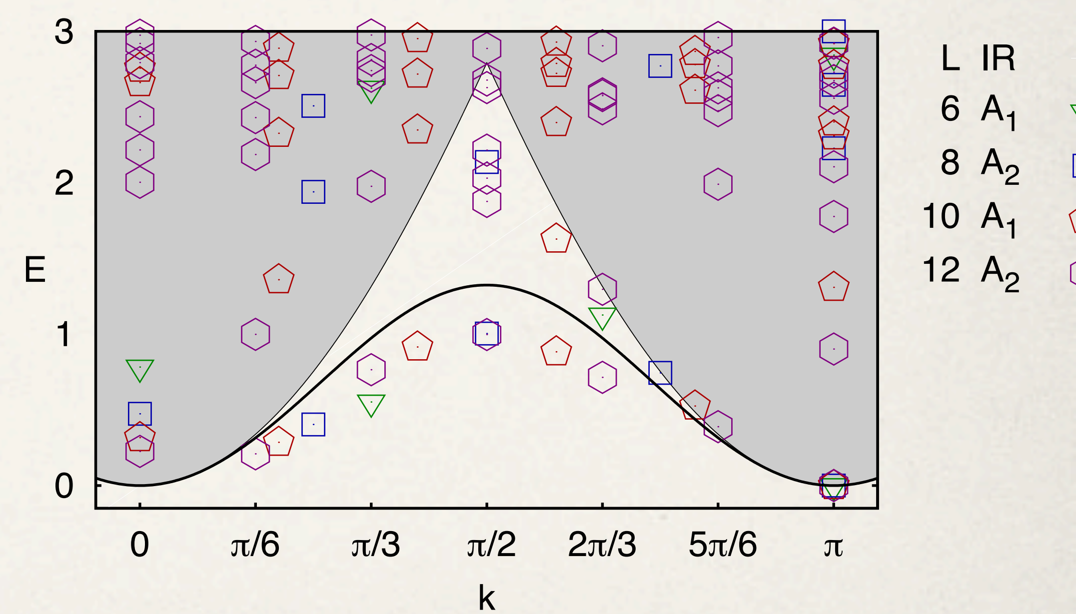




$K_{\Delta} \geq 0$, two exact ground states

1 exact ground state with gapless spectrum at a quantum phase transition point ($K_{\Delta} = 0$)

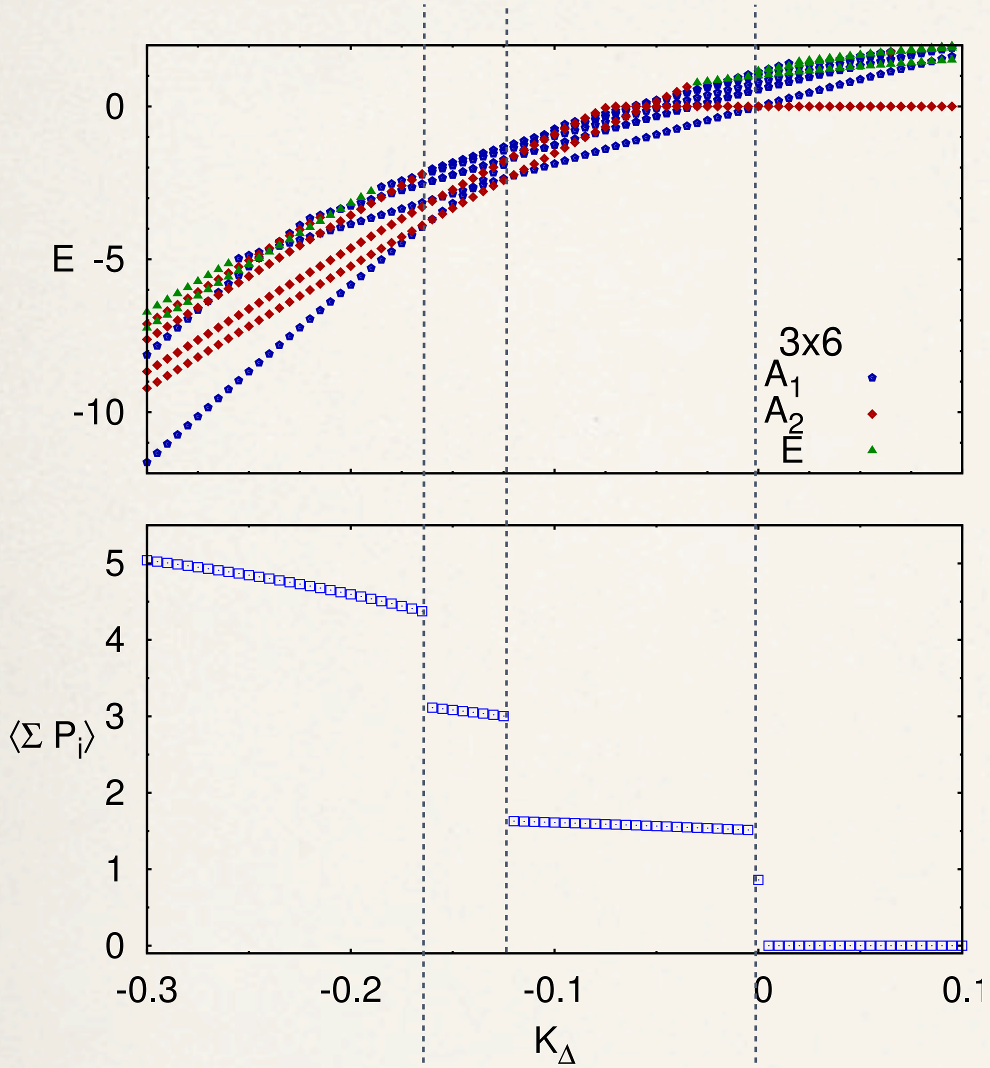




Phys. Rev. Lett **108**, 017205/1-5 (2012)

Thank you for your attention

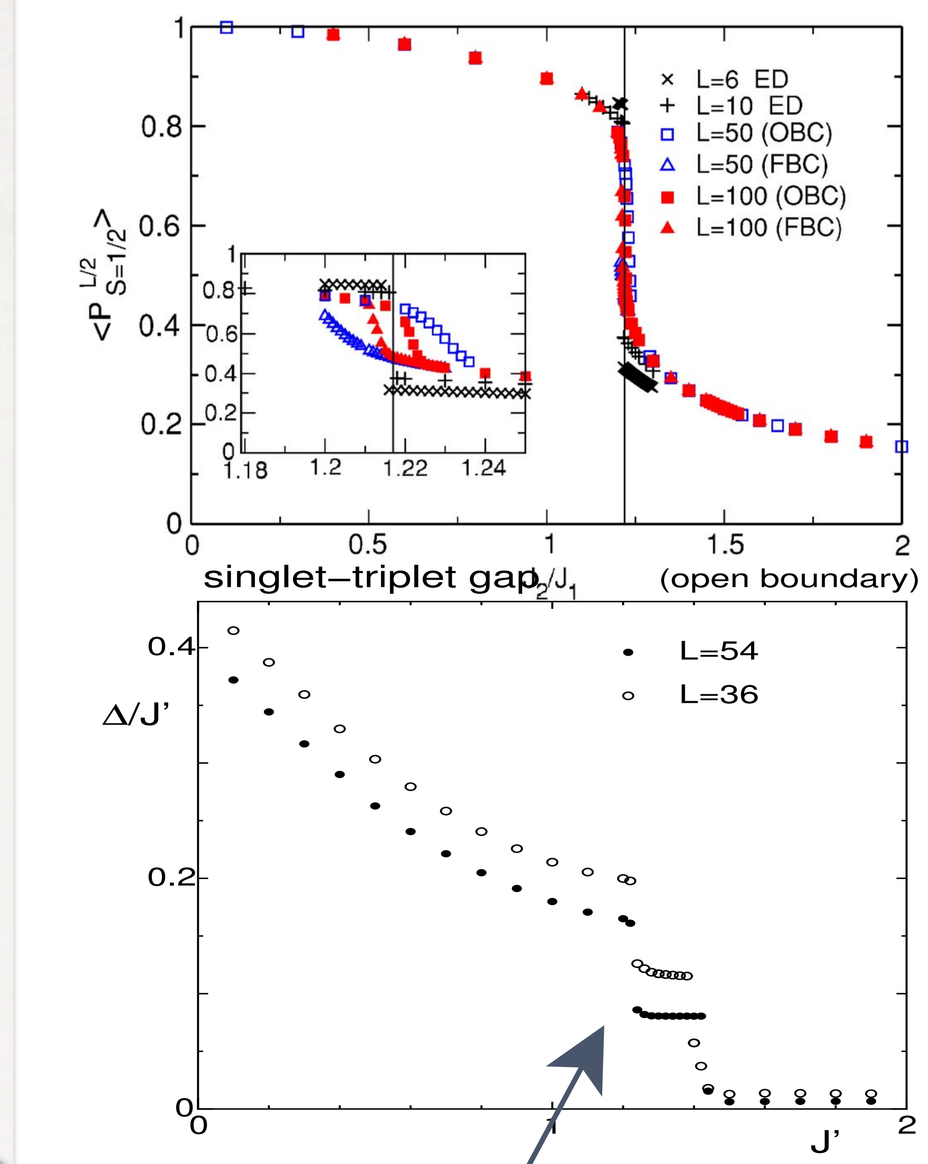
Intermediate phase



no gap S=3/2

no gap

dimerized, gapped



effect of open boundary condition

J.-B. Fouet, A. Läuchli, S. Pilgram, R. M. Noack, and F. Mila PHYSICAL REVIEW B 73, 014409

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