Long-range spin chirality dimer order in the spin $S = 1/2$ Heisenberg chain with modulated Dzyaloshinskii-Moriya interactions (DMI)

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- **Phys.Rev. B 99 205159 (2019);**
- **ArXiv/1909.04618 .**

OUTLINE

- **The model: spin $S = 1/2$ Heisenberg chain with spatially modulated DMI**

$$\mathcal{H} = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \sum_n \mathbf{D}(n) \cdot [\mathbf{S}_n \times \mathbf{S}_{n+1}] \,,$$

Motivation: recent progress in tailoring DMI

- **The spin $S = 1/2$ chain with uniform and staggered DMI**

$$\mathcal{H} = \sum_n \left\{ J\mathbf{S}_n \cdot \mathbf{S}_{n+1} + \mathbf{D} \cdot [\mathbf{S}_n \times \mathbf{S}_{n+1}] \right\} ,$$

$$\mathcal{H} = \sum_n \left\{ J\mathbf{S}_n \cdot \mathbf{S}_{n+1} + (-1)^n \mathbf{D} \cdot [\mathbf{S}_n \times \mathbf{S}_{n+1}] \right\} ,$$

Long history of studies:

I E. Dzyaloshinskii Zh. Eksp. Teor. Fiz. **46** *1420 (1964); ibid* **47**, *992 (1964).*

J.H.H. Perk and H.W. Capel, Physics Letters A **58**, *115 (1976); ibid Physica* **A 92**, *163 (1978).*

A.A. Zvyagin, Fiz. Niz. Temp. **15** *977 (1989); ibid J. Phys.: Cond. Matter.* **3**, *3865 (1991).*

L. Shekhtman, O. Entin-Wohlman, and A. Aharony, Phys. Rev. Lett. **69**, *836 (1992).*

M. Bocquet, F.H.L. Essler, A.M. Tsvelik, and A.O. Gogolin, Phys. Rev. B **64**, *094425 (2001).*

- **Gauge transformation**

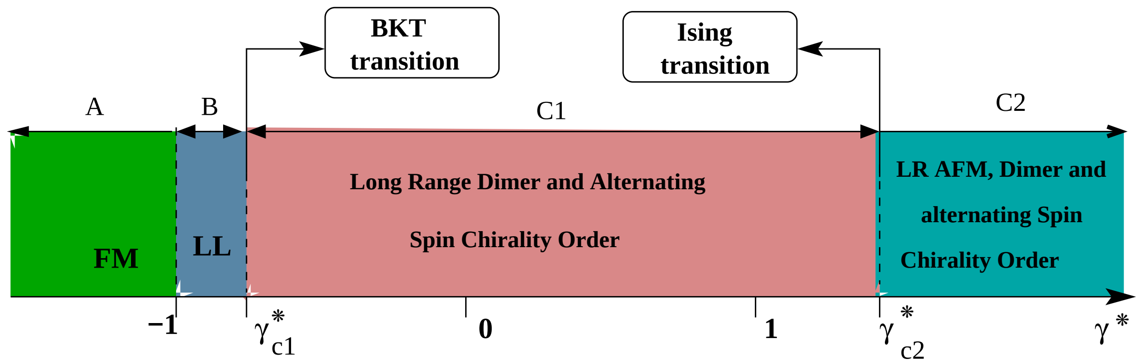
– **The Anisotropic Heisenberg chain with modulated DM interaction**

$$\mathbf{D}(n) = (0, 0, D(n)) \qquad D(n) = D_0 + (-1)^n D_1$$

$$\begin{aligned}
\hat{H} &= J \sum_n \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z\right) + \left(D_0 + (-1)^n D_1\right)\left(S_n^x S_{n+1}^y - S_n^y S_{n+1}^x\right) \\
&= J \sum_n \left[\frac{1}{2}\left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+\right) + \Delta S_n^z S_{n+1}^z\right] \\
&+ \frac{i}{2} \sum_n \left(D_0 + (-1)^n D_1\right)\left(S_n^+ S_{n+1}^- - S_n^- S_{n+1}^+\right) \ .
\end{aligned}$$

- **The Exactly Solvable limit**
- **The Effective Continuum Limit Theory**
- **Numerical (DMRG) Analysys**
- **Summary**

- **Ground state phase diagram**



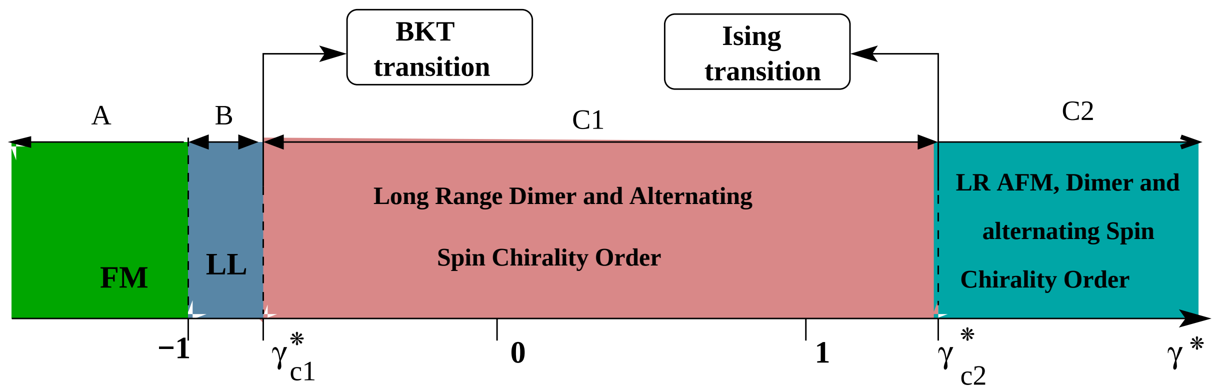
Here the effective anisotropy parameter

$$\gamma^* = J\Delta/\sqrt{J^2 + D_0^2 + D_1^2}.$$

The phase diagram contains the following four phases:

(i) the ferromagnetic phase at $\gamma^* \leq -1$;

(ii) the gapless Luttinger-liquid (LL) phase at $-1 < \gamma^* < \gamma^*_{c1} = -1/\sqrt{2}$;



At $\gamma^* = \gamma^*_{c1}$ the Berezinskii-Kosterlitz-Thouless (BKT) phase transition takes the system into the composite (C1) gapped phase characterized by the coexistence of long-range ordered (LRO) alternating spin dimerization pattern

$$\epsilon(n) = \langle \mathbf{S}_n \cdot \mathbf{S}_{n+1} \rangle \sim const + (-1)^n \epsilon$$

coexisting with long-range alternating pattern of the spin chirality vector

$$\kappa^z_n = \langle [\, \mathbf{S}_n \times \mathbf{S}_{n+1} \,]_z \rangle \sim const + (-1)^n \kappa \,.$$

Finally, at $\gamma^* = \gamma^*_{c2} > 1$ there is an Ising type phase transition into the other composite (C2) gapped phase, characterized by the coexistence of long-range dimerization, chirality and antiferromagnetic

$$\langle S^z_n \rangle \sim const + (-1)^n m$$

modulations.

Additonal motivations from the recent experimental achievements:

Recently it has been demonstrated that DM interaction can be *efficiently tailored* with an substantial efficiency factor by **structural modulations**

O.M. Volkov *et al.*, Scientific Reports **8**, Article number: 866 (2018).

or by **external electric field**

H. Yang *et al.*, Scientific Reports, **8**, Article N: 12356 (2018); W. Zhang, *et al.*, App. Phys. Lett. **113**, 122406 (2018); T. Srivastava *et al.*, Nano Lett. **18**, 4871 (2018).

External electric field induced modulation of the DM interaction can be realized in **spin-driven chiral multiferroic** (MF) systems.

R. Ramesh and N. A. Spaldin, Nat. Mater. **6**, 21 (2007); M. Bibes and A. Barthelemy, Nat. Mater. **7**, 425 (2008); S.-W. Cheong and M. Mostovoy, Nature Materials **6**, 13 (2007).

$$\mathcal{H} \sim J \sum_n \mathbf{P} \cdot [\mathbf{S}_n \times \mathbf{S}_{n+1}] \,,$$

Context of materials useful for electric field controlled quantum information processing

A single spin-1/2 XXX chain with DM interaction. [M.Bocquet et al., Phys. Rev. B **64**, 094425 (2001).]

$$H = J \sum_n \left[\frac{1}{2} \left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+ \right) + S_n^z S_{n+1}^z \right] + i \frac{D}{2} \sum_n \left(S_n^+ S_{n+1}^- - S_n^- S_{n+1}^+ \right) . \quad (1)$$

Theorem: *The model (1) with periodic boundary conditions is equivalent to an XXZ chain with twisted boundary conditions.*

Indeed, performing a local rotation around the z-axis

$$S_n^+ = e^{in\theta}\, \tau_n^+, \qquad S_n^- = e^{-in\theta} \tau_n^-, \qquad S_n^z = \tau_n^z \,,$$

and choosing $\tan\theta = D/J$ gives

$$H = J_{eff} \sum_{n=1}^{L} \left\{ \frac{1}{2} \left(\tau_n^+ \tau_{n+1}^- + \tau_n^- \tau_{n+1}^+ \right) + \Delta_{eff}\, \tau_n^z \tau_{n+1}^z \right\} .$$

Here

$$J_{eff} = \sqrt{J^2 + D^2} \quad and \quad \Delta_{eff} = \frac{J}{J_{eff}} < 1 \,.$$

Using the above mapping we can now express bulk correlation functions of the spin-1/2 chain with DM interaction in terms of correlation functions of an XXZ chain with exchange J_{eff} and anisotropy Δ_{eff}. For example,

$$\langle S_n^+ S_{n+l}^- \rangle_{DM} \quad = \quad e^{-i\,l\,\theta}\,\langle \tau_n^+ \tau_{n+l}^- \rangle_{XXZ}, \qquad \langle S_m^- S_{n+l}^+ \rangle_{DM} = e^{+i\,l\,\theta}\,\langle \tau_n^- \tau_{n+l}^+ \rangle_{XXZ}\,.$$

This allows us to express the dynamical magnetic susceptibility of the model with uniform DMI in terms of the results for the Heisenberg XXZ chain

$$\chi_{\mathsf{DM}}^{+-}(\omega,k) \quad = \quad \chi^{+-}(\omega,k+\theta), \quad \chi_{\mathsf{DM}}^{-+}(\omega,k) = \chi^{-+}(\omega,k-\theta), \qquad \chi_{\mathsf{DM}}^{\mathrm{zz}}(\omega,k) = \chi^{\mathrm{zz}}(\omega,k).$$

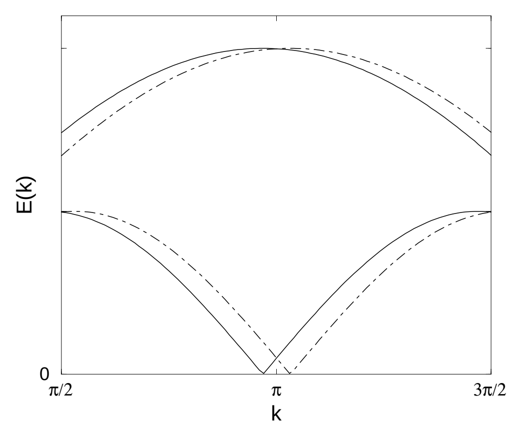


Figure 1: Schematic two-spinon dispersion in the vicinity of $k = \pi$ in the sector $\Delta S^z = \pm 1$ for the isotropic Heisenberg chain with DM interaction. From arXiv:cond-mat/0102138

The XX chain with alternating DM interaction.

$$
\begin{aligned}
\mathcal{H} &= \sum_n \Big[\frac{J}{2}\left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+\right) + J_z\, S_n^z S_{n+1}^z \\
&+ \frac{i}{2}(D_0 + (-1)^n D_1)\left(S_n^+ S_{n+1}^- - S_n^- S_{n+1}^+\right)\Big],
\end{aligned}
$$

where $S_n^+ = S_x^+ \pm iS_y^+$.

Using the Jordan-Wigner transformations [P. Jordan and E. Wigner Z. Phys. **47** 631 (1928).]

$$
\begin{aligned}
S_n^+ &= a_n^\dagger \exp\left(i\pi \sum_{m<n} a_m^\dagger a_m\right), \\
S_n^- &= \exp\left(-i\pi \sum_{m<n} a_m^\dagger a_m\right) a_n, \\
S_n^z &= a_n^\dagger a_n - 1/2,
\end{aligned}
$$

where $a_n^\dagger$ (a_n) is a spinless fermion creation (annihilation) operator on site n.

We rewrite the initial **spin Hamiltonian** in terms of **interacting spinless fermions** in the following way:

$$
\begin{aligned}
\mathcal{H} &= \frac{J}{2}\sum_n \left(a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n\right) \\
&+ \frac{iD_0}{2}\sum_n \left(a_n^\dagger a_{n+1} - a_{n+1}^\dagger a_n\right) \\
&+ \frac{iD_1}{2}\sum_n (-1)^n \left(a_n^\dagger a_{n+1} - a_{n+1}^\dagger a_n\right) \\
&+ J_z \sum_n (a_n^\dagger a_n - 1/2)(a_{n+1}^\dagger a_{n+1} - 1/2)\,.
\end{aligned}
$$

The exactly solvable limit $J_z = 0$.

The Fourier transform

$$a_n = \frac{1}{\sqrt{L}} \sum_k a_k e^{ikn} ,$$

and at $J_z = 0$ we obtain

$$\mathcal{H} = \sum_k \left[\epsilon(k)\, a_k^\dagger a_k + i\Delta(k) a_k^\dagger a_{k+\pi} \right] ,$$

where

$$\begin{aligned} \epsilon(k) &= (J \cos k - D_0 \sin k) = J_{eff} \cos(k + q_0) , \\ \Delta(k) &= D_1 \cos k \end{aligned}$$

and

$$\begin{aligned} J_{eff} &= \sqrt{J^2 + D_0^2} \\ q_0 &= \arctan(D_0/J) . \end{aligned}$$

Thus, in absence of the staggered component of the DM interaction and $(D_1 = 0)$ the excitation spectrum of the model is given by the same dispersion relation as the standard XX chain

$$\mathcal{H}_0 \quad = \quad \sum_k \epsilon(k)\, a_k^\dagger a_k \, ,$$

but for a uniform shift q_0 in the momentum vector due to the uniform part of the DM interaction system is characterized by two Fermi points $k_F^\pm = \pm\frac{\pi}{2} - q_0$, so that in the ground state all states with $\pi/2 \leq |k + q_0| \leq \pi$ are occupied and those with $|k + q_0| < \pi/2$ are empty. The bandwidth is half filled, the total magnetization of the system in the ground state as well as the average value of the on-site spin vanishes

$$m = \frac{1}{L}\sum_n \langle 0|S_n^z|0\rangle = 0\, .$$

The vacuum spin current, determined via the chirality order parameter

$$J_{sp} = \frac{1}{L}\sum_n \langle 0|j_n^z|0\rangle = \frac{2}{\pi}\sin q_0\, .$$

Note that due to the gapless excitation spectrum, all corresponding correlations decay in power-laws and no LRO is present in absence of modulated part of the DM interaction.

At $D_1 \neq 0$, diagonalization of the Hamiltonian (2) is also straightforward. It is convenient to restrict momenta within the reduced Brillouin zone $-\pi/2 < k \leq \pi/2$ and to introduce a new notation $a_{k+\pi} = b_k$. In these terms the Hamiltonian reads

$$\mathcal{H} = {\sum_k}' \left[\epsilon(k) \left(a^\dagger_k a_k - b^\dagger_k b_k\right) + i\Delta(k) \left(a^\dagger_k b_k - b^\dagger_k a_k\right)\right] ,$$

Here prime in the sum means that the summation is taken over the reduced Brillouin zone $-\pi/2 < k \leq \pi/2$. Using the unitary transformation

$$a_k \quad = \quad \cos\phi_k\,\alpha_k + i\sin\phi_k\,\beta_k \;\; b_k = i\sin\phi_k\,\alpha_k + \cos\phi_k\,\beta_k$$

and choosing

$$\tan\left(2\phi_k\right) = -\Delta(k)/\epsilon(k)$$

we obtain

$$\mathcal{H} \quad = \quad \sum_{\pi/2<k\leq\pi/2} E(k) \left(\alpha^\dagger_k \alpha_k - \beta^\dagger_k \beta_k\right)$$

where

$$E(k) \quad = \quad \sqrt{J^2_{eff}\cos^2(k+q_0) + D_1^2\cos^2 k}$$

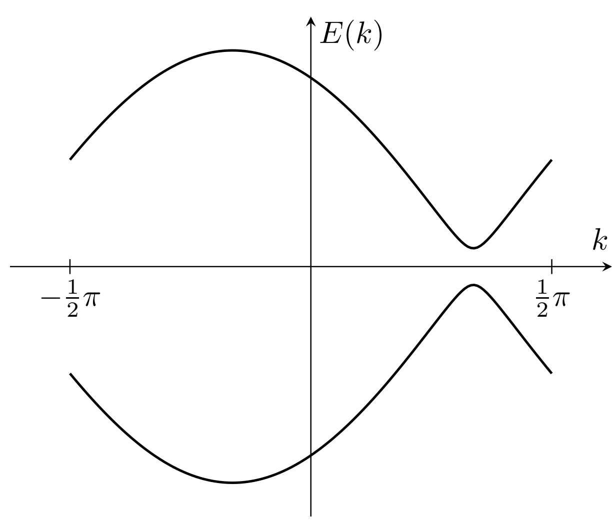
Note that in absence of the uniform component of the DM interaction ($D_0 = 0,\ D_1 \neq 0$), $E(k) = \pm\sqrt{J^2 + D_1^2}\ \cos k$ and therefore the excitation spectrum is gapless, the vacuum spin current $J_{sp} = 0$ and no LRO is present in the ground state.

Only at $D \neq 0,\ D_1 \neq 0$ the spectrum is characterized by a finite excitation gap

$$\begin{aligned}\Delta_{exc} &= J^*\sqrt{2\left(1 - \sqrt{1 - \left(2D_0D_1/J^*\right)^2}\right)} \\ &\simeq 2D_0\, D_1/J^*\,,\end{aligned}$$

where

$$J^* = \sqrt{J^2 + D_0^2 + D_1^2}\,.$$



In the ground state $n_\beta(k) = \langle \beta_k^\dagger \beta_k \rangle = 1$ and $n_\alpha(k) = \langle \alpha_k^\dagger \alpha_k \rangle = 0$. As the result, in the ground state the z-projection of the total spin as well as the staggered part of the on-site magnetization

$$\begin{aligned} M &= \sum_n \langle 0|S_n^z|0\rangle = \frac{L}{2\pi}\int\limits_{-\pi/2}^{\pi/2} [\, n_\beta(k) - 1/2\,] = 0 \\ m &= \frac{1}{L}\sum_n (-1)^n \langle 0|S_n^z|0\rangle = 0\,. \end{aligned}$$

However the staggered transverse spin dimerization and spin current (chirality) order parameters are finite

$$\begin{aligned} \epsilon_\perp &= \frac{1}{L}\sum_n (-1)^n \langle 0|\left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+\right)|0\rangle = -\frac{D_1}{\pi}\int\limits_{-\pi/2}^{\pi/2} \frac{\sin k \cos k}{E(k)}\, dk \\ \kappa &= \frac{i}{L}\sum_n (-1)^n \langle 0|\left(S_n^+ S_{n+1}^- - S_n^- S_{n+1}^+\right)|0\rangle = \frac{D_1}{\pi}\int\limits_{-\pi/2}^{\pi/2} \frac{\cos^2 k}{E(k)}\, dk\,. \end{aligned}$$

It is easy to check by inspection, that both link-located order parameters $\epsilon_\perp \longrightarrow 0$ and $\kappa \longrightarrow 0$ at $D_0 = 0$ and $D_1 \neq 0$.

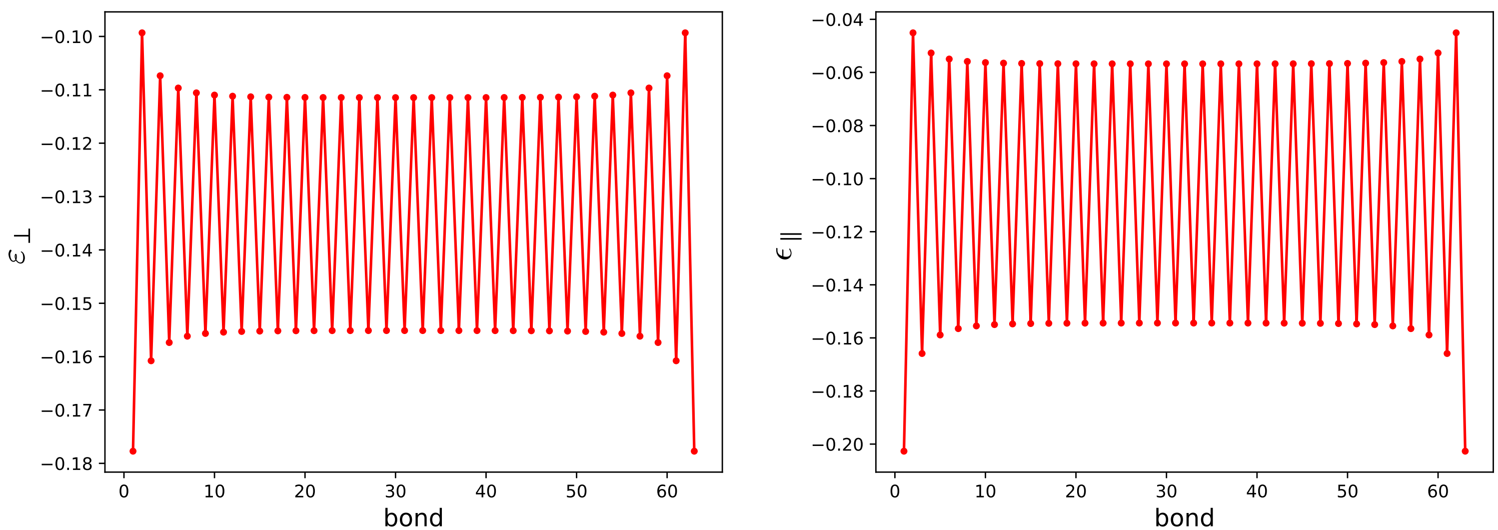


Figure 2: The ground state expectation value distribution along bonds of the transverse and longitudinal part of the nearest-neighbor spin-spin exchange operator $\epsilon_n^\perp$ and $\epsilon_n^\parallel$ as a function of site number. The results correspond to a chain of $L = 64$ sites with OBC, with parameters $J = 1$, $D_0 = \tan(\pi/6)$ and $D_1 = 0.2$.

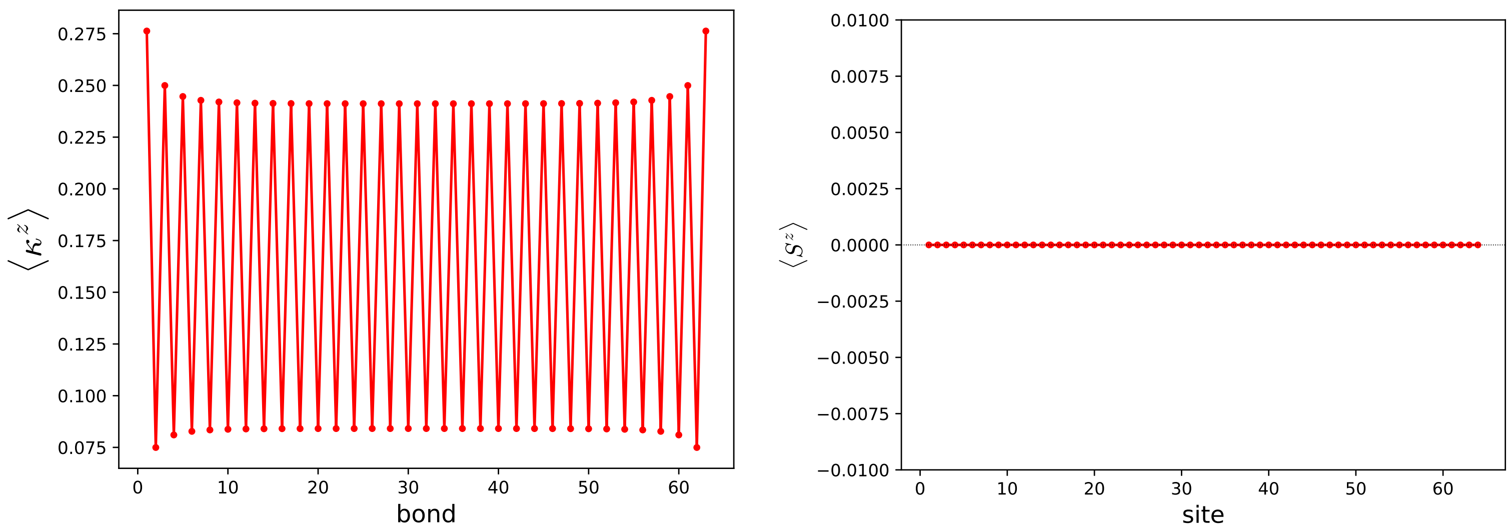


Figure 3: The ground state expectation value distribution along bonds of the of the spin current (chirality) operator j_n^z and of the z component of the spin operator as a function of site number. The results correspond to a chain of $L = 64$ sites with OBC, with parameters $J = 1$, $D_0 = \tan(\pi/6)$ and $D_1 = 0.2$.

Gauging away the DM interaction

Let us first rewrite the Hamiltonian in a way which explicitly takes into account *doubling of the unit cell* by the staggered DMI.

$$\begin{aligned}
\mathcal{H} &= \frac{J}{2}\sum_{m=1}^{N/2}\Big[\ \left(S^+_{2m-1}S^-_{2m}+S^-_{2m-1}S^+_{2m}\right)+\left(S^+_{2m}S^-_{2m+1}+S^-_{2m}S^+_{2m+1}\right)\\
&+\ i\,d_-\left(S^+_{2m-1}S^-_{2m}-S^-_{2m-1}S^+_{2m}\right)+i\,d_+\left(S^+_{2m}S^-_{2m+1}-S^-_{2m}S^+_{2m+1}\right)\\
&+\ 2\,\Delta\,S^z_{2m}\left(S^z_{2m-1}+S^z_{2m+1}\right)\Big]\,.
\end{aligned}$$

where new dimensionless parameters $d_\pm=(D_0\pm D_1)/J$

We introduce new spin variables τ_{2m} and τ_{2m+1} by performing a site-dependent rotation of spins along the chain around the z axis with relative angle ϑ_- for spins at consecutive odd-even sites $(2m-1,2m)$ and ϑ_+ for spins at consecutive even-odd sites $(2m,2m+1)$, so that

$$\begin{aligned}
S^+_{2m-1} &= e^{i(m-1)(\vartheta_-+\vartheta_+)}\ \tau^+_{2m-1}\,,\\
S^+_{2m} &= e^{im\vartheta_-+i(m-1)\vartheta_+}\ \tau^+_{2m}\,,\\
S^+_{2m+1} &= e^{im(\vartheta_-+\vartheta_+)}\ \tau^+_{2m+1}\,,\\
S^z_{2m\pm1} &= \tau^z_{2m\pm1} \qquad S^z_{2m}=\tau^z_{2m}\ .
\end{aligned}$$

Choosing angles $\vartheta_\pm$ such that

$$\tan\vartheta_\pm = d_\pm,$$

one can gauge away the DM contribution and get

$$\mathcal{H} \quad = \quad \tilde{J}\sum_n \Big[\frac{1}{2}(1+(-1)^n\delta)\left(\tau_n^+\tau_{n+1}^- + \tau_n^-\tau_{n+1}^+\right), +\gamma^*\tau_n^z\tau_{n+1}^z\Big], \tag{2}$$

where, at $d_i \ll 1$ ($i = \pm$),

$$\tilde{J} = \frac{1}{2}\left(J_+ + J_-\right) \simeq J^* + \mathcal{O}\left(d_i^4\right),$$
$$\delta\,\tilde{J} = \frac{1}{2}\left(J_+ - J_-\right) \simeq \frac{D_0 D_1}{J^*} + \mathcal{O}\left(d_i^4\right)$$

and

$$\gamma^* = J_z/\tilde{J} \simeq J_z/J^* + \mathcal{O}\left(d_i^4\right) \ .$$

At $J_- \neq J_+$ the Hamiltonian (2) is recognized as a Hamiltonian of the XXZ chain with alternating transverse exchange. Note that the alternation of the transverse exchange $\delta \neq 0$ only for finite $D_1 \neq 0$ and $D_0 \neq 0$. In the following we will discard $\mathcal{O}\left(d_i^4\right)$ corrections.

In the case of uniform DM interaction ($D_1 = 0$) the gauge transformation reduces to the consecutive rotation of spins along the chain around the z axis with respect to the nearest neighbor on the same angle

$$\theta = \arctan\left(D_0/J\right).$$

Because in this limit $J_+ = J_-$ i.e. $\delta = 0$, the effect of the uniform DM interaction reduces to the renormalization of the exchange anisotropy $\gamma \to \gamma^*$ and change of the boundary conditions. Respectively the Heisenberg chain with uniform DM interaction is equivalent to an XXZ chain with twisted boundary conditions. In particular, the excitation spectrum and the bulk correlation functions of a spin-1/2 XXZ Heisenberg chain with DM interaction can be obtained from that of the corresponding XXZ chain

$$\mathcal{H} = J^* \sum_{n=1}^{N} \Big[\frac{1}{2}\left(\tau_n^+ \tau_{n+1}^- + \tau_n^- \tau_{n+1}^+\right) + \gamma^* \tau_n^z \tau_{n+1}^z \Big], \tag{3}$$

taking into account the shift in momentum induced by the mapping and renormalization of the anisotropy parameter

In the case of staggered DM interaction $D(n) = (-1)^n D_1$

$$\vartheta_+ = -\vartheta_- = \vartheta = \arctan\left(D_1/J\right)$$

and the gauge transformation becomes global and corresponds to the rotation of all spins on even sites around the z axis on the same angle θ

$$S^+_{2m} \quad = \quad e^{i\theta}\,\tau^+_{2m},\; S^z_{2m} = \tau^z_{2m+1},$$

while the spins on even sites remain untouched:

$$S^+_{2m-1} \quad = \quad \tau^+_{2m-1},\; S^z_{2m} = \tau^z_{2m}.$$

This gives again the Hamiltonian (3), but with transverse exchange

$$J^* = \sqrt{J^2 + D_1^2}\,.$$

Conclusion:e this Section, gauging away of the DMI maps the initial XXZ spin-chain model with alternating DMI onto the effective spin $\tau = 1/2\ XXZ$ chain with alternating transverse exchange.

The continuum-limit bosonization approach

[*1] A. O. Gogolin, A. A. Nersesyan and A. M. Tsvelik, *Bosonization and strongly correlated systems*, Cambridge University Press (1998).

[*2]T. Giamarchi, *"Quantum Physics in One Dimension"* (Oxford University Press, Oxford, 2004).

To obtain the continuum version of the spin we use the standard bosonization expression of the spin operators [*1]

$$
\begin{aligned}
\tau_n^z &\simeq \sqrt{\frac{K}{\pi}}\partial_x\phi(x) + (-1)^n \frac{a}{\pi\alpha}\sin\sqrt{4\pi K}\phi(x)\,, \qquad (4) \\
\tau_n^\pm &\simeq \frac{b}{\pi\alpha}\cos(\sqrt{4\pi K}\phi)\, e^{\pm i\sqrt{\pi/K}\theta} \\
&- (-1)^n \frac{c}{\pi\alpha}\, e^{\pm i\sqrt{\pi/K}\theta}\,. \qquad (5)
\end{aligned}
$$

Here $\phi(x)$ and $\theta(x)$ are dual bosonic fields, $\partial_t\phi = u\partial_x\theta$, and satisfy the following commutational relation

$$
\begin{aligned}
[\phi(x), \theta(y)] &= i\Theta(y-x)\,, \\
[\phi(x), \theta(x)] &= i/2\,. \qquad (6)
\end{aligned}
$$

Here the non-universal real constants a, b and c depend smoothly on the parameter γ^*, are of the order of unity at $\gamma^* = 0$ expected to be nonzero everywhere at $|\gamma^*| < 1$. The Luttinger liquid parameter is known within the critical line $-1 < \gamma^* < 1$ to be

$$K = \frac{\pi}{2\arccos(-\gamma^*)} .$$

Thus the parameter K decreases monotonically from its maximal value $K \to \infty$ at $\gamma^* \to -1$ (ferromagnetic instability point), is equal to unity at $\gamma^* = 0$ ($J_z = 0$) and reaches the value $K = 1/2$ at $\gamma^* = 1$ (isotropic antiferromagnetic chain). In the case of dominating Ising type anisotropy, at $\gamma^* > 1$, $K < 1/2$.

Using (4)-(5) we finally obtain for the initial lattice Hamiltonian (3):

$$\mathcal{H} = u \int dx \left[\frac{1}{2}(\partial_x \phi)^2 + \frac{1}{2}(\partial_x \theta)^2 + \frac{m_0}{\pi\alpha^2} \cos\sqrt{4\pi K}\phi + \frac{M_0}{\pi\alpha^2} \cos\sqrt{16\pi K}\phi\right], \tag{7}$$

where

$$m_0 \simeq \delta = D_0 D_1 / J^{*\,2} ,$$
$$M_0 \simeq \gamma^* / 2\pi$$

and $u \simeq J^*/K$ stands for the velocity of spin excitation.

Thus the effective continuum-limit version of the initial lattice spin model is given by the **double-frequency sine-Gordon** (DSG) model.

$$\mathcal{H} = u\int dx\,\Big[\frac{1}{2}(\partial_x\phi)^2+\frac{1}{2}(\partial_x\theta)^2+\frac{m_0}{\pi\alpha^2}\cos\sqrt{4\pi K}\phi+\frac{M_0}{\pi\alpha^2}\cos\sqrt{16\pi K}\phi\Big]\,, \qquad (8)$$

[*3] R.K. Boullough, P.J. Caudrey, and H.M Gibbs in *Solitons* Springer-Verlag 1980,pg 107-141.

[*4] G. Delfino and G. Mussardo, Nucl. Phys. B **516**, 675 (1998).

The ground state properties of the DSG model are controlled by the scaling dimensions of the two *cosine* terms

$$d = dim[\cos\sqrt{4\pi K}\phi] = K \qquad d^* = dim[\cos\sqrt{16\pi K}\phi] = 4K$$

present in the Hamiltonian. Each of these *cosine* terms becomes relevant in the parameter range where the corresponding scaling dimensionality $d \leq 2$ or $d^* \leq 2$. Using (7) we find that $d \leq 2$, i.e. the first *cosine* term in (8) is relevant, at $\gamma^* > \gamma^*_{c1} = -\sqrt{2}/2$, while $d^* \leq 2$, i.e. the second *cosine* term in (8), for $\gamma^* > 1$. This gives following four segments of the model parameter range (see Fig.1), where each one corresponds to the different mechanisms of formation of the ground-state properties of the system:

The Ferromagnetic sector $\gamma^* \leq -1$

At $\gamma^* \leq -1$ the system is in the *ferromagnetic phase*, all spins are oriented along the z-axis

$$\langle \tau_n^z \rangle = \langle S_n^z \rangle = 1/2; \langle \tau_n^x \rangle = \langle \tau_n^y \rangle = 0$$

and therefore the effect of the DM interaction is completely suppressed.

The Luttinger-liquid sector $-1 < \gamma^* < \gamma^*_{c1}$

At $-1 < \gamma^* < \gamma^*_{c1}$, $d^* > d > 2$ and therefore both cosine terms in (8) are irrelevant and can be neglected. The gapless long-wavelength excitations of the anisotropic spin chain are described by the standard Gaussian theory with the Hamiltonian

$$\mathcal{H}_0 = u \int dx \left[\frac{1}{2} (\partial_x \phi)^2 + \frac{1}{2} (\partial_x \theta)^2 \right]. \tag{9}$$

In this *critical Luttinger-liquid phase*, all correlations show a power-law decay, with indices smoothly depending on the parameter K

The dimerized sector $\gamma^*_{c1} < \gamma^* \leq 1$

At $\gamma^*_{c1} < \gamma^* \leq 1$, $d < 2$ while $d^* > 2$, therefore the double-frequency cosine term is irrelevant and can be neglected. In this case infrared properties of the system are described by the sine-Gordon model

$$\mathcal{H} = u \int dx \left[\tfrac{1}{2}(\partial_x \phi)^2 + \tfrac{1}{2}(\partial_x \theta)^2 + \tfrac{m_0}{\pi\alpha^2} \cos\sqrt{4\pi K}\phi\right]. \tag{10}$$

With increasing γ^*, the scaling dimensionality of the *relevant cosine* term changes from the marginal value $d = 2$ at $\gamma^* = \gamma^*_{c1}$, to $d = 1/2$ at $\gamma^* = 1$. Thus, at $\gamma^* = \gamma^*_{c1} \simeq -0.7$ the BKT ground state of the system, the excitation gap opens at $\gamma^* = \gamma^*_{c1}$ and remains finite in the whole region $-0.7 < \gamma^* \leq 1$.

Exact solution of the quantum sine-Gordon model
V. E. Korepin and L. D. Faddeev, Theor. Math. Phys. **25**, 1039 (1975).
Al. B. Zamolodchikov, Int. J. Mod. Phys. A **10**, 1125 (1995).
it is known that for arbitrary finite m_0 the gapped excitation spectrum of the Hamiltonian Eq. (10) at $2 > d > 1$ $(-0.7 < \gamma^* \leq 0)$, consists of solitons and antisolitons with masses

$$\mathcal{M}_{sol} \sim \left(m_0/J^*\right)^{\frac{1}{2-d}} = \left(m_0/J^*\right)^{\frac{1}{2-K}},$$

while at $1 > d \geq 1/2$ $(0 < \gamma^* \leq 1)$ in addition, also of soliton-antisoliton bound states ("breathers") with the lowest breather mass

$$\mathcal{M}_{br} = 2\mathcal{M}_{sol} \sin\left(\frac{\pi K}{4 - 2K}\right).$$

The excitation gap is exponentially small at the BKT phase transition point

$$\Delta_{exc} \sim J^* \exp\left(-1/(\gamma^* - \gamma^*_{c1})\right) \ ,$$

it smoothly increases with increasing γ^*, and at $\gamma^* = 0$

$$\Delta_{exc} = 2J^*\mathcal{M}_{sol} = 2m_0 = 2D_0 D_1/J^* \, .$$

Finally, at $\gamma^* = 1$ the gap is

$$\Delta_{exc} = J^*\mathcal{M}_{br} = J^* \left(D_0 D_1/{J^*}^2\right)^{2/3} \ .$$

The gap in the excitation spectrum leads to suppression of fluctuations in the system and the ϕ field is condensed in one of its vacua ensuring the minimum of the dominating potential energy

$$\sqrt{4\pi K}\langle\phi\rangle = \left\{ \begin{array}{lll} \pi & \text{at} & m_0 > 0 \\ 0 & \text{at} & m_0 < 0 \end{array} \right. \ . \tag{11}$$

Trapping of the ϕ field in one of the vacua from the given set leads to suppression of the site-located magnetic degrees of freedom

$$\langle \tau_n^z \rangle = \langle \tau_n^x \rangle = \langle \tau_n^y \rangle = 0.$$

Respectively we obtain, that the site-located magnetic order is also fully suppressed in the initial spin chain system:

$$\langle S_n^z \rangle = \langle S_n^x \rangle = \langle S_n^y \rangle = 0.$$

Moreover, if we consider the link-located degrees of freedom, using (4)-(5) one obtains that the continuum limit bosonized version of the τ-spin chirality operator is given by

$$\kappa_n^{(\tau)} = -i\left(\tau_n^+ \tau_{n+1}^- - h.c.\right) \to \frac{2}{\sqrt{\pi}}\partial_x\theta + (-1)^n \frac{2b}{\pi\alpha}\sin(\sqrt{4\pi K}\phi)$$

and therefore in the gapped phase, where $\sqrt{4\pi K}\langle\phi\rangle = 0$ mod π $\kappa_n^{(\tau)}\rangle = 0$.

However, the bosonized expressions for the staggered parts of the τ-spin longitudinal and transverse nearest-neighbor spin exchange operators

$$\epsilon_\perp^{(\tau)}(n) = \frac{(-1)^n}{2}\left(\tau_n^+ \tau_{n+1}^- + h.c.\right) \sim \frac{a}{2\pi^2\alpha^2}\cos(\sqrt{4\pi K}\phi) \qquad (12)$$

$$\epsilon_z^{(\tau)}(n) = (-1)^n \tau_n^z \tau_{n+1}^z \sim \frac{b}{\pi\alpha}\cos(\sqrt{4\pi K}\phi) \qquad (13)$$

are characterized a finite vacuum expectation value in the gapped phase and therefore, in the given gapped sector of the phase diagram we find the presence of the long-range dimerization pattern in the ground state:

$$(-1)^n \langle\, \epsilon_{\perp}^{(\tau)}(n)\,\rangle \sim (-1)^n \langle\, \epsilon_{z}^{(\tau)}(n)\,\rangle \simeq \epsilon$$

where

$$\epsilon = \langle\, \cos\sqrt{2\pi K}\phi\,\rangle \simeq m_0^K = \left(D_0 D_1/{J^{*}}^{2}\right)^K$$

at weak coupling ($m_0 << J^*$) and becomes of the unit order in the strong coupling, at $m_0 \geq J^*$.

Turning back to initial spins gives that in the gapped phase the initial spin chain shows a long-range dimerization order

$$\frac{1}{L}\sum_n (-1)^n \langle\, \mathbf{S}_n \cdot \mathbf{S}_{n+1}\,\rangle \sim (\cos\vartheta_+ - \cos\vartheta_-)\,\epsilon\,,$$

which coexists with the long-range order pattern of the alternating spin chirality vector

$$\frac{1}{L}\sum_n (-1)^n \langle\, \kappa_n^z \rangle \sim (\sin\vartheta_+ - \sin\vartheta_-)\,\epsilon\,.$$

The Ising type sector $\gamma^* > 1$

At $\gamma^* > 1$ both cosine terms in (8) are relevant and, in principle, have to be considered on equal grounds. Therefore in this case the low-energy sector of the initial spin chain is given in terms of the double sine-Gordon model

$$\mathcal{H} \quad = \quad u \int dx \left[\frac{1}{2}(\partial_x \phi)^2 + \frac{1}{2}(\partial_x \theta)^2 + \frac{m_0}{\pi\alpha^2}\cos\beta\phi + \frac{M_0}{\pi\alpha^2}\cos 2\beta\phi\,\right], \tag{14}$$

with $\beta = \sqrt{4\pi K}$, which describes an interplay between two relevant perturbations to the Gaussian conformal field theory H_0 with the ratio of their scaling dimensions equal to 4.

Since both terms are relevant, acting separately, each leads to the pinning of the field ϕ in corresponding minima, however because these two perturbations have *different parity symmetries*, the field configurations which minimize one perturbation do not minimize the other.

This competition between possible sets of vacuum configurations of the two *cosine* terms is resolved via the presence of the *quantum phase transition* in the ground state. The very presence of the QPT can already be traced performing minimization of the potential

$$\mathcal{V}(\phi) \quad = \quad m_0 \cos\beta\phi + M_0 \cos 2\beta\phi\,, \tag{15}$$

where the transition corresponds to the crossover from a single well to a double well profile of the potential.

Indeed, one can easily obtain, that at $M_0 < m_0/4$ the vacuum expectation value of ϕ field which minimizes $\mathcal{V}(\phi)$ is given by $< \phi >= 0$ and therefore in this case the dimerized phase is realized ground state. However, at $M_0 > m_0/4$, instead of (11) the ϕ field is condensed in the minima

$$\langle \phi \rangle = \phi_0 = \frac{1}{\beta} \arccos{(m_0/4M_0)} \tag{16}$$

and, as the result, in addition to the dimerization pattern

$$(-1)^n \langle \, \epsilon_i^{(\tau)}(n) \, \rangle \sim \langle \, \cos(\sqrt{4\pi K}\phi_0) \rangle \;\; i = \perp, z \tag{17}$$

the ground state of the τ-spin system is characterized by the long range antiferromagnetic order with the amplitude of the staggered magnetization

$$m = (-1)^n \langle \, \tau_n^z \, \rangle \sim \sin\sqrt{4\pi K}\phi_0 \, . \tag{18}$$

Following the analysis [G. Delfino and G. Mussardo, Nucl. Phys. B **516**, 675 (1998)] one can show that the model displays an Ising criticality with **central charge $c = 1/2$ on a quantum critical line**. The critical properties of this transition have been investigated in detail by mapping the DSG model onto the deformed quantum Ashkin-Teller model [M. Fabrizio, A. O. Gogolin, A. A. Nersesyan, Phys. Rev. Lett. **83** 2014 (1999).]

The dimensional arguments based on equating physical masses produced by the two cosine terms separately is usually used to define the critical line. Using (11) one finds

$$\left\{ \begin{array}{ccc} m & = & m_0^{1/(2-K)} \\ M & = & M_0^{1/(2-4K)} \end{array} \right.$$

Equating these two masses we obtain the following expression for the critical value of the chain anisotropy parameter vs. DM coupling:

$$\gamma^*_{c2} = 1 + \left(\frac{D_0 D_1}{J^{*\,2}}\right)^{\frac{2-4K}{2-K}} \quad .$$

Numerical Results

The computations were carried out for finite-length systems with $L = 48, 64, 96$ and 128 sites, using the ALPS library

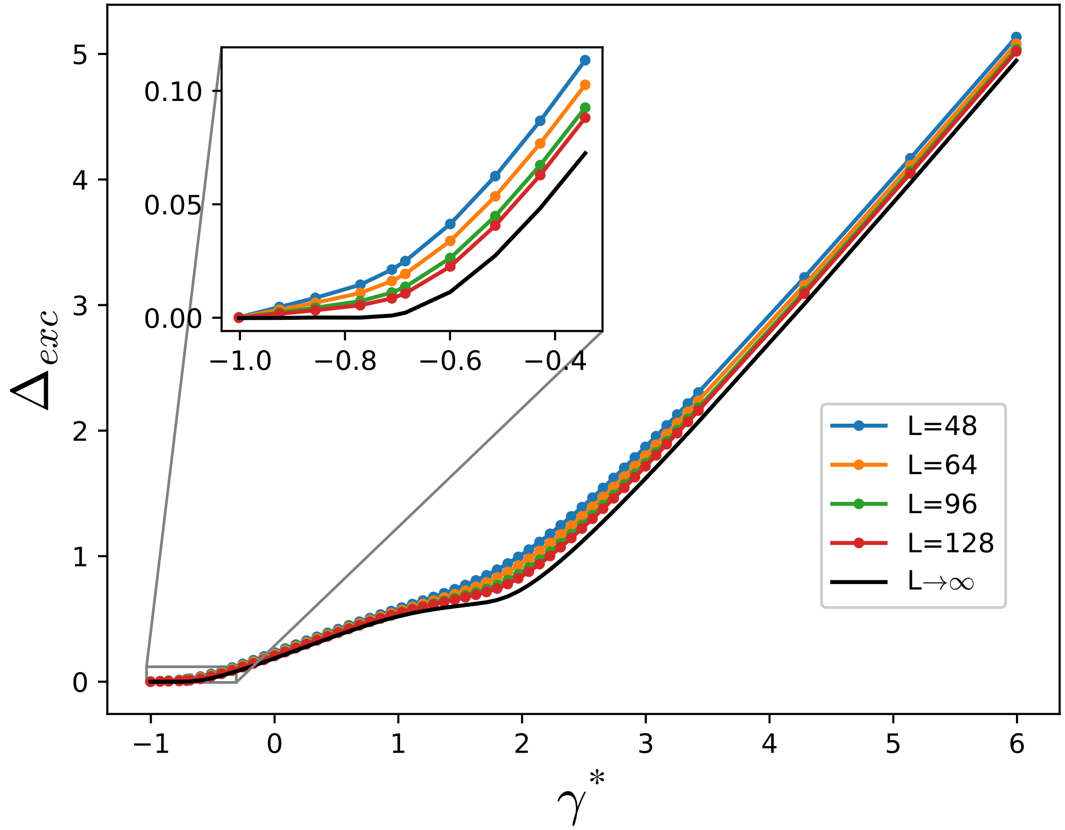
[**1] A.F. Albuquerque et al. (ALPS collaboration), Journal of Magnetism and Magnetic Materials **310**, 1187 (2007).

[**2] B. Bauer et al. (ALPS collaboration), Journal of Statistical Mechanics: Theory and Experiment **05**, P05001 (2011).

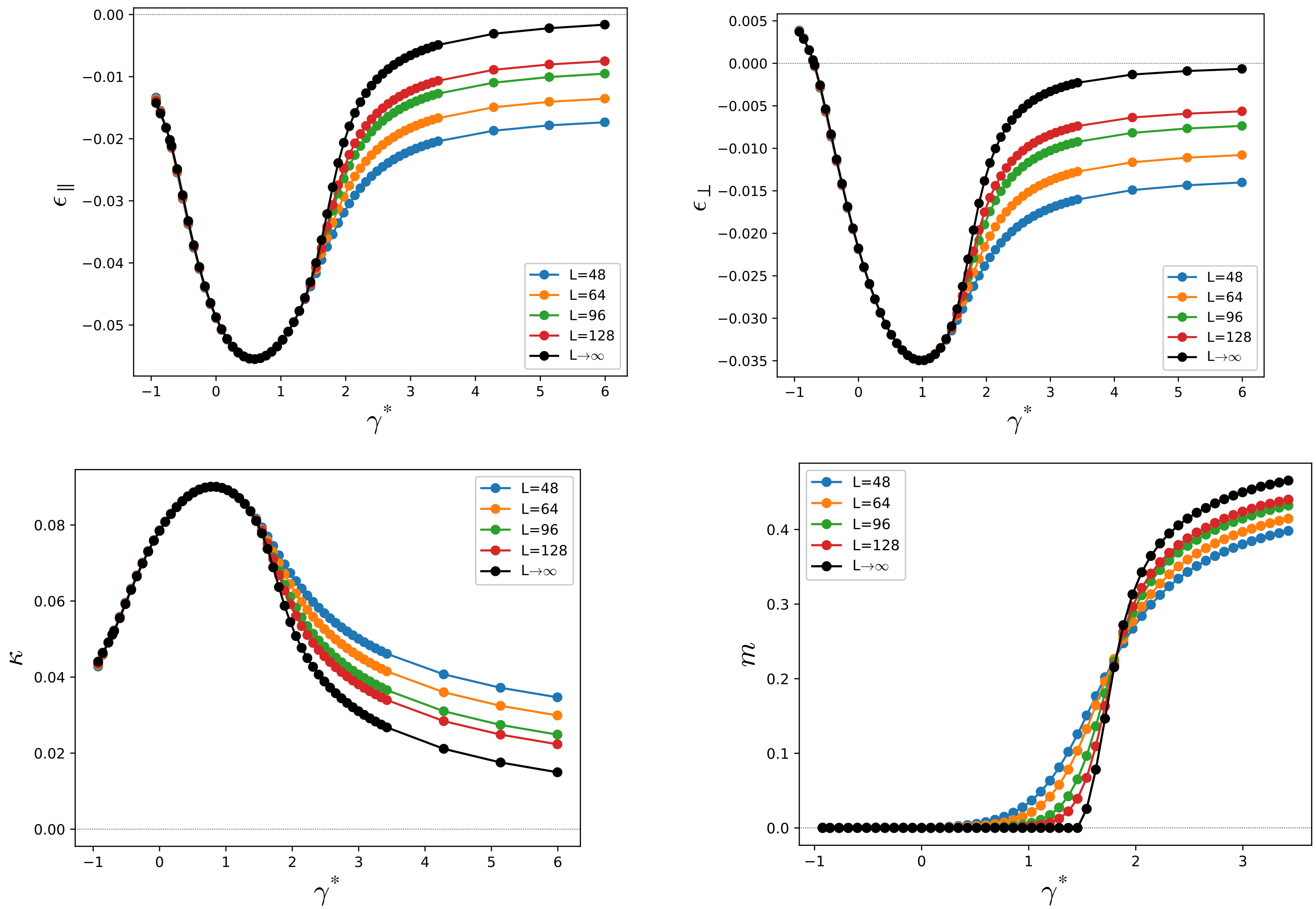
System parameters are set to $J = 1$, $D_0 = tan(\pi/6)$ and $D_1 = 0.2$, while the bare value of the anisotropy Δ is varied providing values of $-1 < \gamma^* \leq 6$. This restricts the ground state analysis to the $S_z^{tot} = 0$ subspace.

Excitation gap.

$$\Delta_{exc} = E_0(N+1) + E(N+1) - 2E(N)\,, \tag{19}$$

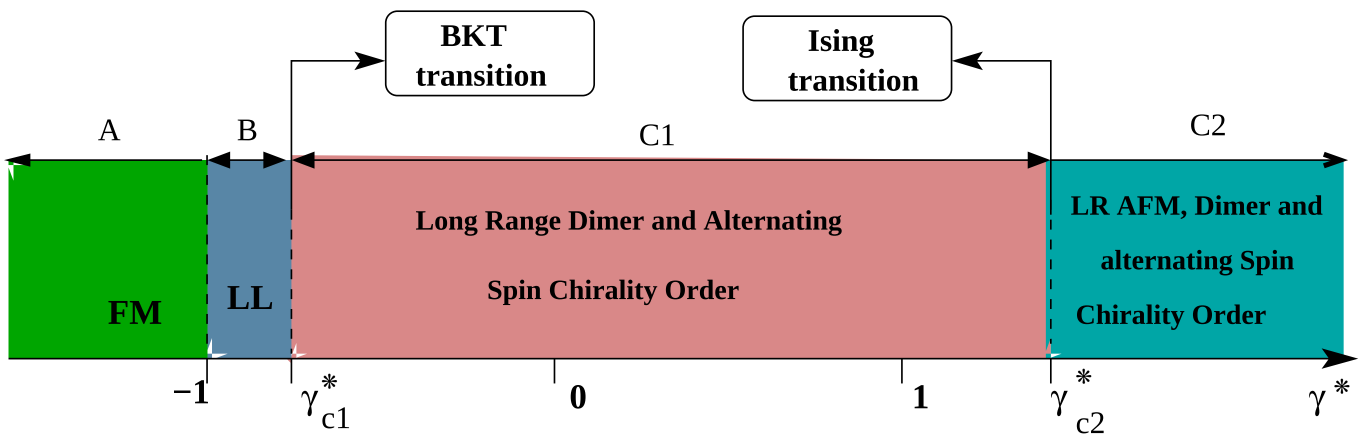


Order Parameters



Summary

We have studied the ground-state properties of the one-dimensional spin $S = 1/2$ XXZ Heisenberg chain with spatially modulated Dzyaloshinskii-Moriya (DM) interaction. Our goal was to describe the interplay between the uniform and staggered parts of the DM interaction which, when acting alone, do not change the excitation spectrum of the system. We have shown that joint effect of the uniform and staggered components of the DM coupling opens a possibility for formation of unconventional gapped phases in the ground-state of the system



Thank you for attention!