Electric field driven flat bands in $S = 1/2$ sawtooth chain.

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Outline

- **Magnetoelectric Effect (MEE)**
  - General points
  - Katsura-Nagaosa-Balatsky (KNB) mechnism
- **Localized magnon states.**
- **Sawtooth chain**
  - Ground states and excitations
  - Flat bands and localized magnons
- **KNB mechanism in sawtooth chain and electric field driven flat bands**
  - Hamiltonian
  - Wide spectrum of flat bands for three couplings
  - Electric field driven flat bands
- **Conclusion**

Magnetoelectric effect

MEE denominates the mutual influence of the electric and magnetic properties in matter. In its most prominent form, MEE can be defined as the magnetic field dependence of (ferro)electric polarization and the electric field dependence of magnetization.

$$\alpha_{ij} = \left(\frac{\partial P_i}{\partial H_j}\right)_{T,\mathbf{E}} = \left(\frac{\partial M_j}{\partial E_i}\right)_{T,\mathbf{H}}$$

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KATSURA-NAGAOSA-BALATSKY (KNB) MECHANISM

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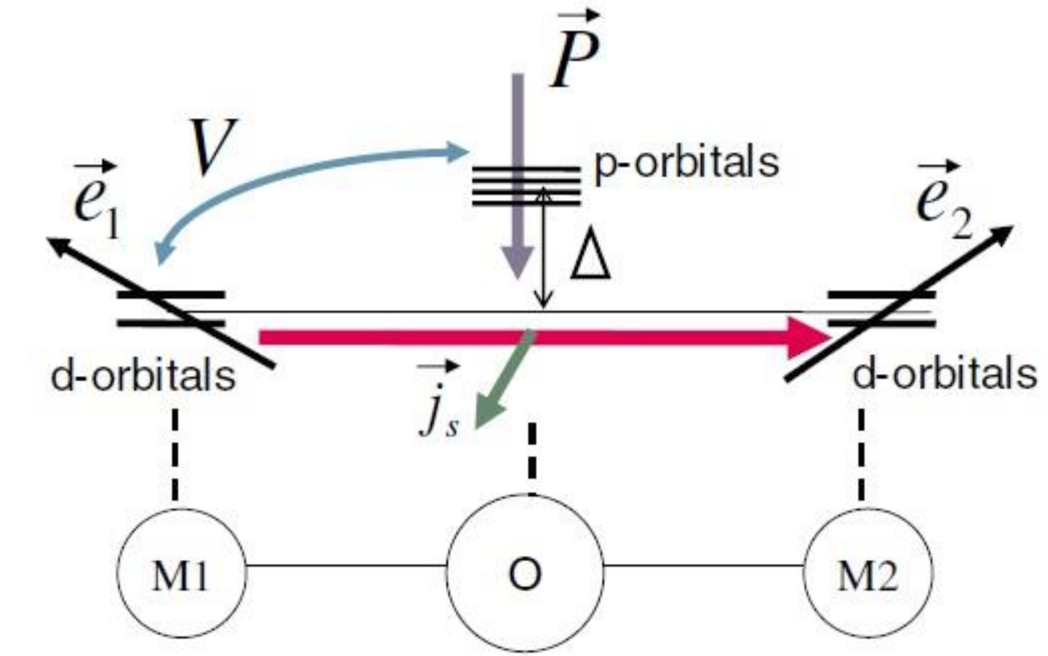

$$H' = H'_{\mathrm{M}} + H'_{\mathrm{O}} + H'_{V},$$

$$H'_{\mathrm{M}} = -U \sum_{a=l,r} (d^{+}_{a,xy} d_{a,xy} + d^{+}_{a,zx} d_{a,zx}),$$

$$H'_{\mathrm{O}} = E_p \sum_{\sigma} (p^{+}_{y\sigma} p_{y\sigma} + p^{+}_{z\sigma} p_{z\sigma}),$$

$$H'_{V} = V(d^{+}_{l,xy} p_{l,y} + d^{+}_{l,zx} p_{l,z} - d^{+}_{r,xy} p_{r,y} - d^{+}_{r,zx} p_{r,z} + \mathrm{H.c.})$$

$$\mathbf{P}_i \sim \mathbf{e}_{ij} \times (\mathbf{S}_i \times \mathbf{S}_j)$$

KNB mechanism in one-dimensional quantum spin models

$$[S_j^a, S_l^b] = i\delta_{jl}\epsilon^{abc}S_j^c, \quad a,b,c = x,y,z$$
$$\mathbf{S}_j \cdot \mathbf{S}_j = \frac{3}{4}$$

$$P_x = 0\,,$$
$$P_y = \gamma\frac{1}{N}\sum_{n=1}^{N}\left(S_n^y S_{n+1}^x - S_n^x S_{n+1}^y\right)$$
$$P_z = \gamma\frac{1}{N}\sum_{n=1}^{N}\left(S_n^z S_{n+1}^x - S_n^x S_{n+1}^z\right)$$

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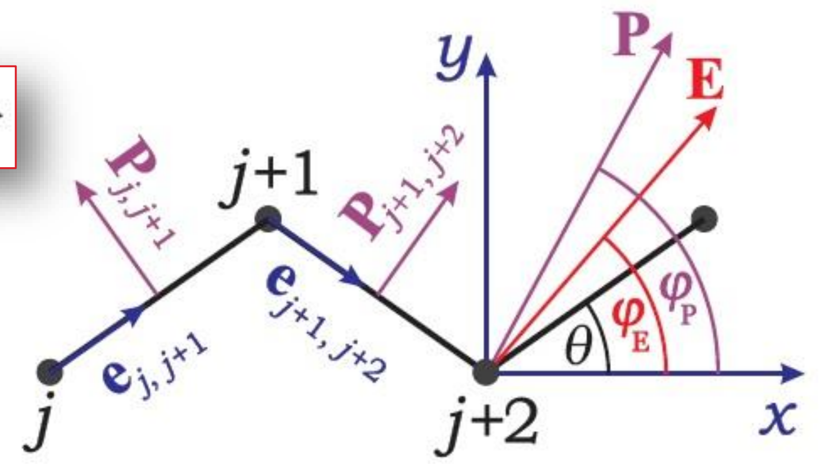
Spin-1/2 XY chain magnetoelectric: Effect of zigzag geometry

$$\mathbf{P}_{j,j+1} = \gamma\left(\cos\theta_j\ \mathbf{e}_x + \sin\theta_j\ \mathbf{e}_y\right) \times \mathbf{S}_j \times \mathbf{S}_{j+1}.$$



The zigzag chain with indicated system axes, electric field vector $\mathbf{E}$, polarization $\mathbf{P}$, bond polarization $\mathbf{P}_{j,j+1}$, and unit vector $\mathbf{e}_{j,j+1}$ pointing from the jth site to the $(j+1)$th site. Here the z component of the bond polarization is equal zero because $\mathbf{E} = (E_x, E_y, 0)$.

$$H = J\sum_{i=1}^{N}\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) - h\sum_{i=1}^{N} S_i^z - J\sum_{i=1}^{N}\mathbf{E}\cdot\mathbf{P}_{i,i+1}.$$

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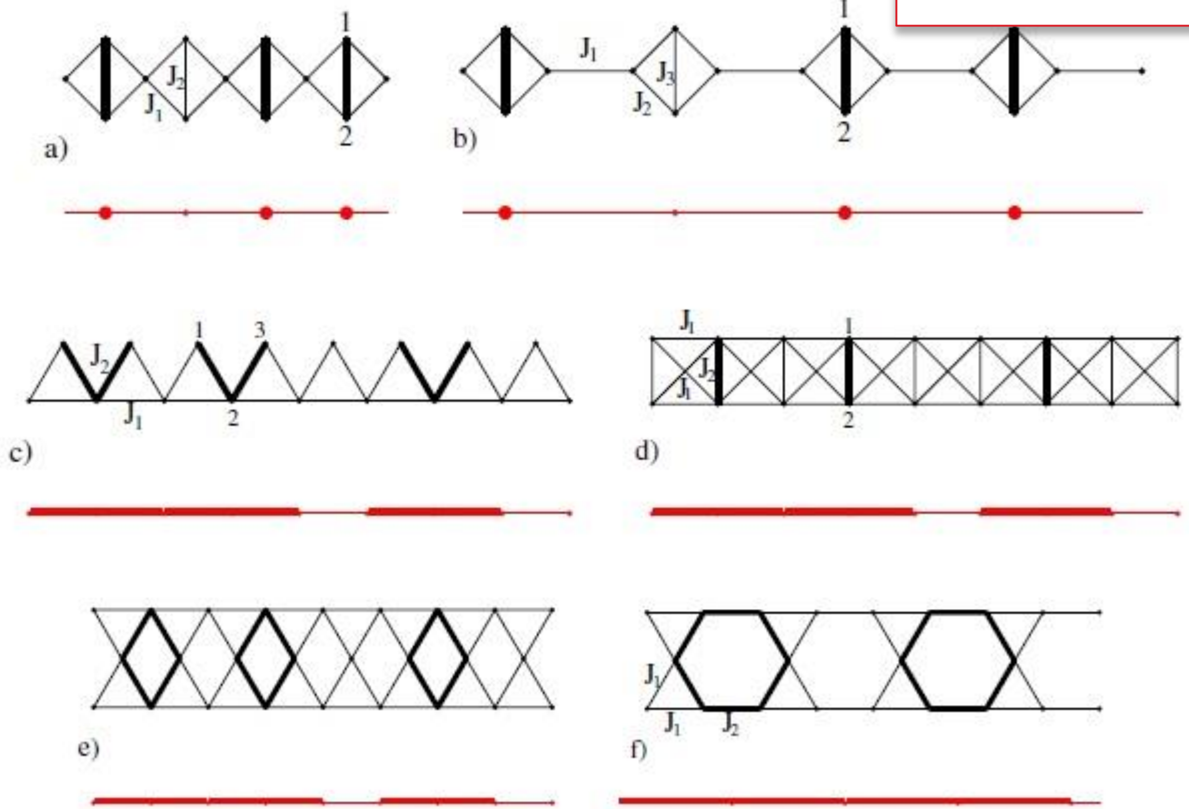
Localized Magnon states

$$|l_j\rangle = \sum_{j \in \mathcal{L}_j} a_j S_j^- |\uparrow\uparrow \ldots \uparrow\rangle$$



Several one-dimensional frustrated quantum spin lattices supporting localized magnon states: the diamond chain [14] (a), the dimer-plaquette chain [15] (b), the sawtooth chain [16] (c), the two-leg ladder (the spins are sitting only on the squares, not on the intersections of the diagonals) [17] (d), and two kagomé-like chains [18,19] (e and f). The trapping cells occupied by localized magnons are shown by fat lines. Below each lattice we show the corresponding auxiliary lattice filled by hard-core objects (monomers (a and b) and dimers (c, d, e and f)).

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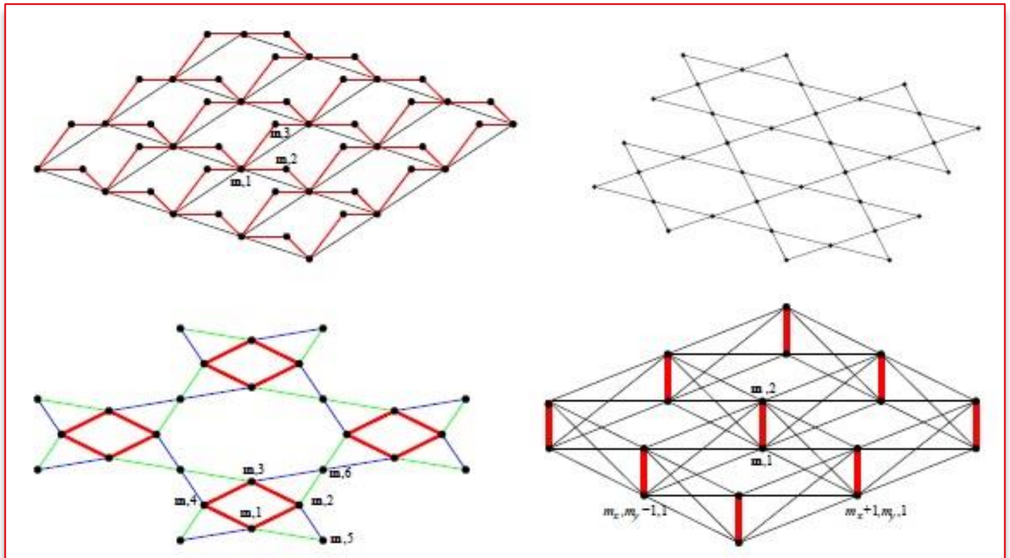
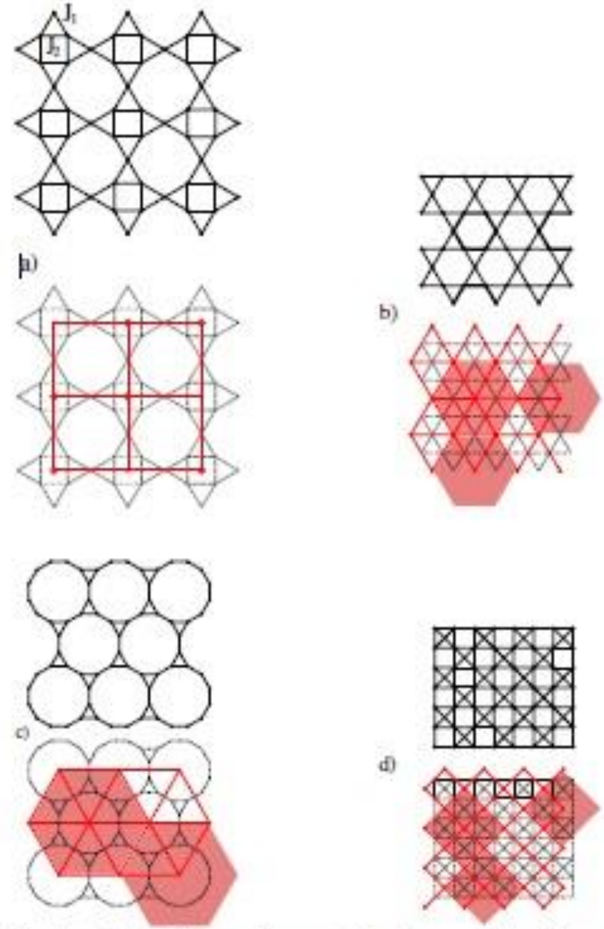
Localized Magnon states





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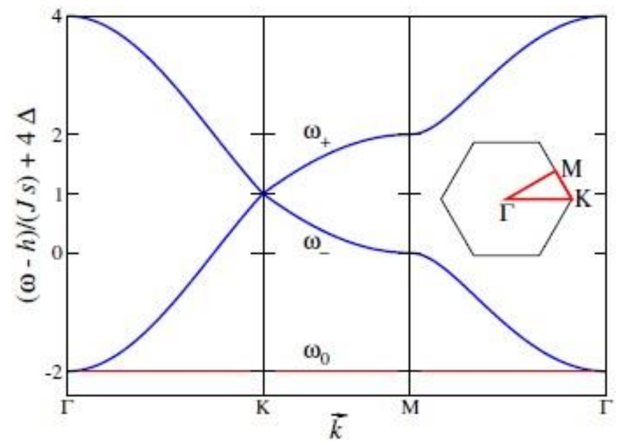
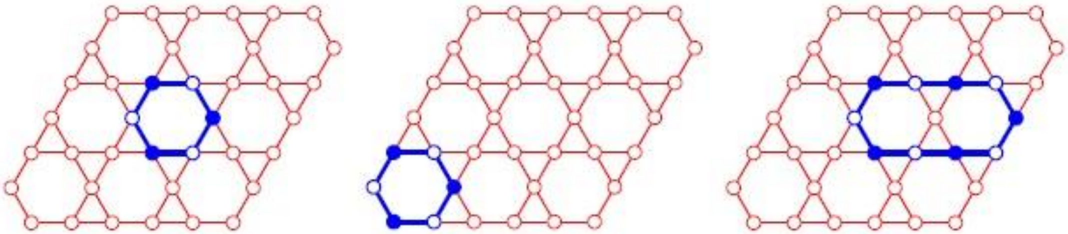
Flat bands. Kagome lattice



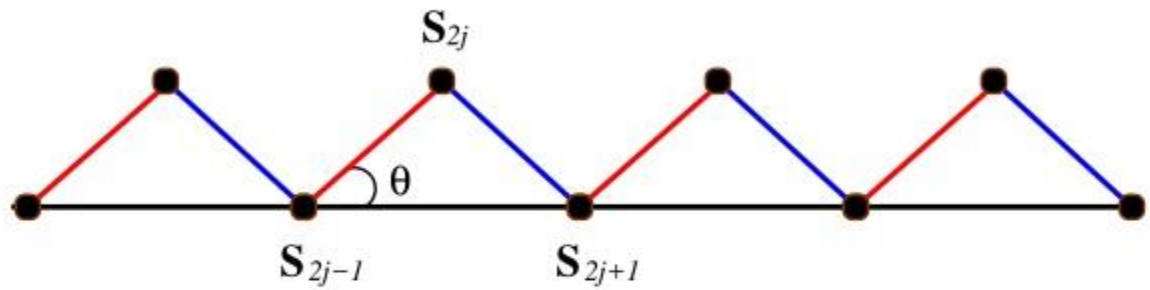
The three bands $\omega_l(\vec{k})$ of single-magnon energies on the kagome lattice along the path in the Brillouin zone shown in the inset. Note that $\omega_0(\vec{k})$ is completely independent of $\vec{k}$.



$$\omega_0(k_x, k_y) = h - J\,s\,(2 + 4\,\Delta),$$

$$\omega_\pm(k_x, k_y) = h + J\,s\left(1 \pm 1\sqrt{1 + 4\,\cos\left(\frac{k_x}{2}\right)\left(\cos\left(\frac{\sqrt{3}\,k_y}{2}\right) + \cos\left(\frac{k_x}{2}\right)\right)} - 4\,\Delta\right)$$

Sawtooth chain (Delta-chain)



$$\mathcal{H} = J_1 \sum_{j=1}^{N/2} \mathbf{S}_{2j-1}\mathbf{S}_{2j+1} + J_2 \sum_{j=1}^{N/2} \mathbf{S}_{2j-1}\mathbf{S}_{2j} + J_3 \sum_{j=1}^{N/2} \mathbf{S}_{2j}\mathbf{S}_{2j+1}$$

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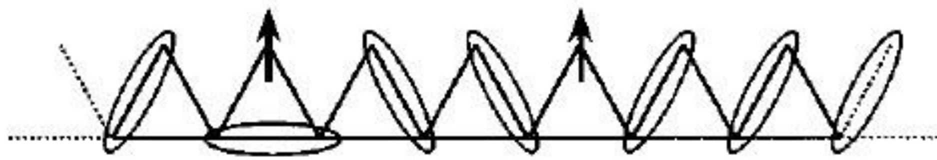
Sawtooth chain (Delta-chain)



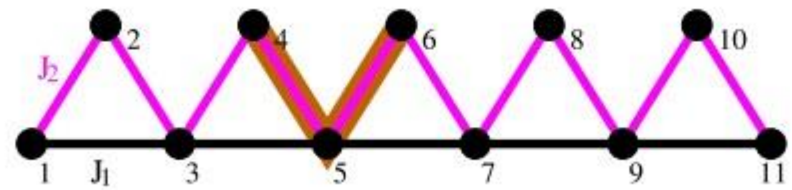
An excited state of the periodic Δ chain. The up spin that has a dimer singlet pair in its triangle is what we call a "kink" and the other one is an "antikink."

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j, \quad (J_1 = J_2 = J_3 \equiv J)$$

$$|S\rangle_{(i,j)} = \frac{1}{\sqrt{2}} \left(| \uparrow_i \downarrow_j \rangle - | \downarrow_i \uparrow_j \rangle \right)$$

$$|GS_L\rangle = \prod_{j=1}^{N/2} |S_{2j-1,2j}\rangle \qquad |GS_R\rangle = \prod_{j=1}^{N/2} |S_{2j,2j+1}\rangle$$

Sawtooth chain (Delta-chain)



$$\mathcal{H} = J_1 \sum_{j=1}^{N/2} \left(S^x_{2j-1} S^x_{2j+1} + S^y_{2j-1} S^y_{2j+1} + \Delta_1 S^z_{2j-1} S^z_{2j+1} \right) + J_2 \sum_{j=1}^{N/2} \mathbf{S}_{2j} \cdot \left(\mathbf{S}_{2j-1} + \mathbf{S}_{2j+1} \right) - B \sum_{j=1}^{N} S^z_j$$

- $J_2 = 2J_1,\ \Delta_1 = 1$
- $J_2 = -2J_1,\ \Delta_1 = 1$
- $J_2 = J_1,\ \Delta_1 = -\frac{1}{2}$

$|l_j\rangle = l_j| \uparrow\uparrow \ldots \uparrow\rangle$

$$l_j = S^-_{2j-1} - 2S^-_{2j-1} + S^-_{2j}, \quad J_2 = 2J_1, \ \Delta_1 = 1$$
$$l_j = S^-_{2j-1} - 2S^+_{2j-1} + S^-_{2j}, \quad J_2 = -2J_1, \ \Delta_1 = 1$$
$$l_j = S^-_{2j-1} - S^+_{2j-1} + S^-_{2j}, \quad J_2 = J_1, \ \Delta_1 = -\frac{1}{2}$$

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KNB mechanism in sawtooth chain

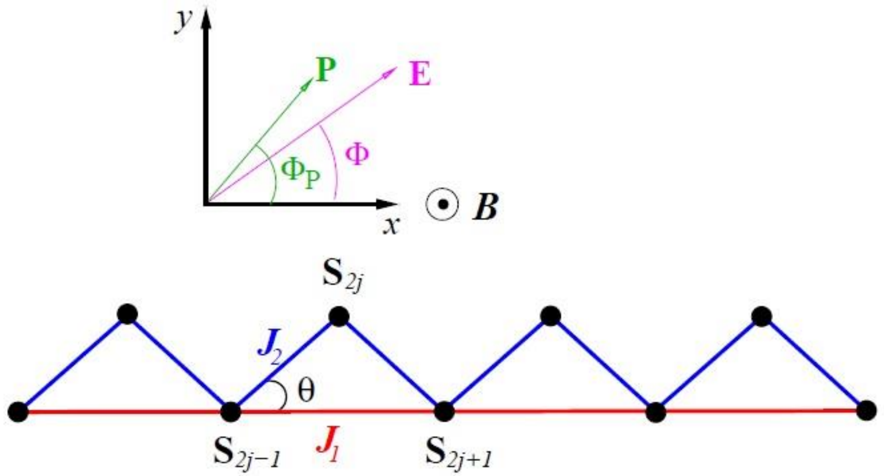


FIG. 1. (Color online) Sketch of the sawtooth chain together with the electric field $\mathbf{E}$, the z-aligned magnetic field H and the resulting electric polarisation $\mathbf{P}$. For the plane defined by

$$-\quad \mathbf{E}\cdot\mathbf{P} = \sum_{j=1}^{N} \left(E_y\cos\theta + (-1)^j E_x \sin\theta\right)\left(S_j^x S_{j+1}^y - S_j^y S_{j+1}^x\right) + \alpha E_y \sum_{j=1}^{N/2}\left(S_{2j-1}^x S_{2j+1}^y - S_{2j-1}^y S_{2j+1}^x\right)$$

KNB mechanism in sawtooth chain

$$\mathcal{H} = \sum_{j=1}^{N/2}\left(\frac{J_1+iD_1}{2}S^+_{2j-1}S^-_{2j+1}+\frac{J_1-iD_1}{2}S^-_{2j-1}S^+_{2j+1}+J_1\Delta_1 S^z_{2j-1}S^z_{2j+1}\right)$$
$$+\sum_{j=1}^{N/2}\left(\frac{J_2+iD_2}{2}S^+_{2j-1}S^-_{2j}+\frac{J_2-iD_2}{2}S^-_{2j-1}S^+_{2j}+J_2\Delta_2 S^z_{2j-1}S^z_{2j}\right)$$
$$+\sum_{j=1}^{N/2}\left(\frac{J_3+iD_3}{2}S^+_{2j}S^-_{2j+1}+\frac{J_3-iD_3}{2}S^-_{2j}S^+_{2j+1}+J_3\Delta_3 S^z_{2j}S^z_{2j+1}\right)-B\sum_{j=1}^{N}S^z_J.$$

$$D_1 = \alpha E\sin\phi,$$
$$D_2 = E(\sin\phi\cos\theta+\cos\phi\sin\theta),$$
$$D_3 = E(\sin\phi\cos\theta-\cos\phi\sin\theta),$$

$$S^\pm_j = S^x_j \pm iS^y_j$$

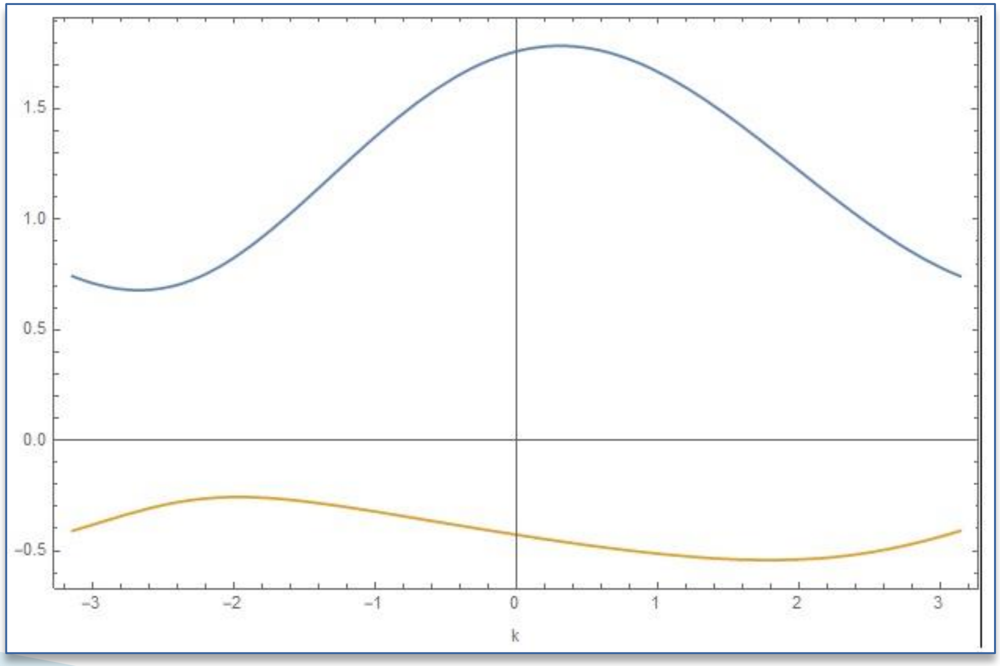
KNB mechanism in sawtooth chain

One-magnon spectrum

$$|1_k\rangle = \sum_{l=0,1} a_l \sum_{j=1}^{N/2} e^{ijk} S^-_{2j+l} |FM\rangle,$$

$$\varepsilon_1^{\pm}(k) = B - \Gamma + \frac{1}{2}\left[\widetilde{J}_1 \cos(k-k_1) \pm \sqrt{\left(J_1\Delta_1 - \widetilde{J}_1\cos(k-k_1)\right)^2 + 2\widetilde{J}_2\widetilde{J}_3\cos(k-k_2-k_3) + \widetilde{J}_2^2 + \widetilde{J}_3^2}\right]$$

$$\Gamma = \frac{1}{2}\left(J_1\Delta_1 + J_2\Delta_2 + J_3\Delta_3\right)$$
$$\widetilde{J}_a = \sqrt{J_2^2 + D_a^2}$$
$$k_a = \arctan\frac{D_a}{J_a}$$
$$a = 1, 2, 3$$



KNB mechanism in sawtooth chain

Flat band conditions

$$\frac{D_1}{J_1} = \frac{\frac{D_2}{J_2} + \frac{D_3}{J_3}}{1 - \frac{D_2 D_3}{J_2 J_3}},$$

$$\left(\frac{\widetilde{J}_2 \widetilde{J}_3}{\widetilde{J}_1} - J_1 \Delta_1 \right)^2 = (J_1 \Delta_1)^2 + \widetilde{J}_2^2 + \widetilde{J}_3^2.$$

For all possible variants of the flat bands Δ_2 and Δ_3 do not affect it and can be chosen arbitrary

Excluding D_1 form the equations

$$(J_2 J_3 - J_1^2 \Delta_1 - D_2 D_3)^2 = J_1^2 (J_1^2 \Delta_1^2 + J_2^2 + J_3^2 + D_2^2 + D_3^2)$$

Flat bands in $J_1 - J_2 - J_3$ XXZ sawtooth chain

$D_1 = D_2 = D_3 = 0$

$$J_1 = \pm \frac{J_2 J_3}{\sqrt{J_2^2 + J_3^2 + 2J_2 J_3 \Delta_1}}$$

$$J_3 = J_2$$
$$J_2 = \pm J_1 \sqrt{2(1+\Delta_1)}$$

- $J_2 = 2J_1,\ \Delta_1 = 1$
- $J_2 = -2J_1,\ \Delta_1 = 1$
- $J_2 = J_1,\ \Delta_1 = -\frac{1}{2}$

$$\varepsilon_1^{+}(k) = B + J_1\left(1 \mp \Delta_2\sqrt{2(1+\Delta_1)}\right) + J_1 \cos k,$$
$$\varepsilon_1^{-}(k) = B - J_1\left(1 + \Delta_1 \pm \Delta_2\sqrt{2(1+\Delta_1)}\right),$$

$$B_{sat} = \begin{cases} \frac{1}{2}\left(J_1(1+\Delta_1) + |J_1(1+\Delta_1)| + 2J_2\Delta_2\right), & J_2^2 < 2J_1^2(1+\Delta_1) \\ J_1\left(1 + \Delta_1 \pm \Delta_2\sqrt{2(1+\Delta_1)}\right), & J_2^2 = 2J_1^2(1+\Delta_1) \\ \frac{1}{2}\left(J_1(\Delta_1 - 1) + 2J_2\Delta_2 + \sqrt{J_1^2(1-\Delta_1)^2 + 4J_2^2}\right), & J_2^2 > 2J_1^2(1+\Delta_1) \end{cases}$$

Flat bands in $J_1 - J_2 - J_3$ XXZ sawtooth chain

$$J_1 = \pm \frac{J_2 J_3}{\sqrt{J_2^2 + J_3^2 + 2J_2 J_3 \Delta_1}}$$

$$\varepsilon_1^+(k) = B + \frac{1}{2}\left(\sqrt{J_2^2 + J_3^2 + 2J_2J_3\Delta_1} - J_2\Delta_2 - J_3\Delta_3\right) + \frac{J_2J_3}{\sqrt{J_2^2 + J_3^2 + 2J_2J_3\Delta_1}}(\cos k - \Delta_1),$$

$$\varepsilon_1^-(k) = B - \frac{1}{2}\left(\sqrt{J_2^2 + J_3^2 + 2J_2J_3\Delta_1} + J_2\Delta_2 + J_3\Delta_3\right).$$

$$B_{sat} = \begin{cases} \frac{1}{2}\left(J_1(\Delta_1 - 1) + J_2\Delta_2 + J_3\Delta_3 + \sqrt{J_1^2(\Delta_1-1)^2 + (J_2+J_3)^2}\right), & J_1 < \frac{J_2J_3}{\sqrt{J_2^2+J_3^2+2J_2J_3\Delta_1}} \\ \frac{1}{2}\left(J_2\Delta_2 + J_3\Delta_3 + \sqrt{J_2^2 + J_3^2 + 2J_2J_3\Delta_1}\right), & J_1 = \frac{J_2J_3}{\sqrt{J_2^2+J_3^2+2J_2J_3\Delta_1}} \\ \frac{1}{2}\left(J_1(\Delta_1 + 1) + J_2\Delta_2 + J_3\Delta_3 + \sqrt{J_1^2(\Delta_1+1)^2 + (J_2-J_3)^2}\right), & J_1 > \frac{J_2J_3}{\sqrt{J_2^2+J_3^2+2J_2J_3\Delta_1}} \end{cases}$$

Flat bands in $J_1 - J_2 - J_3$ XXZ sawtooth chain

$$\varepsilon_1^+(k) = B - J_1\Delta_1 - \frac{J_2}{2}\left(\Delta_2 + \frac{J_1\Delta_3 - J_2}{J_2^2 - J_1^2}\left(J_1\Delta_1 + \sqrt{J_1^2(\Delta_1^2 - 1) + J_2^2}\right)\right) + J_1\cos k,$$

$$\varepsilon_1^-(k) = B - \frac{J_2}{2}\left(\Delta_2 + \frac{J_1\Delta_3 + J_2}{J_2^2 - J_1^2}\left(J_1\Delta_1 + \sqrt{J_1^2(\Delta_1^2 - 1) + J_2^2}\right)\right).$$

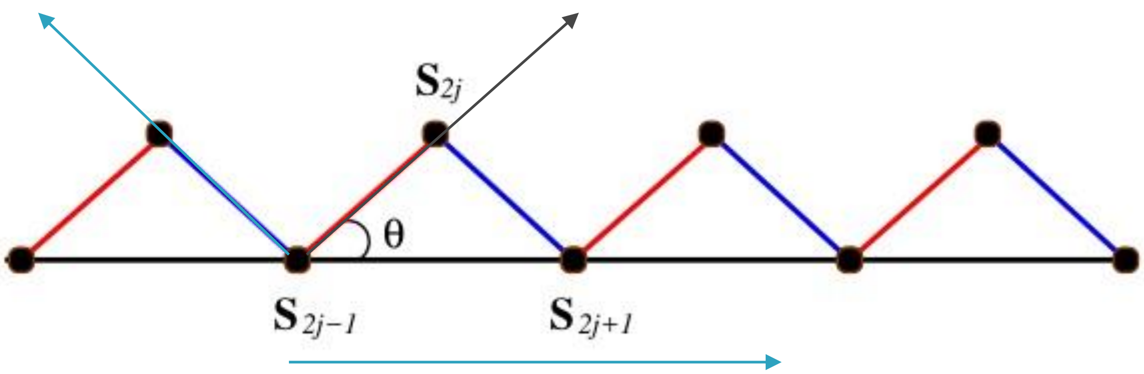
$$B_{sat} = \begin{cases} \frac{1}{2}\left(J_1(\Delta_1 + 1) + J_2\Delta_2 + J_3\Delta_3 + \sqrt{J_1^2(\Delta_1 + 1)^2 + (J_2 - J_3)^2}\right), & J_3 < J_3^{fb} \\ \frac{J_2}{2}\left(\Delta_2 + \frac{J_1\Delta_3 + J_2}{J_2^2 - J_1^2}\left(J_1\Delta_1 + \sqrt{J_1^2(\Delta_1^2 - 1) + J_2^2}\right)\right), & J_3 = J_3^{fb} \\ \frac{1}{2}\left(J_1(\Delta_1 - 1) + J_2\Delta_2 + J_3\Delta_3 + \sqrt{J_1^2(\Delta_1 - 1)^2 + (J_2 + J_3)^2}\right), & J_3 > J_3^{fb} \end{cases}$$

$$J_3^{fb} = \frac{J_1 J_2}{J_2^2 - J_1^2}\left(J_1\Delta_1 + \sqrt{J_1^2(\Delta_1^2 - 1) + J_2^2}\right)$$

Flat bands in $J1-J2-J3$ XXZ sawtooth chain with KNB mechanism

$$D_1 = \alpha E \sin\phi,$$
$$D_2 = E(\sin\phi\cos\theta + \cos\phi\sin\theta),$$
$$D_3 = E(\sin\phi\cos\theta - \cos\phi\sin\theta),$$

$$\frac{D_1}{J_1} = \frac{\frac{D_2}{J_2} + \frac{D_3}{J_3}}{1 - \frac{D_2 D_3}{J_2 J_3}},$$
$$\left(\frac{\widetilde{J}_2\widetilde{J}_3}{\widetilde{J}_1} - J_1\Delta_1\right)^2 = (J_1\Delta_1)^2 + \widetilde{J}_2^2 + \widetilde{J}_3^2.$$



Direction of the electric field corresponding to the system symmetries
$\phi = 0, \theta, \pi-\theta, \pi$

Flat bands in $J1 - J2 - J3$ XXZ sawtooth chain with KNB mechanism

$$\phi = 0, \Rightarrow D_1 = 0, D_2 = -D_3 = E\sin\theta$$

$$E = \pm\frac{\sqrt{2J_1^2(1+\Delta_1) - J_2^2}}{\sin\theta}$$

$$J_1 = J_2 = J_3 \equiv J, \quad \Delta_1 = 1$$

$$E = \pm\frac{\sqrt{3}J}{\sin\theta}$$

$$B_{sat} = \begin{cases} J_1(1+\Delta_1) + \frac{J_2(\Delta_2+\Delta_3)}{2}, & E \leq 2J_1^2(1+\Delta_1) - J_2^2 \\ \frac{1}{2}\left(J_1(\Delta_1 - 1) + J_2(\Delta_2+\Delta_3) + \sqrt{J_1^2(1-\Delta_1)^2 + 4J_2^2 + 4E^2\sin^2\theta}\right), & E > 2J_1^2(1+\Delta_1) - J_2^2 \end{cases}$$

Flat bands in $J1 - J2 - J3$ XXZ sawtooth chain with KNB mechanism

$$\phi = \theta, \Rightarrow D_1 = \alpha E \sin\theta, \quad D_2 = 2E\sin\theta\cos\theta, \quad D_3 = 0$$
$$\phi = \pi - \theta, \Rightarrow D_1 = \alpha E \sin\theta, \quad D_2 = 0, \quad D_3 = 2E\sin\theta\cos\theta$$

$$J_1 = \frac{2\cos\theta}{\alpha} J_2$$

$$\frac{D_1}{J_1} = \frac{\frac{D_2}{J_2} + \frac{D_3}{J_3}}{1 - \frac{D_2 D_3}{J_2 J_3}},$$
$$\left(\frac{\widetilde{J}_2\widetilde{J}_3}{\widetilde{J}_1} - J_1\Delta_1\right)^2 = (J_1\Delta_1)^2 + \widetilde{J}_2^2 + \widetilde{J}_3^2.$$

$$E = \frac{\sqrt{4\cos^2\theta\left(\cos\theta\left(J_3^2 - J_1^2\right) - \alpha J_1 J_3 \Delta_1\right) - \alpha^2 J_3^2}}{2\alpha\sin\theta\cos\theta}$$

$$E = \frac{\sqrt{4\cos^2\theta - 2\alpha^2(1+\Delta_1)}}{\alpha^2\sin\theta} J_1$$

Conclusion

- The model of $S = 1/2$ XXZ sawtooth chain with KNB mechanism is constructed
- A series of novel one-magnon flat bands is obtained for the pure sawtooth chain (without DM terms) with three couplings.
- It was figured out that only axial anisotropy within the basal line relevant for the flat band formation.
- Two class of electric field driven flat band are obtained for the special orientation of the electric field.
- Saturation magnetic field is obtained for all regimes.

Thank you for attention !