Quantum phase transition between two gapless phases in quasi 1D materials

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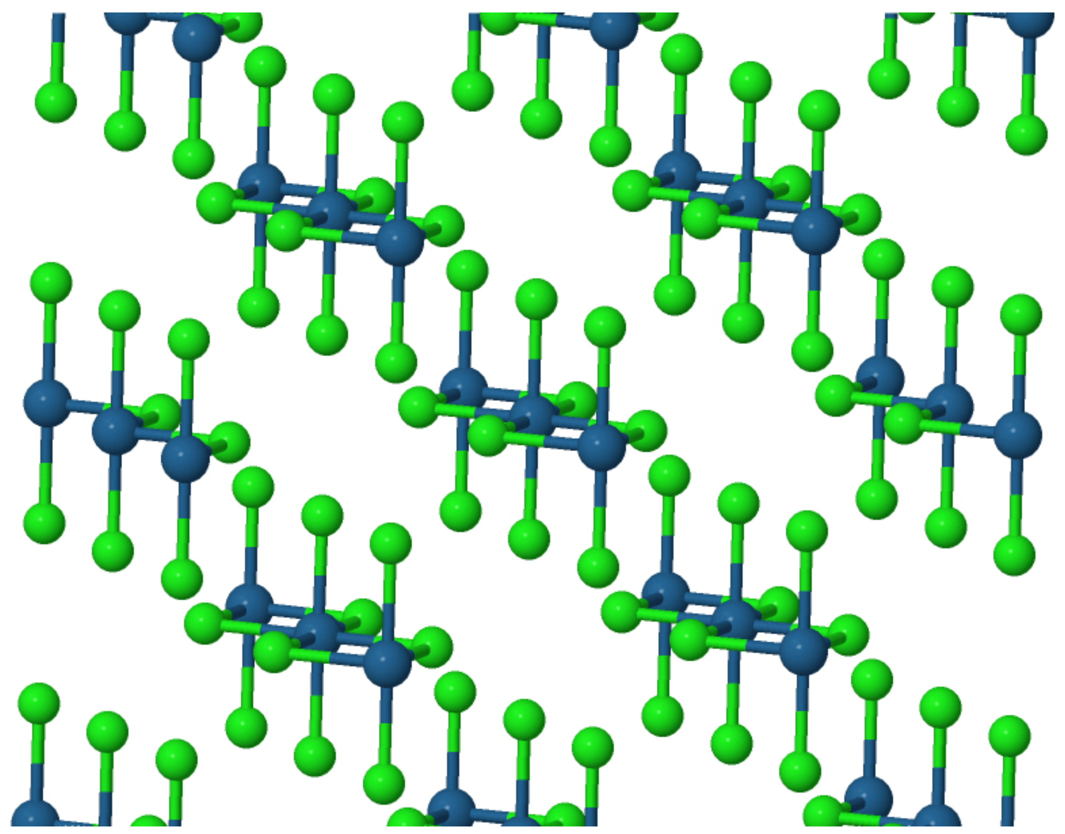
Introduction

Question: **How does a gapped vs gapless quasi 1D magnetic system respond to magnetic field?**

Quasi 1D Crystal:

$OsCl_4$



Spin Orbit Coupling + Coulomb Interaction + d-Orbital Occupancy

$$\Downarrow$$

$$H = H_{BLBQ} + h\sum_i S_i^z, \quad \text{with } H_{BLBQ} = \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \beta(\mathbf{S}_i \cdot \mathbf{S}_j)^2$$

[A spin-1 bilinear-biquadratic (BLBQ) interactions as a function of an applied magnetic field h]

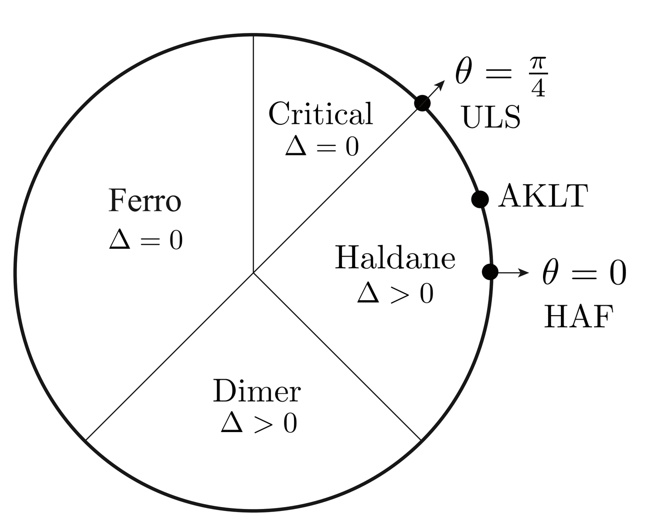
Static and dynamical structure factors:

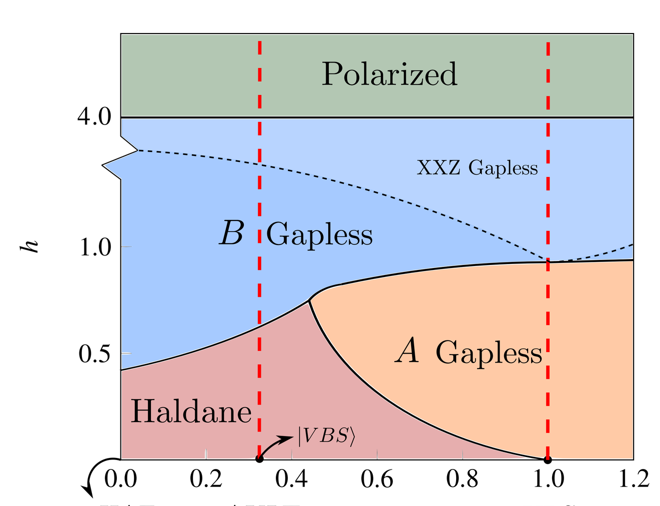
$$S(q) = \frac{1}{L^2}\sum_{i,j} e^{iq(r_i - r_j)}\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle, \quad S^{\alpha\beta}(q,\omega) = \frac{1}{L}\sum_r e^{-iqr}\int_{-\infty}^{\infty} dt\, \langle S_0^\alpha(t) S_r^\beta(0)\rangle\, e^{i\omega t}$$

and entanglement entropy are calculated by density matrix renormalization group:

$$\rho_A = \mathrm{Tr}_B\left[|g.s.\rangle\langle g.s.|\right], \quad S_{vN} = -\mathrm{Tr}\left[\rho_A \log(\rho_A)\right]$$

Phase Diagram:





Relation to d^4 Mott insulators [1]:

$$H_{d^4} = H_{hop} + \sum_i (H_{i,U} + H_{i,SOC})$$

By second order perturbation of H_{hop}:

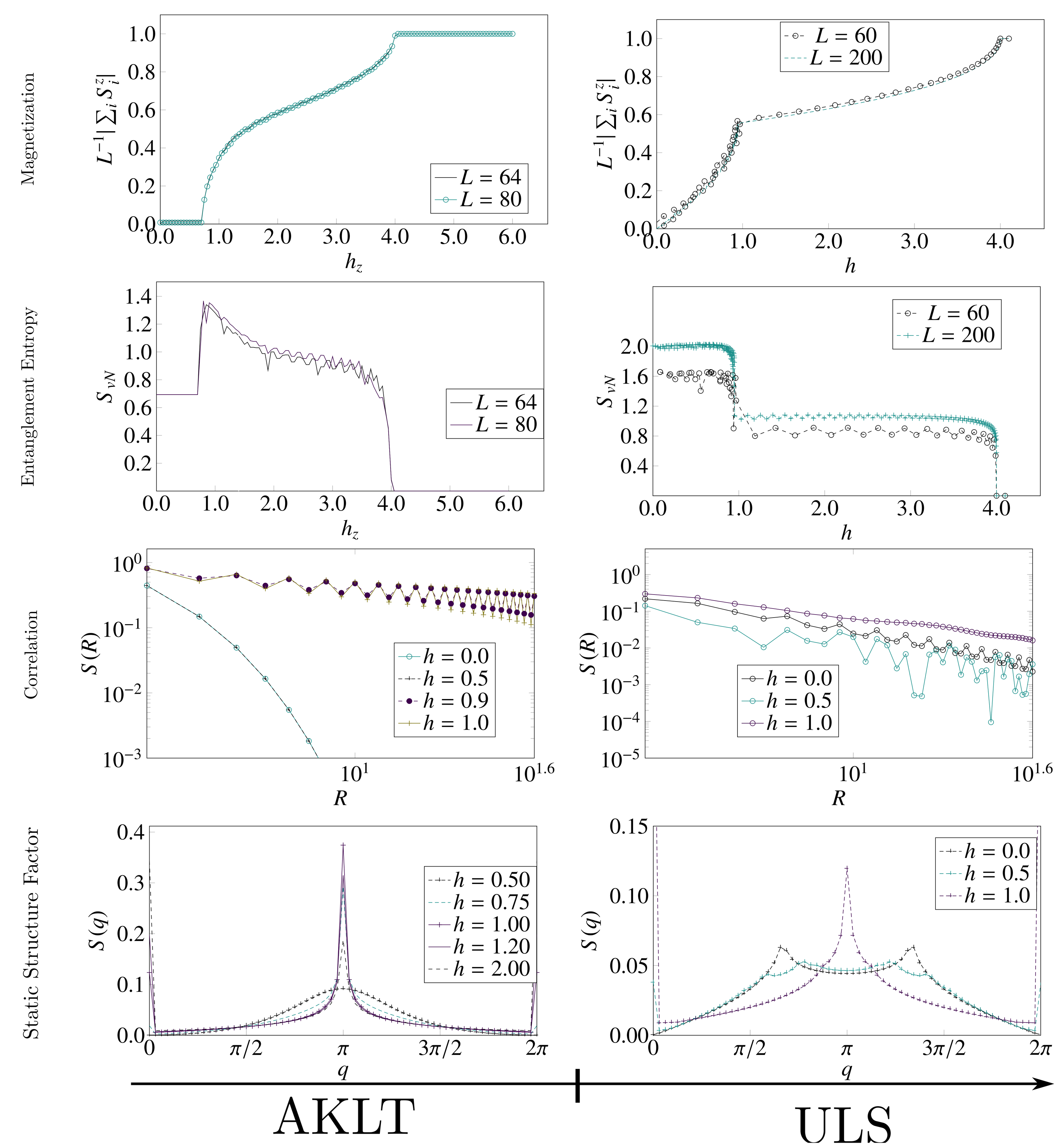
$$H_{d4} \approx -J_{FM}\sum_{\langle ij \rangle}(\mathbf{S}_i \cdot \mathbf{S}_j)\mathcal{P}(\mathbf{L}_i + \mathbf{L}_j = 1) + \lambda\sum_i \mathbf{L}_i \cdot \mathbf{S}_i$$

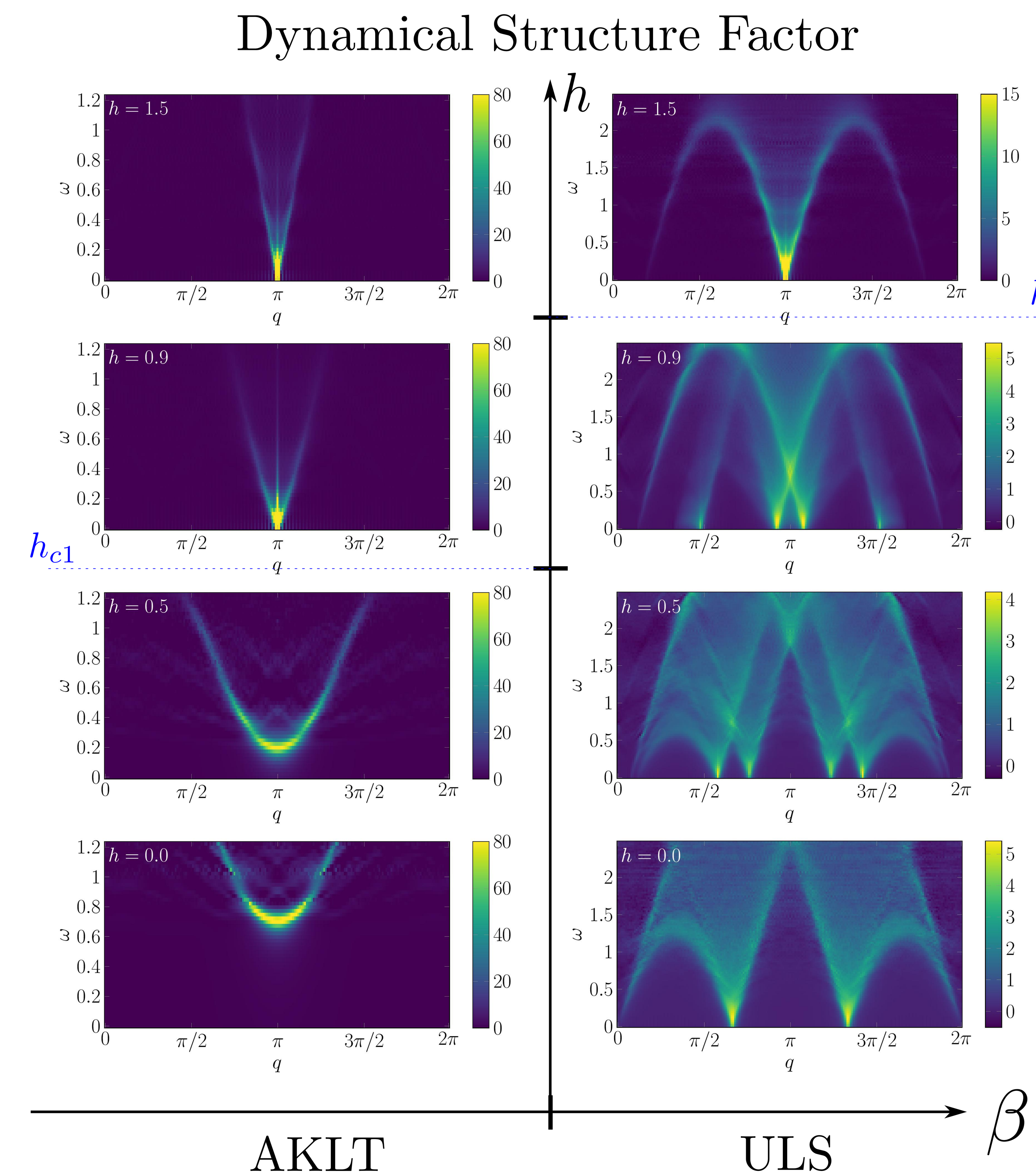
Under mean field approximation, the orbital can be described by effective $\mathcal{S} = 1$ chain:

$$H_{d^4}^{\mathrm{MFT}} = J_{eff}\sum_{\langle ij \rangle}\mathcal{S}_i \cdot \mathcal{S}_j + (\mathcal{S}_i \cdot \mathcal{S}_j)^2 + h_{eff}\sum_i \mathcal{S}_i^z \simeq H_{ULS} + h\sum_i S_i^z$$

with $J_{eff} \simeq J_{FM}\sum_{\langle ij \rangle}\langle \mathcal{S}_i \cdot \mathcal{S}_j \rangle/2$ and $h_{eff} = \lambda\sum_{\langle ij \rangle}\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$

Static and Dynamical Response





ULS Hamiltonian in its slave fermions form $\mathbf{S}_i \equiv \psi_i^\dagger \mathbf{S}_i \psi_i$ with $\psi_i = (d_{i,1}, d_{i,0}, d_{i,-1})$:

$$H_{ULS} - const = \sum_{\langle ij \rangle}\mathbf{S}_i \cdot \mathbf{S}_j + (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - const = -\sum_{\langle ij \rangle; mm'} d_{i,m}^\dagger d_{j,m} d_{j,m'}^\dagger d_{i,m'}$$

with 3 conserved charges with flavor $m = -1, 0, 1$, and respectively 3 Fermi momenta k_m:

$$[\hat{N}_m, H_{ULS}] \equiv \left[\sum_i d_{i,m}^\dagger d_{i,m}, H_{ULS}\right] = 0, \quad \sum_{m=-1,0,1} k_m = \pi$$

At $h = 0$, 3 bands are degenerate, hence $k_{-1,0,1} = \pi/3$. As SU(3) is broken by a field, k_0 remains intact, yet k_1, k_{-1} changes by $k_{1,-1} = \pi/3 \pm h/v$. Hence the soft modes bifurcates:

$$k_1 + k_0 = 2\pi/3 - h/v, \quad k_0 + k_{-1} = 2\pi/3 + h/v\cdot$$

Low energy spinons of the SU(3) model can be approximated by a pair of chiral fermions:

$$d_{i,m} \approx f_{L,m}(x)e^{-ik_m x} + f_{R,m}(x)e^{ik_m x}$$

where $f_{L,m}$ and $f_{R,m}$ respectively denote left and right chiral fermion annihilation operators relevant for m-spinon with momenta $k_m = \pi/3$. Therefore, in the low energy sector for $h \ll vk_m$, the magnon excitation can be approximated by

$$S^+(x) \approx f_{R,1}^\dagger f_{L,0}e^{-i(k_1+k_0)x} + f_{L,1}^\dagger f_{R,0}e^{i(k_1+k_0)x} + f_{R,0}^\dagger f_{L,-1}e^{-i(k_0+k_1)x} + f_{L,-1}^\dagger f_{R,0}e^{i(k_1+k_0)x}$$

Increasing h towards h_{c1} leads to the reduction of fermi momentum k_1 and the de-population of spinon of $m = 1$ type. Its complete de-population happens at $h = h_{c1}$. Upon entering the B-phase, all excitation channels in S^+ relevant for $f_{R/L,1}$ vanish, and the only modes left are those with $k_1 + k_0 = k_0 = \pi$

Conclusion

1. For both AKLT and ULS model, magnetic field does not polarize them directly, but induces a gapless intermediate phase.
2. AKLT goes through a gapped-gapless transition at $h_{c1} \approx 0.8$ and polarizes at $h_{c2} = 4$.
3. ULS goes through a gapless-gapless transition at $h_{c1} \approx 0.94$ at which the 4-soft modes are reduced to 1 soft mode at $q = \pi$, and polarizes at $h_{c2} = 4$.

Acknowledgements & References

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