Field driven quantum phase transitions in spin-1 quasi 1D materials

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Introduction

Motivation:

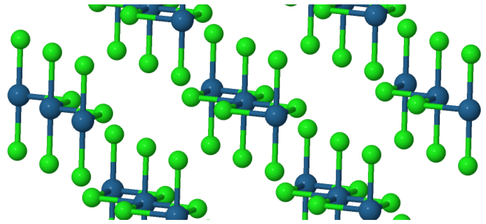
Explore phases with fractionalized excitations in low dimensions generated by frustration.

Candidate Materials for J=1:

$CsNiCl_3$, $LiVGe_2O_6$, $OsCl_4$, Ba_2YIrO_6, La_2ZnRuO_6

Quasi 1D Crystal:

$OsCl_4$



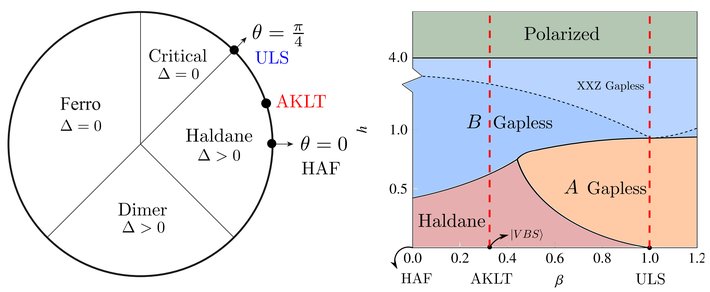
Spin Orbit Coupling + Coulomb Interaction + d-Orbital Occupancy

$$\Downarrow$$

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

Bilinear-biquadratic (BLBQ) interactions with magnetic field

Phases:

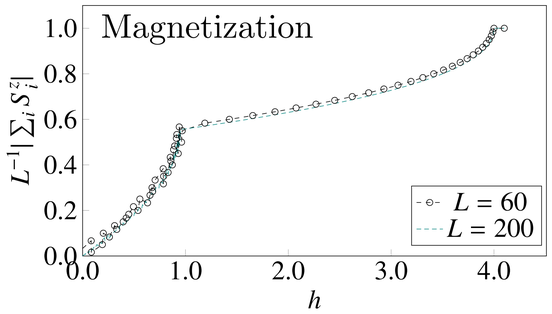


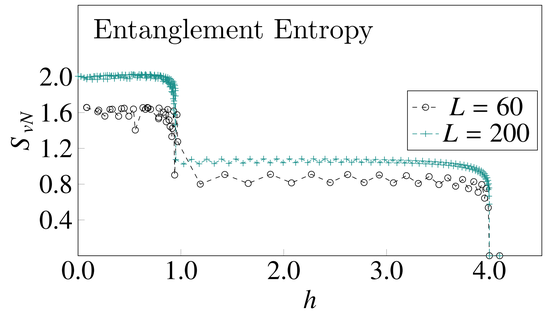
$$\vec{S}_{\text{bond}} = \vec{S}_1 + \vec{S}_2 \qquad S_{\text{bond}} = 2, 1, 0$$

$+\mathcal{P}^{(2)}$: S_{bond} favors $S = 0, 2$ $\Rightarrow$ AKLT (frustration-free)

$-\mathcal{P}^{(1)}$: S_{bond} favors $S = 1$ $\Rightarrow$ ULS (frustrated)

Static and Dynamical Response of ULS Model

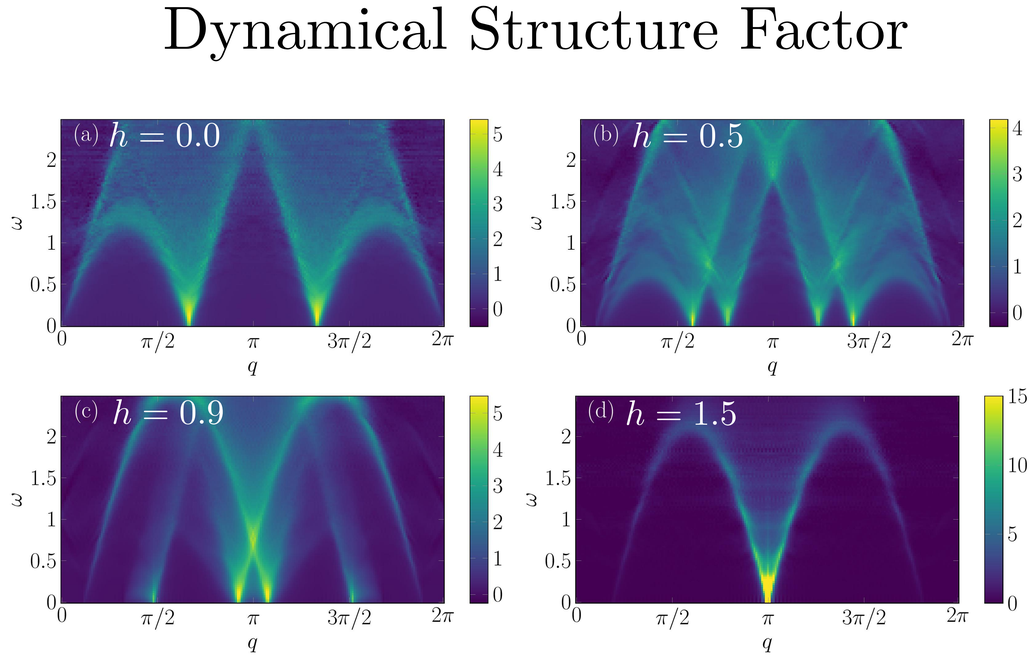




Entanglement entropy are calculated by density matrix renormalization group:

$$\rho_A = \mathrm{Tr}_B\left[\,|g.s.\rangle\langle g.s.|\,\right],$$

$$S_{vN} = -\,\mathrm{Tr}\left[\rho_A \log(\rho_A)\right]$$



Dynamical structure factors:

$$S^{\alpha\beta}(q,\omega) = \frac{1}{L}\sum_r e^{-iqr}\int_{-\infty}^{\infty} dt\,\langle S_0^\alpha(t) S_r^\beta(0)\rangle\, e^{i\omega t}$$

Conclusion

1. Magnetic field does not directly polarize the AKLT and ULS model, 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 $h_{c2} = 4$.
4. Mechanism for gapless-to-gapless transition can be understood by depletion of spinon fermi surfaces.

Acknowledgements & References

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