Dynamics of the S=1/2 Heisenberg Antiferromagnet on the Triangular Lattice

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(i) Dynamical structure factor

[**Drescher**, Vanderstraeten, Moessner, FP, arXiv:2209.03344 (in print)]


Drescher


Vanderstraeten


Moessner

(ii) Spin-Peierls instability

[**Seifert**, **Willsher**, **Drescher**, FP, Knolle, arXiv:2307.12295]


Seifert


Willsher


Drescher


Knolle

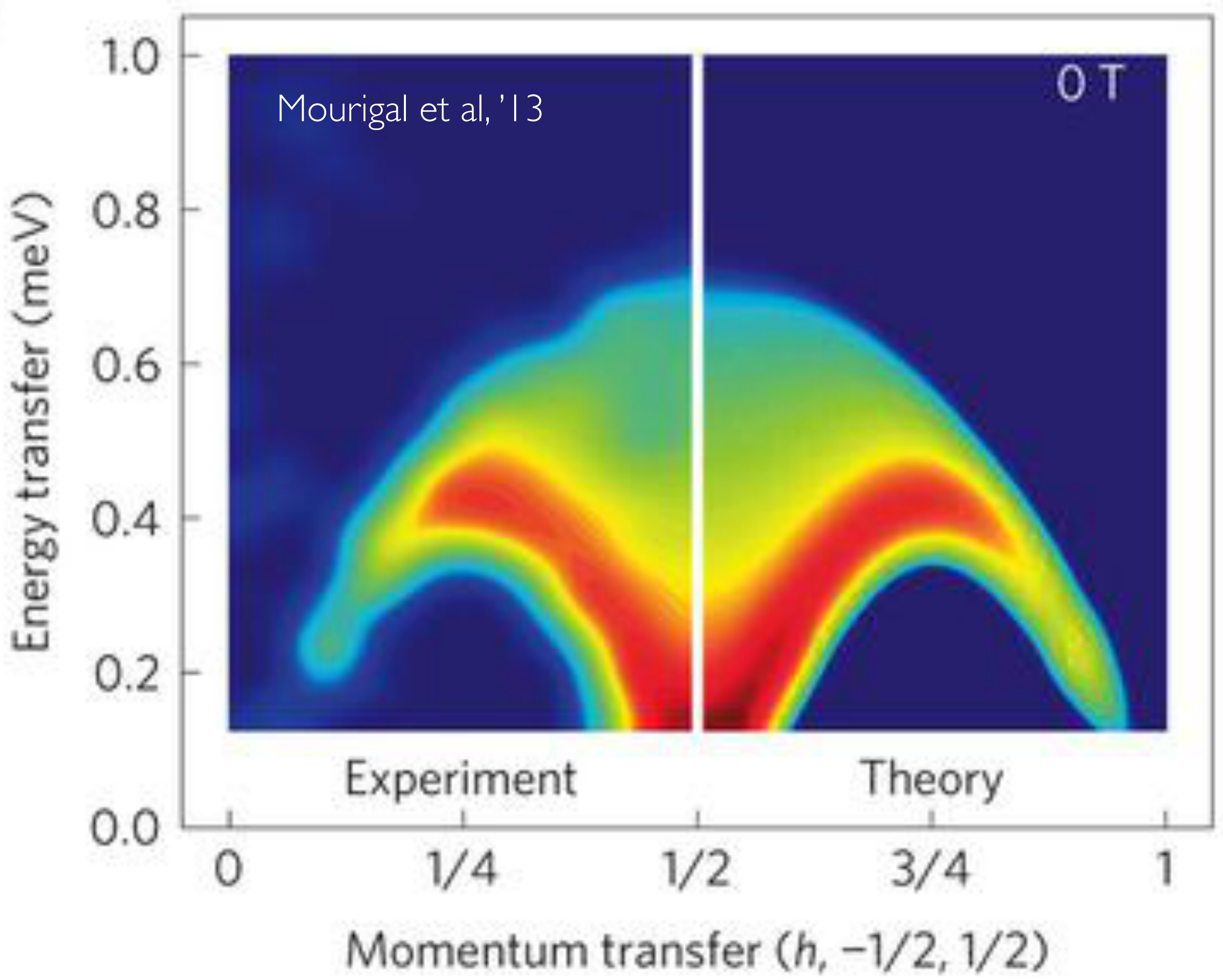
Fractionalization and Emergent Gauge Fields in Quantum Matter
ICTP Dec. 5 2023

Dynamical structure factor of Quantum Spin Liquids (QSL)

1D quantum spin liquid: Fractional **spinon excitations** in the Heisenberg antiferromagnetic chain

$S = 1$

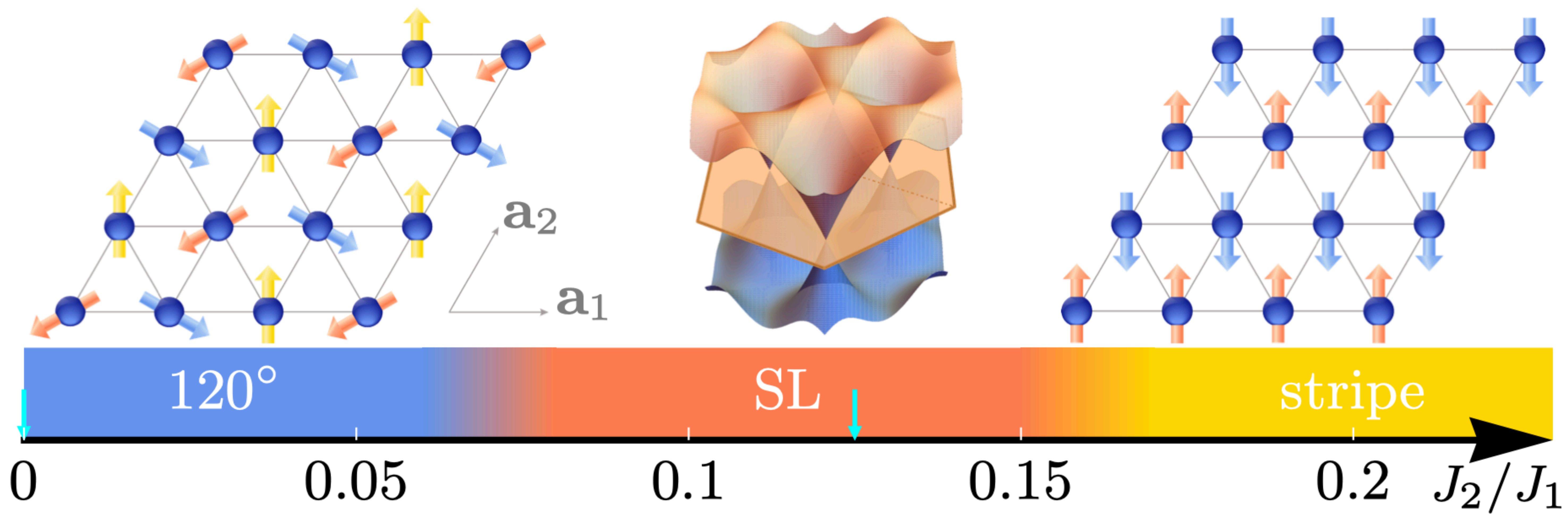
Dynamical structure factor: $$S(\vec{q},\omega) = \sum_n \left| \langle \psi_n | S^+_{\vec{q}} | \psi_0 \rangle \right|^2 \delta(\omega + \omega_0 - \omega_n)$$



QSLs candidate: Triangular lattice Heisenberg materials

$J_1 - J_2$ model on the triangular lattice

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



[Zhu and White '15, …]

- Many Candidate Materials: $Ba_3CoSb_2O_9$, $YbMgGaO_4$, $YbZn_2GaO_5$, …

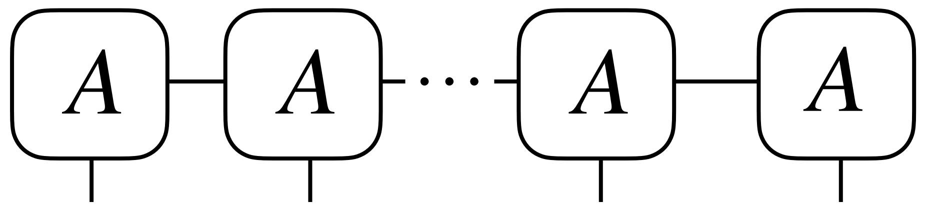
Towards 2D quantum spin systems

Density Matrix Renormalization Group (DMRG)

to efficiently simulate 1D quantum systems [White '92, Schollwoeck '11]

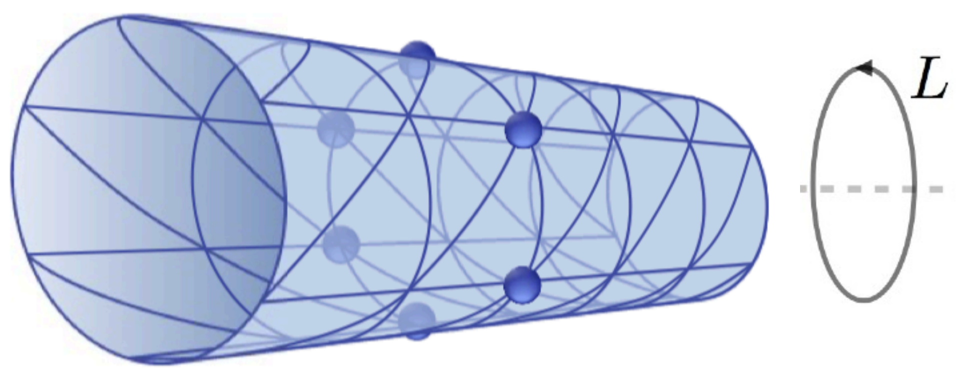
$$|\psi\rangle = \sum_{\{j_n\}} \psi_{\sigma_1,\sigma_2,\ldots,\sigma_N} |\sigma_1, \sigma_2, \ldots, \sigma_N\rangle, \quad \sigma_n = \pm 1$$

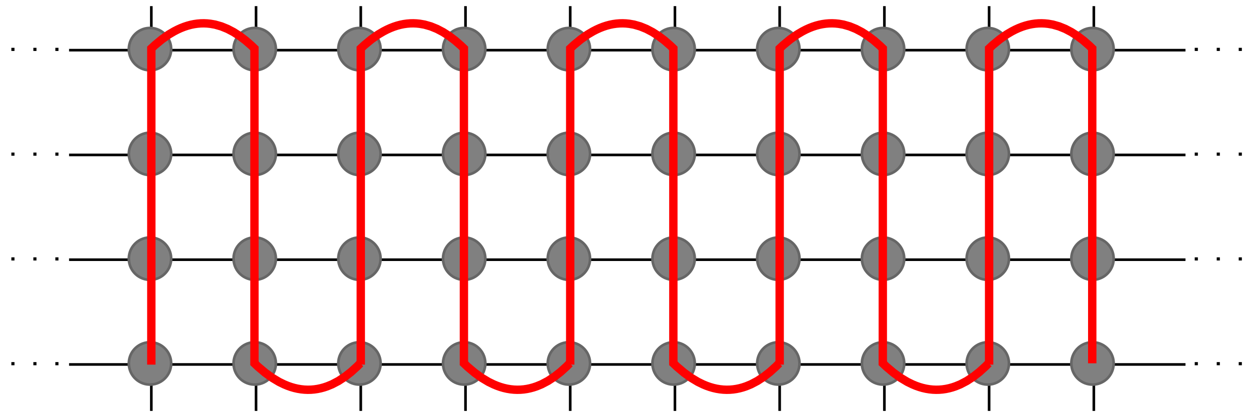
$$\psi_{\sigma_1,\sigma_2,\sigma_3,\ldots,\sigma_N} \approx \sum_{\alpha_1,\alpha_2,\ldots,\alpha_{N-1}}^{\chi} A^{\sigma_1}_{\alpha_1} A^{\sigma_2}_{\alpha_1,\alpha_2} \cdots A^{\sigma_N}_{\alpha_{N-1}} =$$



$$\boxed{2^N \rightarrow N2\chi^2}$$

DMRG of 2D systems on cylinders





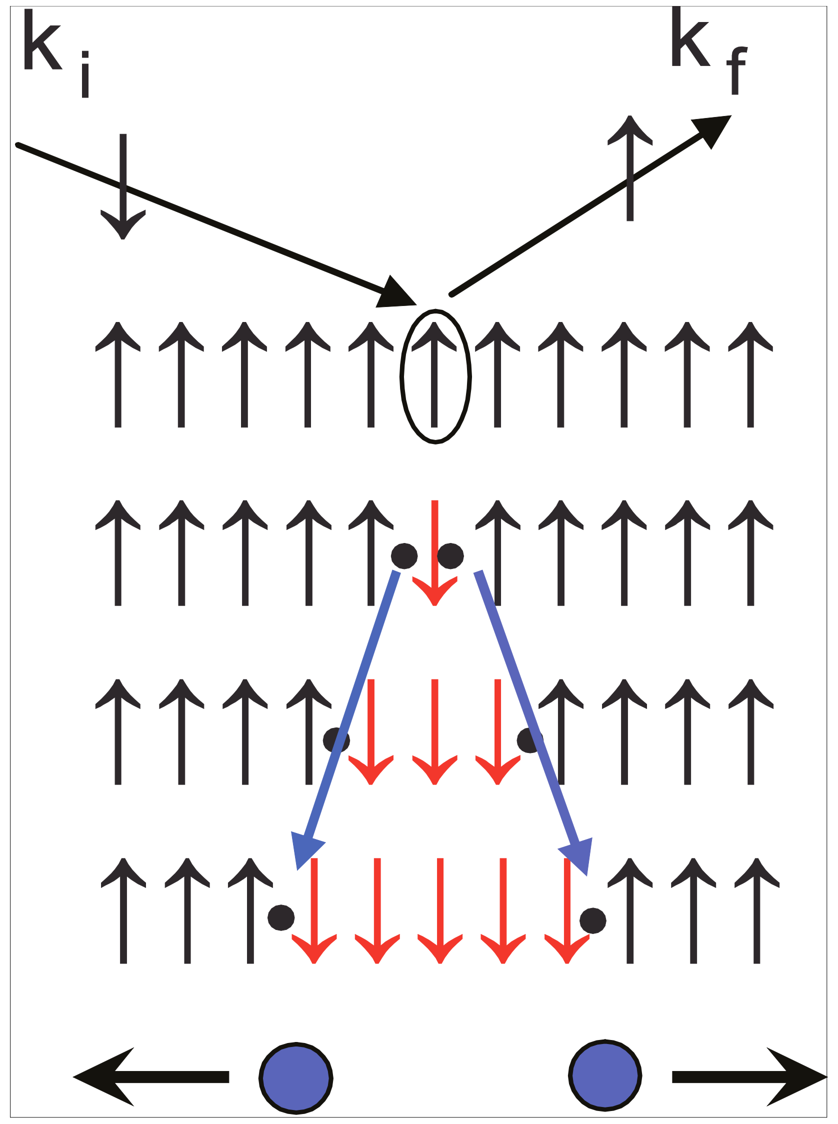
- 2D physics at the cost of **long range interactions** in 1D representation!
  [Stoudenmire and White '12]
- Long ($L_x \rightarrow \infty$) cylinders with moderate circumferences ($L_y \approx 10$)

Dynamics of quantum spin systems

Numerical calculation of the **dynamical structure factor**

$$S(k,\omega) = \sum_x \int_{-\infty}^{\infty} dt e^{-i(kx+\ \omega t)} C(x,t)$$

with $C(x,t) = \langle \psi_0 | S_x^+(t) S_0^-(0) | \psi_0 \rangle$

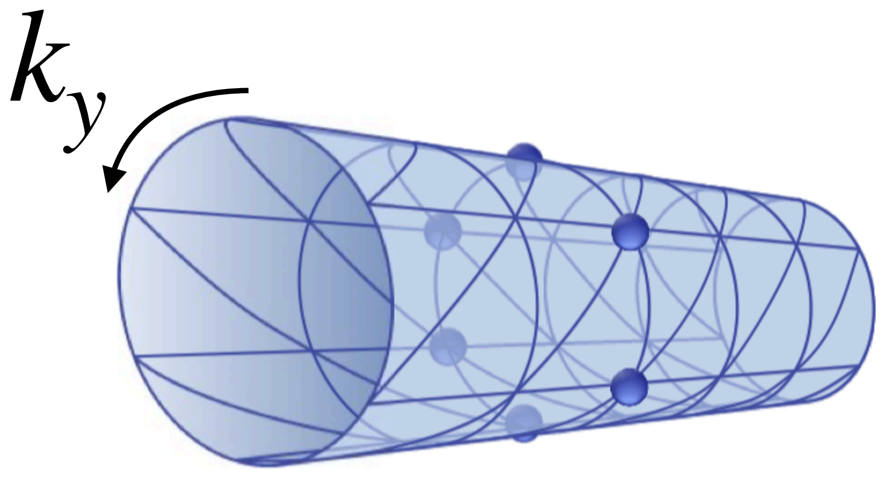


(1) Find the ground state $|\psi_0\rangle$: DMRG

(2) Time evolve $S_0^\alpha |\psi_0\rangle$ to obtain $C(x,t)$

[Zaletel, Mong, Karrasch, Moore, FP '15]

k_y resolved $\hat{S}^-_{n_1}(k_y) = \frac{1}{\sqrt{L_y}} \sum_{j=0}^{L_y-1} e^{\mathrm{i}\, j\cdot k_y} \hat{S}^-_{n_1\cdot \mathbf{a}_1 + j\cdot \mathbf{a}_2}$

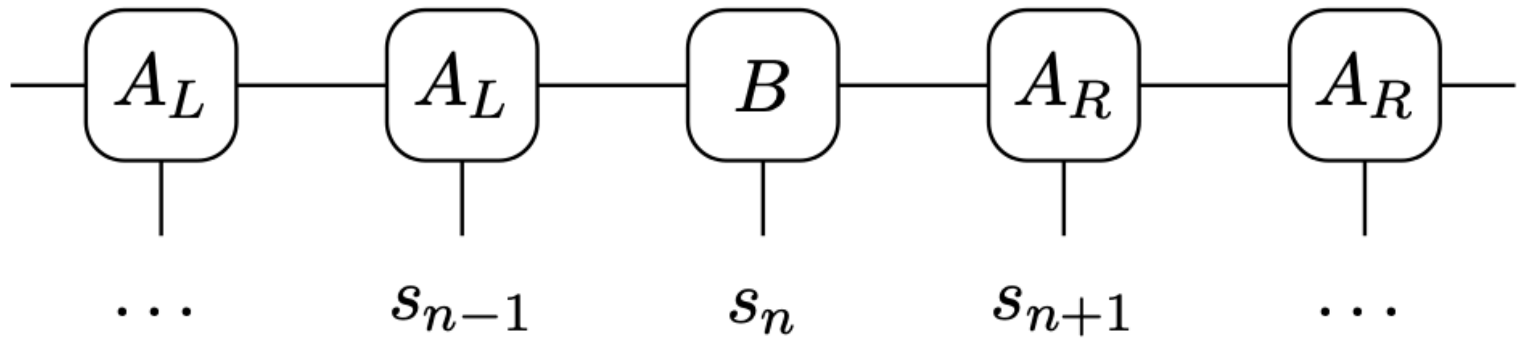


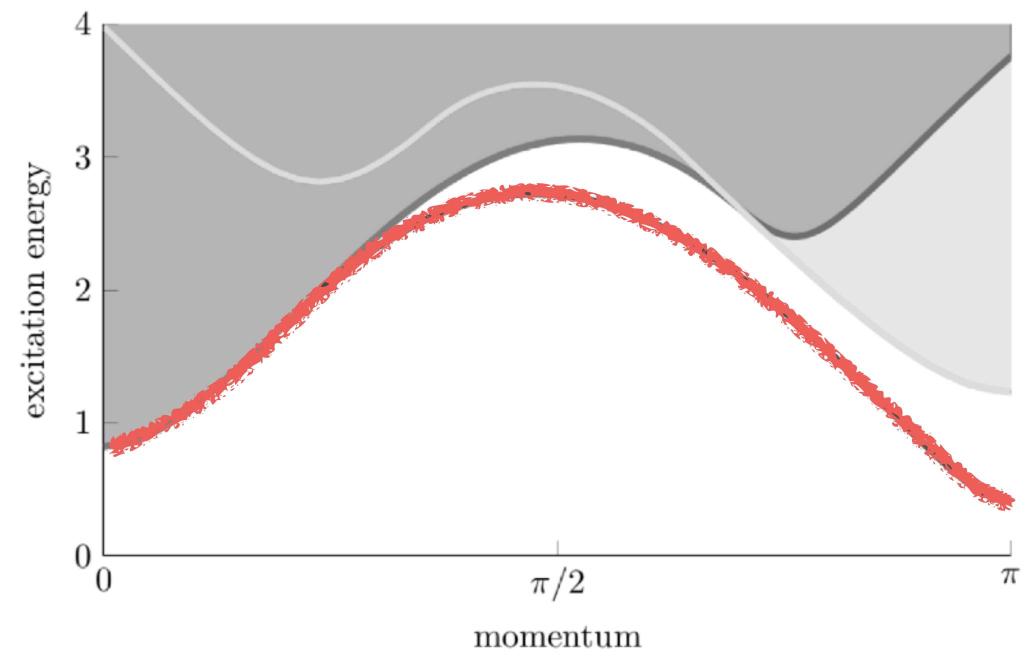
- Slow growth of entanglement: Long times!

Dynamics of quantum spin systems

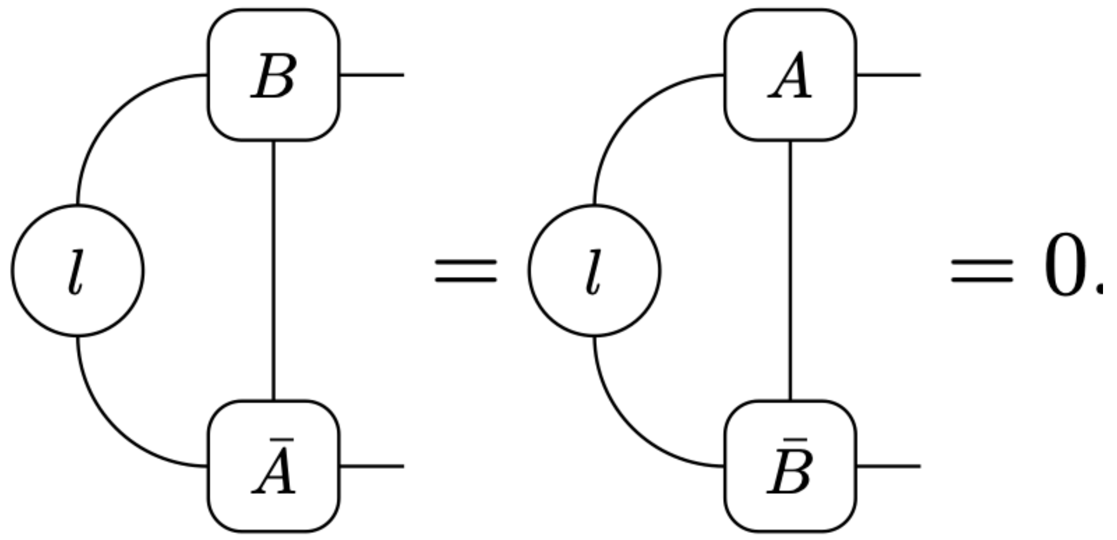
Quasi particle ansatz [Haegeman et al, '13]

$|\psi_k(B)\rangle = \sum_n e^{ikn} \ldots$



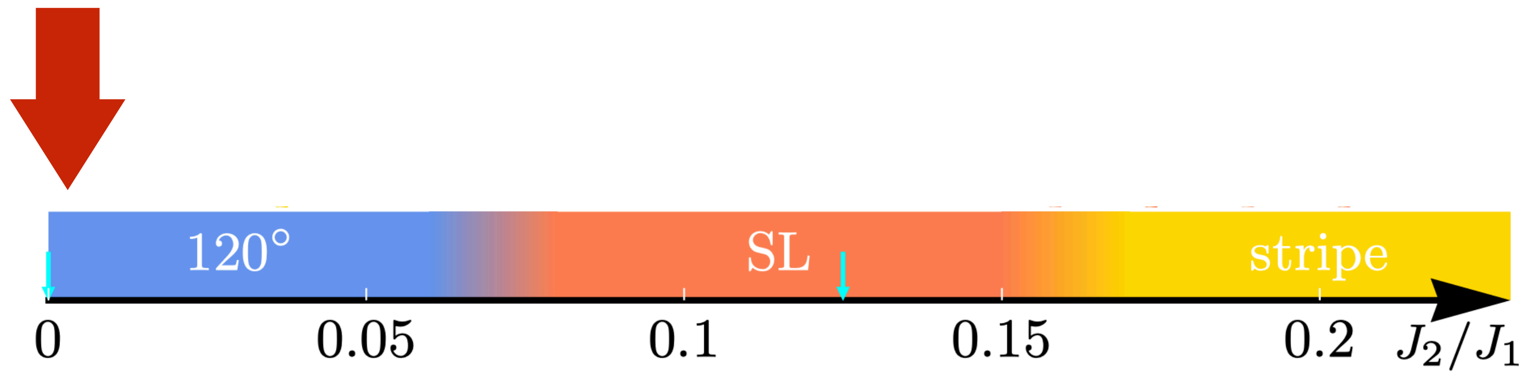


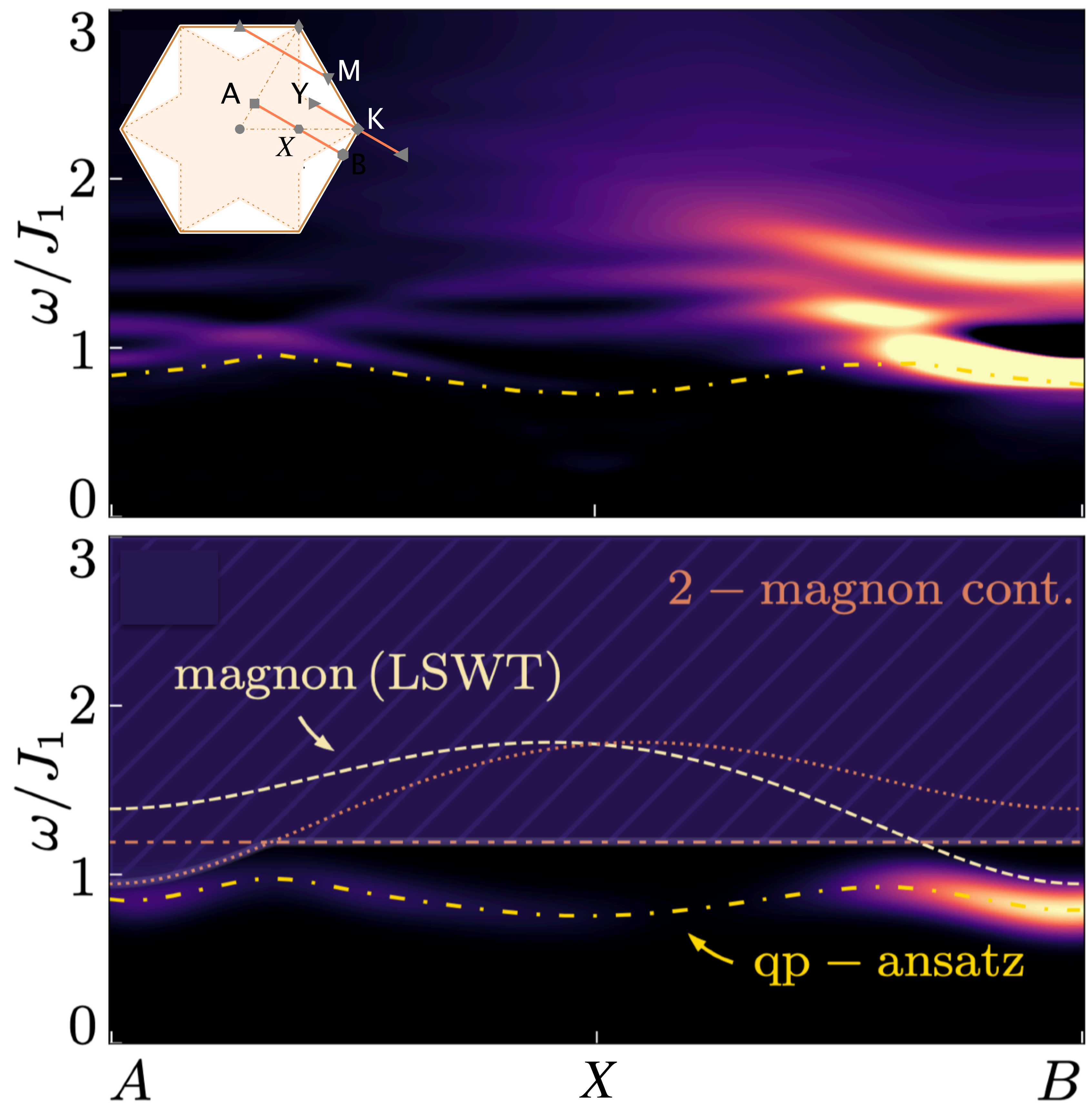
- Gauge fixing ensures a state **orthogonal to GS**
- B contains all the variational parameters and perturbs the ground state

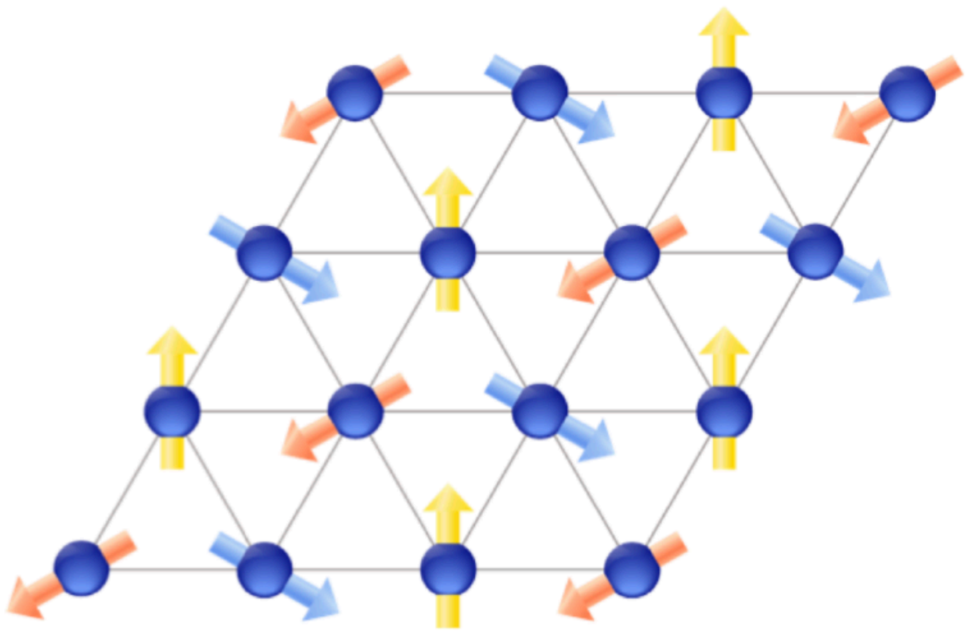


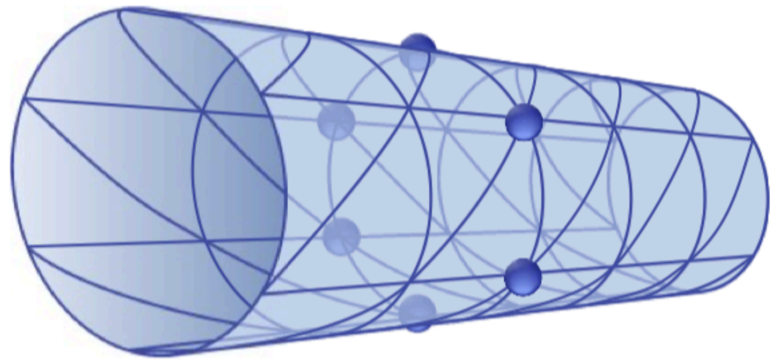
Dynamics of the triangular lattice Heisenberg model

Heisenberg model with $J_2 = 0$: 120° order









$L = 6$

- Magnon repelled from continuum: Decay prevented

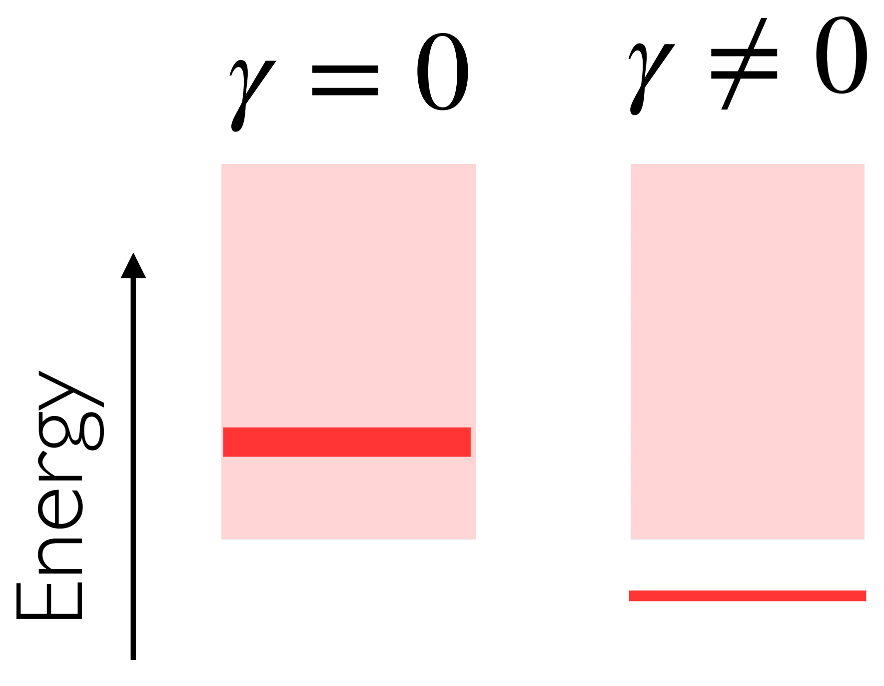
[Zheng et al. '06, Chernyshev et al, '06, '09, '13]

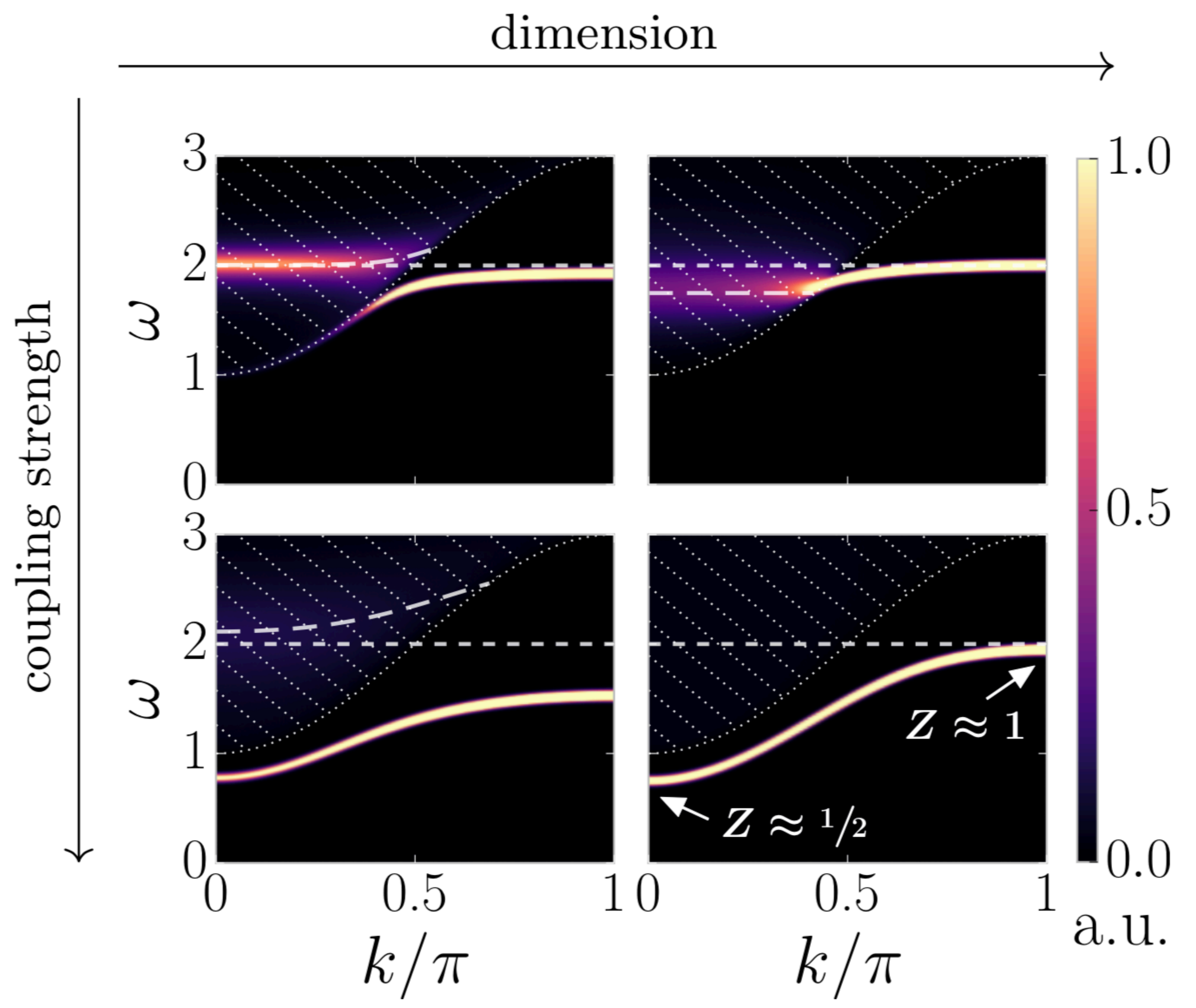
[**Drescher**, Vanderstraeten, Moessner, FP, arXiv:2209.03344]
[Verresen, Moessner, FP, Nat. Phys. **15**, 750 (2019)]

Strong interactions prevent quasiparticle decay

$$\hat{H} = E_b\,|\psi\rangle\langle\psi| + \int \mathrm{d}\alpha\, \Big(E_\alpha |\varphi_\alpha\rangle\langle\varphi_\alpha| + \gamma\,|\psi\rangle\langle\varphi_\alpha| + \gamma\,|\varphi_\alpha\rangle\langle\psi| \Big),$$

$$\hat{H} = \left(\begin{array}{c|ccc} E_b & \gamma & \cdots & \gamma \\ \hline \gamma & \ddots & & \\ \vdots & & (E_\alpha)_{\alpha\in\mathbb{R}} & \\ \gamma & & & \ddots \end{array}\right)$$





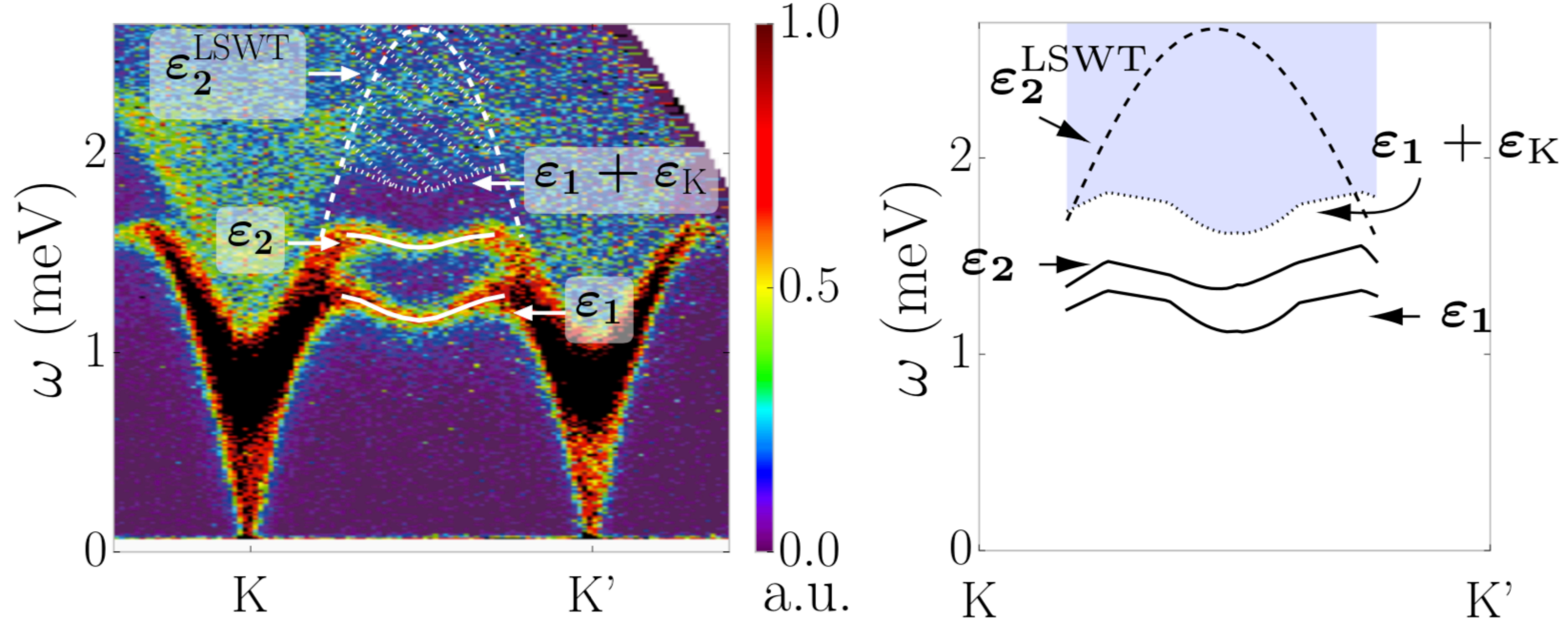
- **Sharp onset:** QP below the continuum for any $\gamma \neq 0$
- **Soft onset:** QP below the continuum for $\gamma > \gamma_0$

[cf. Gaveau and Schulman '95]

[Verresen, Moessner, FP, Nat. Phys. **15**, 750 (2019)]

Dynamics of the triangular lattice Heisenberg model

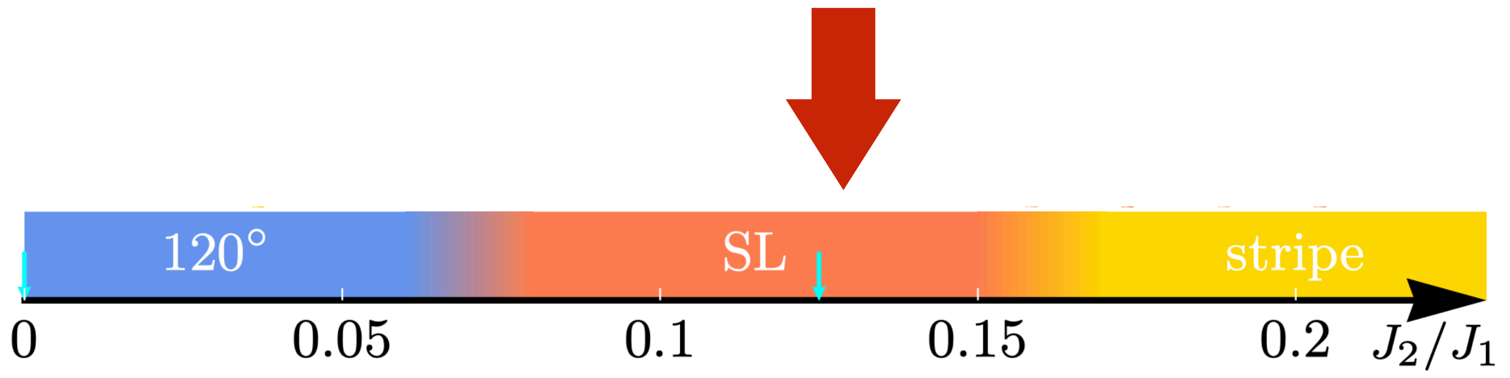
Inelastic neutron scattering for $Ba_3CoSb_2O_9$ [Ito et al. '17]



- Magnon repelled from continuum: **Decay prevented**

[Verresen, Moessner, FP, Nat. Phys. **15**, 750 (2019)]

Dirac QSL



$J_1 - J_2$ Heisenberg model in QSL regime

- Parton construction $\vec{S}_i = \frac{1}{2} f^{+}_{i,\alpha} \sigma_{\alpha,\beta} f_{i,\beta}$ with $f^{\dagger}_{i\uparrow} f_{i\uparrow} + f^{\dagger}_{i\downarrow} f_{i\downarrow} = 1$

  Mean-field $\mathscr{H} = -\sum_{i,j,\alpha} \left(\chi_{ij} f^{\dagger}_{i\alpha} f_{j\alpha} + \mathrm{h.c.} \right)$

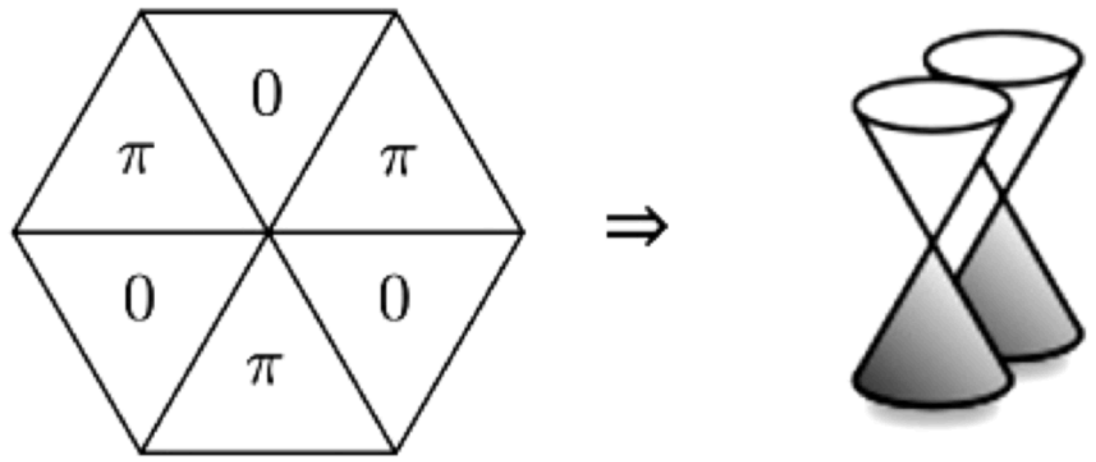
  Local gauge redundancy $f_{j,\alpha} \to e^{i\phi_j} f_{j,\alpha}$

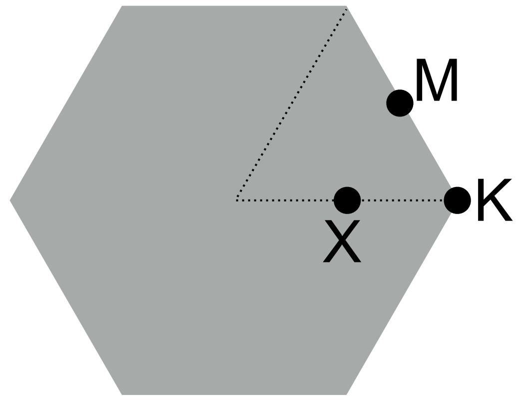
- Staggered flux: Dirac fermions QED_3, $N = 4$
  [Song et al '19, Wietek et al. '23]

  Fermion bilinear at M-points

  Singlet monopoles at X-Points

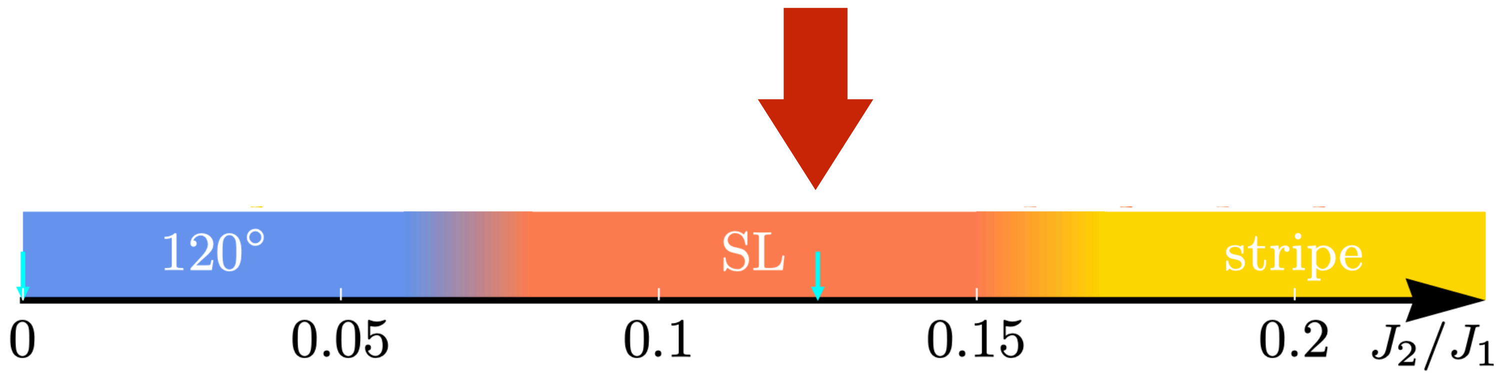
  Triplet monopoles at K-points

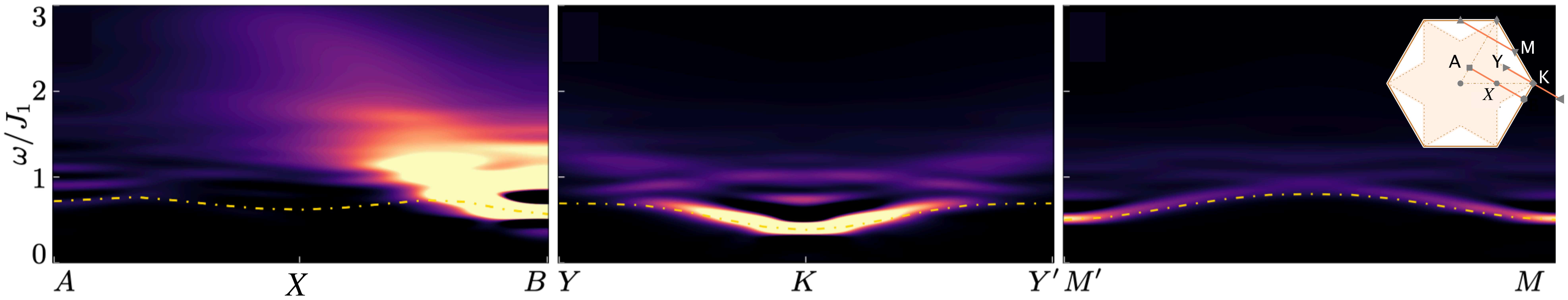




Dynamics of the triangular lattice Heisenberg model

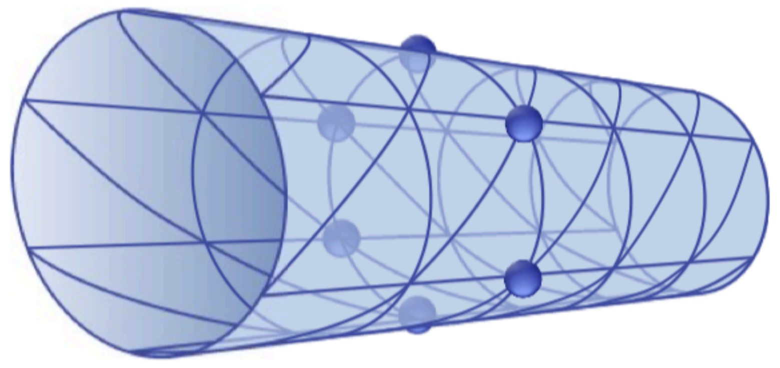
Heisenberg model with $J_2/J_1 = 0.125$: QSL





[see also Sherman et al '23]

- Triplet monopole (K) and Fermion (M) excitations [Song et al '19]
- Agreement with VMC using Dirac QSL ansatz [Ferrari, Becca '19]

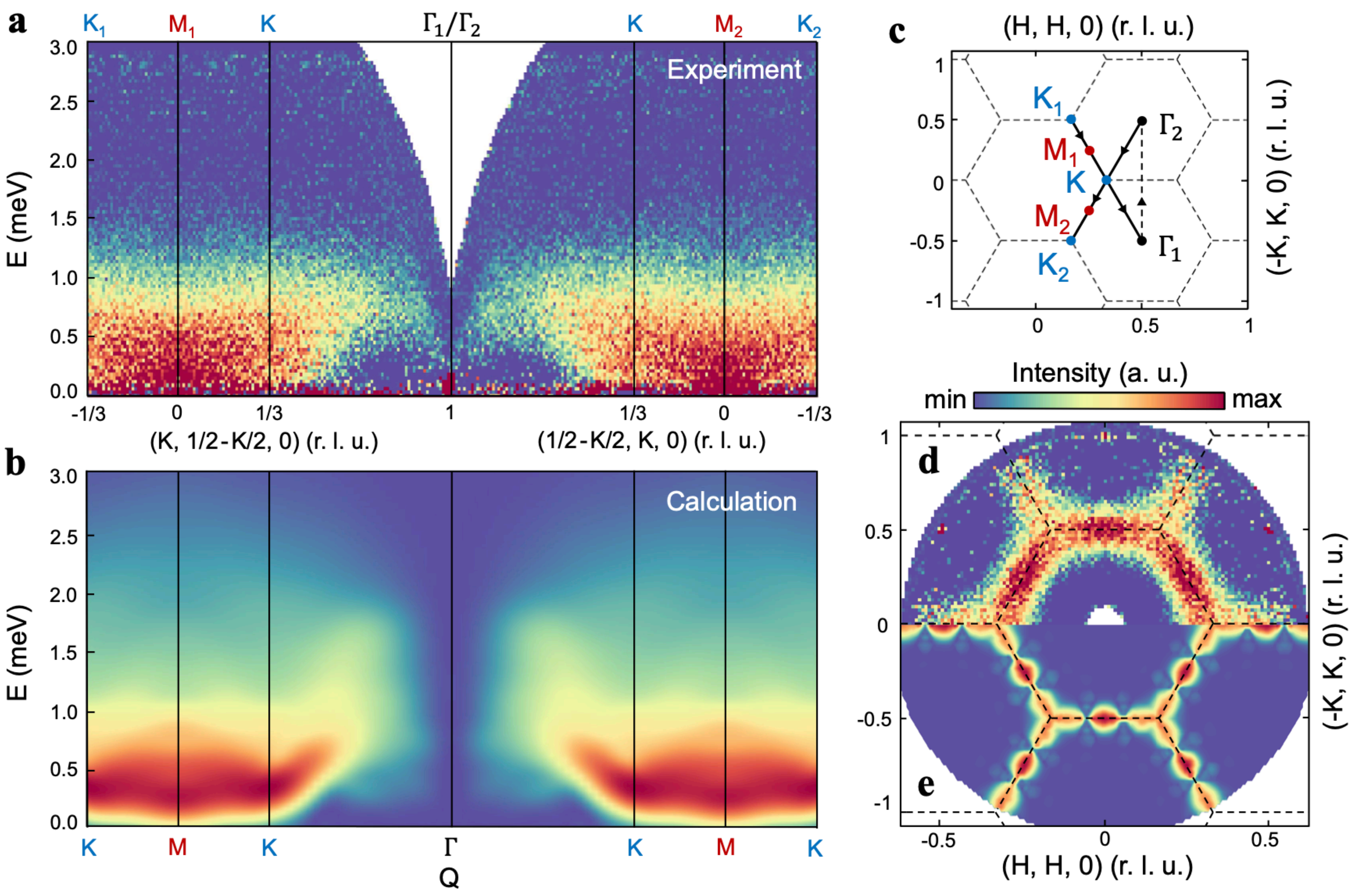


$L = 6$

[Drescher, Vanderstraeten, Moessner, FP, arXiv:2209.03344]

Sinatures of U(1) Dirac QSL in $YbZn_2GaO_5$

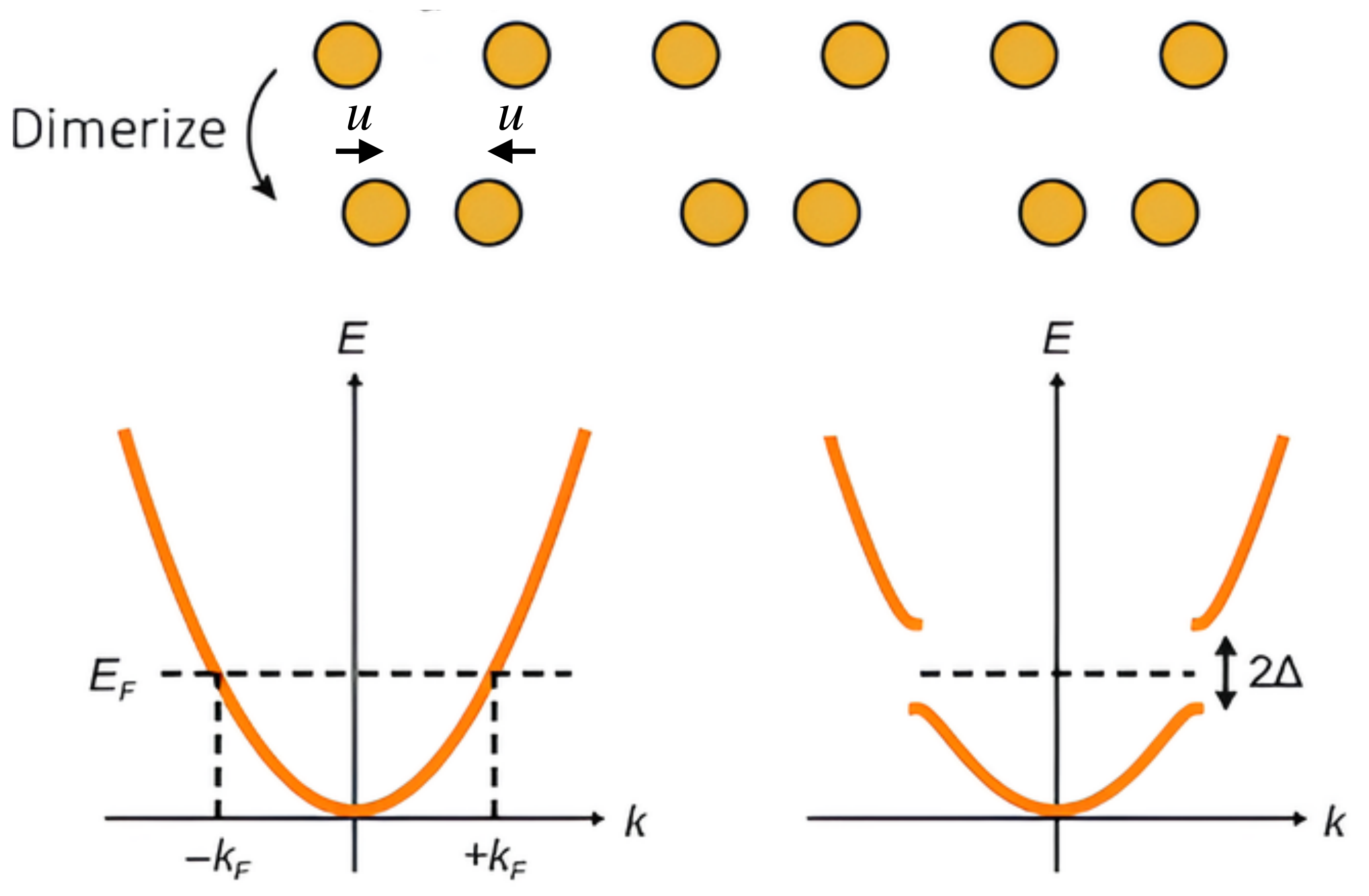
Dirac QSL with gapless excitations at M and K points [Xu et al, '23]



Spin-Peierls instability of the U(1) Dirac QSL

Warmup: **Peierls instability in spin-1/2 chain:**

- AF Heisenberg chain is gapless and disordered
- Infinitesimally weak coupling to lattice deformations leads to dimerization and gap



Free Fermions $E(u) = \dfrac{K}{2}u^2 - \eta u^2 \ln u$

Interacting $E(u) = \dfrac{K}{2}u^2 - \eta u^\chi,$

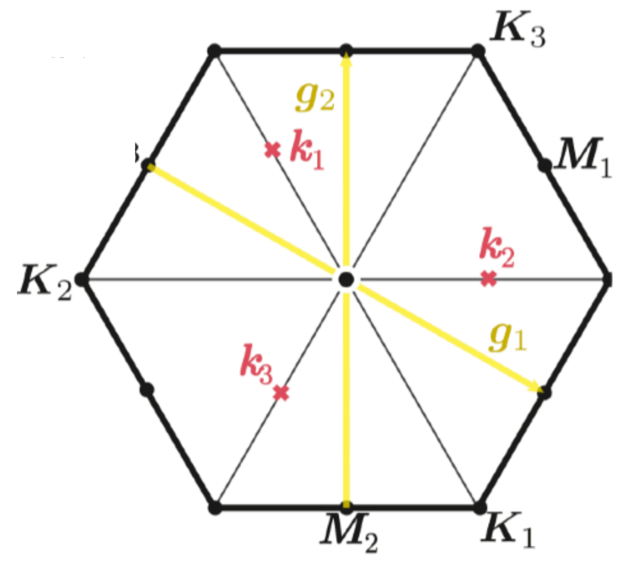
(e.g., $\chi = 4/3$ for Heisenberg)

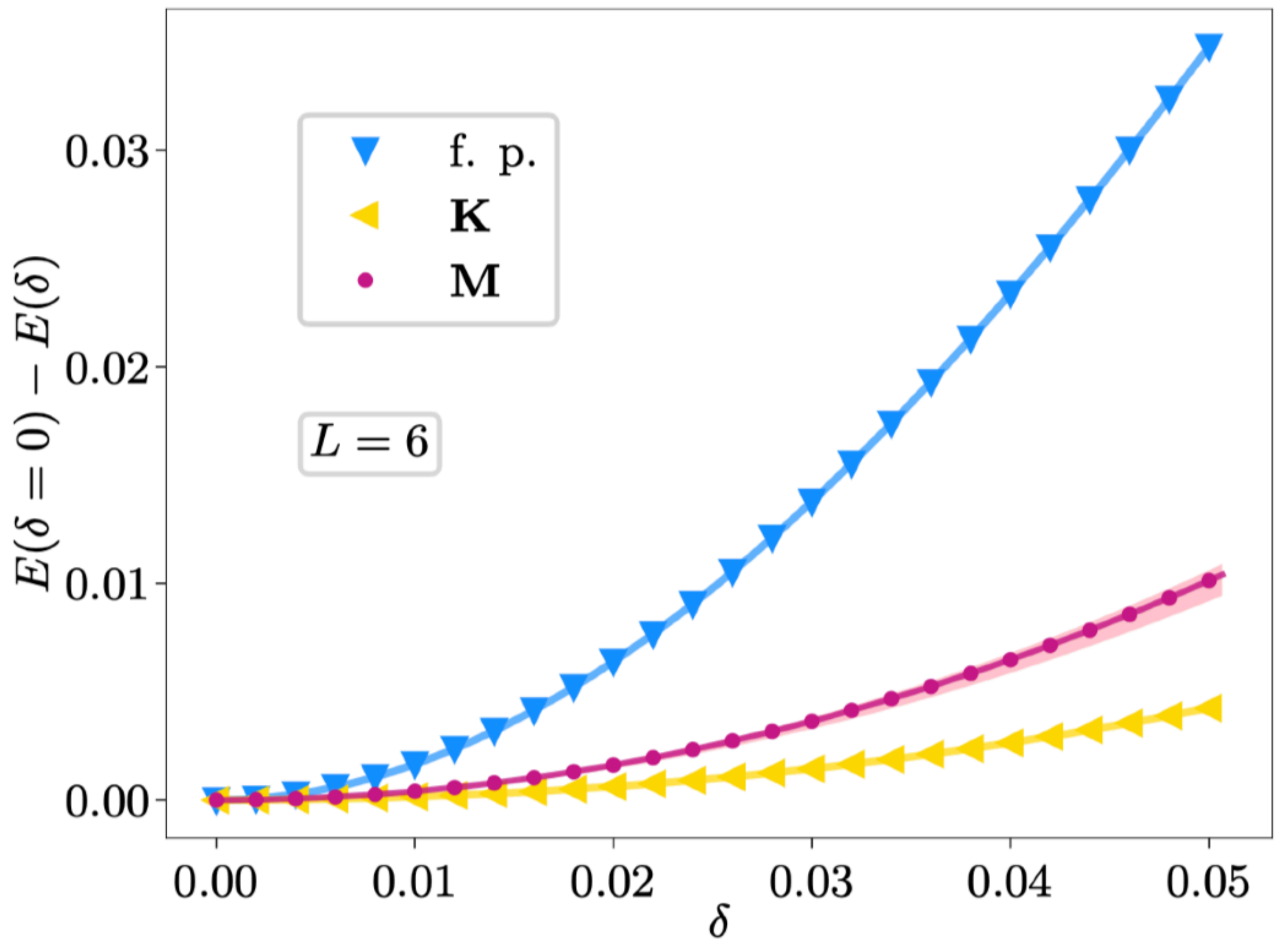
☞ P89 on Thursday by Willsher

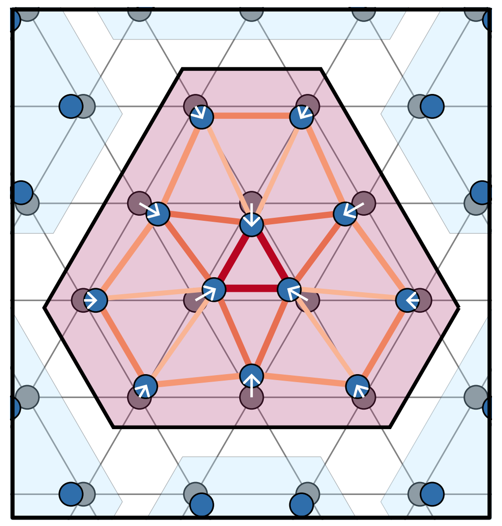
Spin-Peierls instability of the U(1) Dirac QSL

Coupling U(1) Dirac QSL to lattice distortions

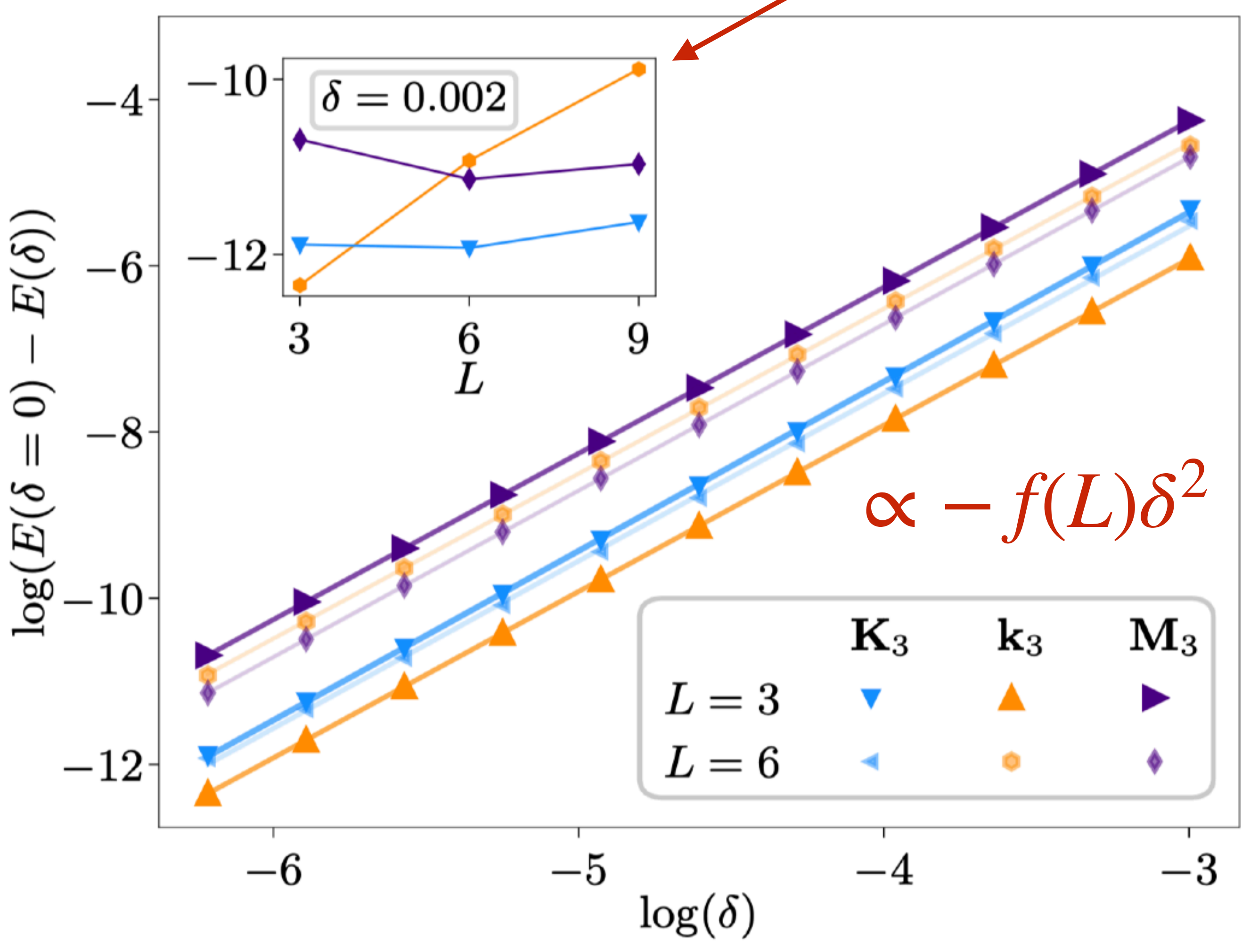
- Relevant and symmetry allowed interaction between monopoles and lattice distortion at $k_a = -K_a/2$
- Minimization of effective action: 12-site VBS-ordered state







Strong L dependence for k_3



☞ P89 on Thursday by Willsher

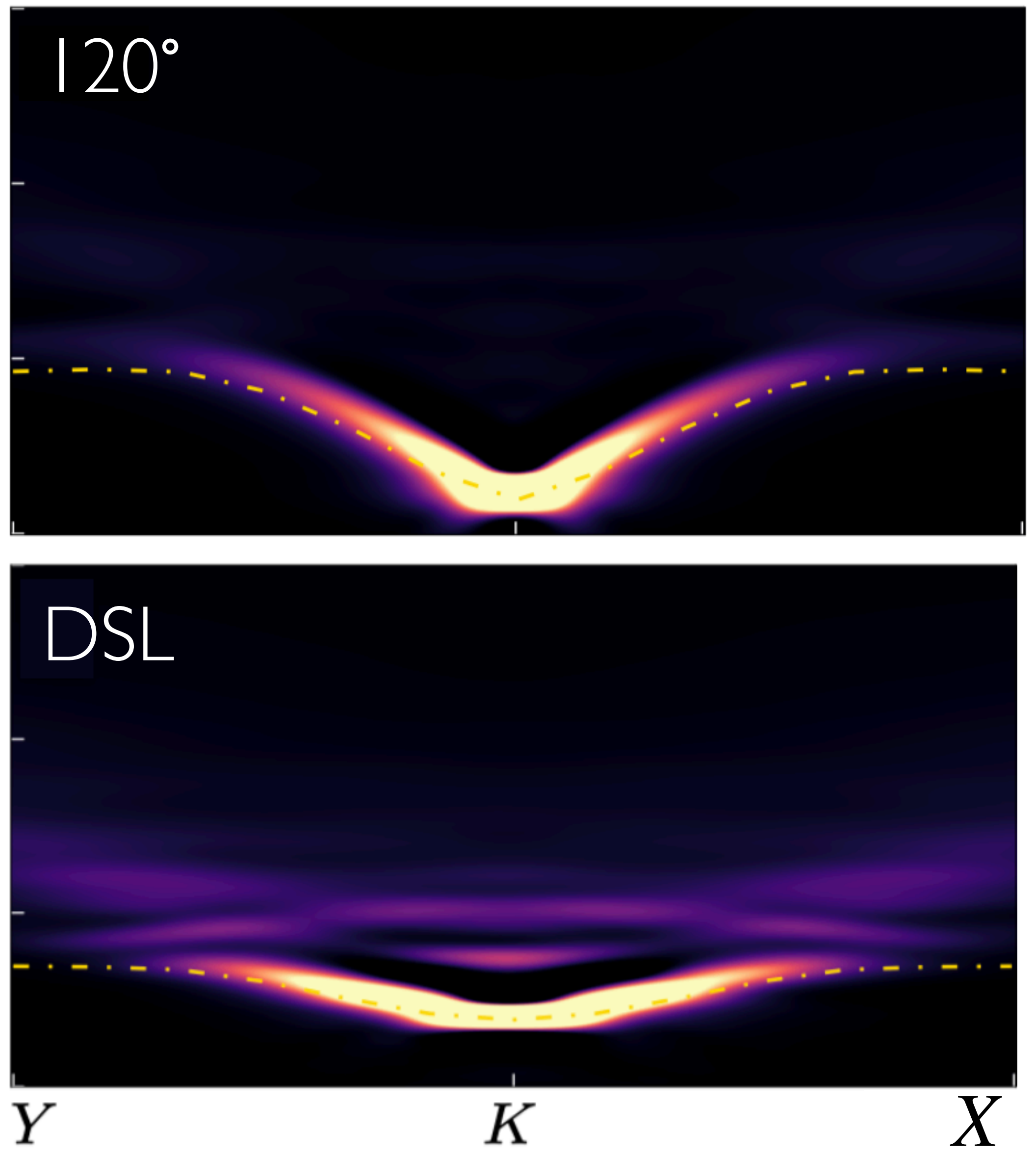
[Seifert, Willsher, Drescher, FP, Knolle, arXiv:2307.12295]

Summary

Dynamical properties of adjacent phases on the triangular lattice

- DMRG dynamics
  - Avoided magnon-decay for 120° order
  - Candidate QSL: Supportive of U(1) DSL

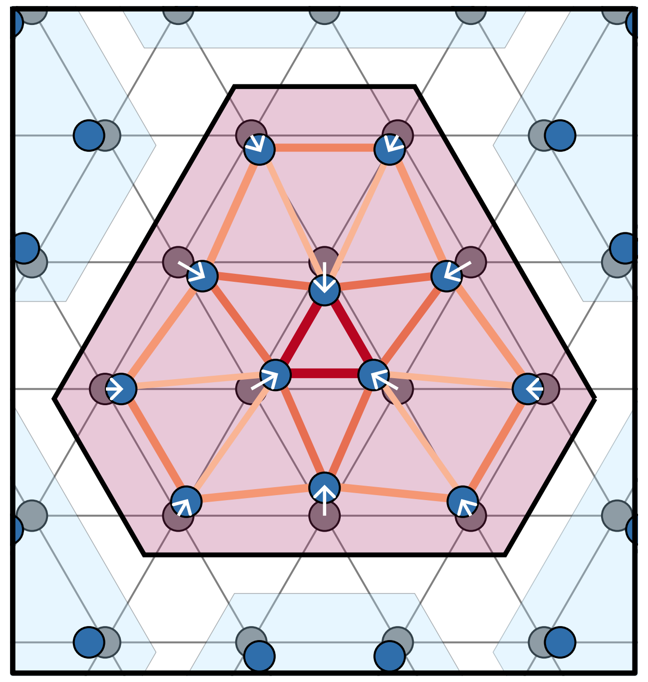
[**Drescher**, Vanderstraeten, Moessner, FP, arXiv:2209.03344 (in print)]



- Spin-Peierls instability of the U(1) DSL

[**Seifert**, **Willsher**, **Drescher**, FP, Knolle, arXiv:2307.12295]

☞ **P89 on Thursday by Willsher**




Drescher


Vanderstraeten


Moessner

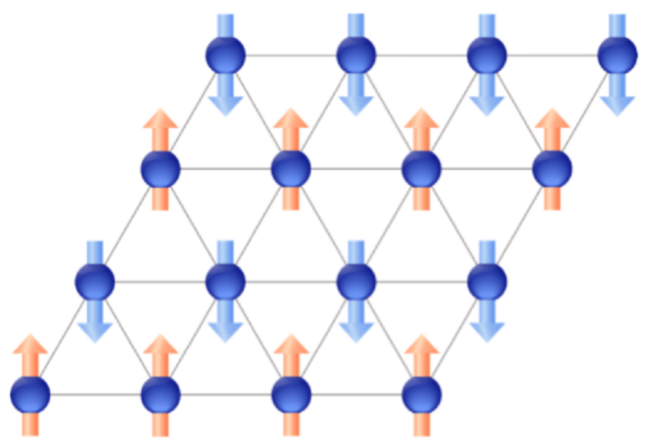

Seifert

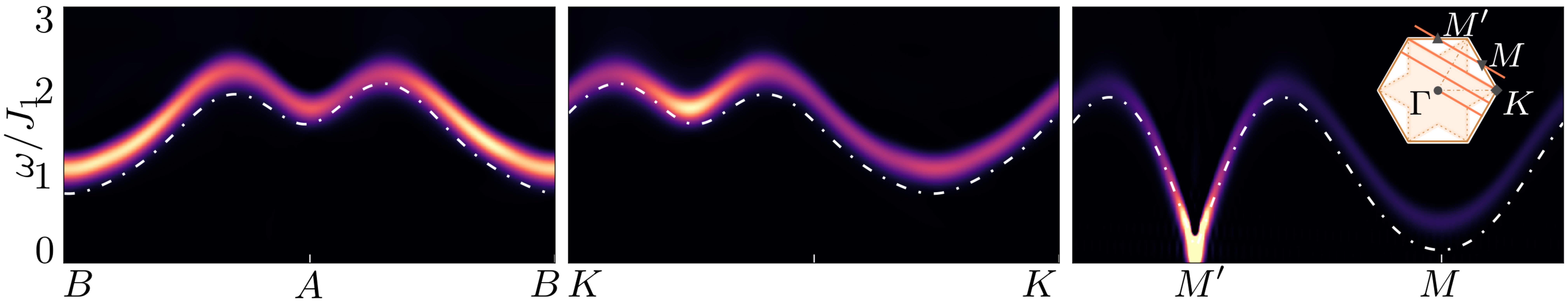

Willsher


Knolle

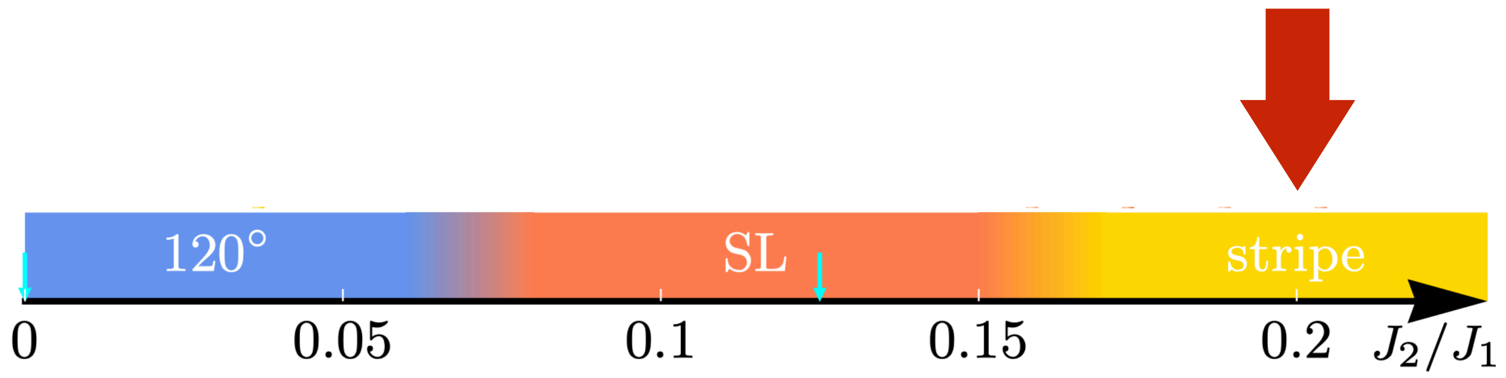
Dynamics of the Heisenberg model: Triangular lattice

Heisenberg model with $J_2/J_1 = 0.55$: Stripe order





- Good agreement with spin wave calculations



[**Drescher**, Vanderstraeten, Moessner, FP, arXiv:2209.03344]