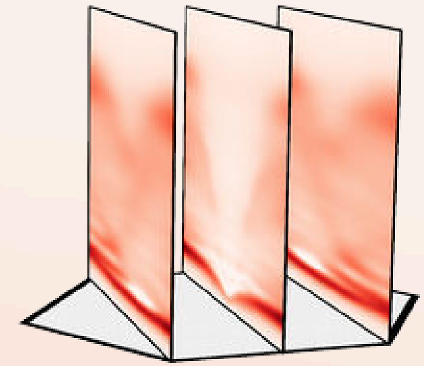
Dynamics of the Kitaev-Heisenberg Model



Ruben Verresen [1,2]

With **Matthias Gohlke** [1], **Roderich Moessner** [1] and **Frank Pollmann** [2]

[1] Max-Planck-Institute for the Physics of Complex Systems (Dresden)

[2] Technical University of Munich

@ Benasque 2017

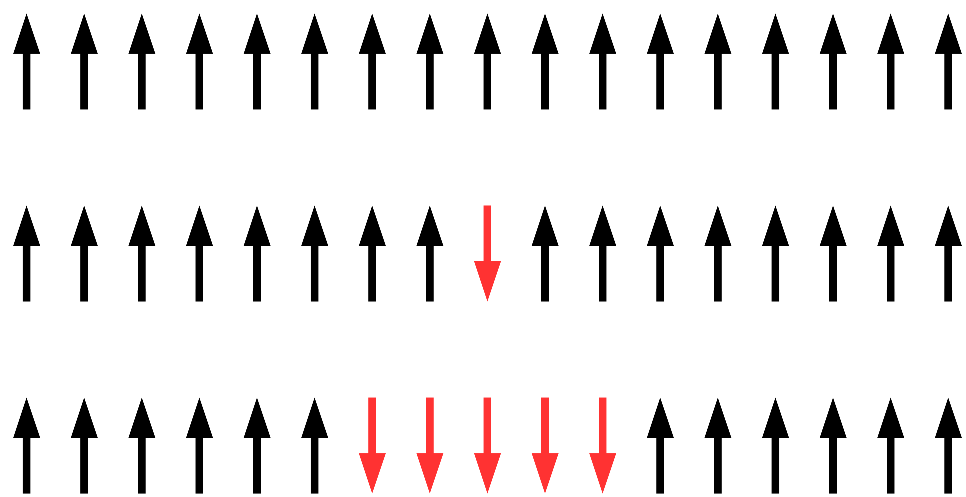
Excited about Excitations

Quantum phases of matter → interesting excitations

E.g. fractionalization

= quasi-particle cannot be created locally

$$H = -\sum \sigma_n^z \sigma_{n+1}^z$$



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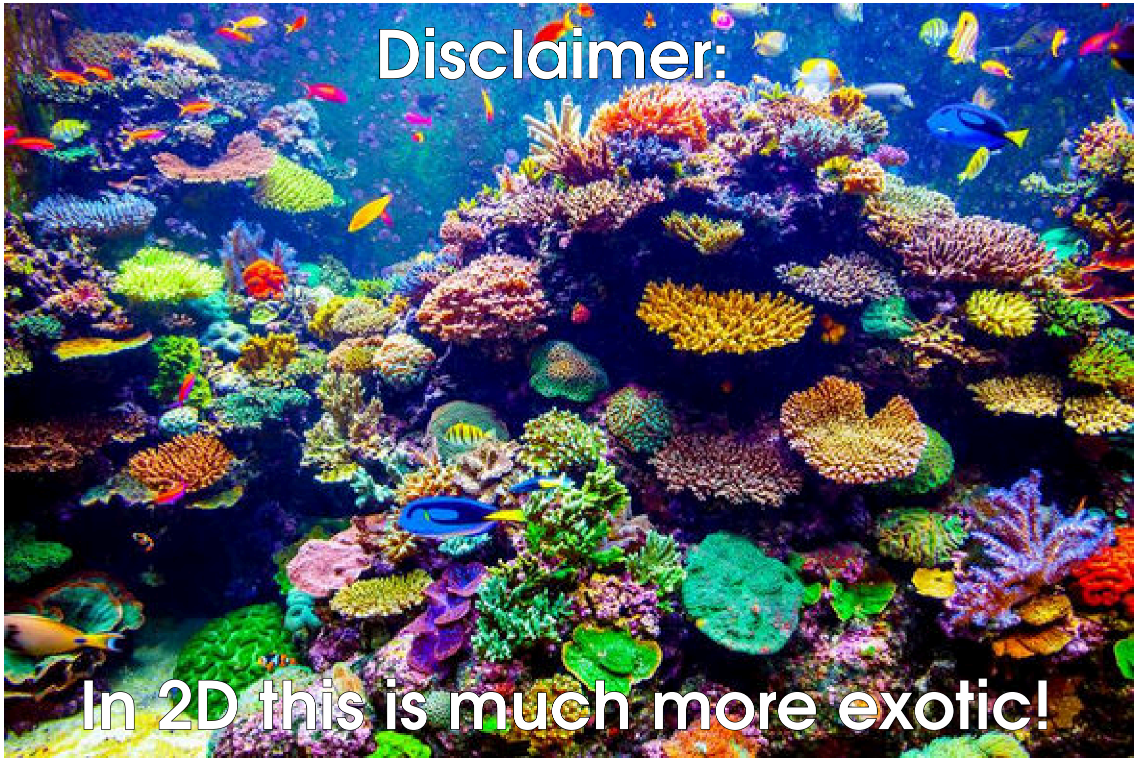
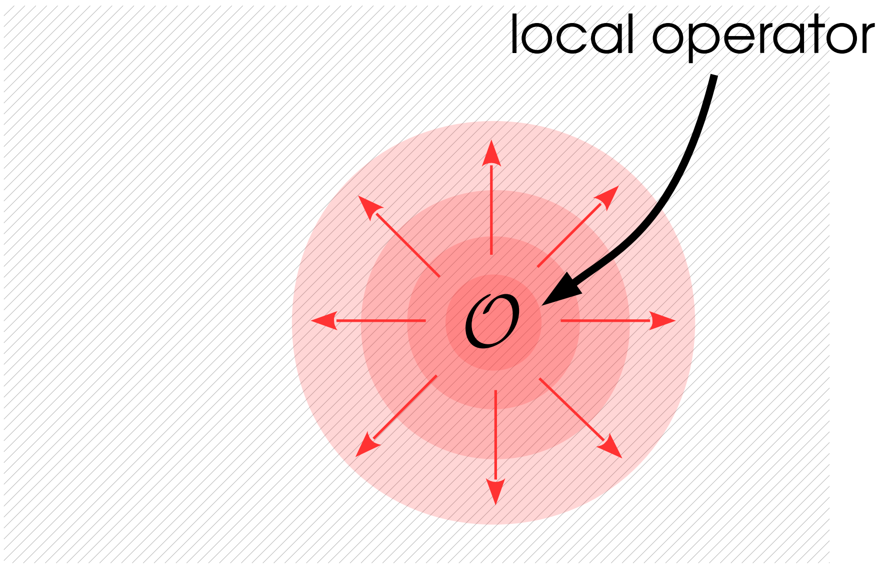


Spectral Function

Question:

" *How many eigenstates with energy* ω *and momentum* $\boldsymbol{k}$ *are in* $\mathcal{O}\,|0\rangle$ *?* "



Answer:

$$\mathcal{S}(\boldsymbol{k},\omega) = \sum_n \delta(\omega-\omega_n)\,\delta(\boldsymbol{k}-\boldsymbol{k}_n)\,|\langle n|\mathcal{O}|0\rangle|^2$$

$=$ Fourier transform of $\langle \mathcal{O}(\boldsymbol{r},t)\,\mathcal{O}(\mathbf{0},0)\rangle$

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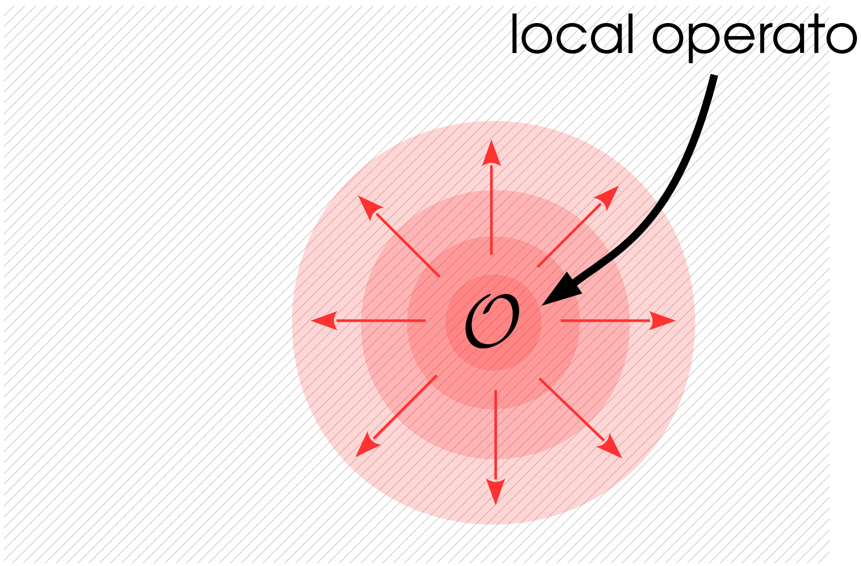


Answer:

Physical meaning

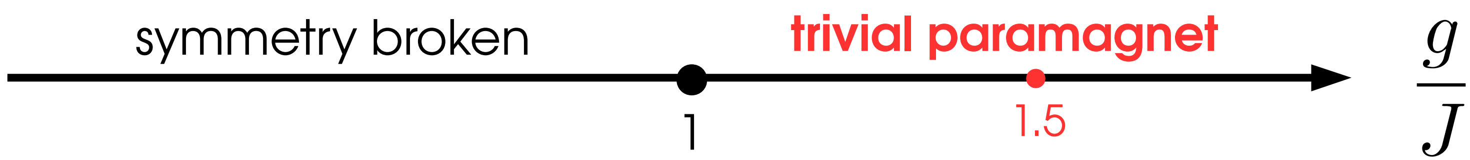
$$\mathcal{S}(\boldsymbol{k},\omega) = \sum_n \delta(\omega-\omega_n)\,\delta(\boldsymbol{k}-\boldsymbol{k}_n)\,|\langle n|\mathcal{O}|0\rangle|^2$$

$=$ Fourier transform of $\langle \mathcal{O}(\boldsymbol{r},t)\;\mathcal{O}(\boldsymbol{0},0)\rangle$

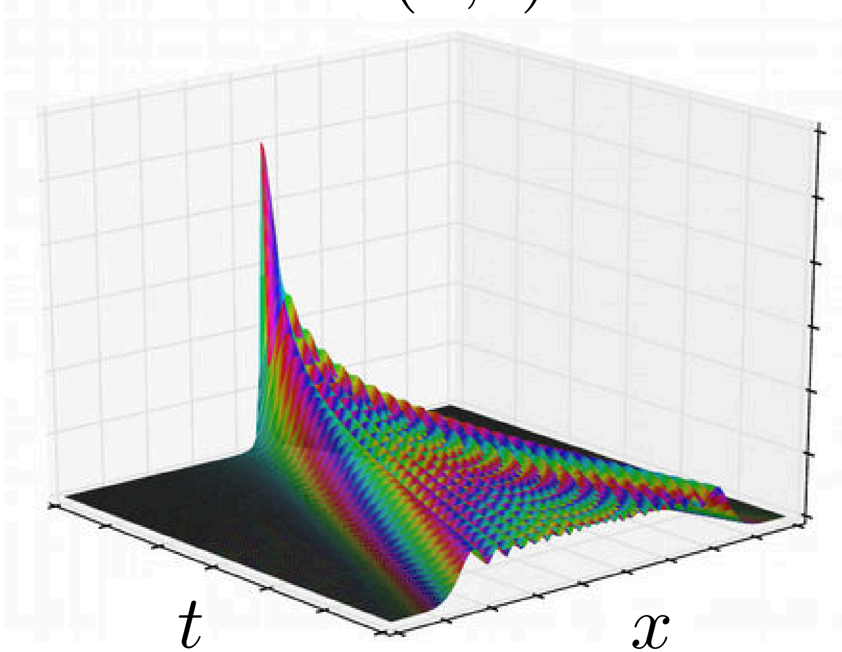
How to obtain it

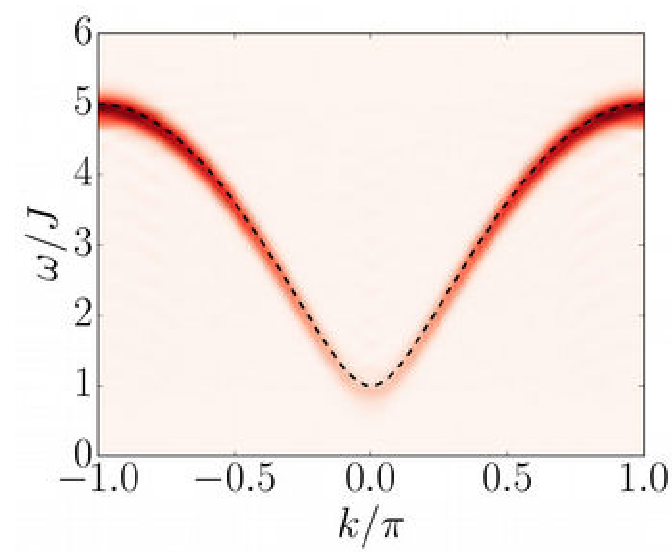
Spectral Function: Examples $(\mathcal{O} = \sigma^y)$

$$H = \sum \left(-J\sigma_n^z\sigma_{n+1}^z + g\sigma_n^x\right)$$



$C(x,t)$ $\xrightarrow{\text{Fourier}}$ $\mathcal{S}(k,w)$





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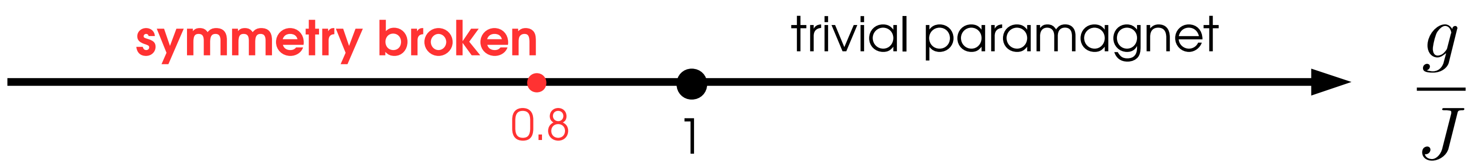

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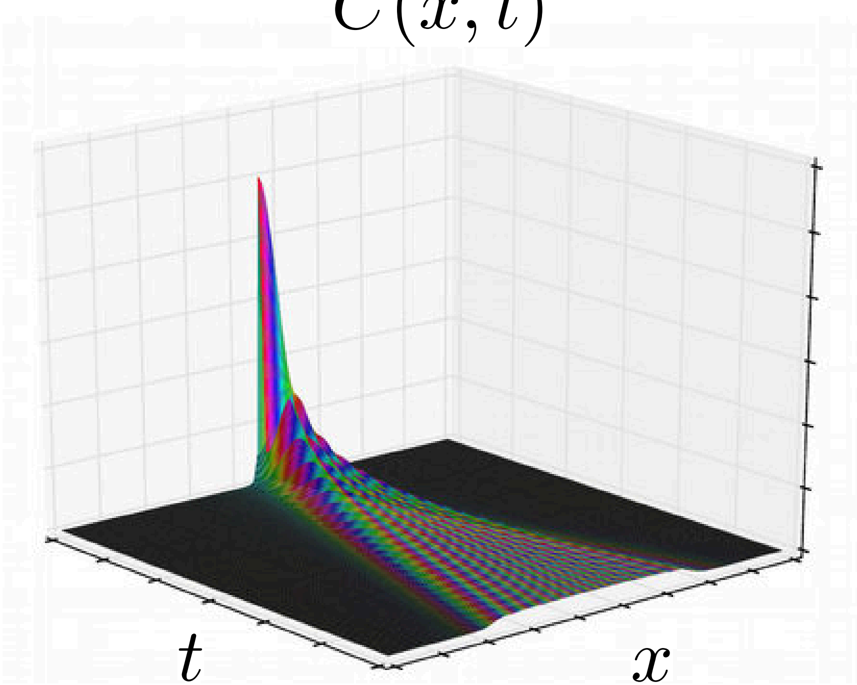
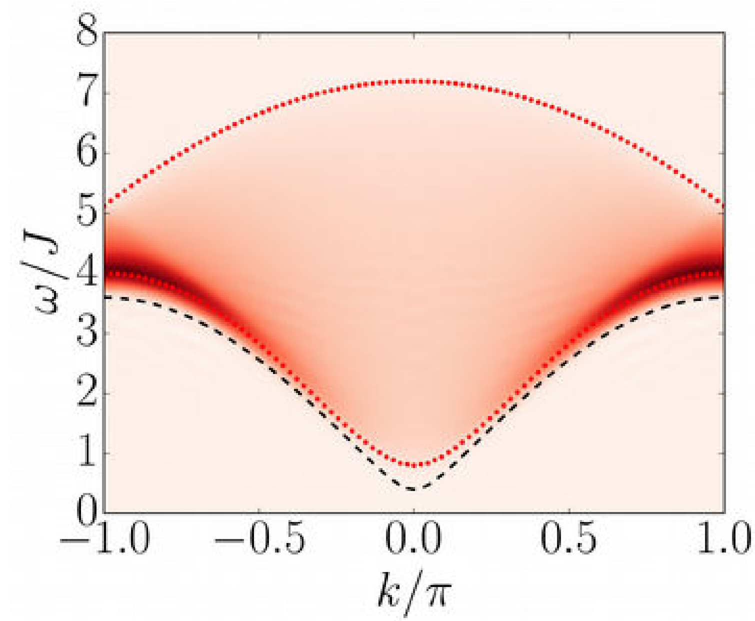


Fourier

$\mathcal{S}(k,w)$



Spectral Function: Summary

$$\mathcal{S}(\boldsymbol{k},\omega) = \frac{1}{2\pi} \sum_{\mathbf{r}} \int_{-\infty}^{\infty} e^{i(\omega t - \boldsymbol{k}\cdot\boldsymbol{r})} \langle \boldsymbol{S}_{\boldsymbol{r}}(t) \cdot \boldsymbol{S}_{\mathbf{0}}(0) \rangle \, \mathrm{d}t$$

Information about

→ spectrum of the Hamiltonian (Lehmann repres.)

$$\mathcal{S}(\boldsymbol{k},\omega) = \sum_{n} \delta(\omega - \omega_n)\, \delta(\boldsymbol{k} - \boldsymbol{k}_n)\, |\langle n|\boldsymbol{S}_{\mathbf{0}}|0\rangle|^2$$

→ are quasi-particles local or not (fractionalization)

→ quasi-particle lifetime, etc...

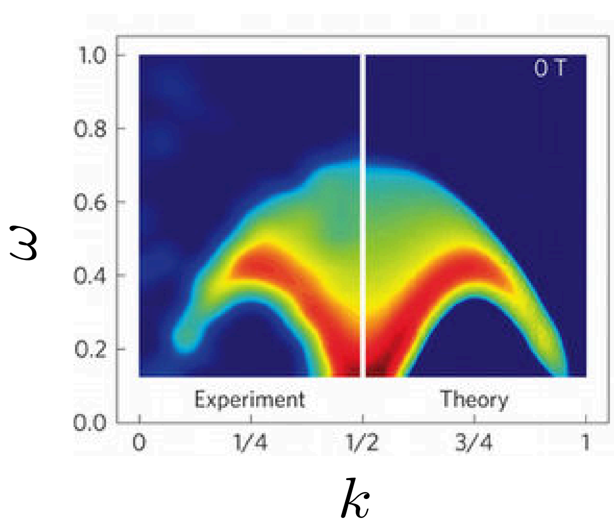
Spectral Function: Experiment

$$\mathcal{S}(\boldsymbol{k},\omega) = \frac{1}{2\pi}\sum_{\mathbf{r}}\int_{-\infty}^{\infty} e^{i(\omega t - \boldsymbol{k}\cdot\boldsymbol{r})}\langle \boldsymbol{S}_{\boldsymbol{r}}(t)\cdot\boldsymbol{S}_{\mathbf{0}}(0)\rangle\,\mathrm{d}t$$

Measurable through inelastic neutron scattering !

1D

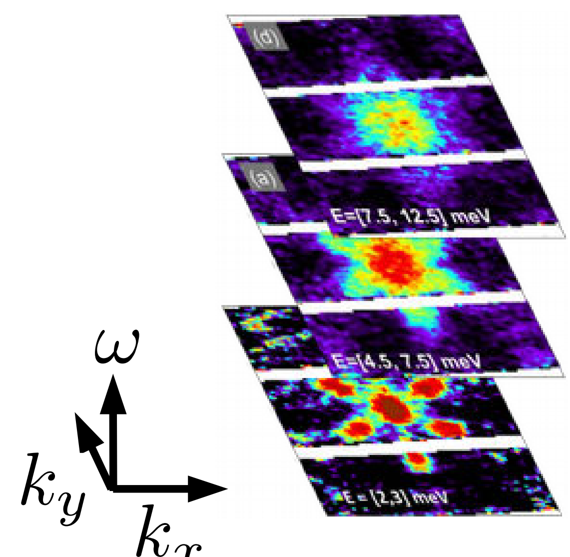
$$H = -\sum_n \boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1}$$



Mourigal et al. (2013)

2D

$$\alpha - \mathrm{RuCl}_3$$



Banerjee et al. (2016)

Spectral Function: Experiment

$$\mathcal{S}(\boldsymbol{k},\omega) = \frac{1}{2\pi}\sum_{\mathbf{r}}\int_{-\infty}^{\infty} e^{i(\omega t - \boldsymbol{k}\cdot\boldsymbol{r})}\,\langle \boldsymbol{S}_{\boldsymbol{r}}(t)\cdot\boldsymbol{S}_{\mathbf{0}}(0)\rangle\,\mathrm{d}t$$

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1D | 2D

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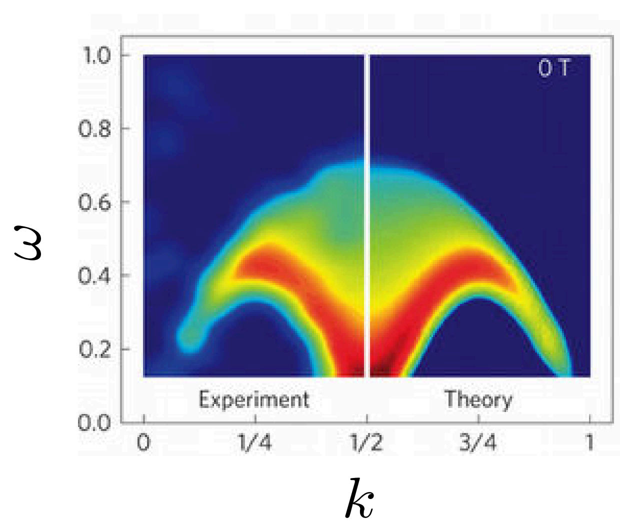

Mourigal et al. (2013)

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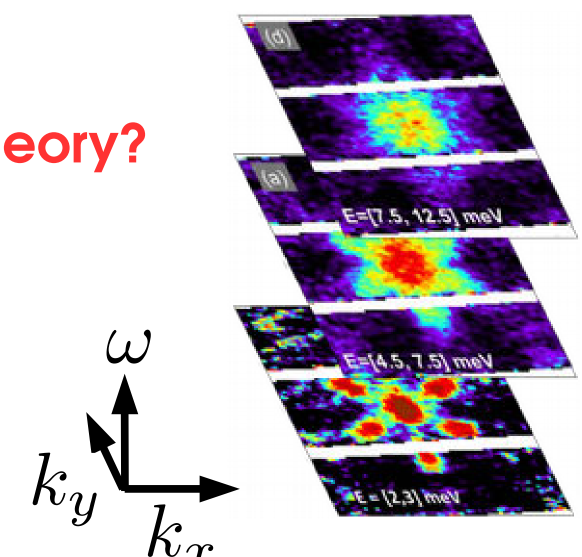
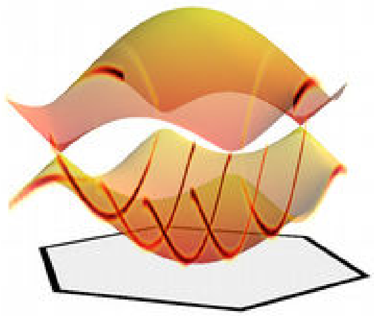
Theory?



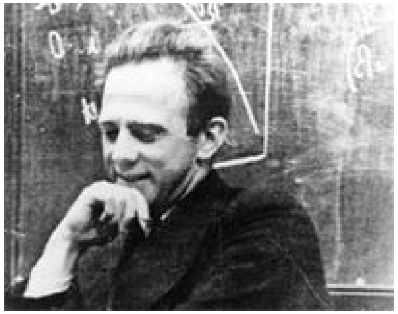
Banerjee et al. (2016)

A Very Short Outline

- Numerical method for calculating dynamic correlations for two-dimensional systems



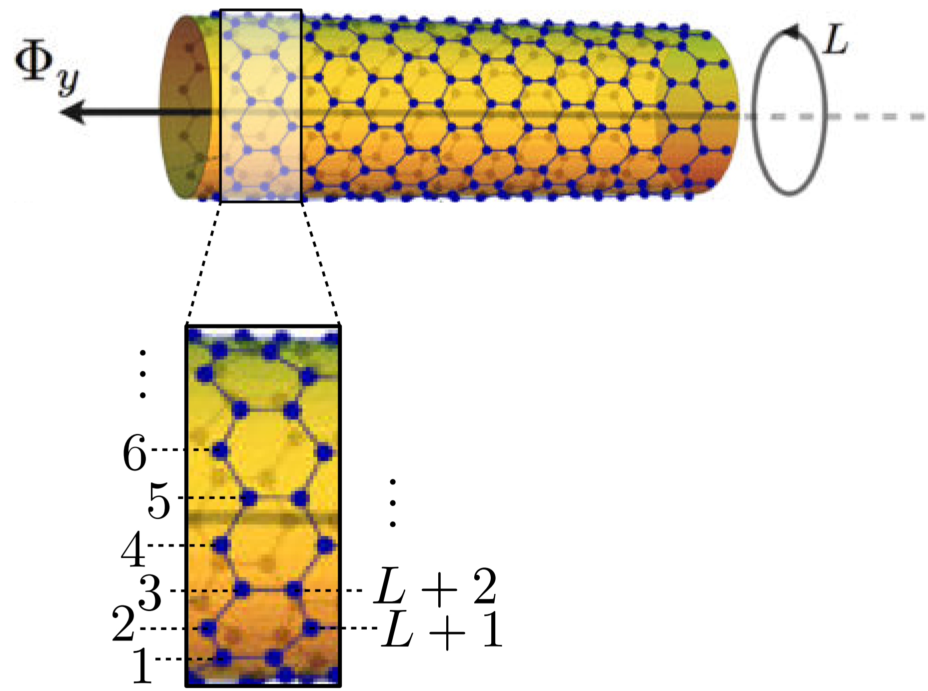
- Application to the Kitaev-Heisenberg model



"proximate spin liquids"?

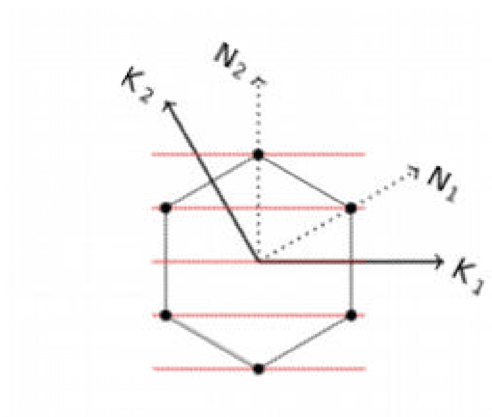
2D in a 1D jacket

Real space:



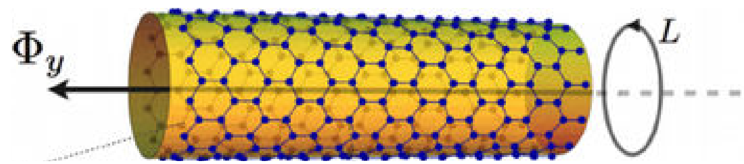
$(L \leq 12)$

Momentum space:



(cylinder by Adolfo Grushin)

Cylinder: 1D or 2D?



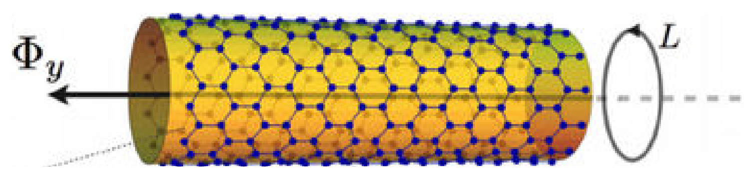
$$H = \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} S^x_{\boldsymbol{i}} S^x_{\boldsymbol{j}} + S^y_{\boldsymbol{i}} S^y_{\boldsymbol{j}} + \Delta S^z_{\boldsymbol{i}} S^z_{\boldsymbol{j}}$$

$SU(2)$

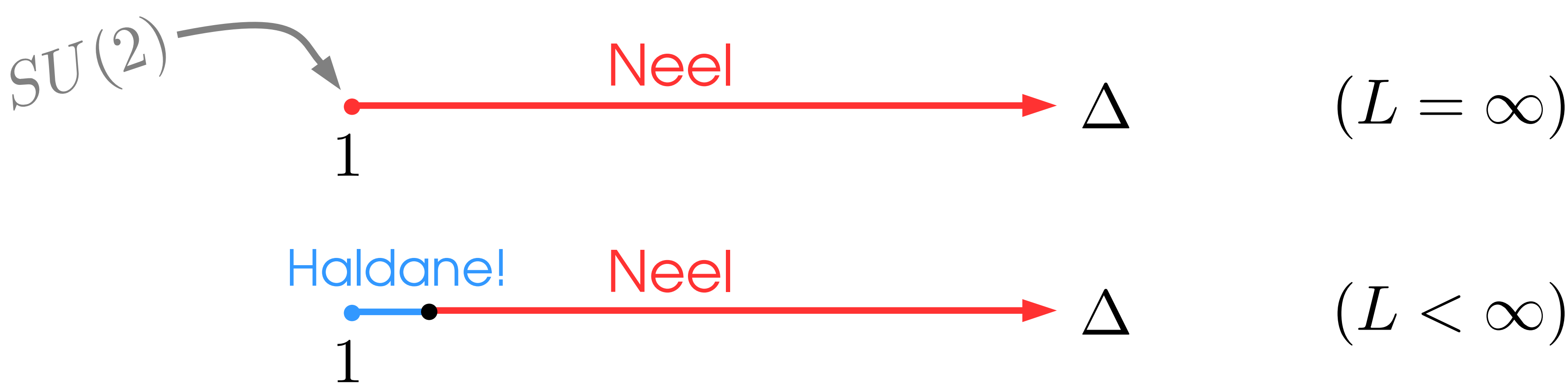
Neel

$1 \longrightarrow \Delta \qquad (L = \infty)$

Cylinder: 1D or 2D?



$$H = \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} S^x_{\boldsymbol{i}} S^x_{\boldsymbol{j}} + S^y_{\boldsymbol{i}} S^y_{\boldsymbol{j}} + \Delta S^z_{\boldsymbol{i}} S^z_{\boldsymbol{j}}$$



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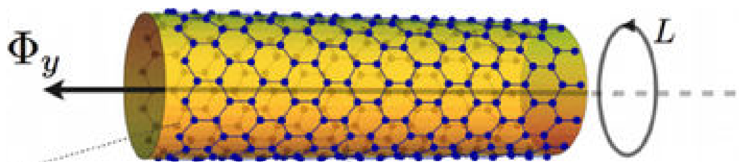


Compared to exact diagonalization:

Similar care needed when extrapolating

Advantages:

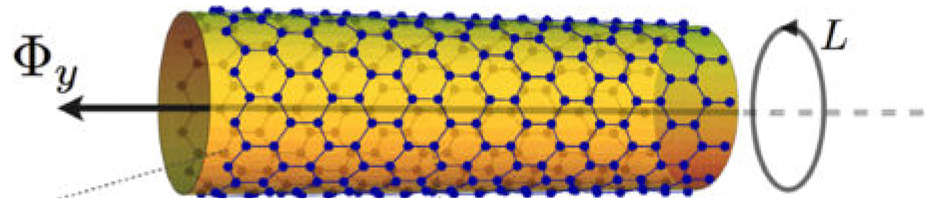
→ larger system sizes

→ continuous momentum

→ (much) longer times

Method to Obtain $\mathcal{S}(\boldsymbol{k},\omega)$ in 2D

Physics:



$(L \leq 12)$

Numerical ingredients:

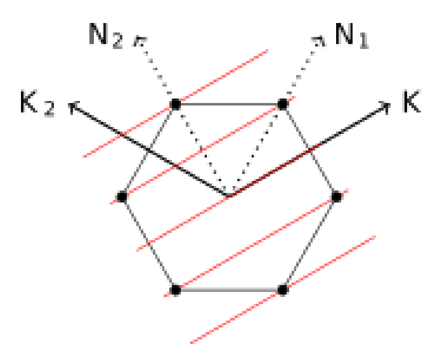
→ For ground state:

Density Matrix Renormalization Group (DMRG) (*)

→ For time evolution:

Matrix Product Operator (MPO) method (**)

We obtain: $C(\boldsymbol{r},t) \xrightarrow{\text{Fourier}} \mathcal{S}(\boldsymbol{k},w)$



(*) White, PRL 69, 2863 (1992)

(**) Zaletel, Mong, Karrasch, Moore, Pollmann; PRB 91, 165112 (2015)

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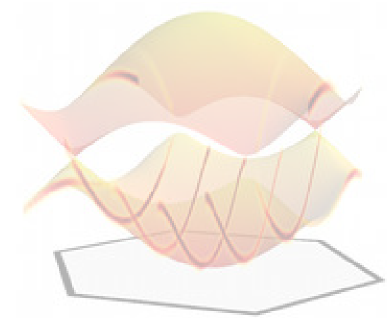

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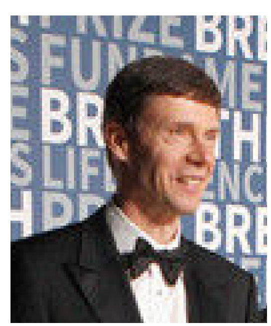
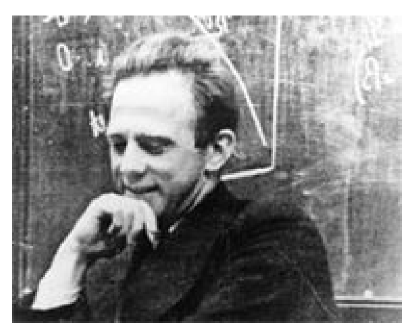
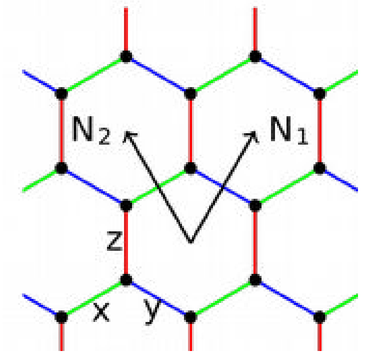



"proximate spin liquids"?

Kitaev (Honeycomb) Model

$$H = \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle_x} S^x_{\boldsymbol{i}} S^x_{\boldsymbol{j}} + \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle_y} S^y_{\boldsymbol{i}} S^y_{\boldsymbol{j}} + \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle_z} S^z_{\boldsymbol{i}} S^z_{\boldsymbol{j}}$$



Exactly soluble model (2006):

$$S^\gamma = c^\dagger_a \, \sigma^\gamma_{ab} \, c_b \dashrightarrow c_a = \gamma_a + i\tilde{\gamma}_a$$

cf. Yasir Iqbal's talk

half → gauge field

half → majoranas

→ spin liquid ground state

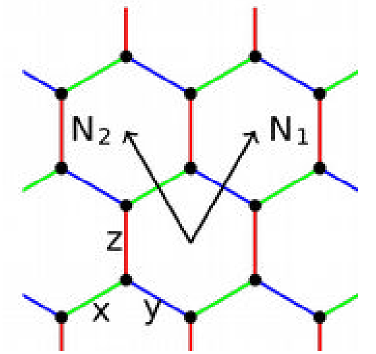
→ fractionalization:

one spin = two gapped fluxes and gapless majorana

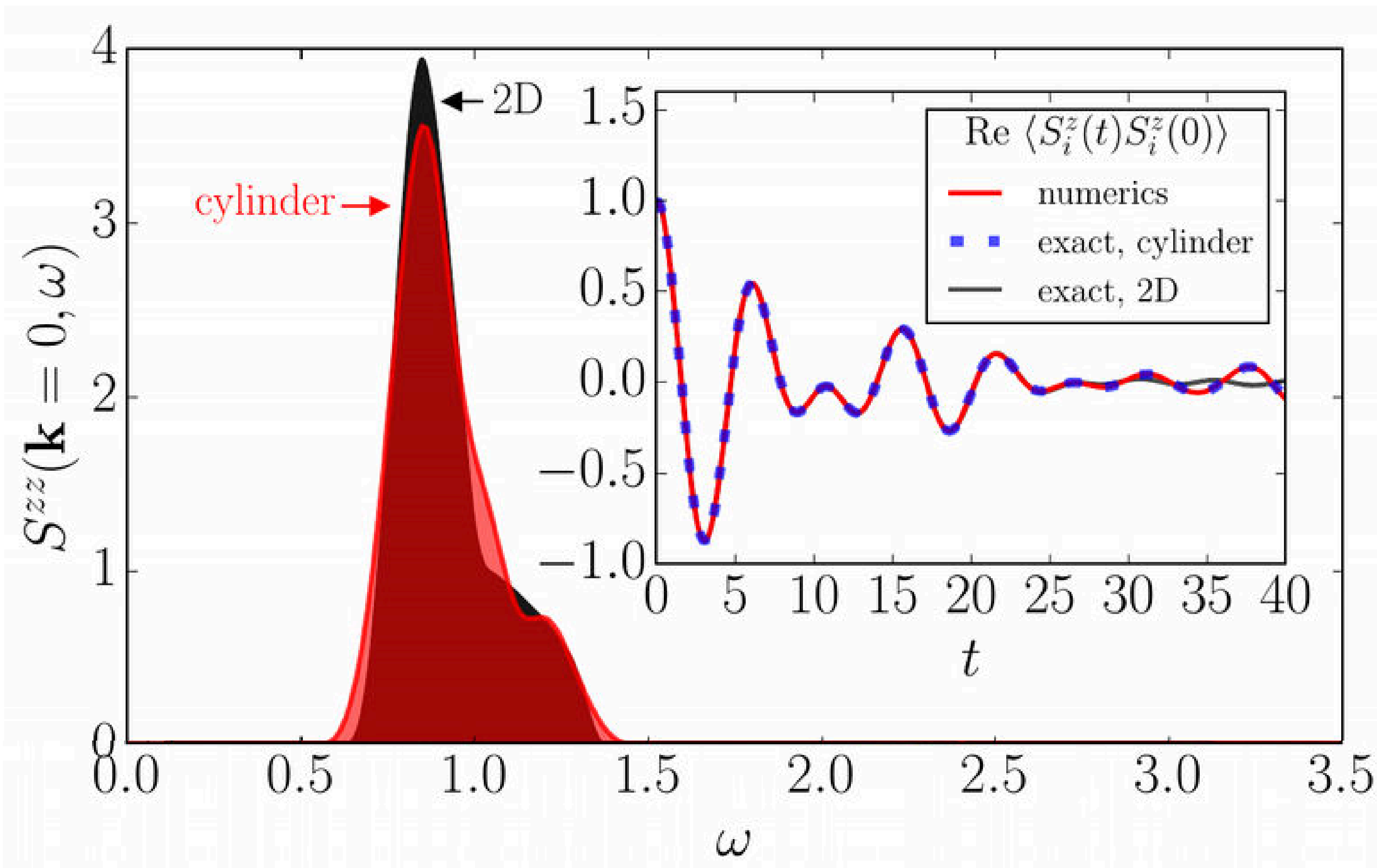
→ gapped $\mathcal{S}(\boldsymbol{k}, w)$ (Knolle et al., \`13)

Dynamics of the gapped Kitaev Model

$$H = -\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle_\gamma} J_\gamma S^\gamma_{\boldsymbol{i}} S^\gamma_{\boldsymbol{j}} \qquad (J_x = 6J_y = 6J_z)$$

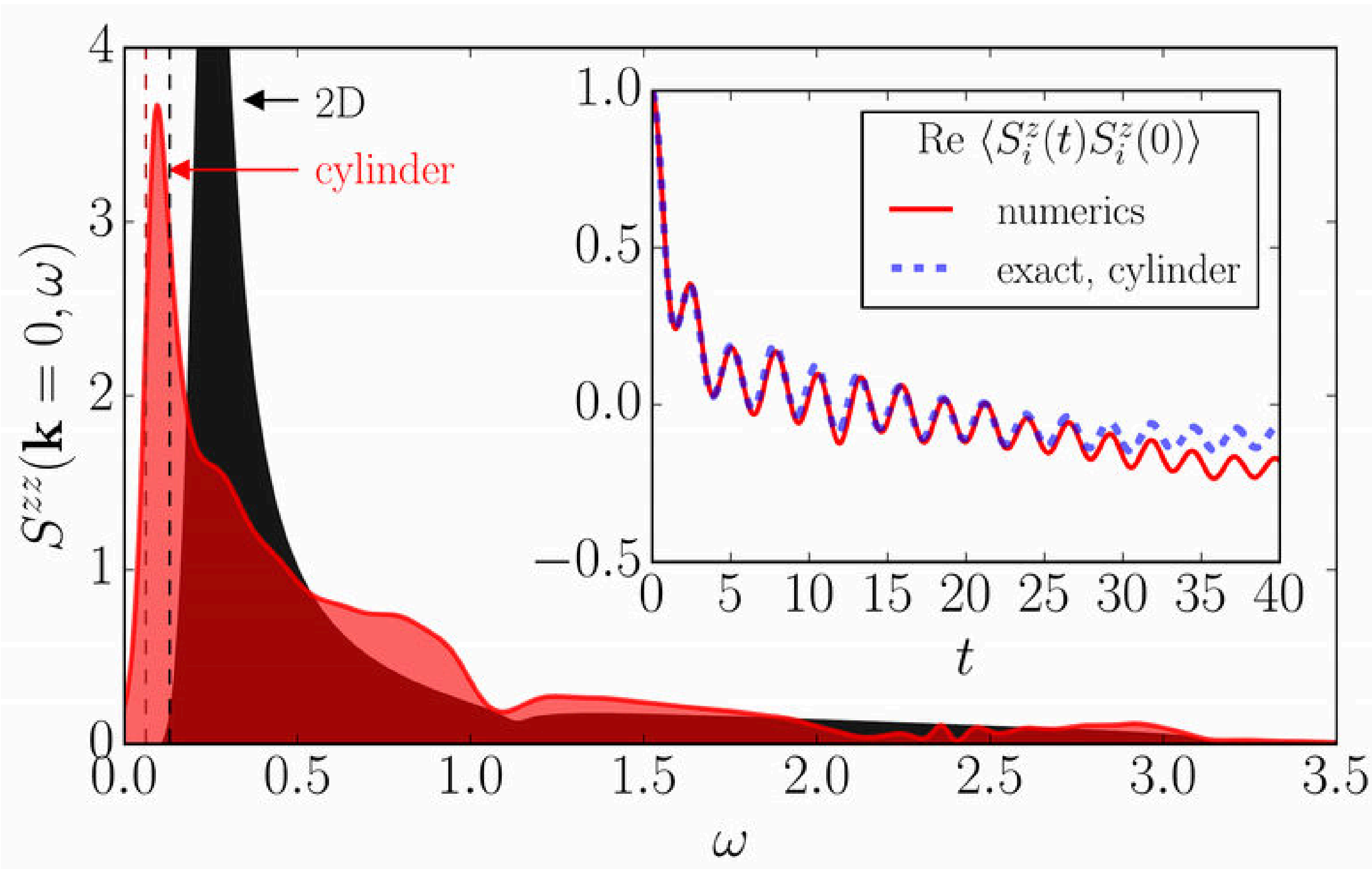


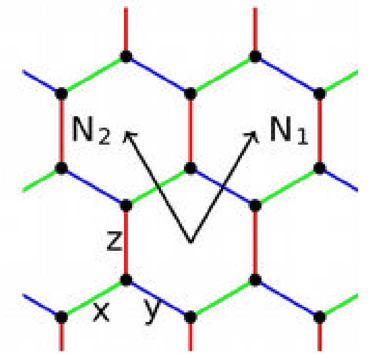
Benchmark: gapped Kitaev model $(L_{\rm circ} = 10)$



Dynamics of the Kitaev-Heisenberg Model

Benchmark: gapless Kitaev model $(L_{\rm circ} = 6)$





Kitaev-Heisenberg Model

$$H = 2\sin\alpha \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle_\gamma} S_{\boldsymbol{i}}^{\gamma} S_{\boldsymbol{j}}^{\gamma} + \cos\alpha \sum_{\boldsymbol{i},\boldsymbol{j}} \boldsymbol{S_i} \cdot \boldsymbol{S_j}$$

→ relevance for A_2IrO_3 and $\alpha{-}RuCl_3$

(Chaloupka, Jackeli, Khaliullin, `10)

→ various works on ground state phase diagram

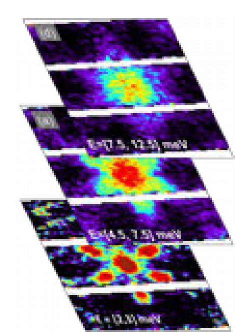
(Chaloupka et al., Iregui et al., Jiang et al., Sela et al., Shinjo et al.)

→ $\mathcal{S}(\boldsymbol{k}, w)$? Perturbative results, low energies

(Song, You, Balents, `16; also recent E.D.: Gotfryd et al, `16)

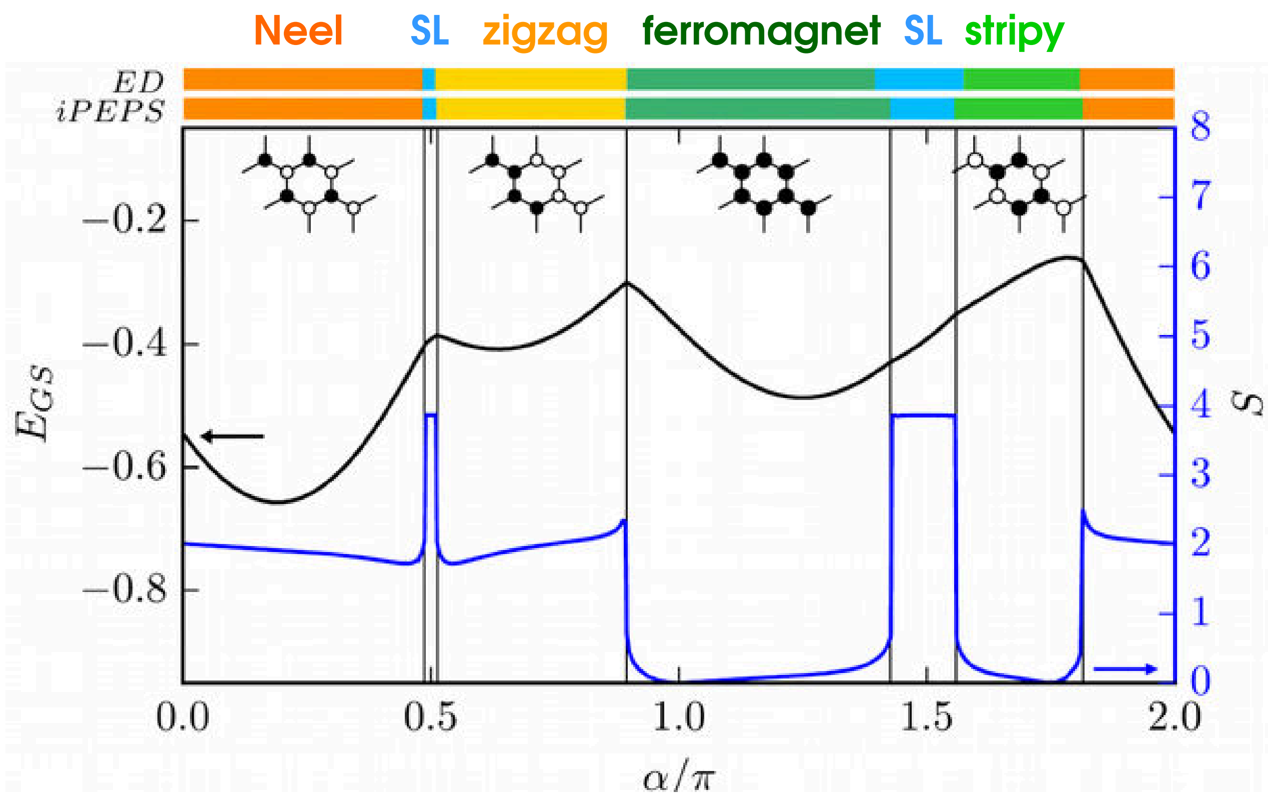
→ experiments: “proximate spin liquids”

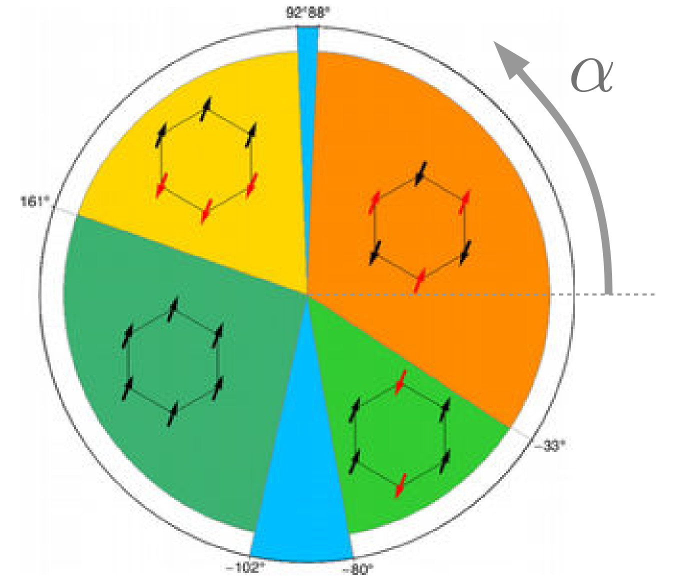
(Banerjee et al., `16; Suzuki et al., `15)



Kitaev-Heisenberg Model

$$H = {\color{red}2\sin\alpha} \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle_\gamma} S^\gamma_{\boldsymbol{i}} S^\gamma_{\boldsymbol{j}} + {\color{red}\cos\alpha} \sum_{\boldsymbol{i},\boldsymbol{j}} \boldsymbol{S}_{\boldsymbol{i}} \cdot \boldsymbol{S}_{\boldsymbol{j}}$$

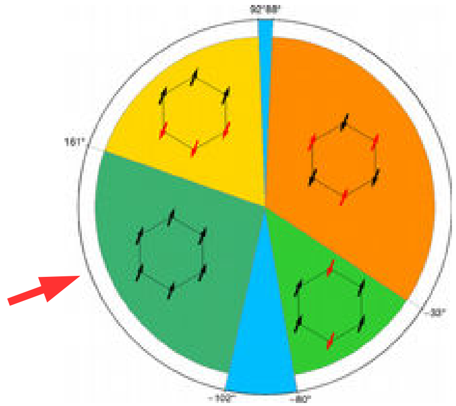




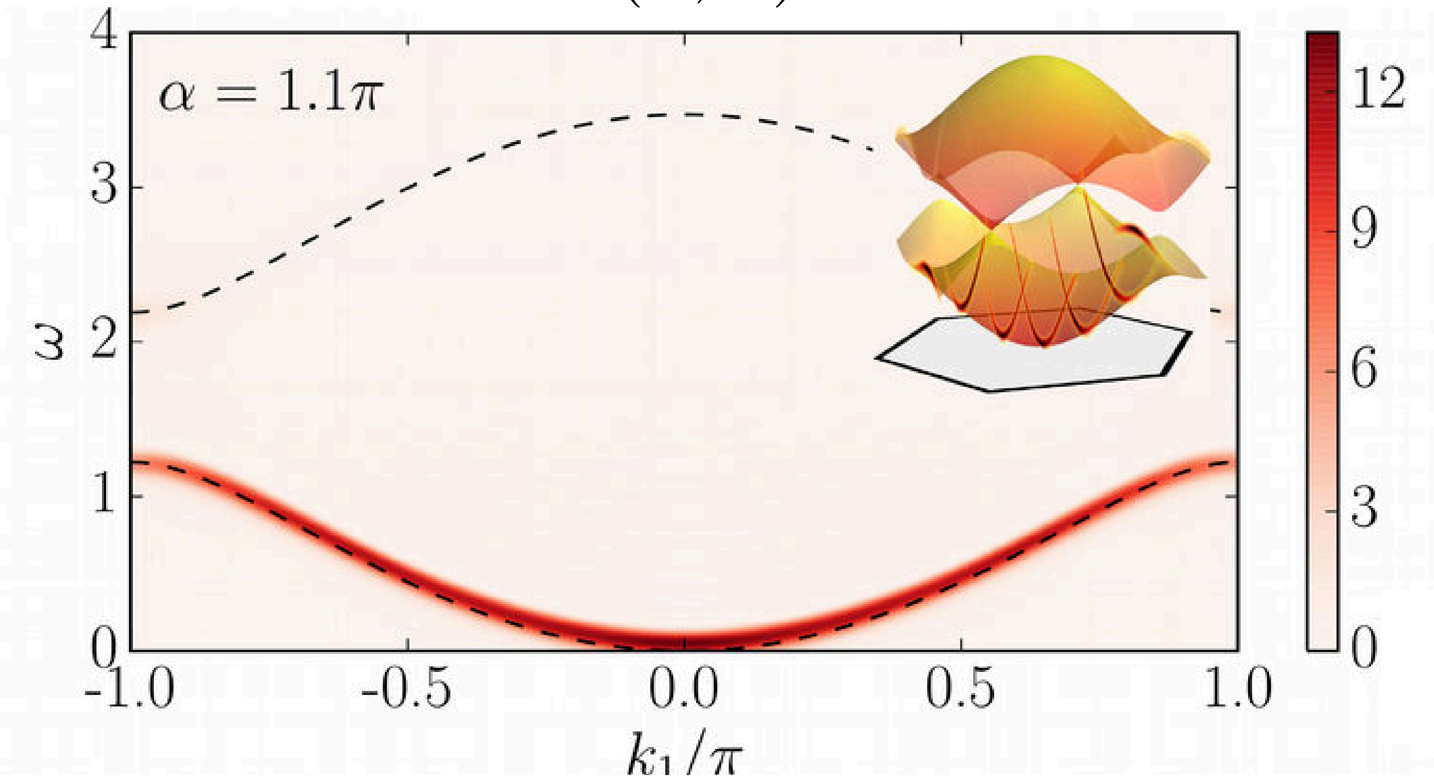
(Image from Iregui, Corboz, Troyer '14)

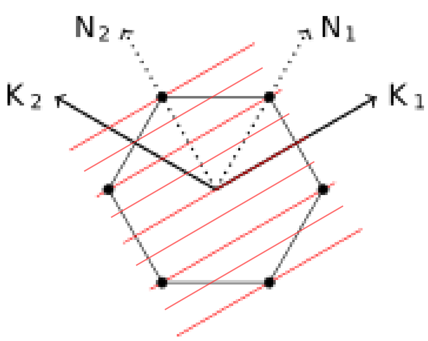
Dynamics of the Kitaev-Heisenberg Model

Ferromagnet with $J_{\mathrm{Kitaev}} = 0.65\ J_{\mathrm{Heis}}$
$(L_{\mathrm{circ}} = 12)$



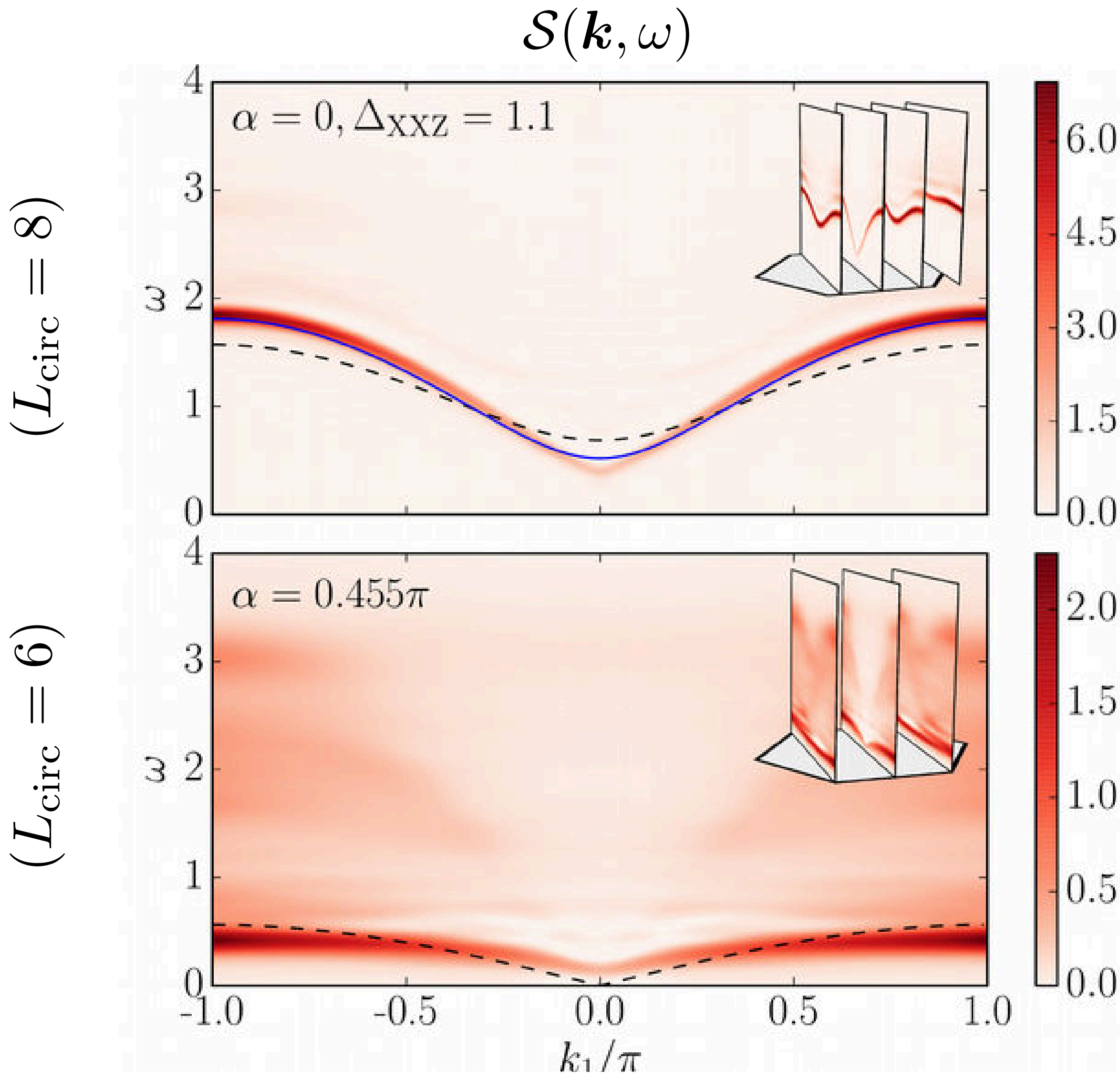
$\mathcal{S}(\boldsymbol{k}, \omega)$

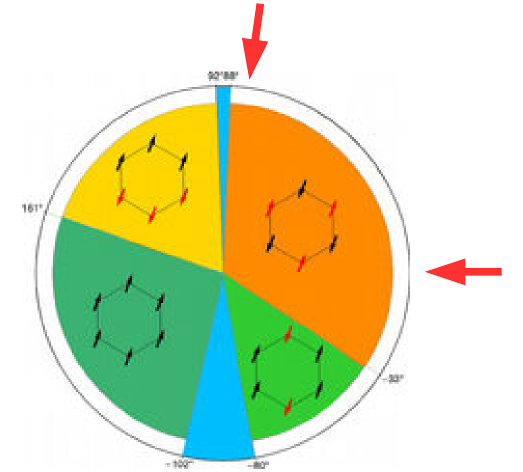


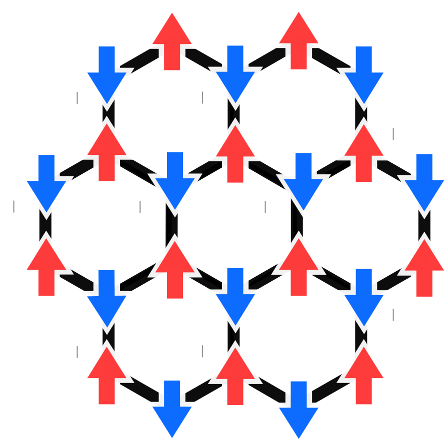


Dynamics of the Kitaev-Heisenberg Model

Neel states: approaching the spin liquid

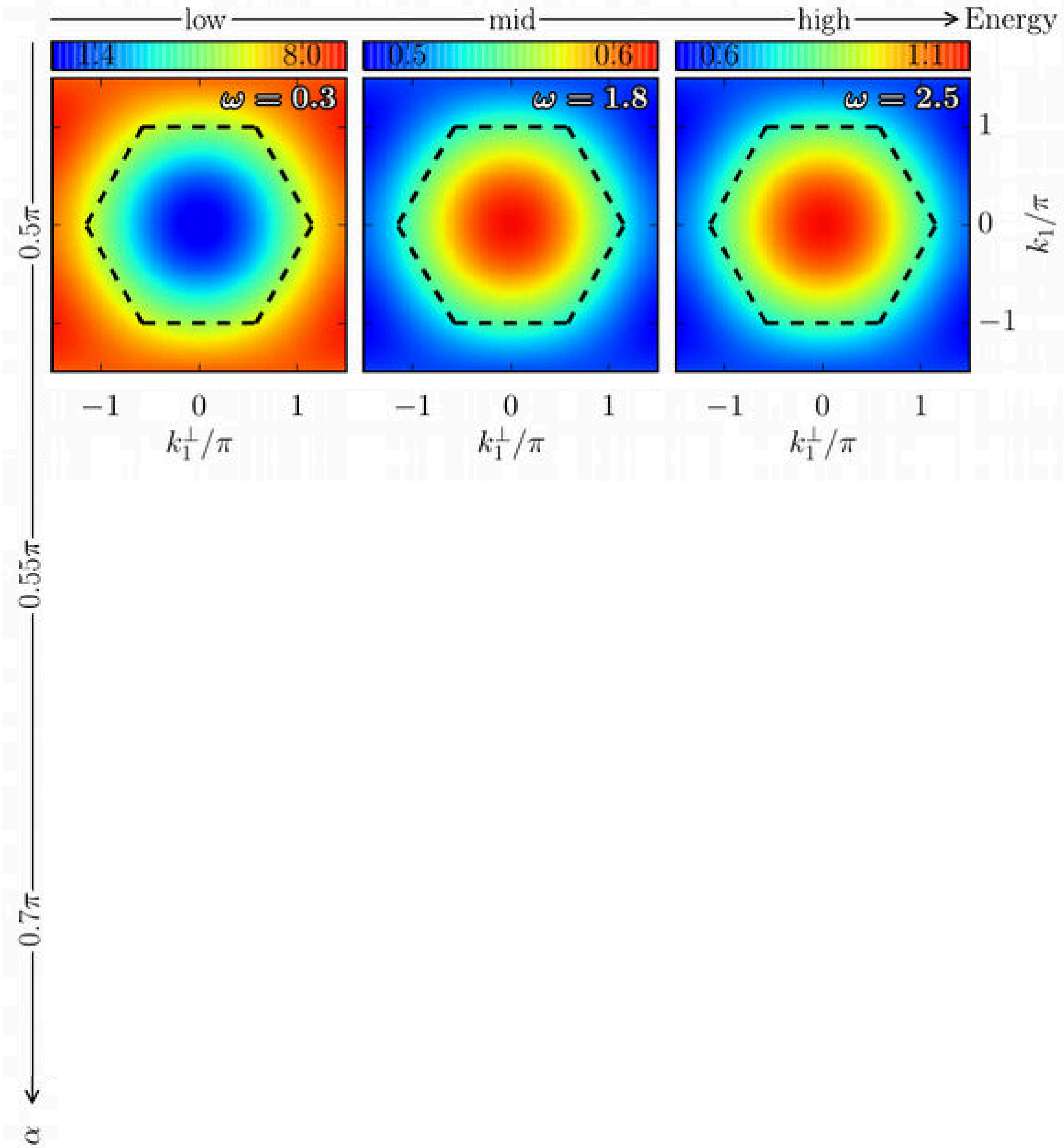


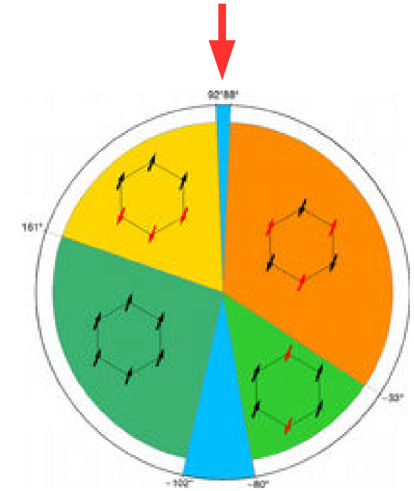


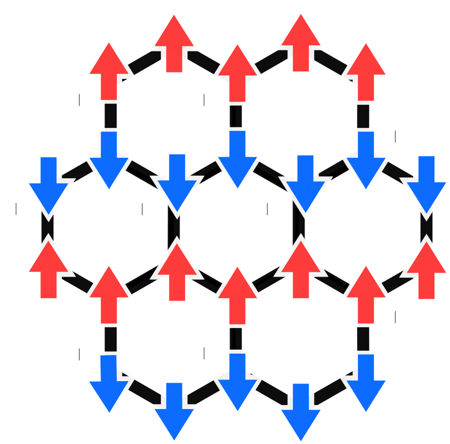


Dynamics of the Kitaev-Heisenberg Model

Zigzag phase: proximate spin liquid? $(L_{\text{circ}} = 12)$







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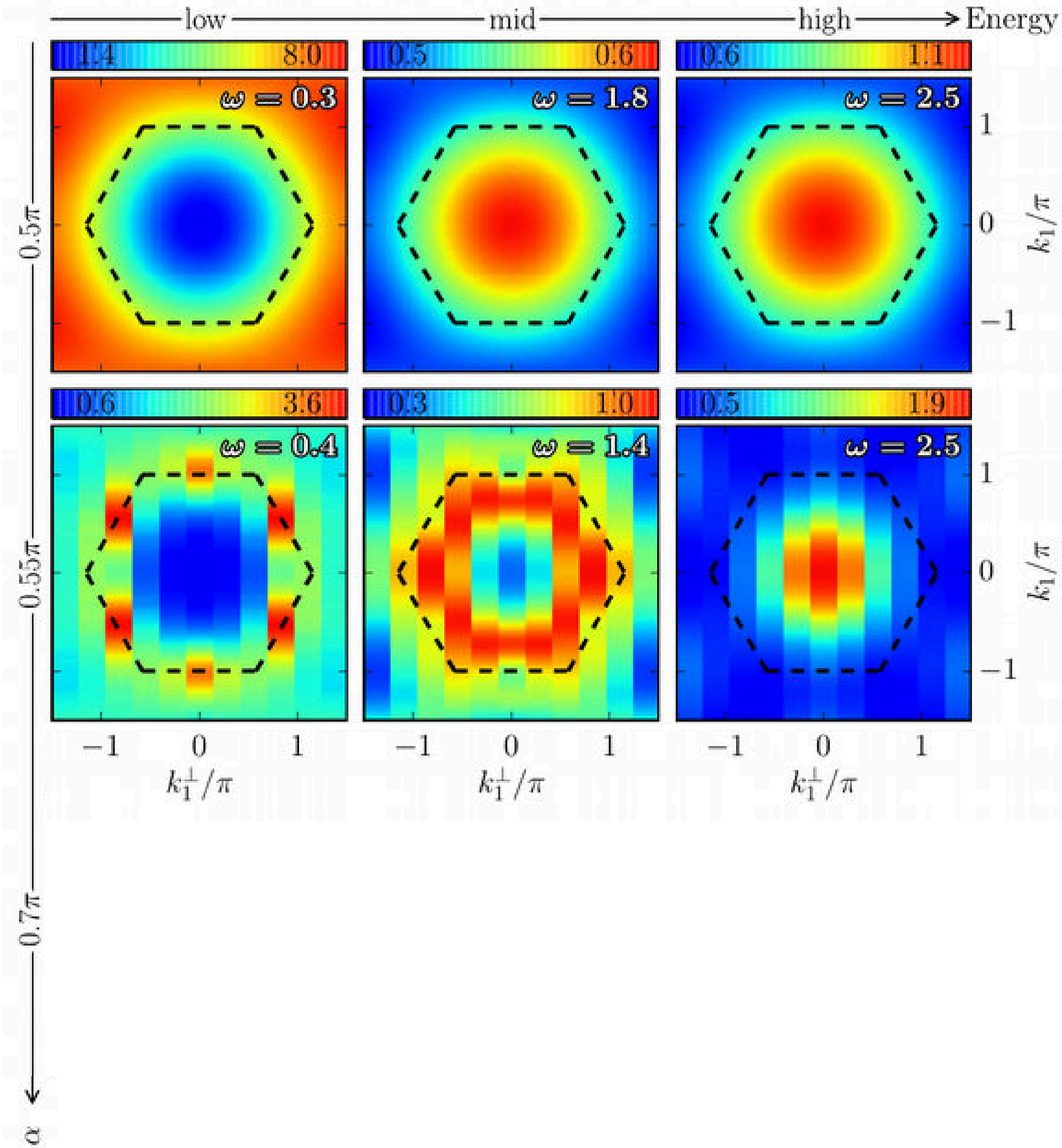

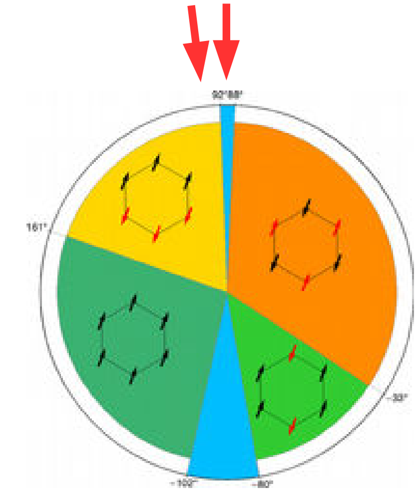

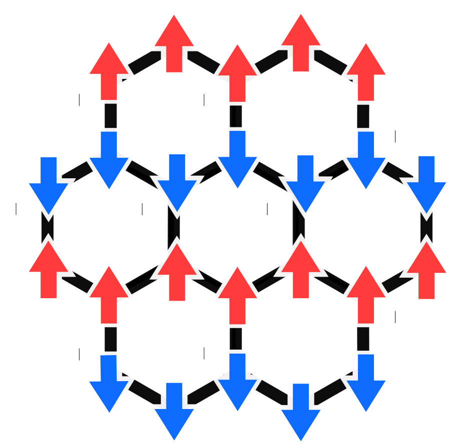

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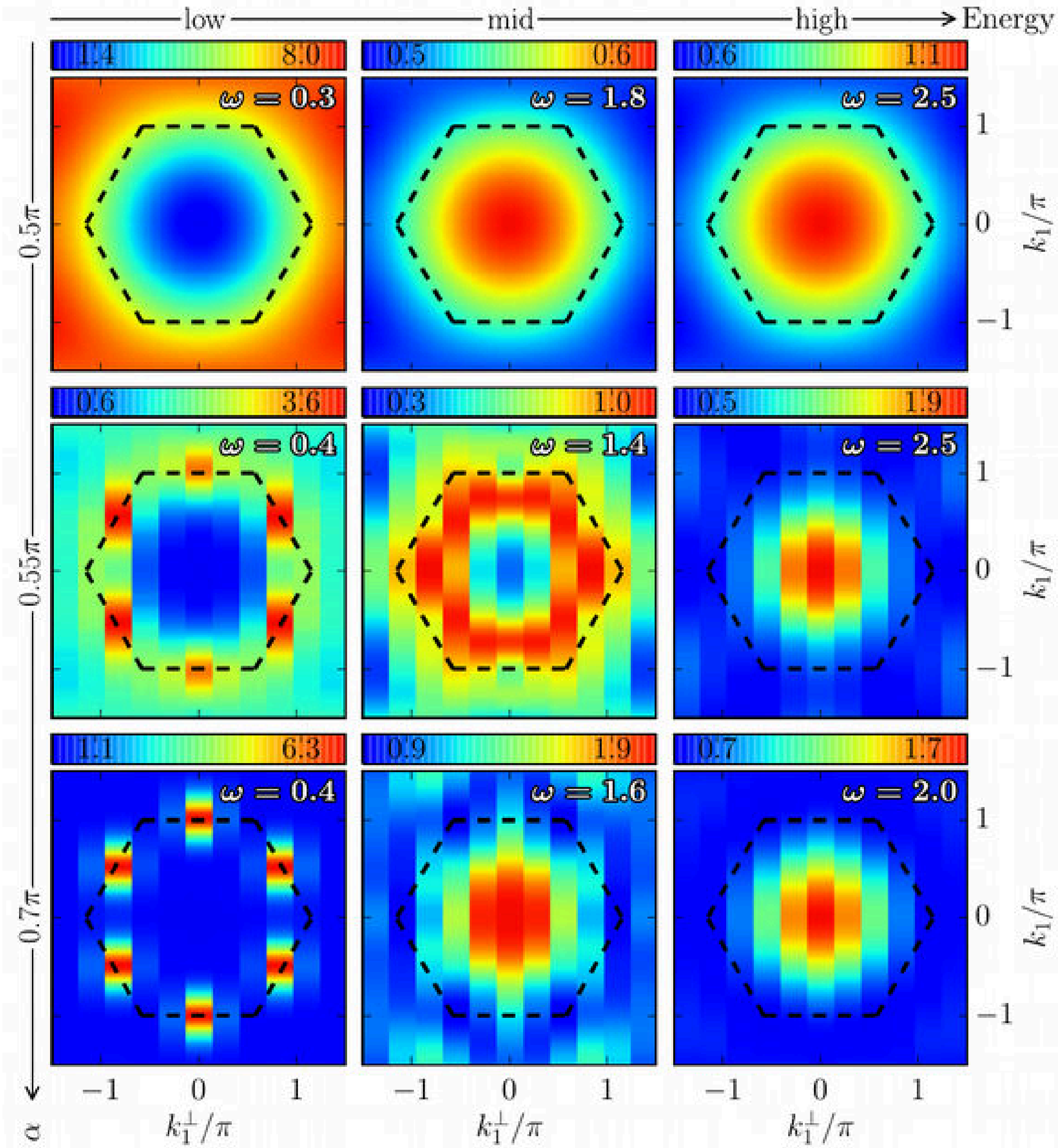

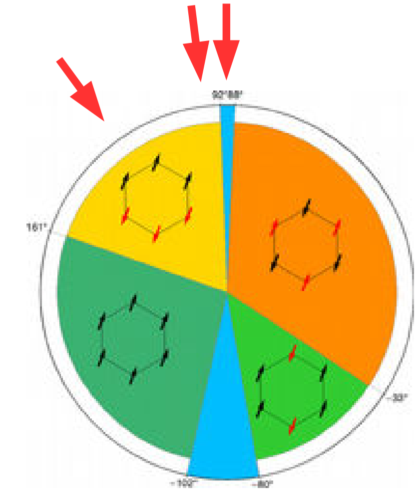

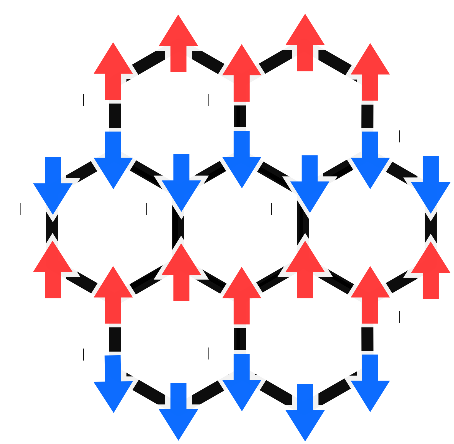

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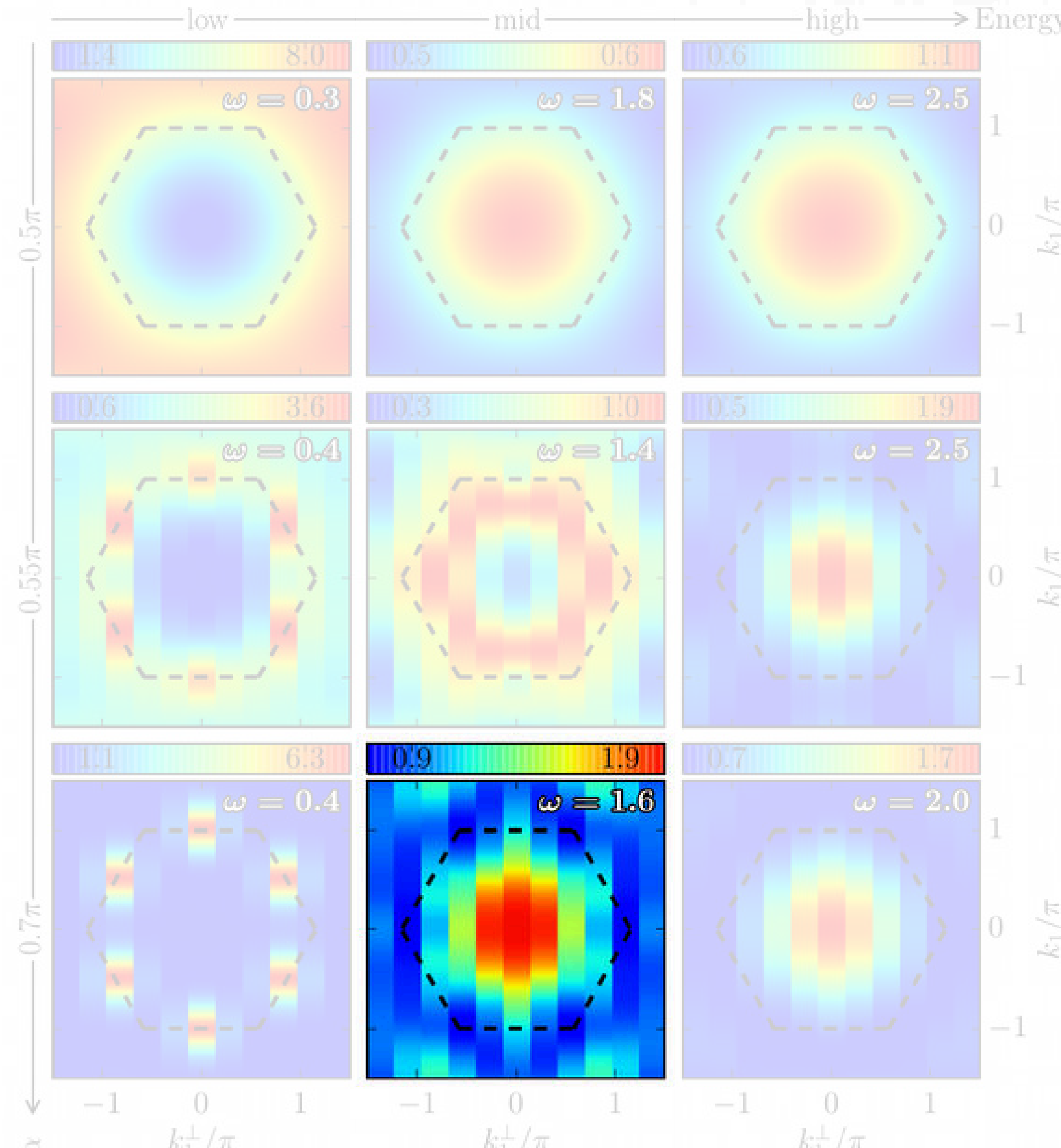
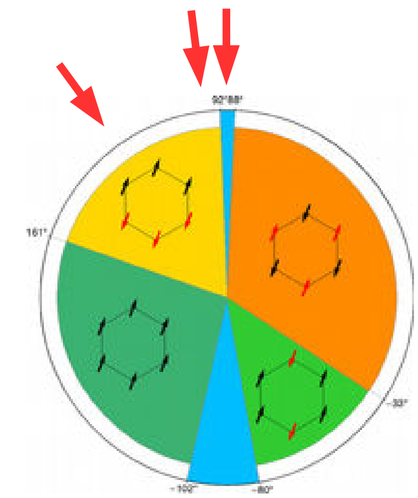
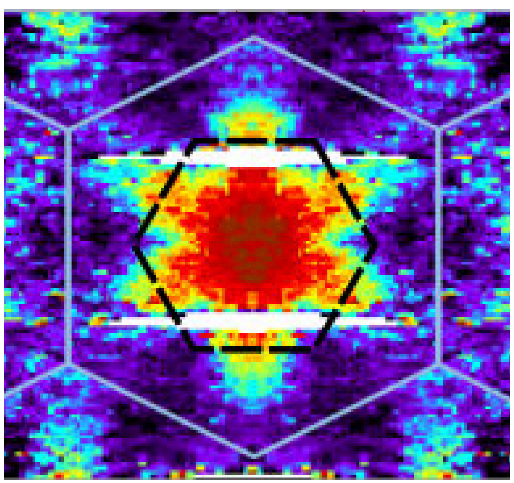
Zigzag phase: proximate spin liquid? $(L_{\mathrm{circ}} = 12)$





$\alpha-\mathrm{RuCl_3}$



(Banerjee et al., `16)

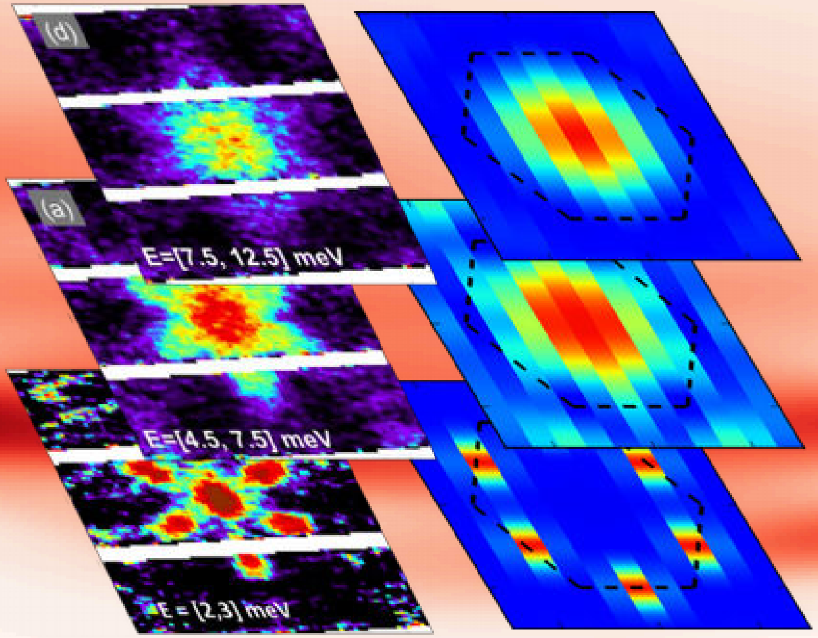
Summary

Obtaining $S(\boldsymbol{k},\omega)$ for two-dimensional systems

Application to Kitaev-Heisenberg model
→ anomalous features of $\alpha{-}\mathrm{RuCl}_3$

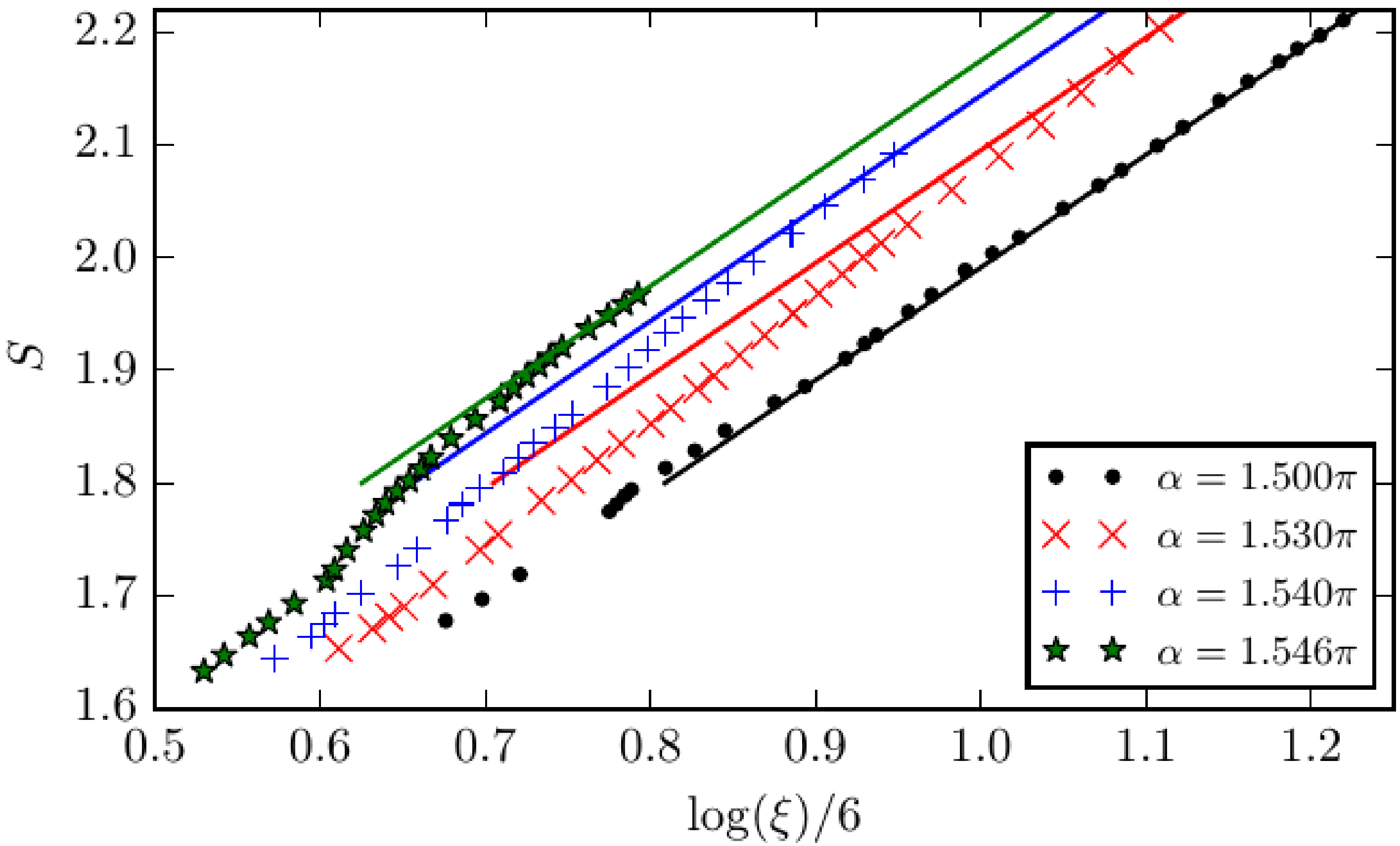
Exciting questions
waiting to be attacked…

How can a spin wave fractionalize?
Spin wave anomalies on other lattices?
Signatures of non-abelian anyons?
How does 1D become 2D?
…

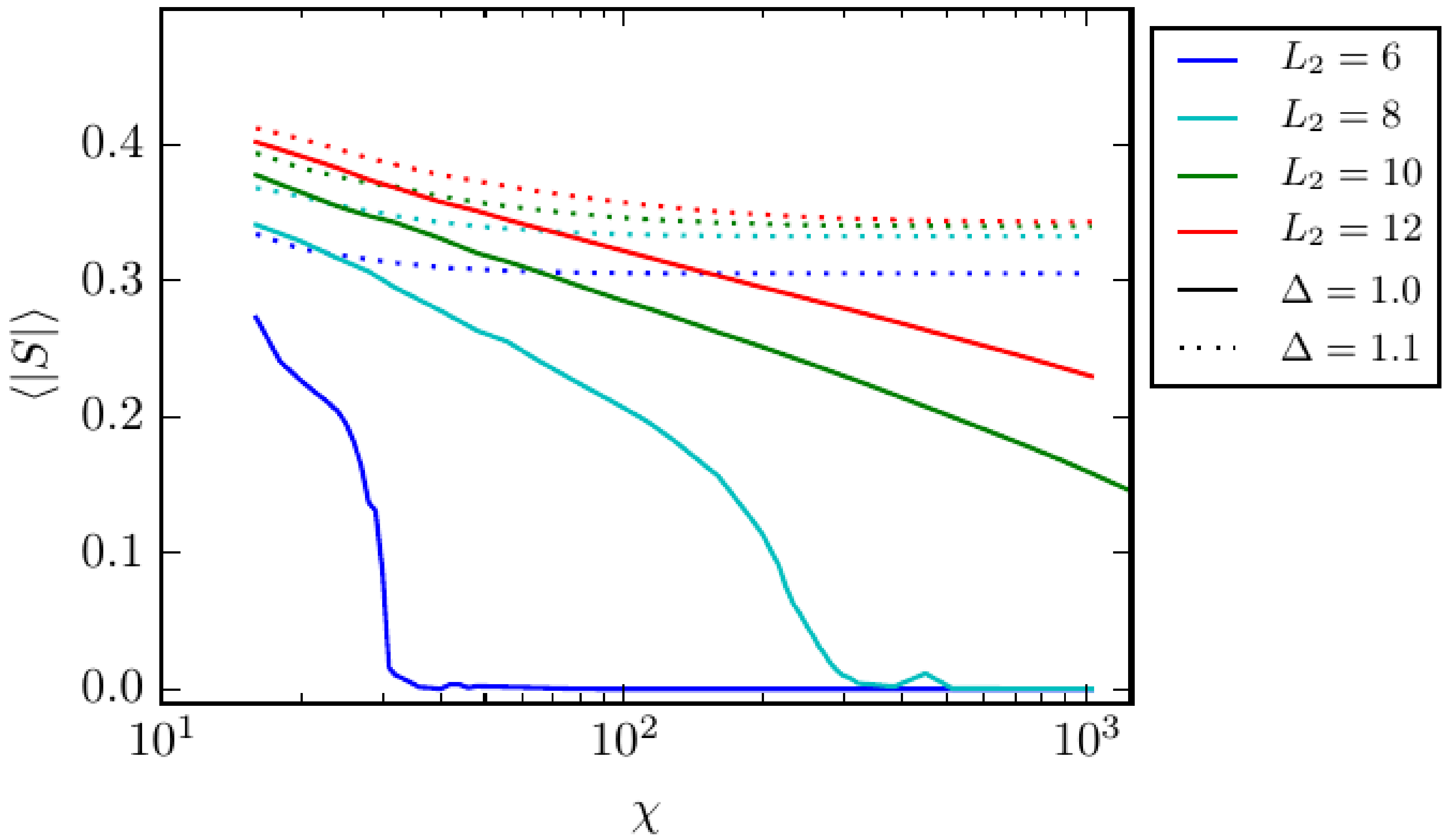


Ruben Verresen
With Matthias Gohlke, Roderich Moessner and Frank Pollmann

Gapless Cylinder



Coleman and 1D vs. 2D



Broadness in Zig-Zag Phase