quasi-particle pictures from continuous unitary transformations

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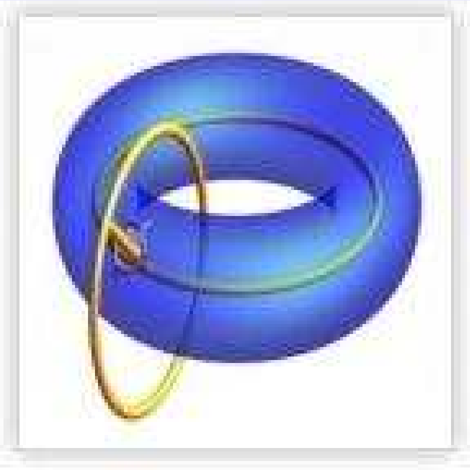

Entanglement in Strongly Correlated Systems

The study of entanglement in strongly correlated systems has lived a series of important advances in recent years, in turn underpinning a better understanding of the quantum properties of matter. Concerning numerics, examples of these are e.g. new numerical methods based on tensor networks, as well as advances in quantum Monte Carlo, exact diagonalizations, and **continuous unitary transformations**....

overview

- **continuous unitary transformations (CUTs)**
  spirit
  quasi-particle pictures
- **perturbative CUTs (pCUTs)**
  transverse-field Ising model on the three-dimensional Swedenborgite lattice
- **graph-based CUTs (gCUTs)**
  generalized notion of linked-cluster theorem
  quasi-particle decay
- **momentum-space CUTs**
  magnon and Higgs particles in an ordered quantum magnet

numerical tools for quantum-lattice models

- **exact diagonalization (ED)**
- **quantum Monte Carlo (QMC)**
- **tensor-network approaches**
  DMRG, iPEPS, ...
- **...**

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- **exact diagonalization (ED)**
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  DMRG, iPEPS, ...
- **...**
- **continuous unitary transformations (CUTs)**
  linked-cluster expansions (LCEs)
  non-perturbative LCEs

continuous unitary transformations (CUTs)

CUT	$\mathcal{H}(\ell) = U(\ell)\mathcal{H}U^\dagger(\ell)$
flow equation	$\frac{d\mathcal{H}(\ell)}{d\ell} = [\eta(\ell), \mathcal{H}(\ell)]$
effective model	$\mathcal{H}(\ell = \infty) = \mathcal{H}_{\text{eff}}$

'94 Wegner
'93/94 Glazek/Wilson

infinite hierarchy of coupled equations

truncation schemes necessary!

see also works by Wegner, Stein, Toda, Mielke, Kehrein, ...

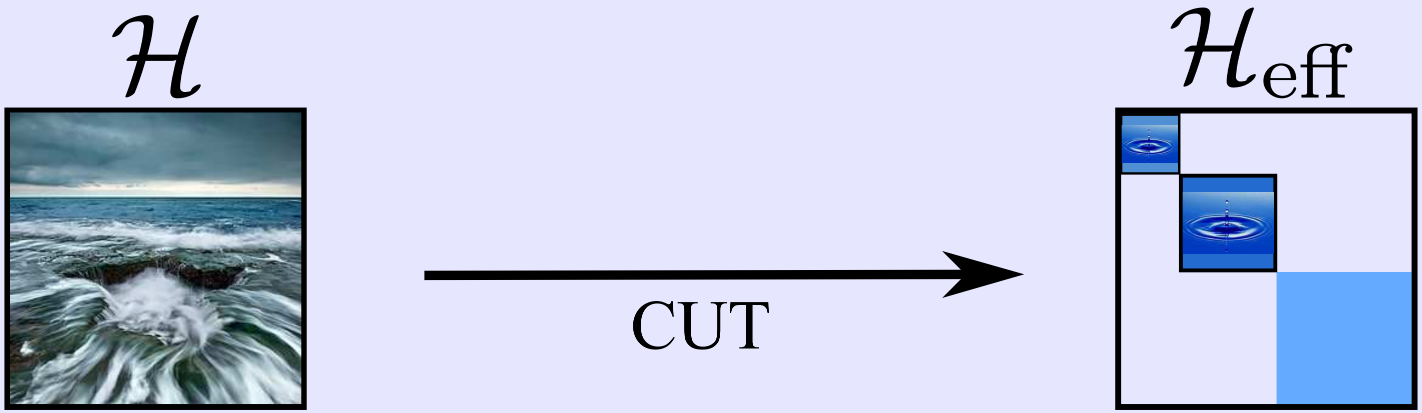
effective models and quasi-particles

photobucket.com

correlated system

low energy

quasi-particle conserving CUT



- counting operator $\mathcal{Q}$ with $\mathcal{Q}|i\rangle = q_i|i\rangle$
- quasi-particle generator

$$\eta^{\mathcal{Q}}_{i,j} = \text{sgn}(q_i - q_j)\mathcal{H}_{i,j}$$

- quasi-particle conserving effective Hamiltonian with $[\mathcal{Q}, \mathcal{H}_{\text{eff}}] = 0$

'97 Stein
'98 Mielke
'00 Knetter/Uhrig

truncation schemes

perturbative CUT

high-order series expansions
thermodynamic limit

Knetter/Uhrig, EPJB (2000)
Knetter/KPS/Uhrig, J. Phys. A (2003)
Coester/KPS, PRE (2015)

graph-based CUT

combine graph theory with CUTs
thermodynamic limit

Yang/KPS, EPL (2011)
Coester/Clever/Herbst/Capponi/KPS, EPL (2015)
Coester/KPS (2016)

self-similar CUT

operator flow
thermodynamic limit

Heidbrink/Uhrig, PRL (2002)
Fischer/Duffe/Uhrig, NJP (2010)
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Powalski/Uhrig/KPS, PRL (2015)

see also posters by David Schneider and Serkan Sahin!

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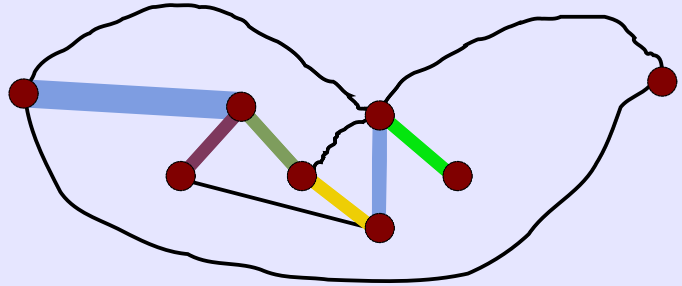
set up

- consider lattice of supersites ● (spin, dimer, ...)



- rewrite exactly $\mathcal{H} = \mathcal{H}_0 + \sum_{j=1}^{N_\lambda} \lambda_j \mathcal{V}^{(j)}$

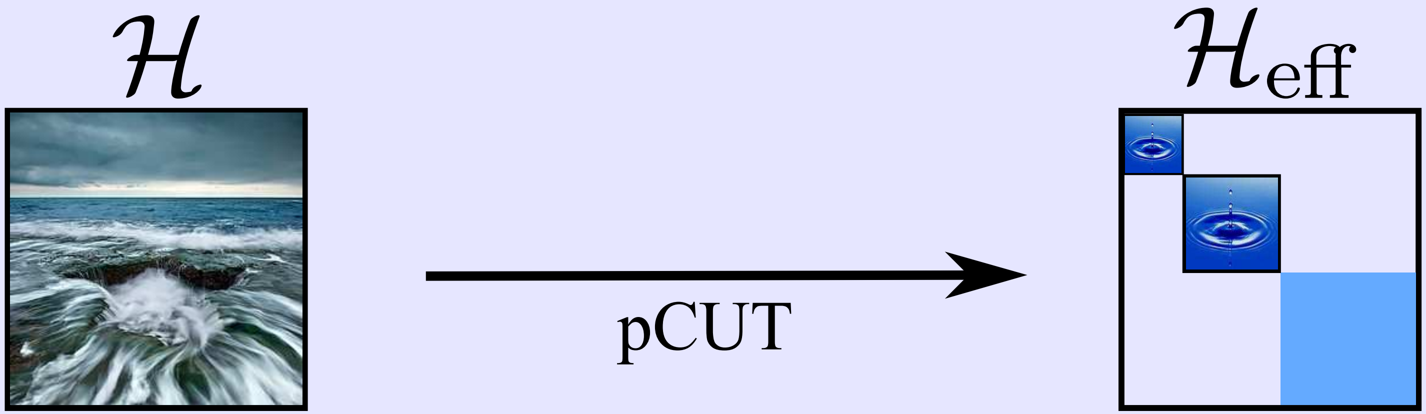
- unperturbed part diagonal in supersites

$$\mathcal{H}_0 = E_0 + \mathcal{Q} \quad \text{mit} \quad \mathcal{Q} \equiv \sum_i \hat{n}_i \equiv \sum_{i,\alpha} \hat{f}^\dagger_{i,\alpha} \hat{f}_{i,\alpha}$$

- interaction $\mathcal{V}^{(j)}$ couples supersites (colors)

$$\mathcal{H} = \mathcal{H}_0 + \sum_{n=-N}^{N} T_n \quad \text{mit} \quad [\mathcal{Q}, T_n] = nT_n$$

perturbative CUT



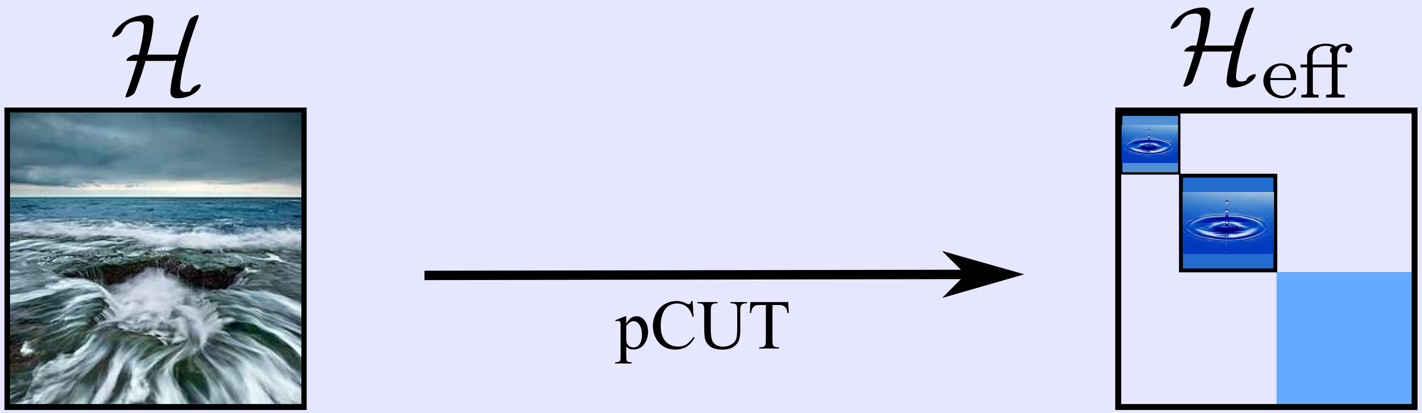
- if spectrum of $\mathcal{H}_0$ is equidistant in

$$\mathcal{H} = \mathcal{H}_0 + \sum_{n=-N}^{N} T_n \quad \text{with} \quad [\mathcal{Q}, T_n] = nT_n$$

- then perturbative CUT yields model-independently

$$\mathcal{H}_{\text{eff}}(\{\lambda_j\}) = \mathcal{H}_0 + \sum_{\sum_j k_j = k}^{\infty} \lambda_1^{k_1} \ldots \lambda_{N_\lambda}^{k_{N_\lambda}} \sum_{|\underline{m}|=k\ \sum_i m_i = 0} C(\underline{m}) T(\underline{m})$$

perturbative CUT



- model-independent effective Hamiltonian

$$\mathcal{H}_{\text{eff}}(\{\lambda_j\}) = \mathcal{H}_0 + T_0 + T_1 T_{-1} - T_{-1} T_1 + \frac{1}{2} T_2 T_{-2} - \frac{1}{2} T_{-2} T_2 \ldots$$

- $\mathcal{H}_{\text{eff}}$ not normal-ordered (model-dependent part!)

$\longrightarrow$ pCUT as a linked-cluster expansion

pCUT as a linked-cluster expansion

divide in finite clusters

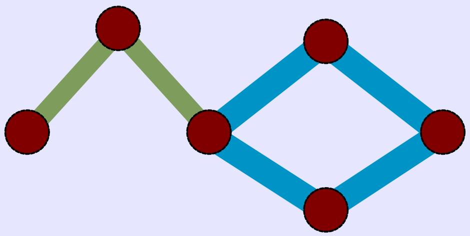
and embed in thermodynamic limit

linked-cluster expansions (LCEs)

- quantum many-body problem

$$\mathcal{H} = \mathcal{H}_0 + \lambda V$$

- lattice with sites and links



- focus on zero temperature

linked-cluster expansions (LCEs)

Goal

- calculate high-order series expansion (order 10-20) in λ

$$\mathcal{H} = \mathcal{H}_0 + \lambda V$$

- use extrapolation schemes to
  - access quantum critical regime
  - determine properties of elementary excitations

linked-cluster expansions (LCEs)

Extensive quantities

- e.g. ground-state energy per site (also entanglement entropies)

$$\epsilon_0 \equiv \frac{E_0}{N} = \sum_{\mathcal{G}_\nu} c(\mathcal{G}_\nu)\epsilon(\mathcal{G}_\nu)$$

  - sum over linked clusters $\mathcal{G}_\nu$

- reduced energies via subcluster subtractions

$$\epsilon(\mathcal{G}_\nu) = E(\mathcal{G}_\nu) - \sum_{\mathcal{G}_{\nu'} \in \mathcal{G}_\nu} c(\mathcal{G}_{\nu'}/\mathcal{G}_\nu)\epsilon(\mathcal{G}_{\nu'})$$

linked-cluster expansions (LCEs)

Excitations

- quasi-particles, e.g. magnons, triplons, anyons, ...
- momentum $\vec{k}$, dispersion $\omega(\vec{k})$
  - one quasi-particle dispersion — '96 Gelfand
  - two quasi-particle interaction — '00 Trebst et al.
'01 Zheng et al.
'01 Knetter/KPS/Uhrig
  - spectral densities — '01 Knetter et al..
'01 KPS/Knetter/Uhrig
  - topological order / anyons — '08- Dusuel/Vidal/KPS

linked-cluster expansions (LCEs)

Properties

- thermodynamic limit
- scales well with increasing dimensions
- perturbative, but extrapolations

linked-cluster expansions LCEs

Properties

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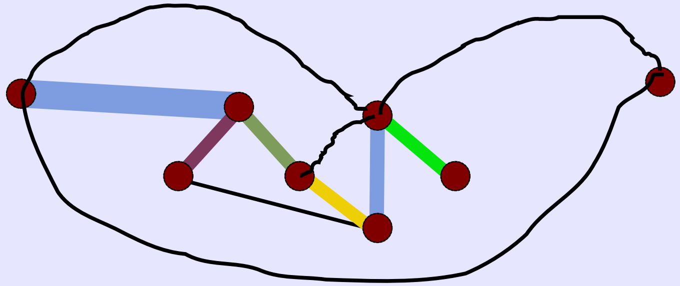
Challenges

- systems with various couplings
- long-range interactions
- disorder
- non-perturbative extensions



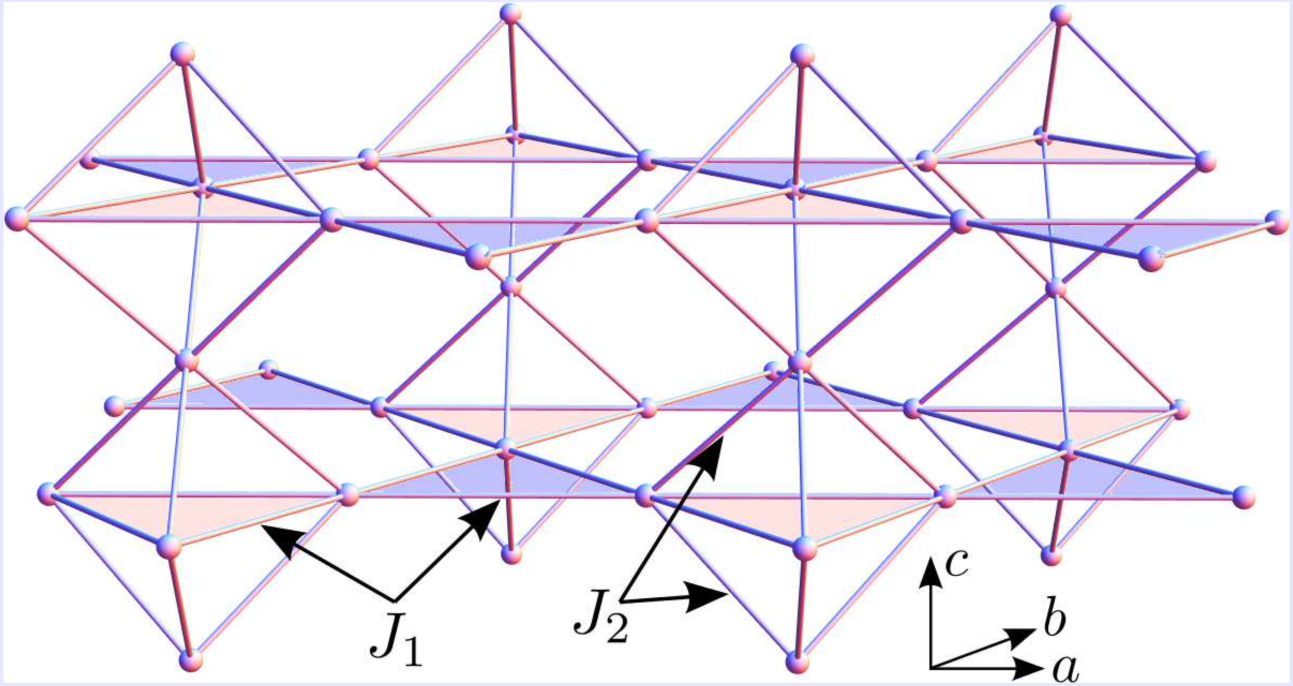
→ white graphs

Coester/KPS, PRE (2015)

TFIM on the Swedenborgite lattice

Sikkenk/Coester/Fritz/KPS (2016)

- sweden borgites



$CaBaCo_2Fe_2O_7$

$YBaCo_4O_7$

(not Ising spins)

- transverse field Ising model
- limits

h = 0 pure Ising (classical)

$J_1 = 0$ TFIM on quasi 1d chains

$J_2 = 0$ TFIM kagome lattice

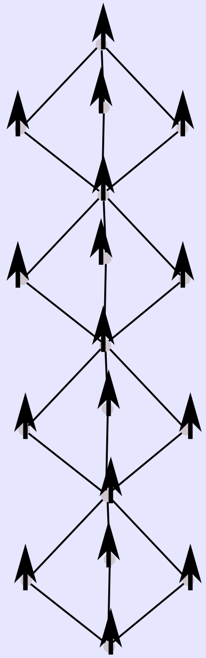
Buhrandt/Fritz, PRB (2014)

Powalski/Coester/Moessner/KPS, PRB (2013)

decoupled chains on the Swedenborgite lattice ($J_1 = 0$)

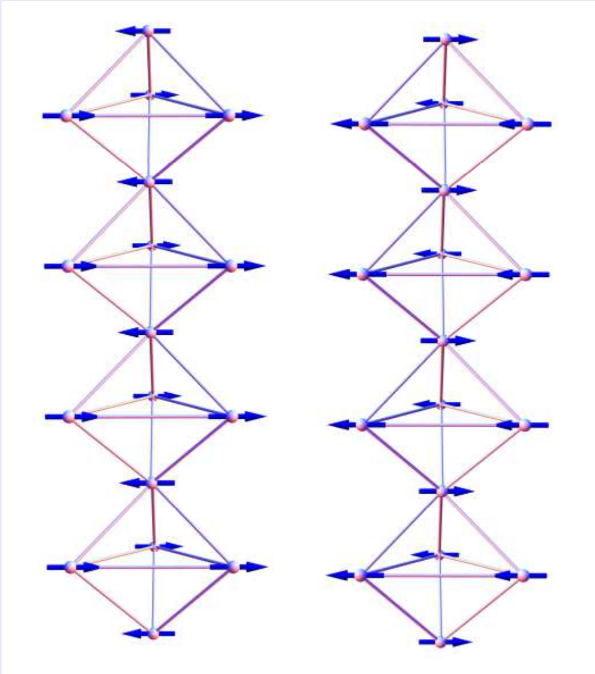
- unfrustrated TFIM on quasi-1d chain
- quantum phase transition in 2d Ising universality class

polarized state



$J_2 = 0$

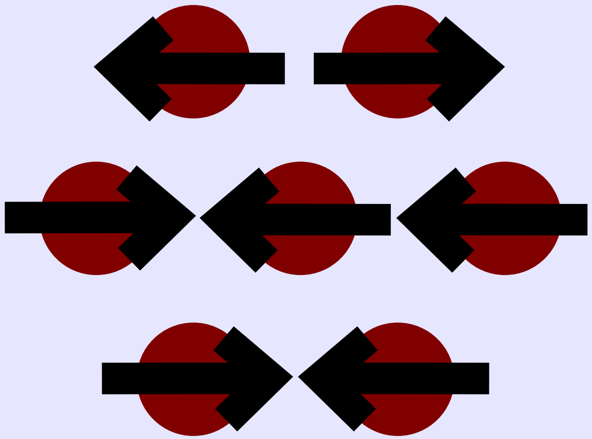
Ising macro-spin



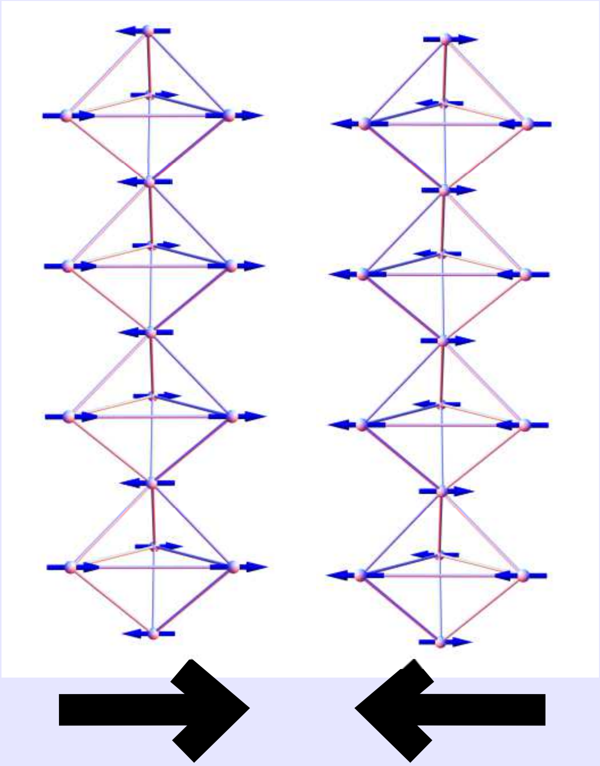
$h = 0$

decoupled chains on the Swedenborgite lattice ($J_1 = 0$)

- $h = 0$: atomic limit for Ising macro-spins
- Ising macro-spins build effective triangular lattice



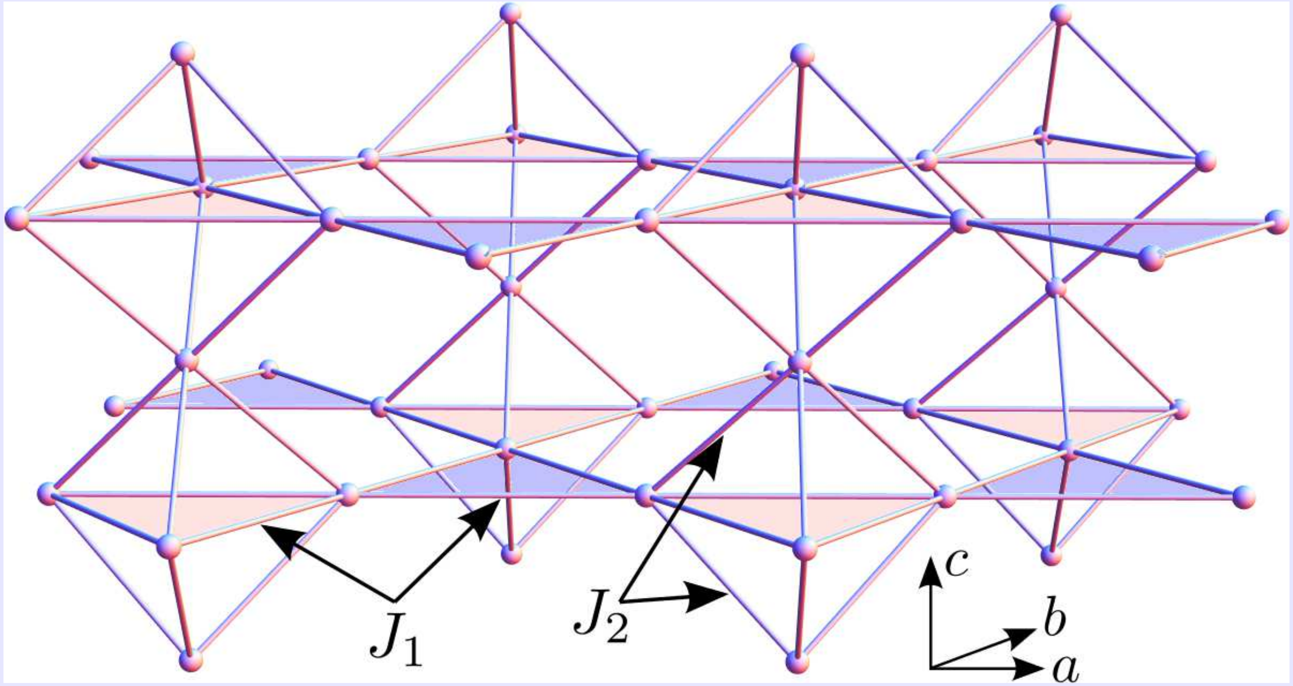
Ising macro-spin



TFIM on the Swedenborgite lattice

Sikkenk/Coester/Fritz/KPS (2016)

- sweden borgites



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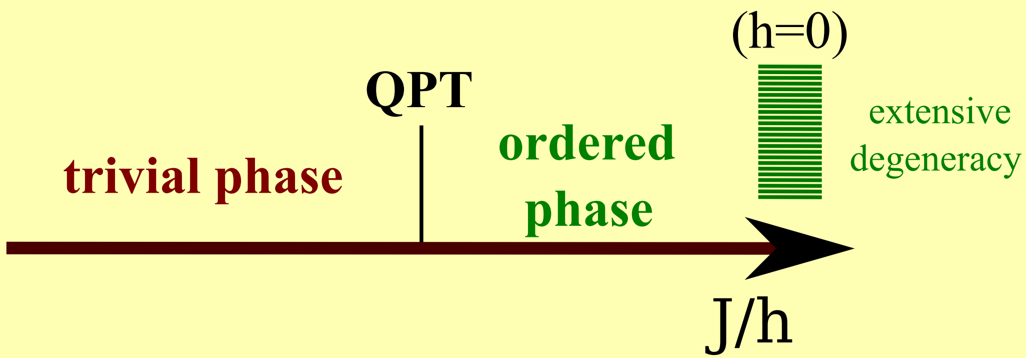
Buhrandt/Fritz, PRB (2014)

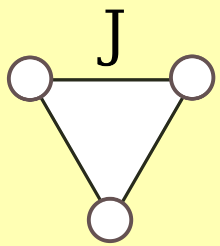
Powalski/Coester/Moessner/KPS, PRB (2013)

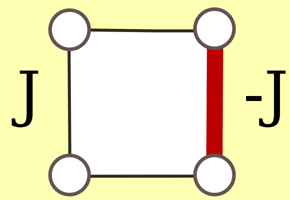
fully frustrated Ising models

$$H = \sum_{<i,j>} J_{ij}\,\sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x$$

- h=0: extensively many ground states
- J=0: fully polarized phase (trivial)
- generically "order by disorder"





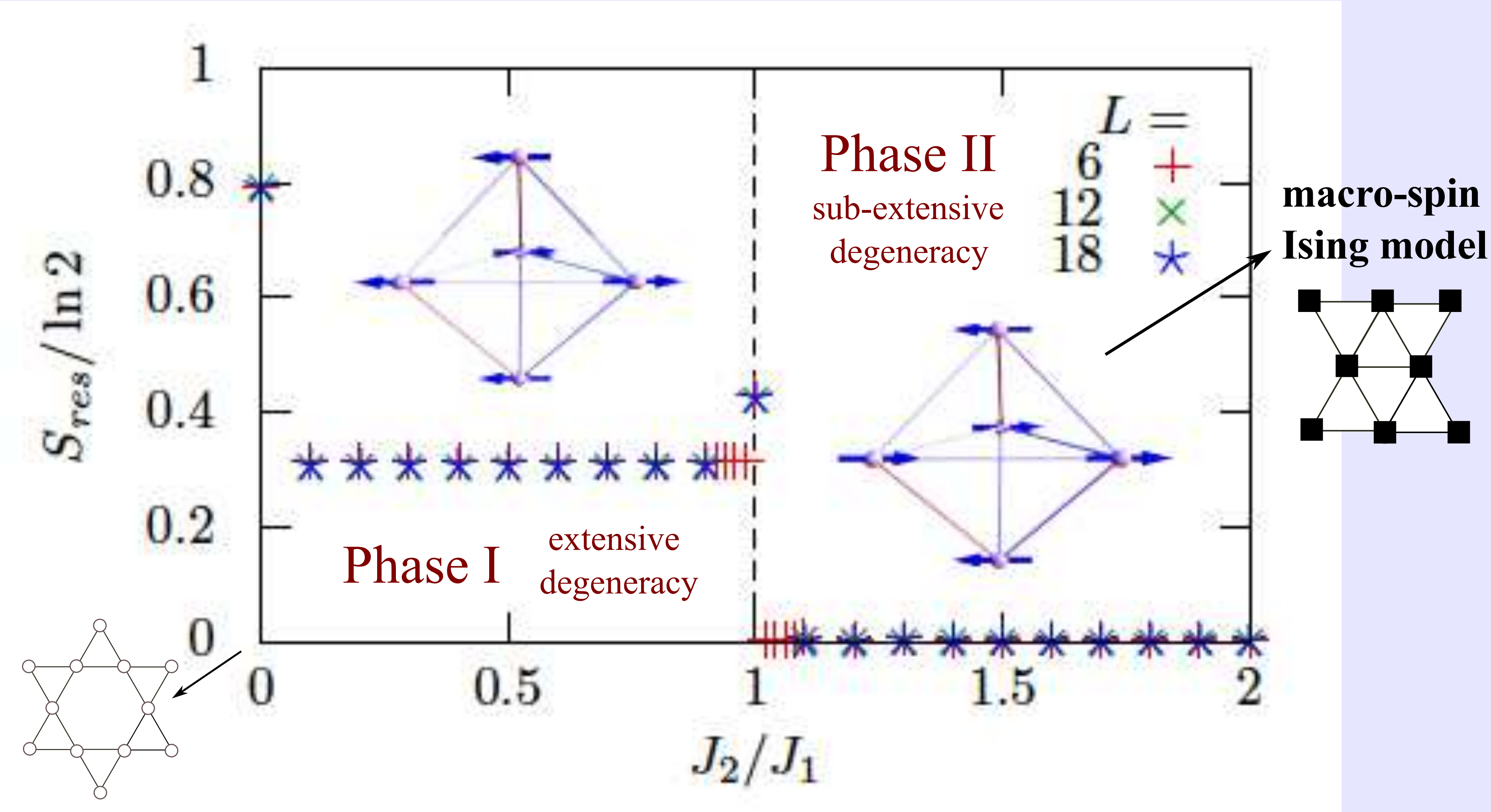


Moessner/Sondi/Chandra, PRL (2000)
Moessner/Sondi, PRB (2001)

Ising model on the Swedenborgite lattice ($h = 0$)

Buhrandt/Fritz, PRB (2014)

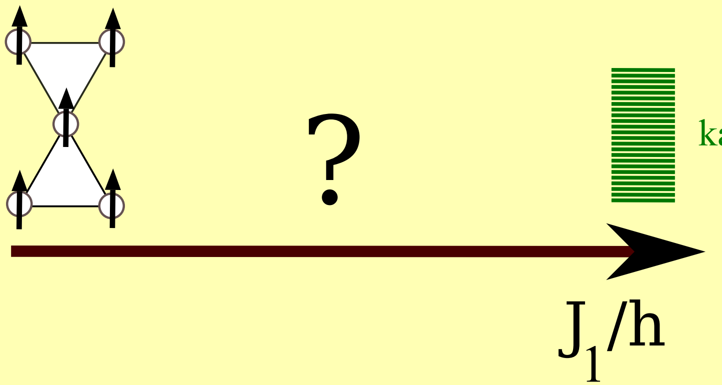
- two classical spin liquids I and II

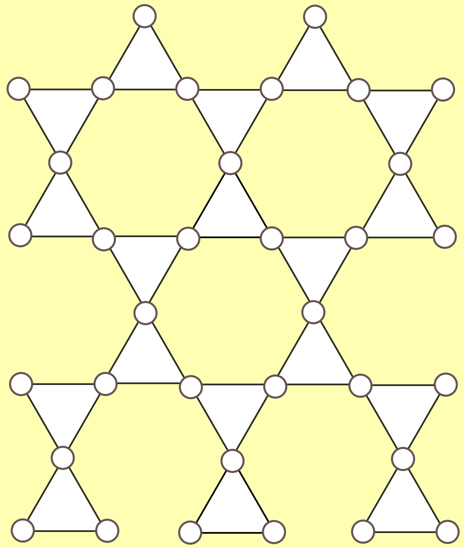


kagome ice in a transverse field ($J_2 = 0$)

$$H = J_1 \sum_{<i,j>} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x$$

- h=0: infinitely many ground states (kagome ice)
- J_1=0: fully polarized phase





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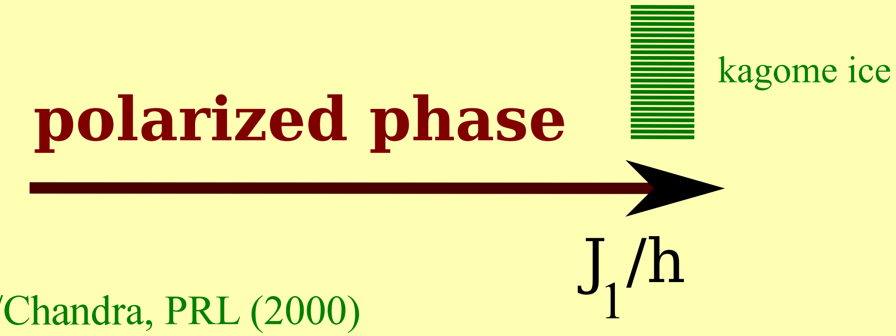
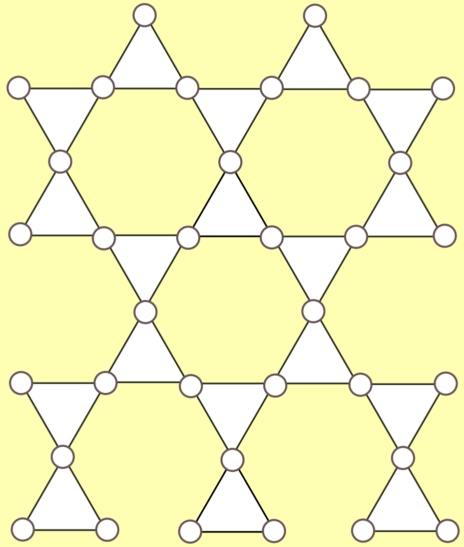
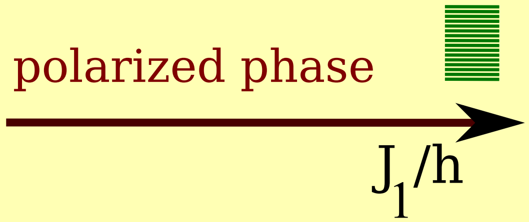




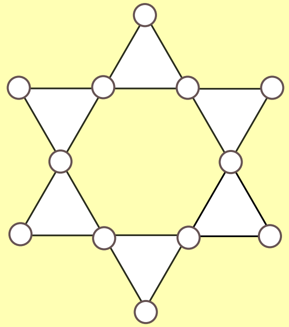
Moessner/Sondi/Chandra, PRL (2000)
Moessner/Sondi, PRB (2001)

disorder by disorder ($J_2 = 0$)

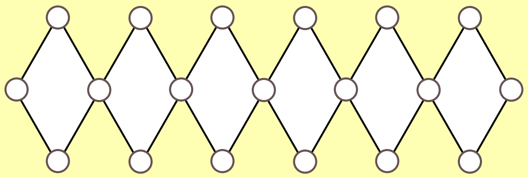
$$H = J_1 \sum_{<i,j>} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^x$$



- disorder by disorder scenario for kagome TFIM
  Powalski/Coester/Moessner/KPS, PRB (2013)

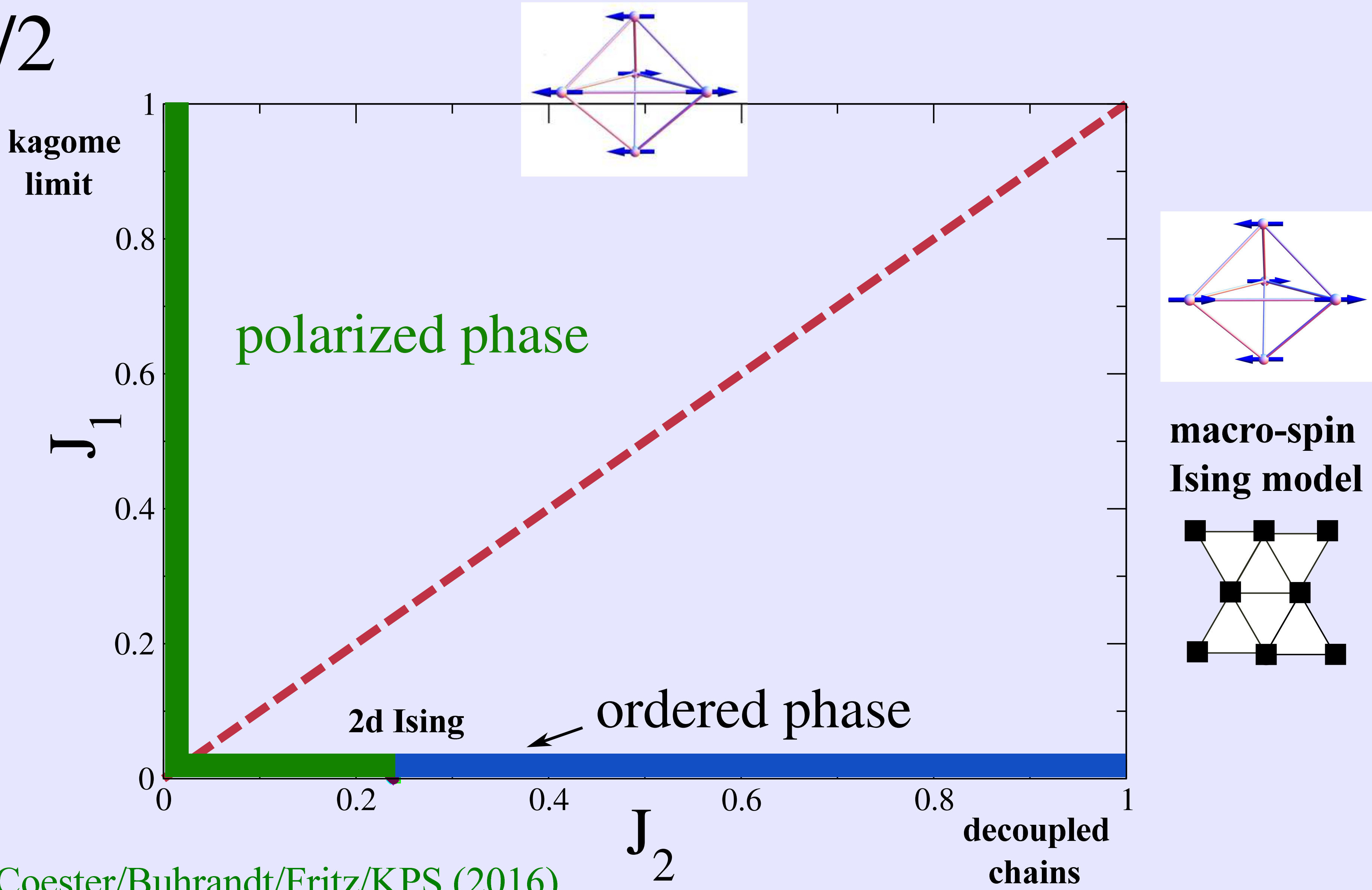


- disorder by disorder for fully-frustrated diamond chain can be deduced analytically
  Coester/Malitz/Fey/KPS, PRB (2013)



TFIM on the Swedenborgite lattice

h=1/2



Sikkenk/Coester/Buhrandt/Fritz/KPS (2016)

LCEs on the Swedenborgite lattice

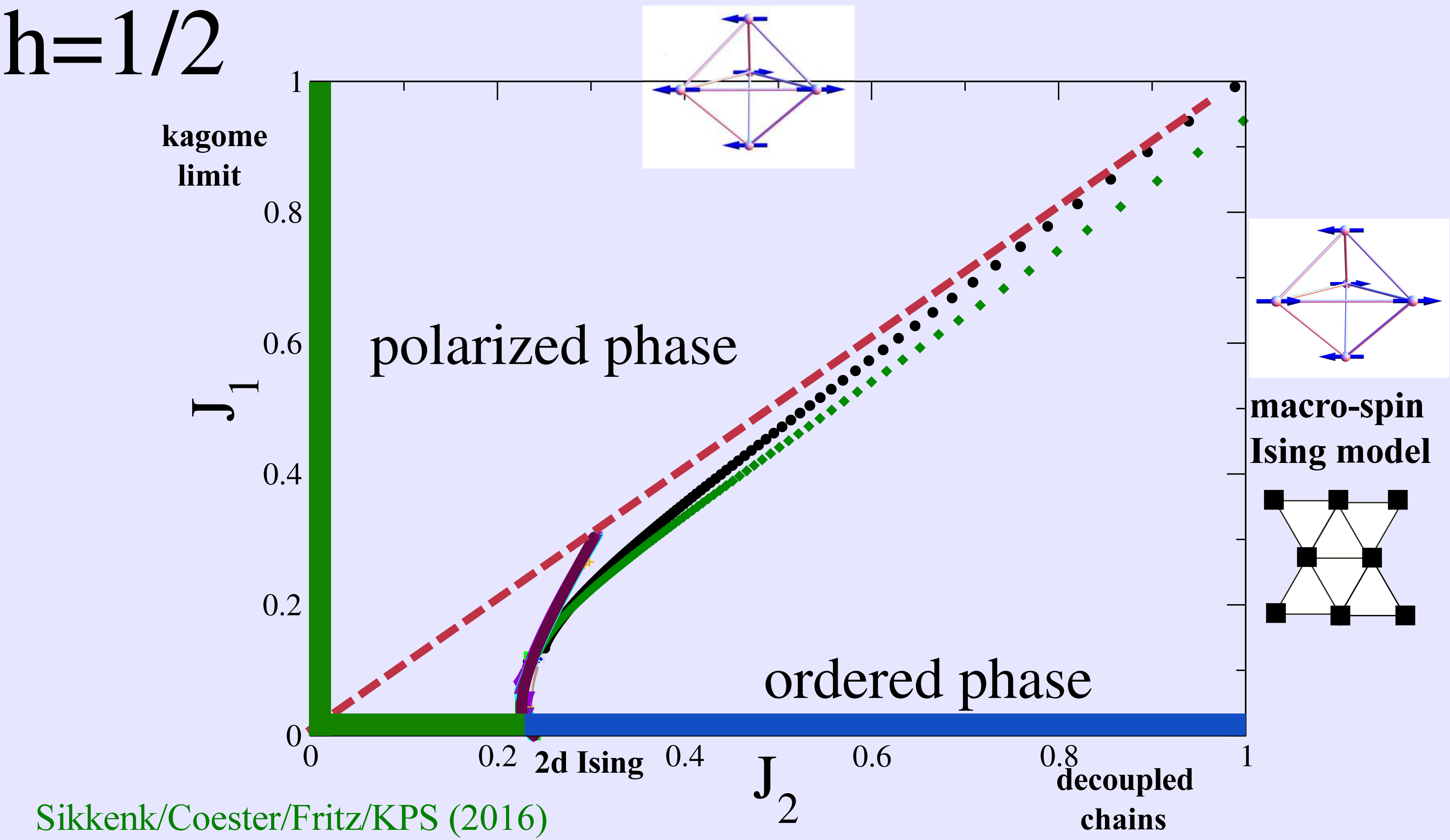
$$\mathcal{H} = h \sum_i \sigma_i^x + J_1 \sum_{\langle i,j \rangle \in \text{same layer}} \sigma_i^z \sigma_j^z + J_2 \sum_{\langle i,j \rangle \in \text{different layer}} \sigma_i^z \sigma_j^z$$

- high-field expansion in J_1 and J_2 up to order 11
- linktypes = "color"
- white-graph expansion

ignore color for generating topologically distinct graphs, but do an optimal bookkeeping!

Coester/KPS, PRE (2015)

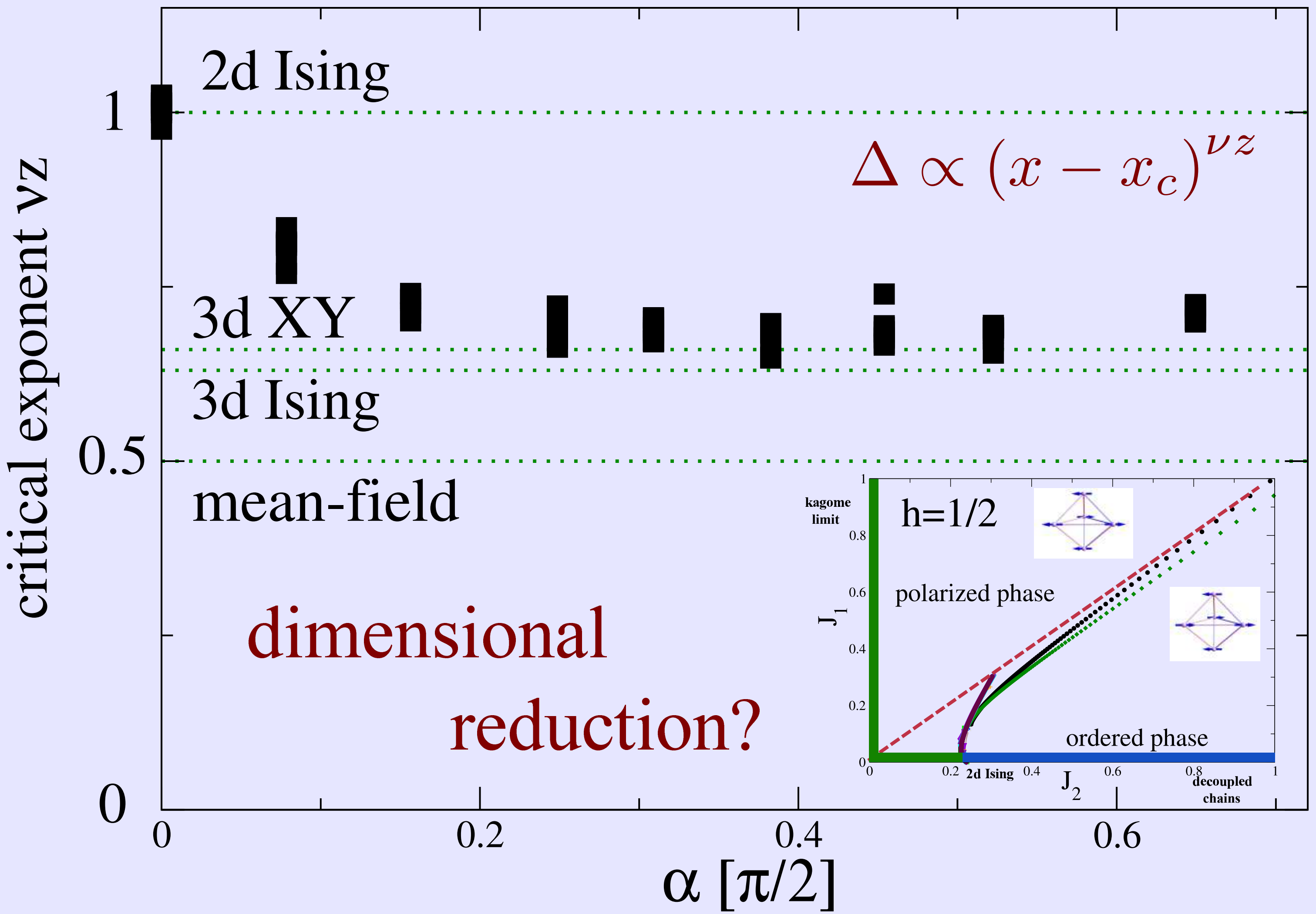
TFIM on the Swedenborgite lattice



Sikkenk/Coester/Fritz/KPS (2016)

TFIM on the Swedenborgite lattice

Sikkenk/Coester/Fritz/KPS (2016)



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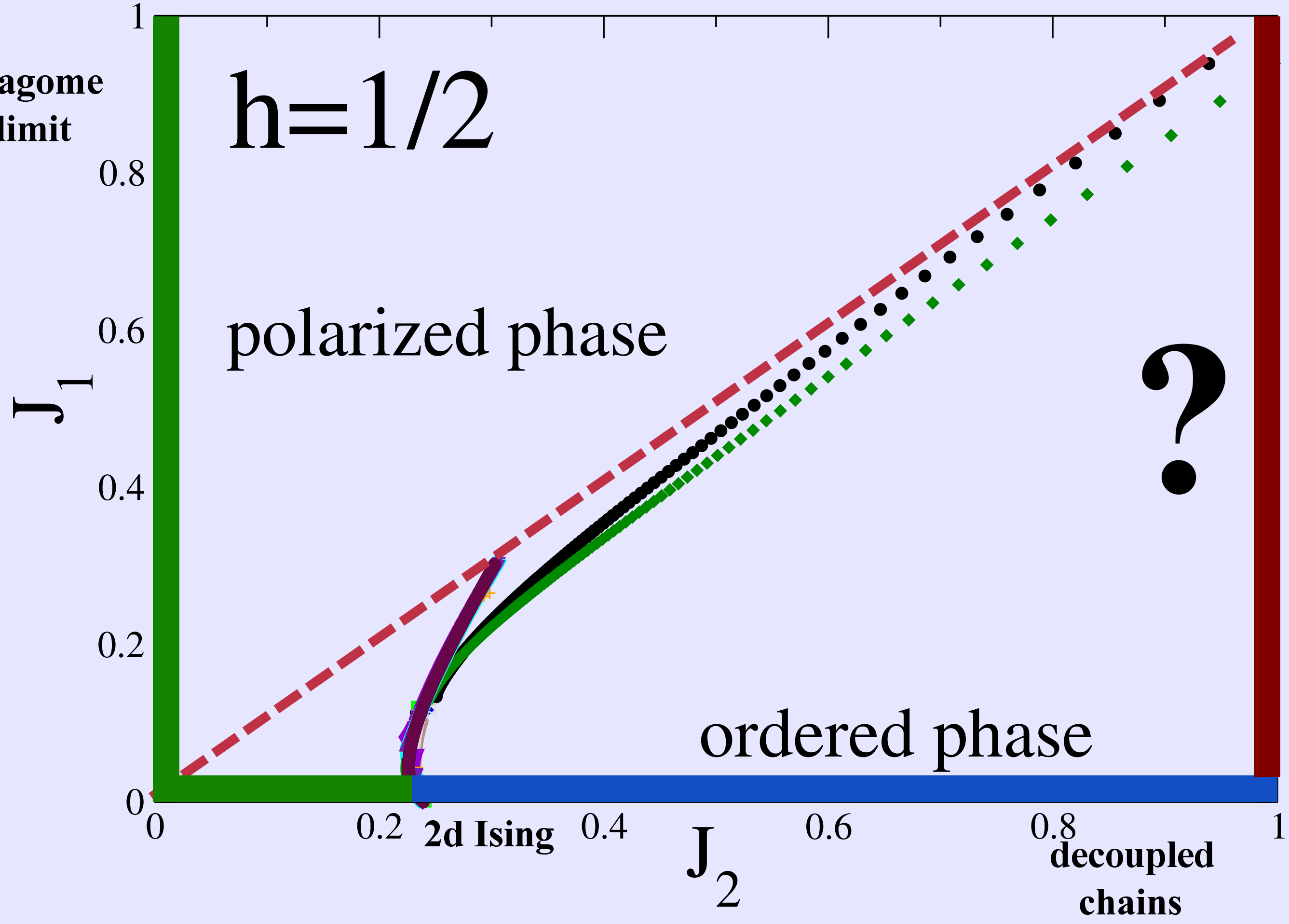
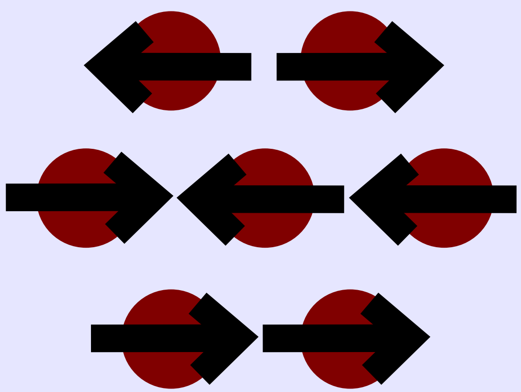


Sikkenk/Coester/Fritz/KPS (2016)

degenerate macro spins

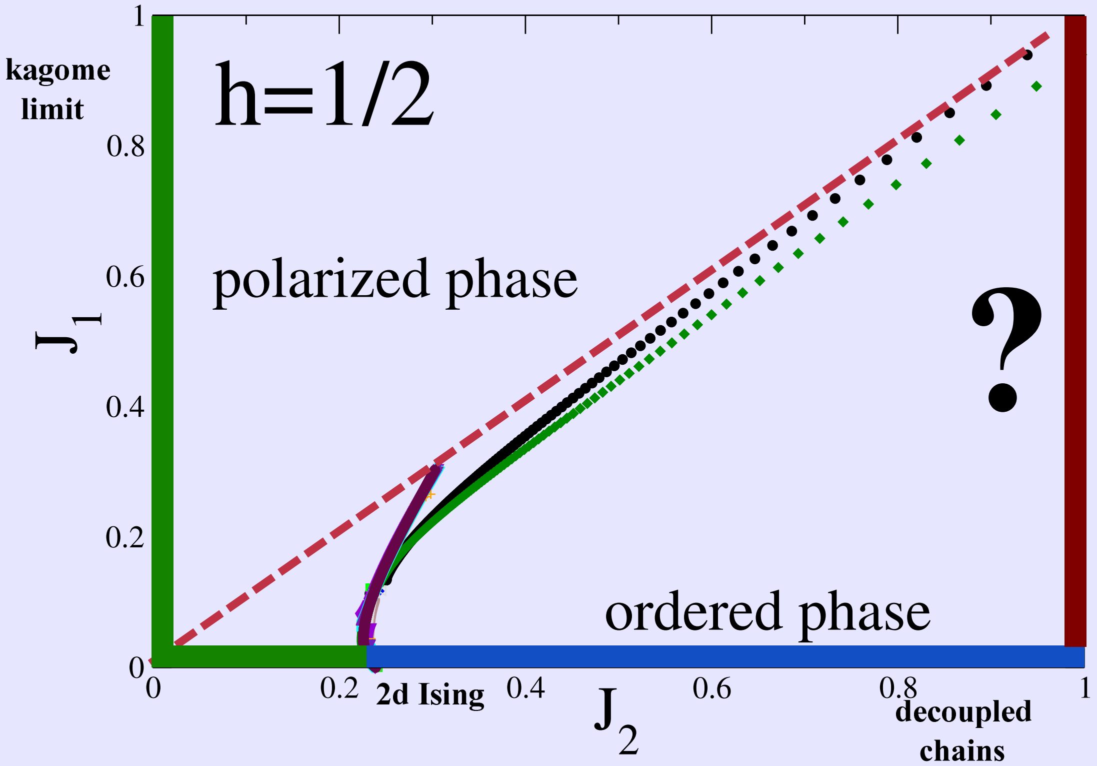
$J_2 > J_1 \gg h$



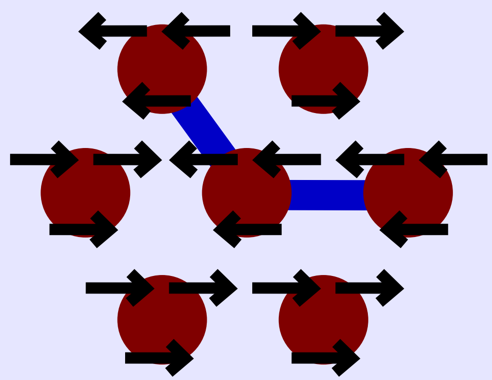
ground states of triangular Ising model

TFIM on the Swedenborgite lattice

$J_2 > J_1 \gg h$ degenerate macro spins



- effective **diagonal 2d** classical dimer model in frustrated links



Sikkenk/Coester/Fritz/KPS (2016)

TFIM on the Swedenborgite lattice

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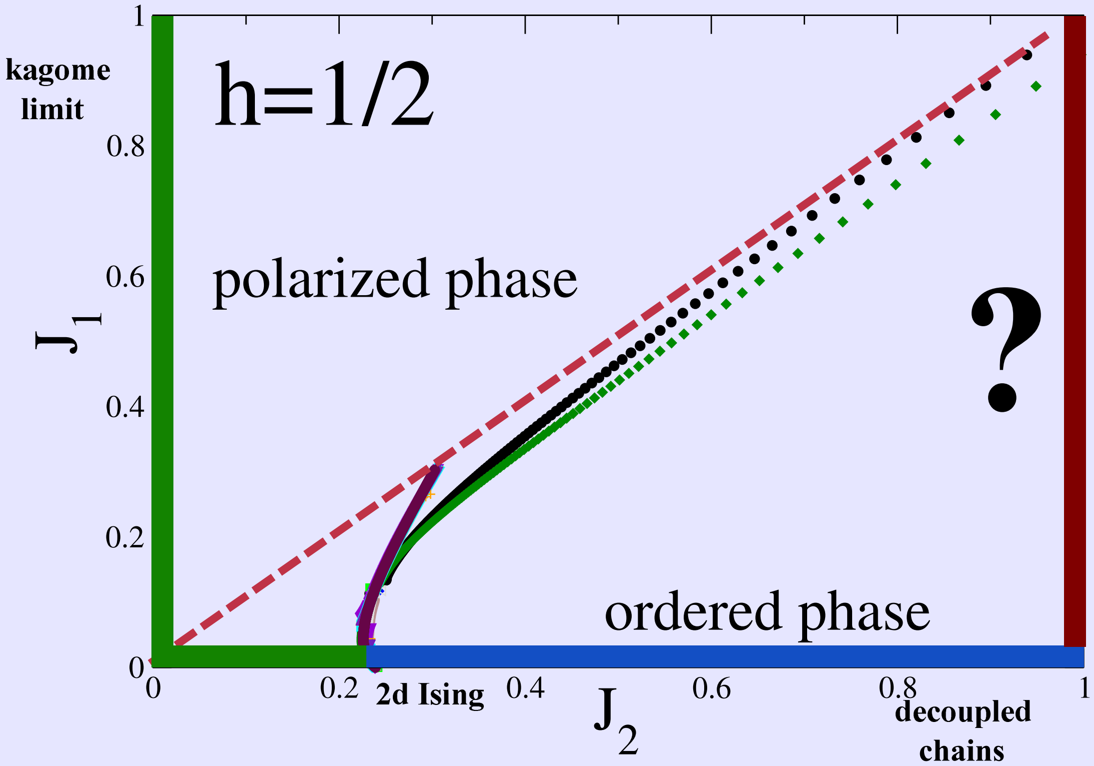
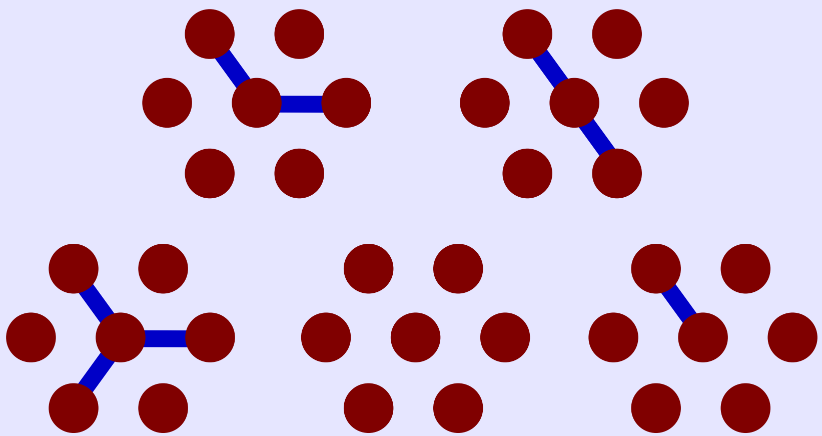


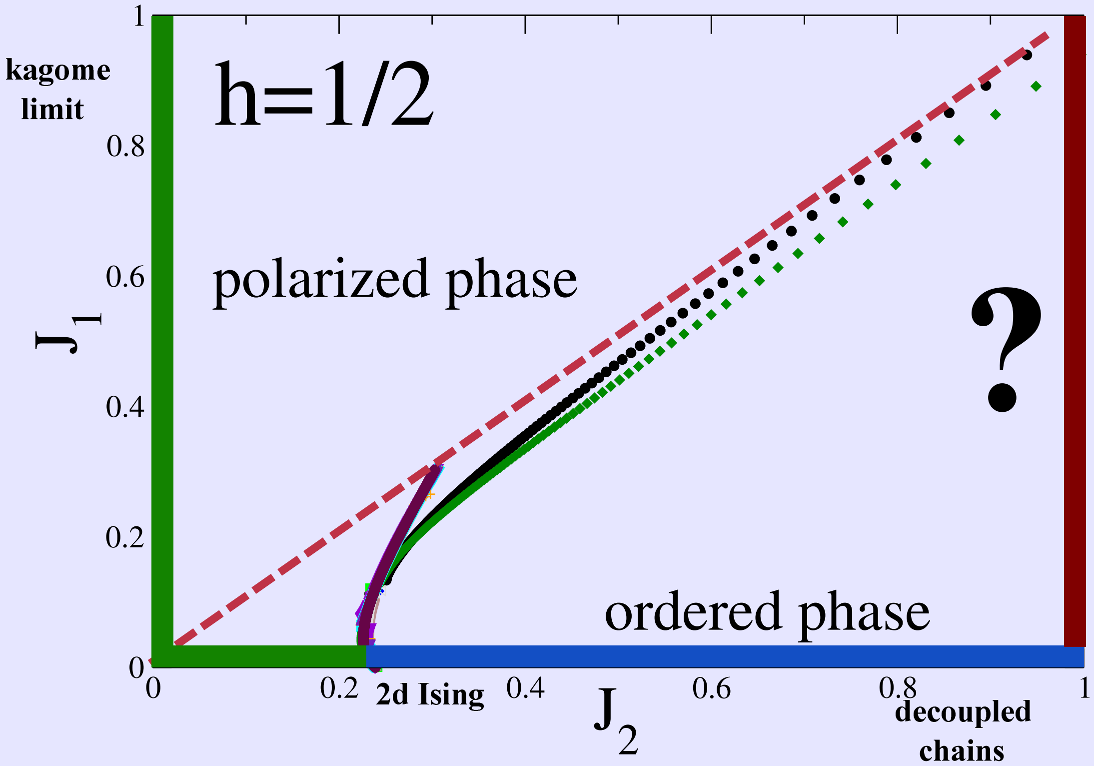
- effective **diagonal 2d** classical dimer model in frustrated links
- all configurations stay degenerate in $\mathcal{O}(h^2)$



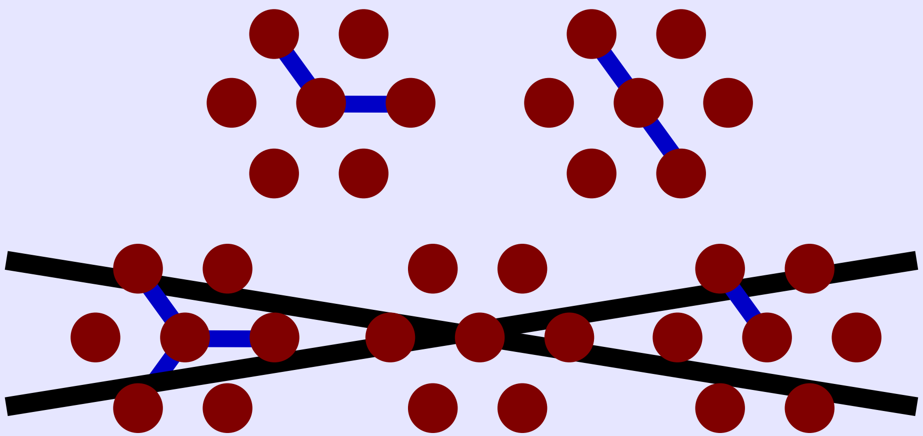
Sikkenk/Coester/Fritz/KPS (2016)

TFIM on the Swedenborgite lattice

$J_2 > J_1 \gg h$ degenerate macro spins



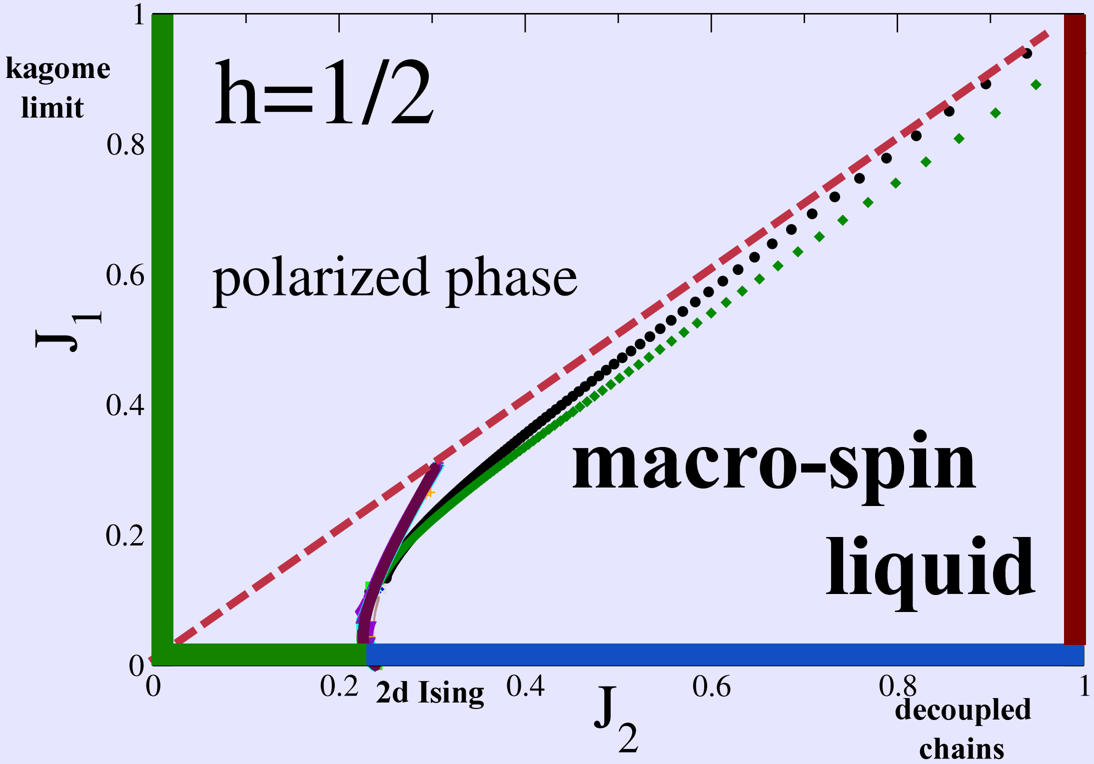
- effective **diagonal 2d** classical dimer model in frustrated links
- configurations with 2 frustrated links in $\mathcal{O}(h^4)$



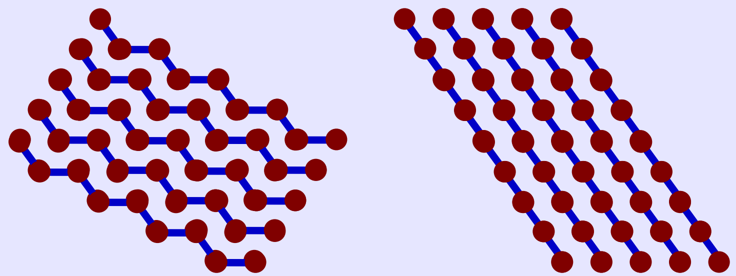
Sikkenk/Coester/Fritz/KPS (2016)

TFIM on the Swedenborgite lattice

$J_2 > J_1 \gg h$ degenerate macro spins



- effective **diagonal 2d** classical dimer model in frustrated links
- emergent stripe structures sub-extensively degenerate



- exact degeneracy on finite clusters and at least up $\mathcal{O}(h^{10})$

Sikkenk/Coester/Fritz/KPS (2016)

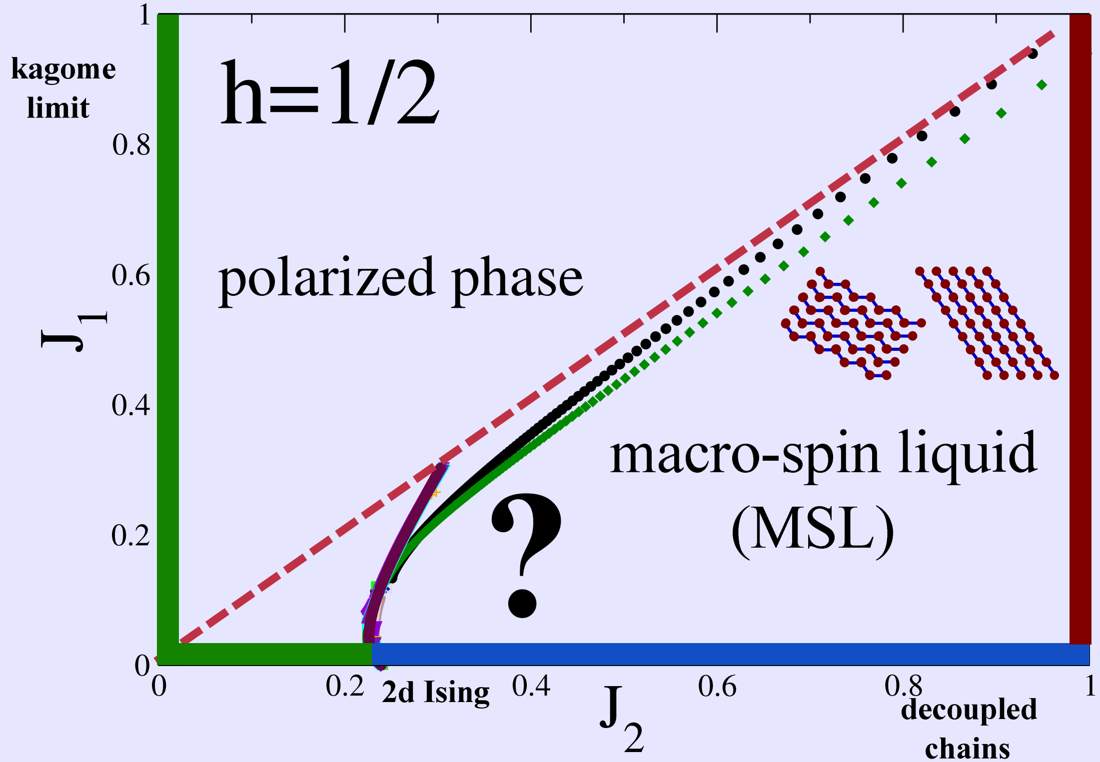
TFIM on the Swedenborgite lattice

Sikkenk/Coester/Fritz/KPS (2016)

- white graphs efficient
- disorder by disorder
- dimensional reduction (2+1)d from high-field expansion
- effective **diagonal** **2d** classical dimer model in terms of macro-spins

↓

dimensional reduction (3+1)d to 2d



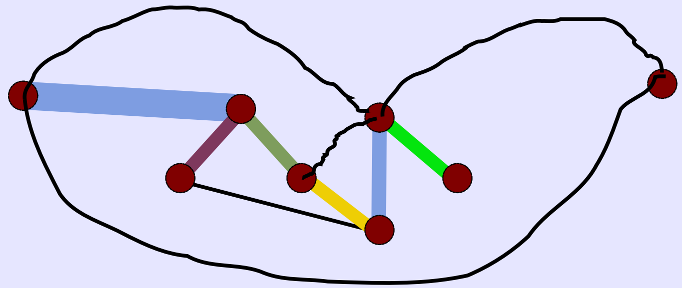
perturbative CUTs and LCEs

Properties

- thermodynamic limit
- scales well with increasing dimensions
- perturbative, but extrapolations

Challenges

- systems with various couplings
- long-range interactions
- disorder
- **non-perturbative extensions**



→ white graphs

Coester/KPS, PRE (2015)

truncation schemes

perturbative CUT

high-order series expansions
thermodynamic limit

Knetter/Uhrig, EPJB (2000)
Knetter/KPS/Uhrig, J. Phys. A (2003)
Coester/KPS, PRE (2015)

graph-based CUT

combine graph theory with CUTs
thermodynamic limit

Yang/KPS, EPL (2011)
Coester/Clever/Herbst/Capponi/KPS, EPL (2015)
Coester/KPS (2016)

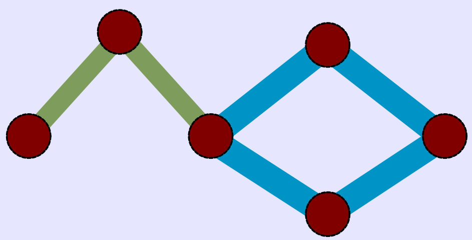
self-similar CUT

operator flow
thermodynamic limit

Heidbrink/Uhrig, PRL (2002)
Fischer/Duffe/Uhrig, NJP (2010)
Krull/Drescher/Uhrig, PRB (2013)
Powalski/Uhrig/KPS, PRL (2015)

non-perturbative linked-cluster expansions (NLCEs)

- do graph expansion as before
- calculate non-perturbatively (e.g. ED) on graphs!



divide in finite clusters
and embed in thermodynamic limit

non-perturbative linked-cluster expansions (NLCEs)

see also poster by Dominik Ixert !

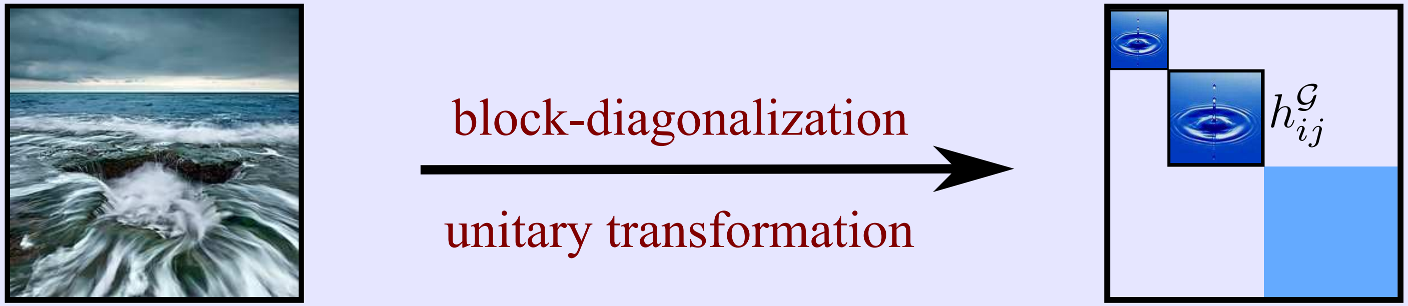
History and developments

- ground-state energy for lattice gauge theories (ED) — '84 Irving/Hamer
- thermodynamic quantities for quantum spin models (ED) — '06 Rigol/Bryant/Singh
- **excitations and effective models (gCUT)** — '11 Yang/KPS, '15 Coester/Clever/Herbst/Capponi/KPS
- entanglement entropies (ED,DMRG) — '13 Kallin/Hyatt/Singh/Melko, '14 Stoudenmire/Gustainis/Johal/Wessel/Melko
- quantum quenches and many-body localization in the thermodynamic limit (ED) — '14 Rigol, '15 Tang/Iyer/Rigol

graph-based CUTs

Idea

- generate topologically distinct graphs
- solve flow-equation on each graph $\partial_l \mathcal{H}^{\mathcal{G}_\nu} = [\eta^{\mathcal{G}_\nu}, \mathcal{H}^{\mathcal{G}_\nu}]$



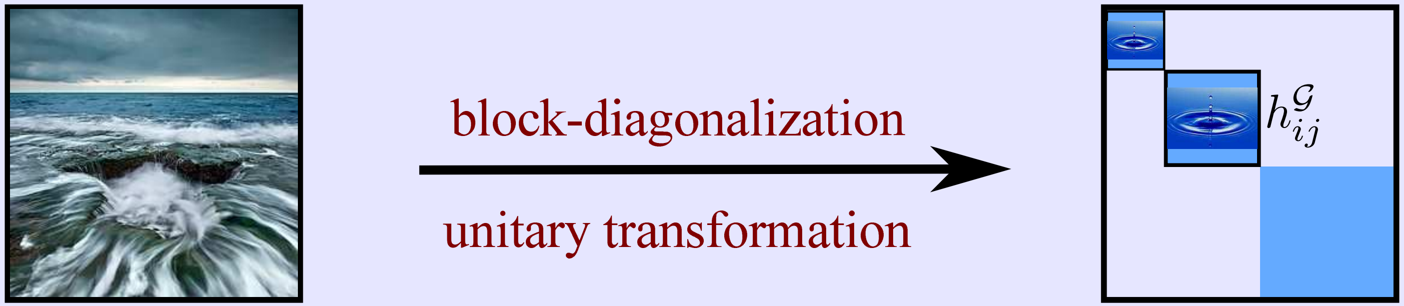
block-diagonal
in particle-number operator

Yang/KPS EPL (2011)

graph-based CUTs

Idea

- generate topologically distinct graphs
- solve flow-equation on each graph $\partial_l \mathcal{H}^{\mathcal{G}_\nu} = [\eta^{\mathcal{G}_\nu}, \mathcal{H}^{\mathcal{G}_\nu}]$



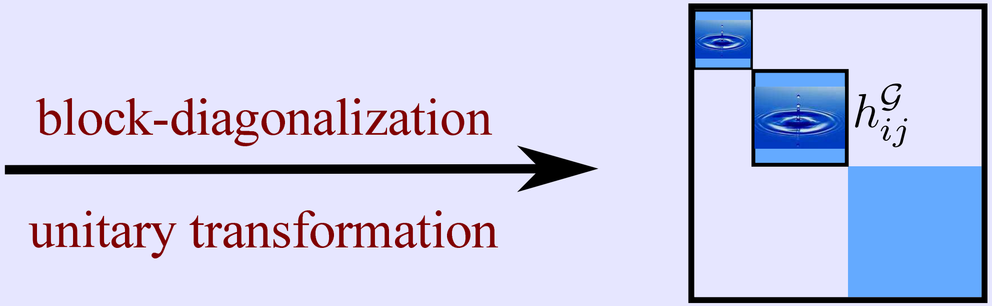
- subgraph subtractions for matrix elements (gse, hopping elements, ...)
- embedding in the thermodynamic limit

Yang/KPS EPL (2011)

graph-based CUTs

Idea

- generate topologically distinct graphs
- solve flow-equation on each graph $\partial_l \mathcal{H}^{\mathcal{G}_\nu} = [\eta^{\mathcal{G}_\nu}, \mathcal{H}^{\mathcal{G}_\nu}]$



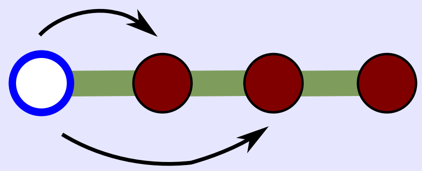
- on graph numerically exact solution of CUT (finite matrices ...)
- for ground-state energy: just identical to NLCE with ED
- convergence expected for finite correlation length

Yang/KPS EPL (2011)

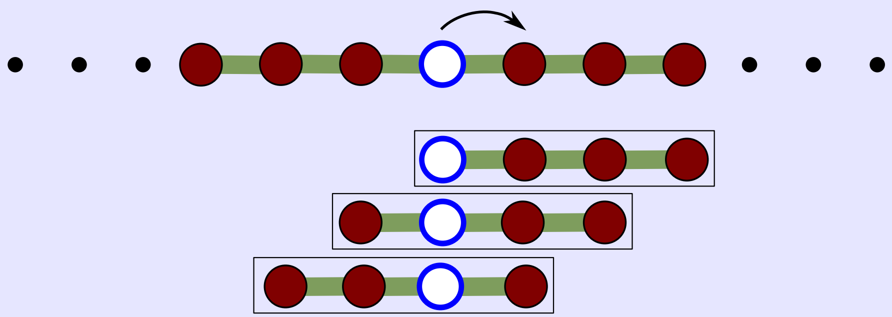
graph-based continuous unitary transformations (gCUTs)

one-particle dispersion

- hopping matrix $h_{ij}^{\mathcal{G}}$ on each cluster



- embedding restores translation symmetry

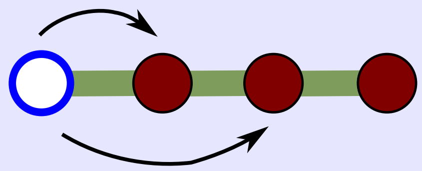


- Fourier transformation yields $\omega(\vec{k})$

graph-based continuous unitary transformations (gCUTs)

one-particle dispersion

- hopping matrix $h_{ij}^{\mathcal{G}}$ on each cluster



- embedding restores translation symmetry

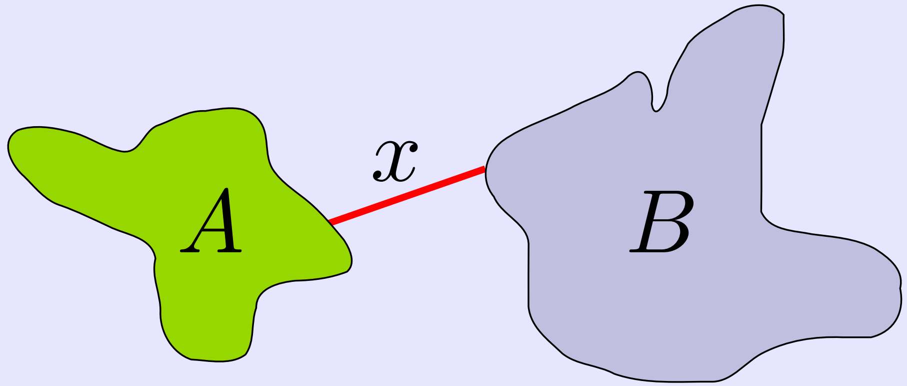
?

really true non-perturbatively?

graph-based continuous unitary transformations (gCUTs)

- $\mathcal{H} = \mathcal{H}_0 + \lambda V$

- consider two clusters

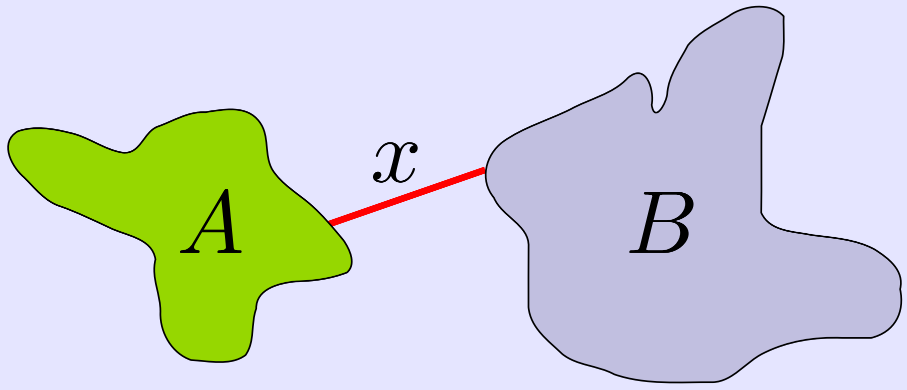


Coester/Clever/Herbst/Capponi/KPS EPL (2015)

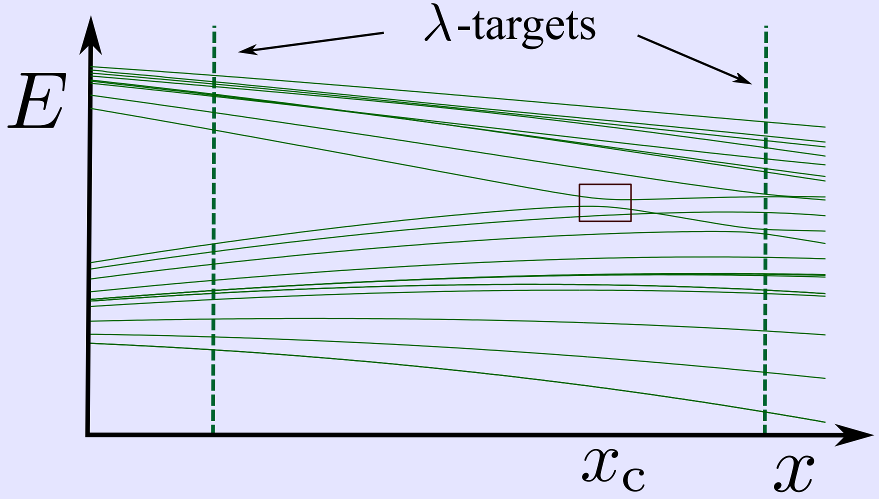
graph-based continuous unitary transformations (gCUTs)

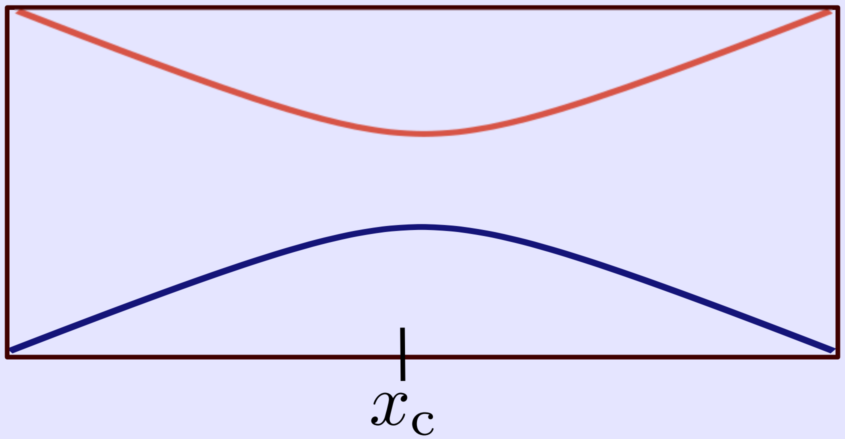
Coester/Clever/Herbst/Capponi/KPS EPL (2015)

- consider two clusters



- anti-level crossings

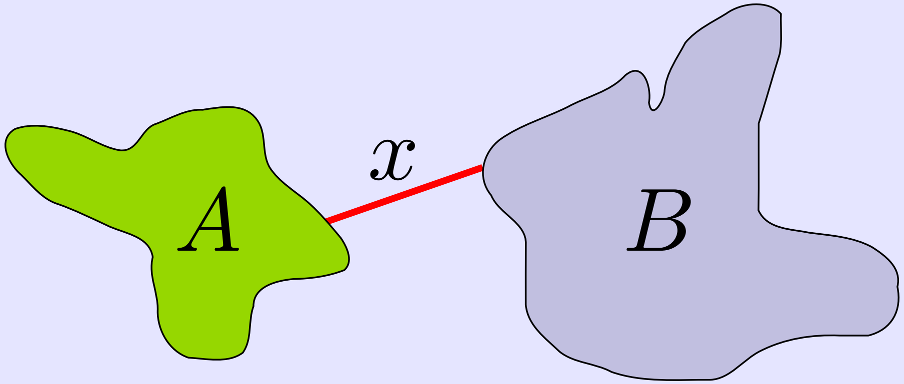


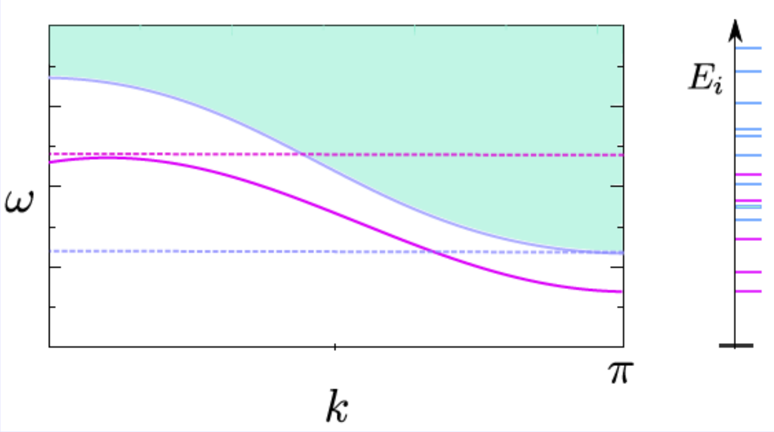


graph-based continuous unitary transformations (gCUTs)

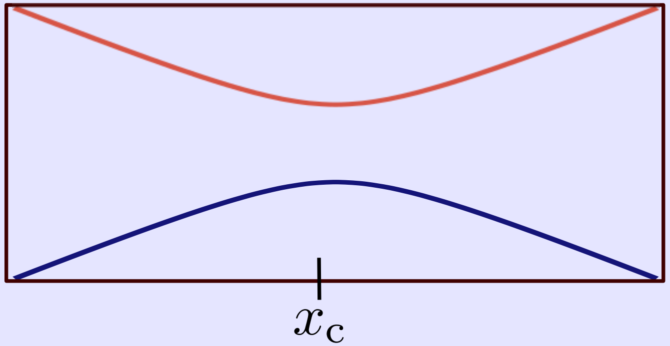
Coester/Clever/Herbst/Capponi/KPS (2015)

- consider two clusters





- artificial anti-level crossings (assume no true decay, "pseudo-decay")

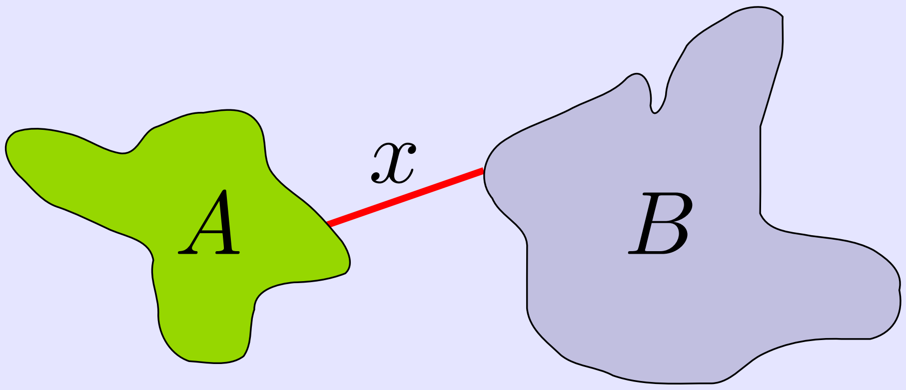


- drastic change of hopping elements
- non-perturbative effect
- relation to intruder states in quantum chemistry Malrieu et al. (1985)
- breakdown of conventional NLCE

graph-based continuous unitary transformations (gCUTs)

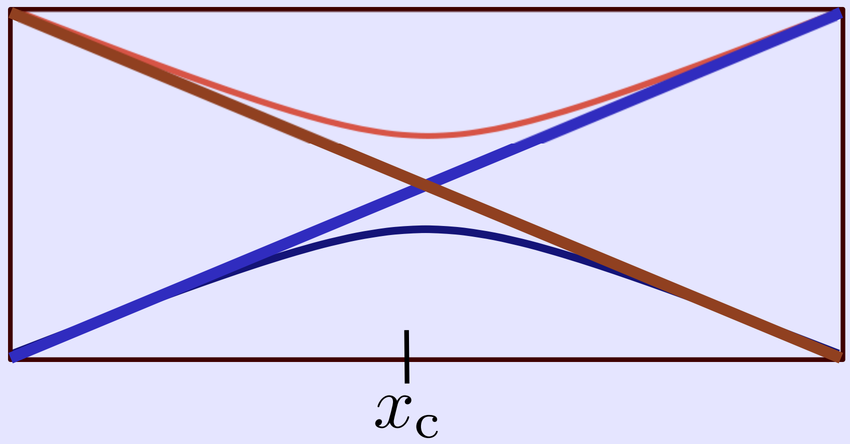
Coester/Clever/Herbst/Capponi/KPS (2015)

- consider two clusters



- need level crossing!

generalized notion of cluster additivity needed!

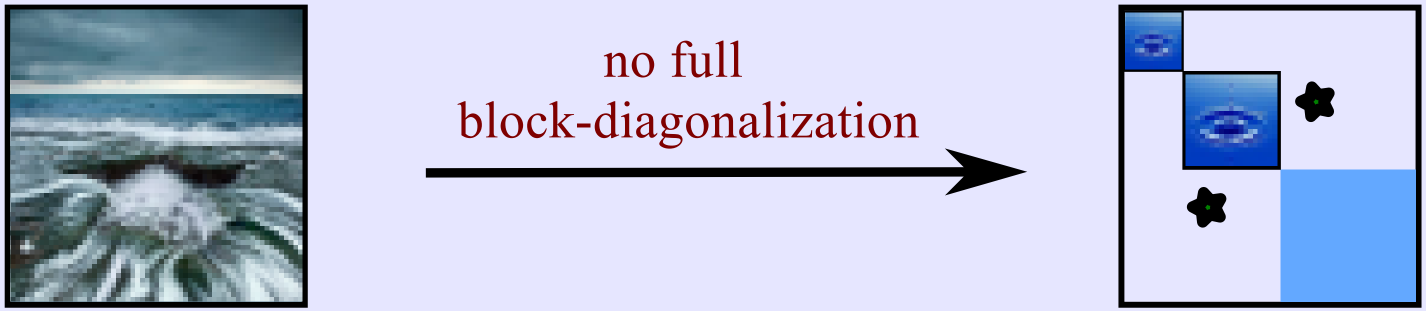


graph-based continuous unitary transformations (gCUTs)

Coester/Clever/Herbst/Capponi/KPS (2015)

generalized cluster additivity

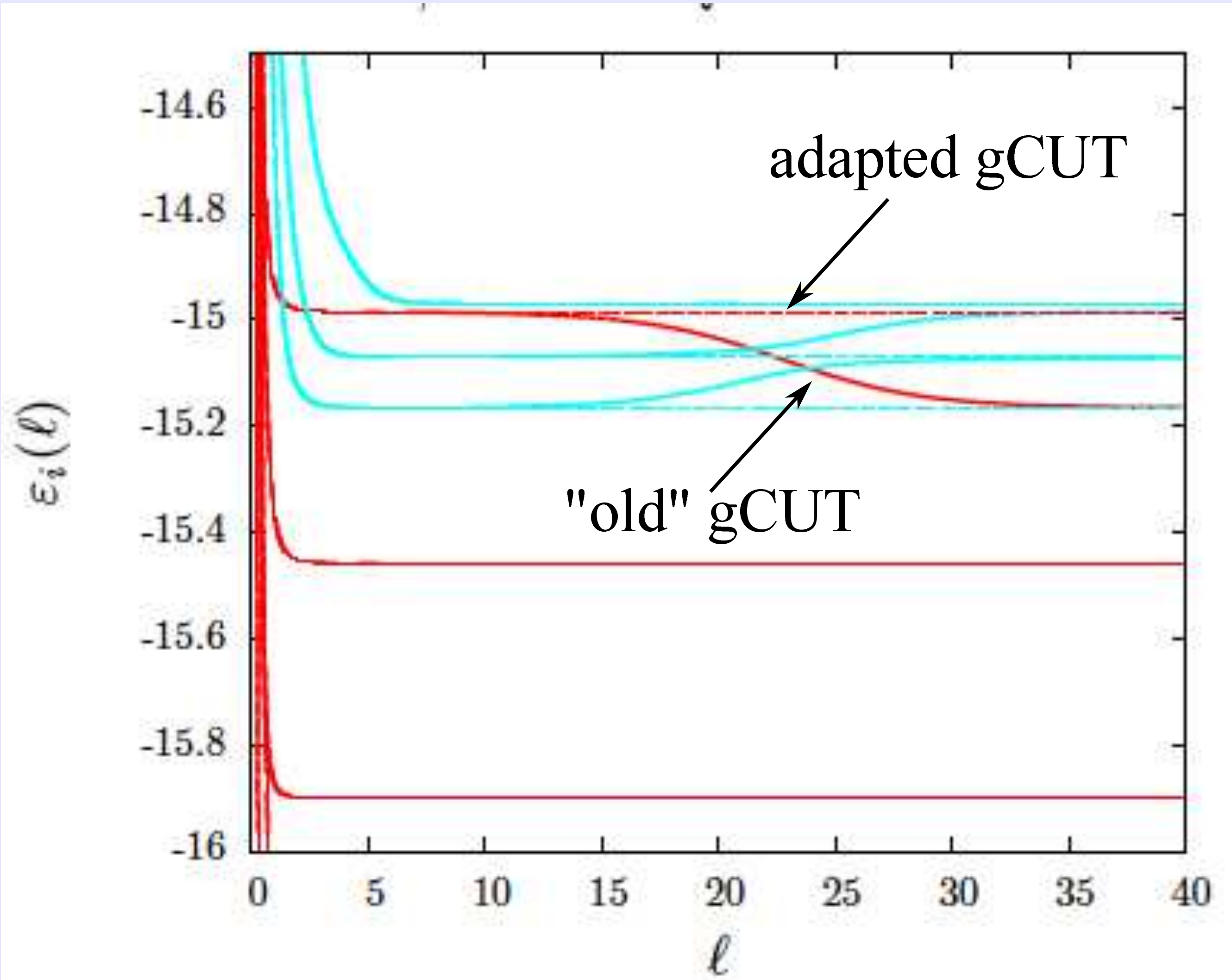
- reduced graph symmetry yields artificial entanglement
- one has to disentangle such levels
- adapted graph-based CUTs



- beyond the paradigm of using exact eigenvectors!

graph-based continuous unitary transformations (gCUTs)

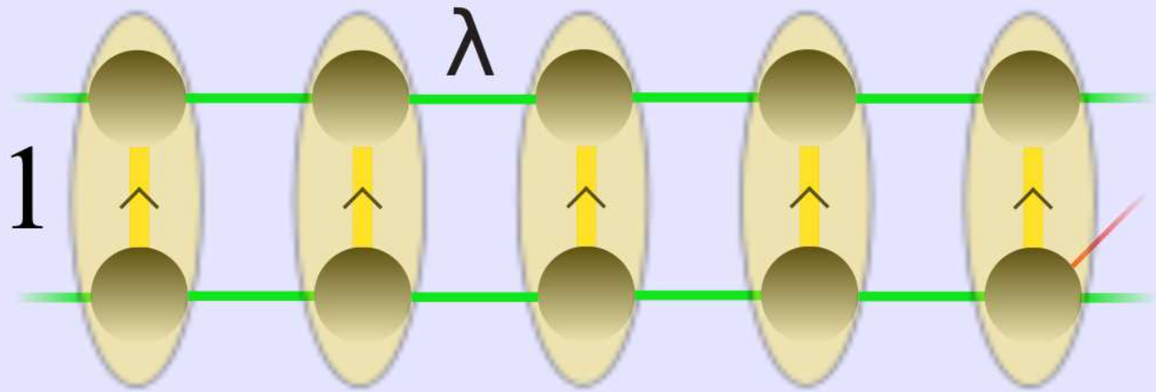
Coester/Clever/Herbst/Capponi/KPS (2015)



flow axis gives freedom which one can use!

graph-based continuous unitary transformations (gCUTs)

two-leg Heisenberg ladder

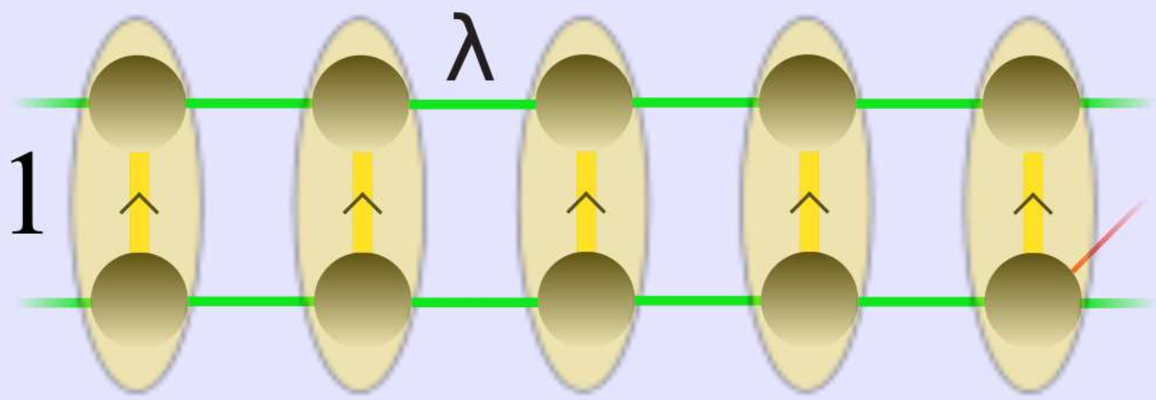


- $\lambda = 0$: product state of singlets, excitations local triplets
- finite λ: triplon quasi-particles, finite dispersion

'03 KPS/Uhrig

graph-based continuous unitary transformations (gCUTs)

two-leg Heisenberg ladder

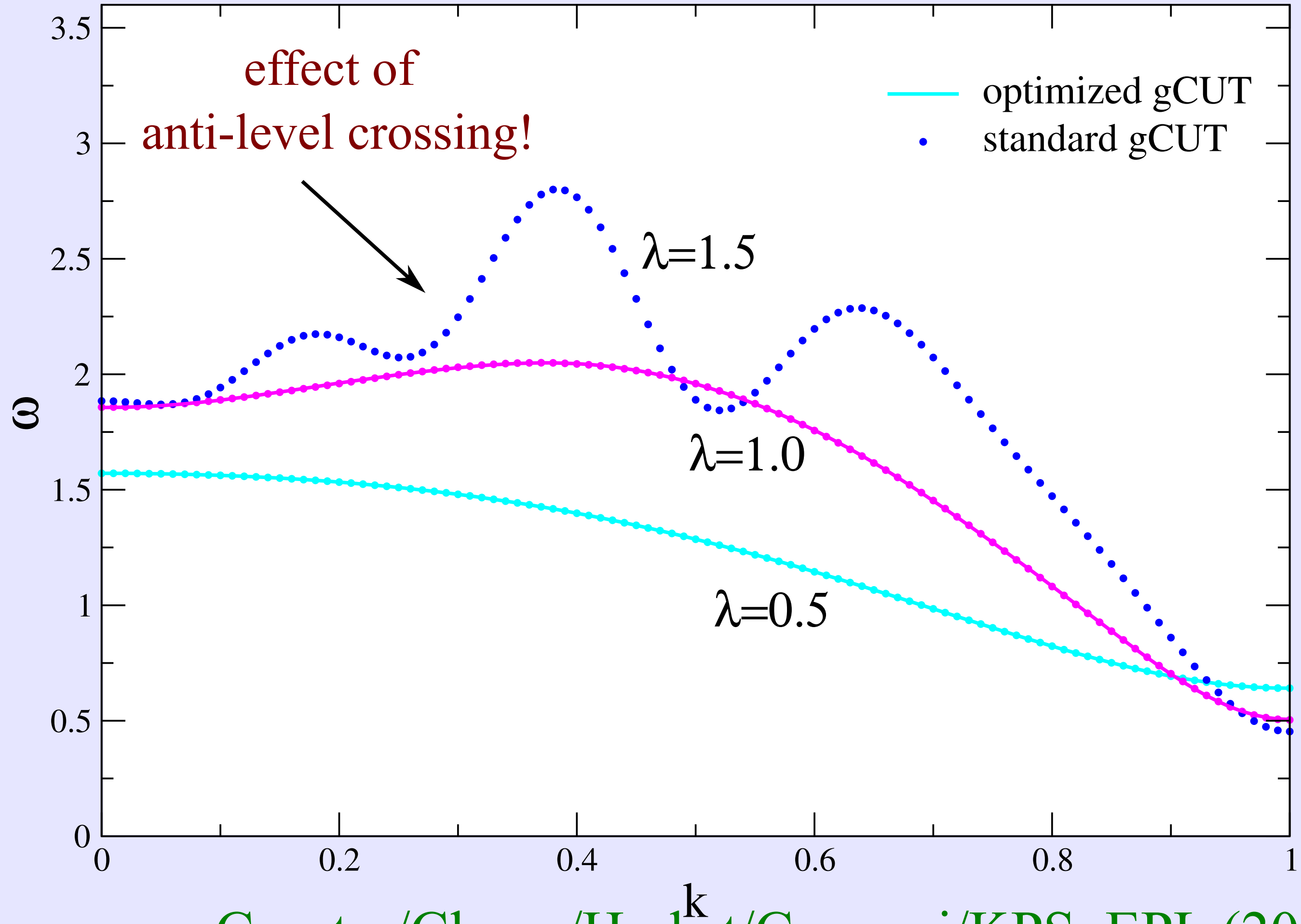


- apply standard and optimized gCUTs
- consider graphs up to 12 dimers

Coester/Clever/Herbst/Capponi/KPS, EPL (2015)

graph-based continuous unitary transformations (gCUTs)

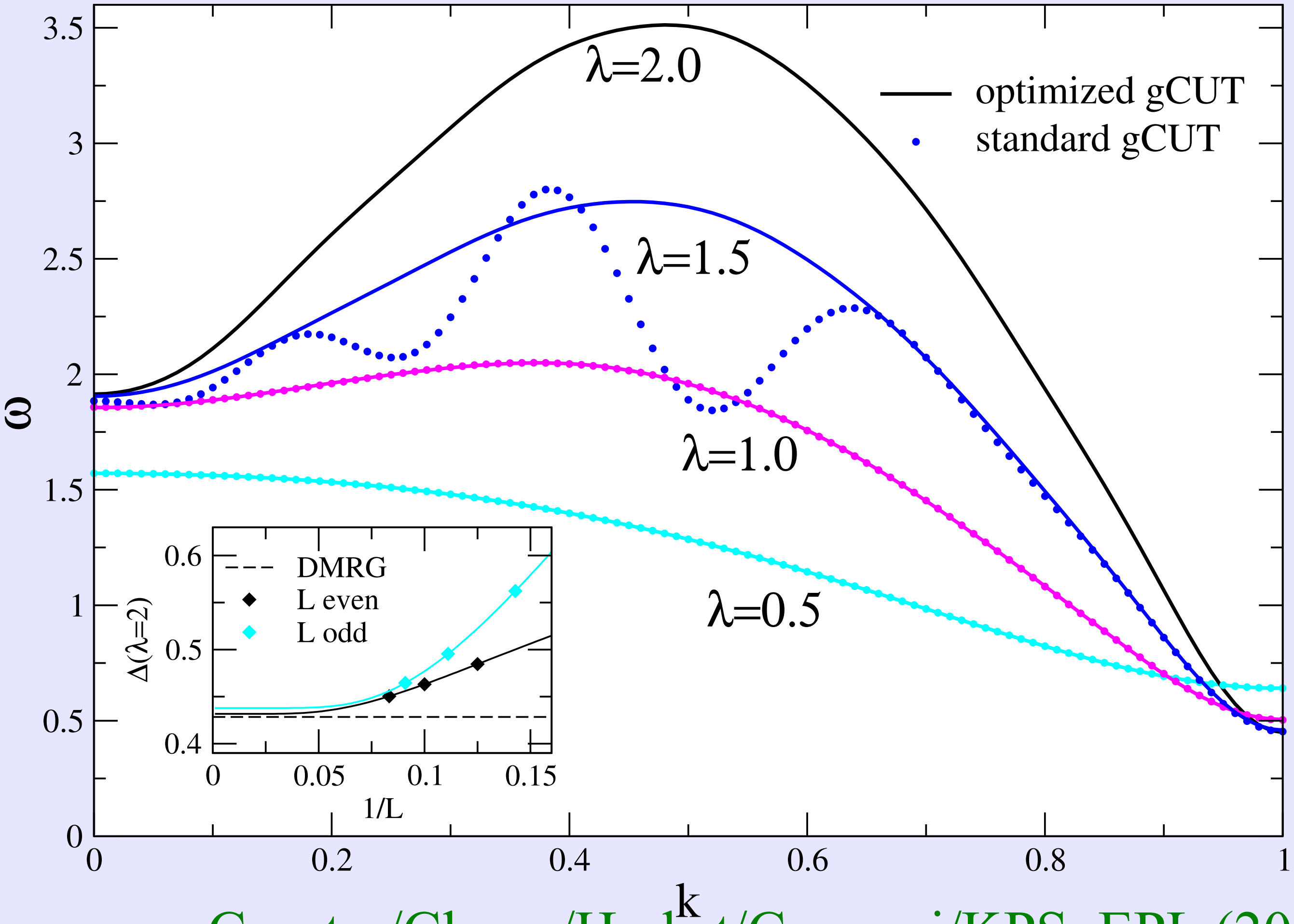
two-leg Heisenberg ladder



Coester/Clever/Herbst/Capponi/KPS, EPL (2015)

graph-based continuous unitary transformations (gCUTs)

two-leg Heisenberg ladder

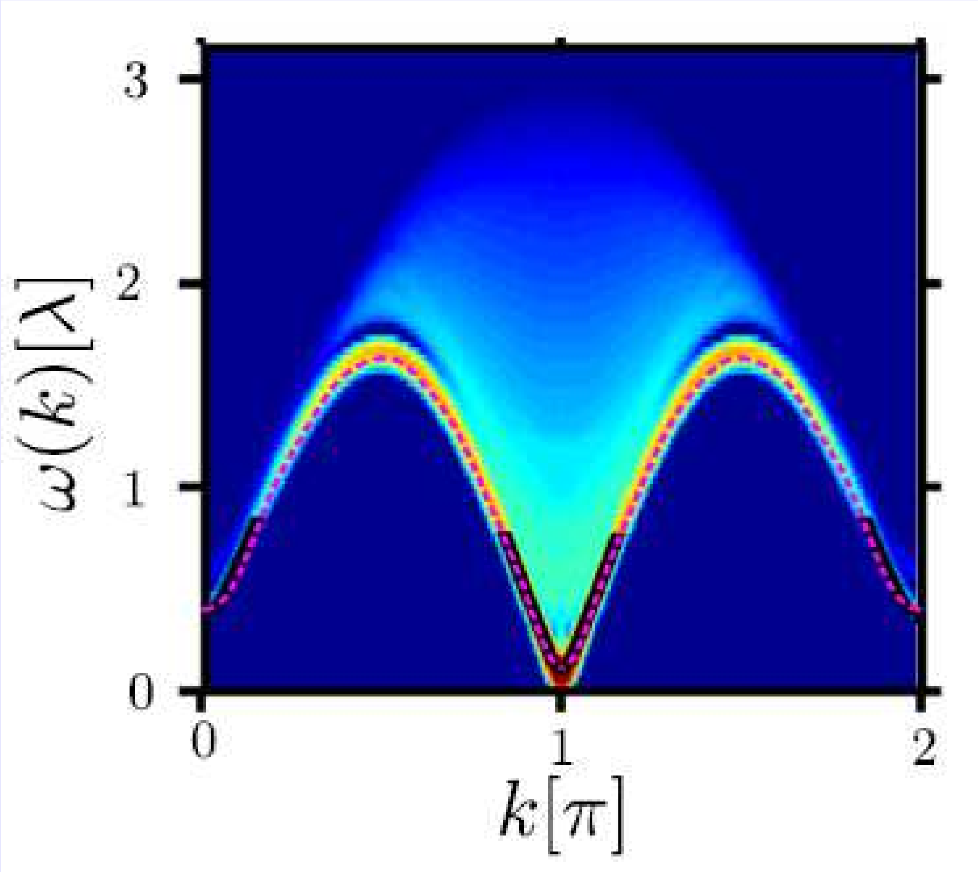


Coester/Clever/Herbst/Capponi/KPS, EPL (2015)

graph-based continuous unitary transformations (gCUTs)

two-leg Heisenberg ladder

$\lambda = 5$



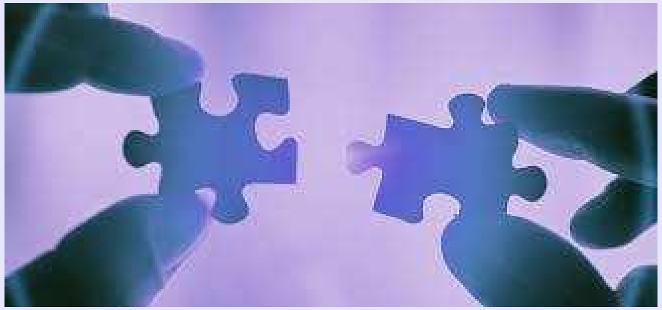
comparison

gCUT/DMRG

DMRG data from Schmidinger et al., PRB (2013)

Coester/KPS (2016)

summary - graph-based CUTs



non-perturbative LCEs

- for excited states, fundamental challenge due to reduced symmetry of graphs (intruder states)
- generalized notion of cluster additivity
- challenge can be solved with graph-based CUTs (also possible for true quasi-particle decay!)

truncation schemes

perturbative CUT

high-order series expansions
thermodynamic limit

Knetter/Uhrig, EPJB (2000)
Knetter/KPS/Uhrig, J. Phys. A (2003)
Coester/KPS, PRE (2015)

graph-based CUT

combine graph theory with CUTs
thermodynamic limit

Yang/KPS, EPL (2011)
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Coester/KPS (2016)

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operator flow
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Heidbrink/Uhrig, PRL (2002)
Fischer/Duffe/Uhrig, NJP (2010)
Krull/Drescher/Uhrig, PRB (2013)
Powalski/Uhrig/KPS, PRL (2015)

set up

- pCUT/gCUT good for gapped quantum phases

  $\longrightarrow$ gapless phases ? (here: ordered magnets)

- momentum space

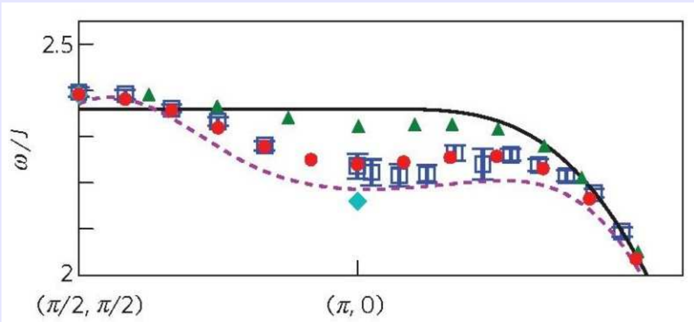
$$\mathcal{H} = E_0 + \sum_k \omega_k b_k^\dagger b_k + \sum_k \Gamma_k \left(b_k^\dagger b_{-k}^\dagger + \text{h.c.} \right) + \ldots$$

- truncation scheme?

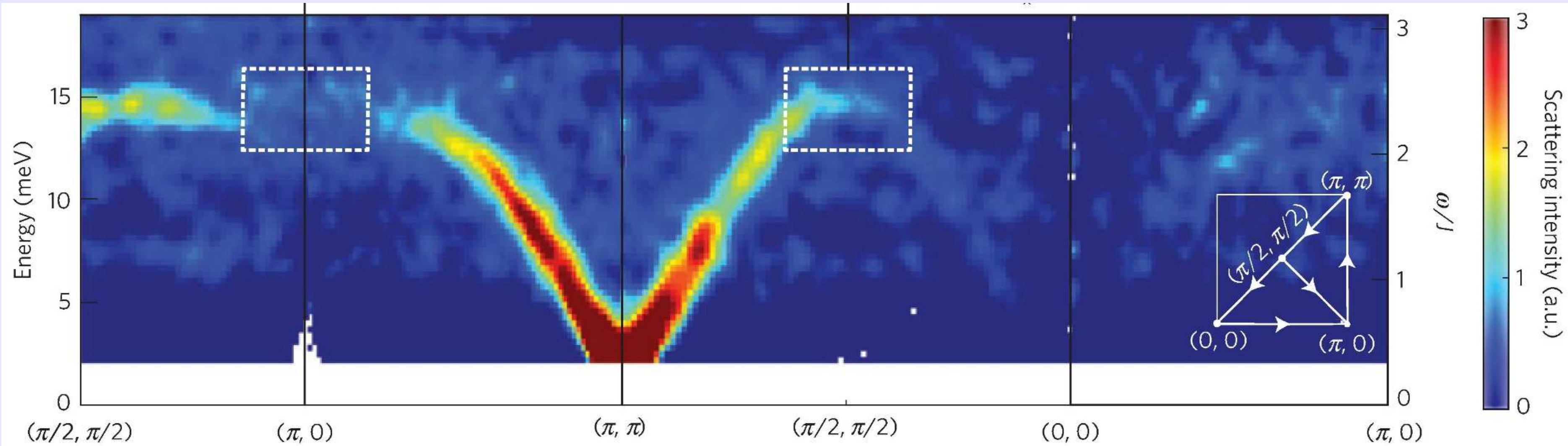
  $\longrightarrow$ idea: scaling dimension d of operators $k_i \to \lambda k_i$

$$\left(\begin{array}{ll} d=1 & \text{self-consistent mean-field theory} \\ d=2 & \text{beyond} \end{array} \quad \begin{array}{l} \text{square lattice spin-1/2} \\ \text{Heisenberg model} \end{array} \right)$$

Fractional spinons in the square lattice Heisenberg ?



spin wave theory
magnon perturbation up to $1/S^3$
spinon calculation
experiment
series expansion around Ising limit
quantum Monte Carlo

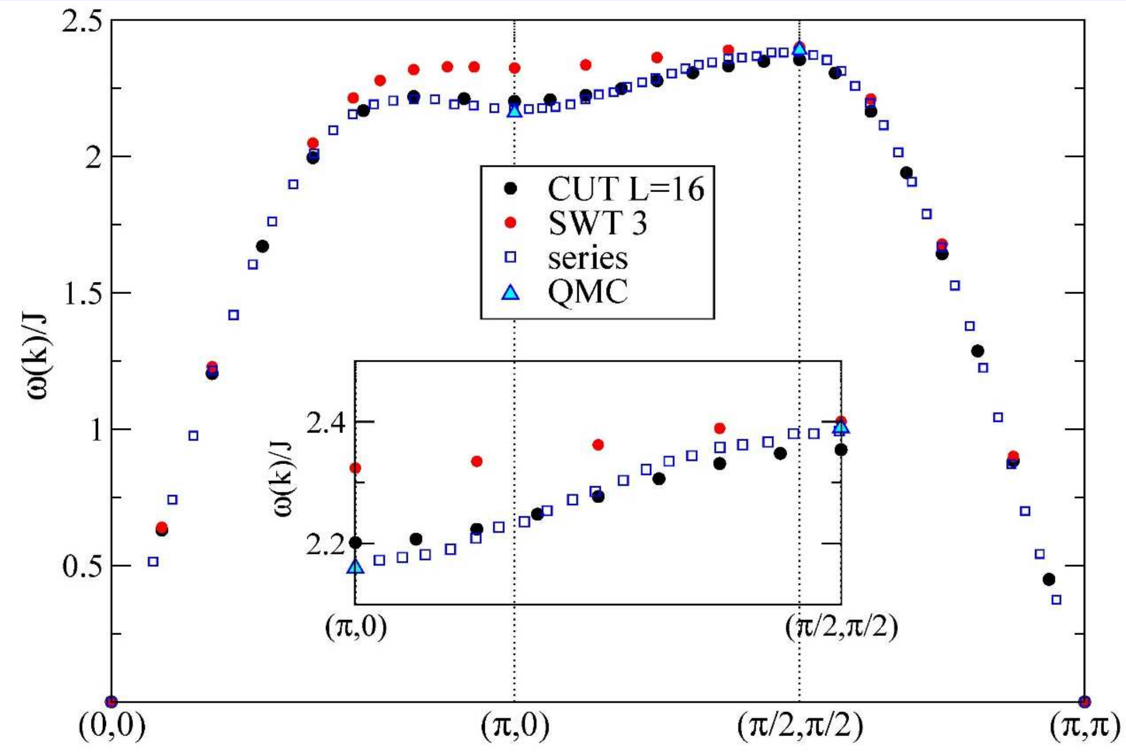


$\mathrm{Cu(DCOO)_2 4D_2O}$

Dalla Piazza et al., Nat. Phys. (2015)

momentum space CUTs

quantitative magnon description



roton minimum
from magnon-Higgs scattering

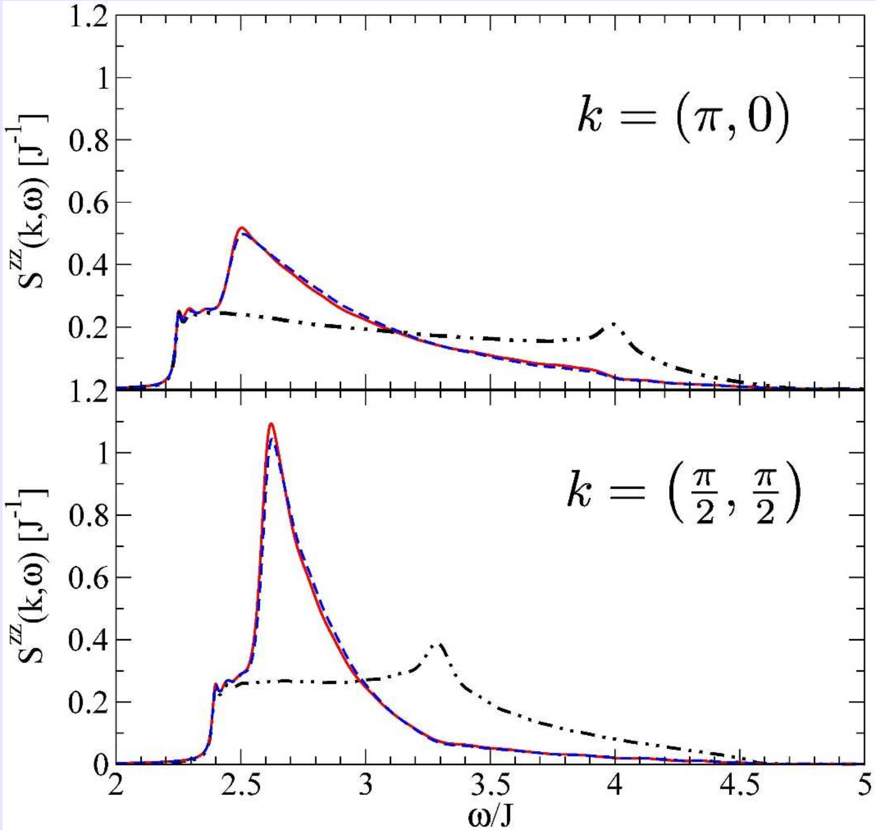
$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

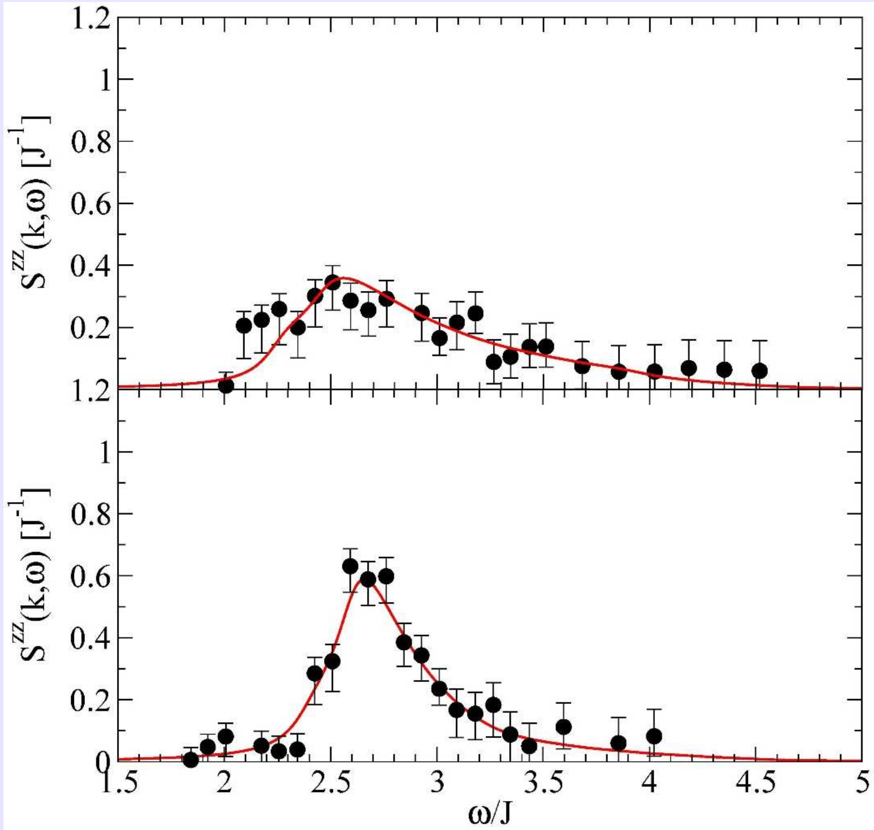
- **square lattice, spin 1/2**
- **Dyson-Maleev representation**
- **CUT in momentum space**
- **truncation based on scaling dimensions**

Powalski/Uhrig/KPS, PRL (2015)

momentum space CUTs

longitudinal dynamic structure factor





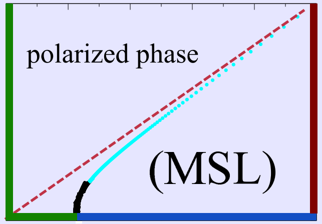
"Higgs" resonance

Powalski/Uhrig/KPS, PRL (2015)

summary

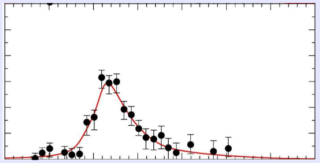
- **continuous unitary transformations (CUTs)**
  spirit
  quasi-particle pictures

- **perturbative CUTs (pCUTs)**
  transverse-field Ising model on the three-dimensional Swedenborgite lattice



- **graph-based CUTs (gCUTs)**
  generalized notion of linked-cluster theorem
  quasi-particle decay

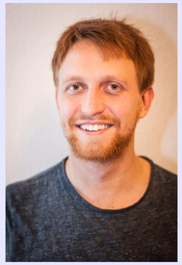
- **momentum-space CUTs**
  magnon and Higgs particles in an ordered quantum magnet



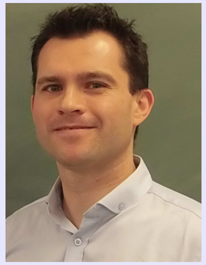
collaborators

- **pCUTs - Swedenborgites**

Kris Coester (Dortmund)
Tycho Sikkenk (Utrecht)
Lars Fritz (Utrecht)



Kris



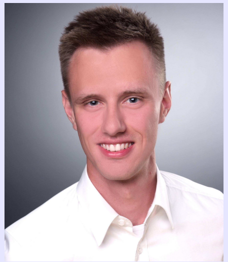
Lars

- **gCUTs**

Kris Coester (Dortmund)
Frederik Herbst (Dortmund)
Sebastian Clever (Dortmund)
Sylvain Capponi (Toulouse)

Kris

Frederik



Sebastian

Sylvain

- **momentum-space CUTs**

Michael Powalski (Dortmund)
Götz Uhrig (Dortmund)

Michael

Götz


to be continued...