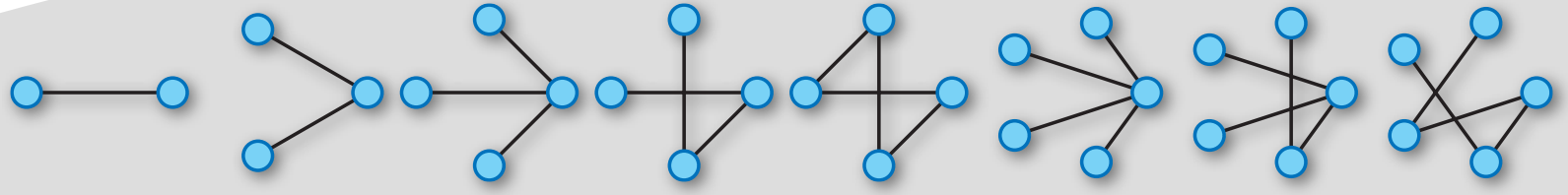
Linked-Cluster Expansions for Quantum Many-Body Systems

Boulder Summer School 2010

Simon Trebst



Lecture overview

- **Why series expansions?**
- **Linked-cluster expansions**
  - From Taylor expansions to linked-cluster expansions
  - Why linked clusters?
  - Series analysis, (Padé) approximants
- **Things to calculate, examples**
  - ground-state properties
  - tracking (various) excited states
- **Alternative approaches**
- **References**

Some history

High-temperature series expansions for classical models.

$$\exp(-\beta H) = 1 - \beta H + \frac{(\beta)^2}{2!} H^2 + \ldots$$

Series expansions gave the first indications of universal exponents.

This led to the development of renormalization group techniques and the discovery of universality.

Starting in the late 80's series expansion techniques were expanded to quantum systems including **zero-temperature** expansions.

Series expansions at T=0

Focus in this lecture: High-order perturbation expansions in some coupling parameter at zero temperature.

$$H = H_0 + \lambda H_1$$

unperturbed Hamiltonian

some perturbation

Taylor expansion, e.g. for ground-state energy

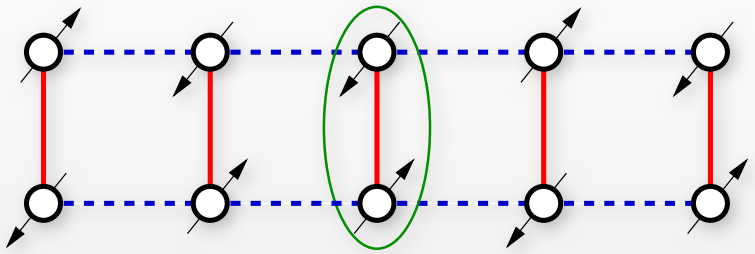
$$E(\lambda) = E_0 + E_1\lambda^1 + E_2\lambda^2 + \ldots + E_n\lambda^n + O(\lambda^{n+1})$$

High-order series expansions (T=0)

Taylor expansion, e.g. for ground-state energy

$$E(\lambda) = E_0 + E_1\lambda^1 + E_2\lambda^2 + \ldots + E_n\lambda^n + O(\lambda^{n+1})$$

Toy model: One-dimensional spin ladder



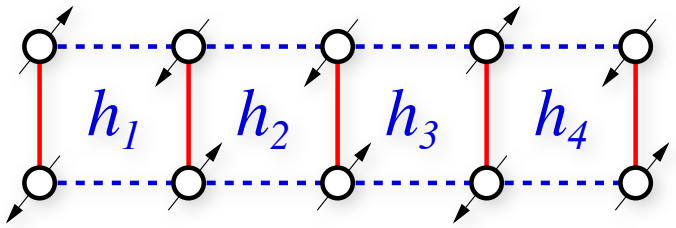
$$\lambda = J_{||}/J_{\perp}$$

$$H = H_0 + \lambda H_1 = J_{\perp} \sum_i \left\{ \vec{S}_i \cdot \vec{S}'_i + \lambda \left(\vec{S}_i \cdot \vec{S}_{i+1} + \vec{S}'_i \cdot \vec{S}'_{i+1} \right) \right\}$$

Multivariable expansions

The perturbation H_1 is a sum of local interaction terms h_k

$$H_1 = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = \sum_k h_k$$

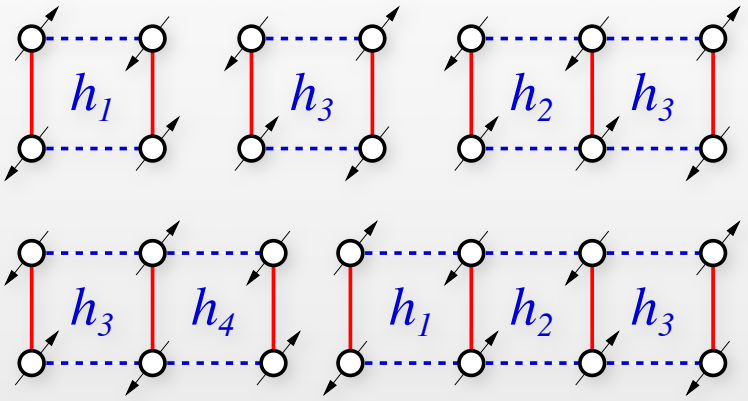


Associate each term h_k with a coefficient λ_k
and (multi-)expand the ground-state energy

$$E(\{\lambda_k\}) = \sum_{\{n_k\}} e\{n_k\} \prod_k \lambda_k^{n_k}$$

$$= \sum_C W_{[E]}(C)$$

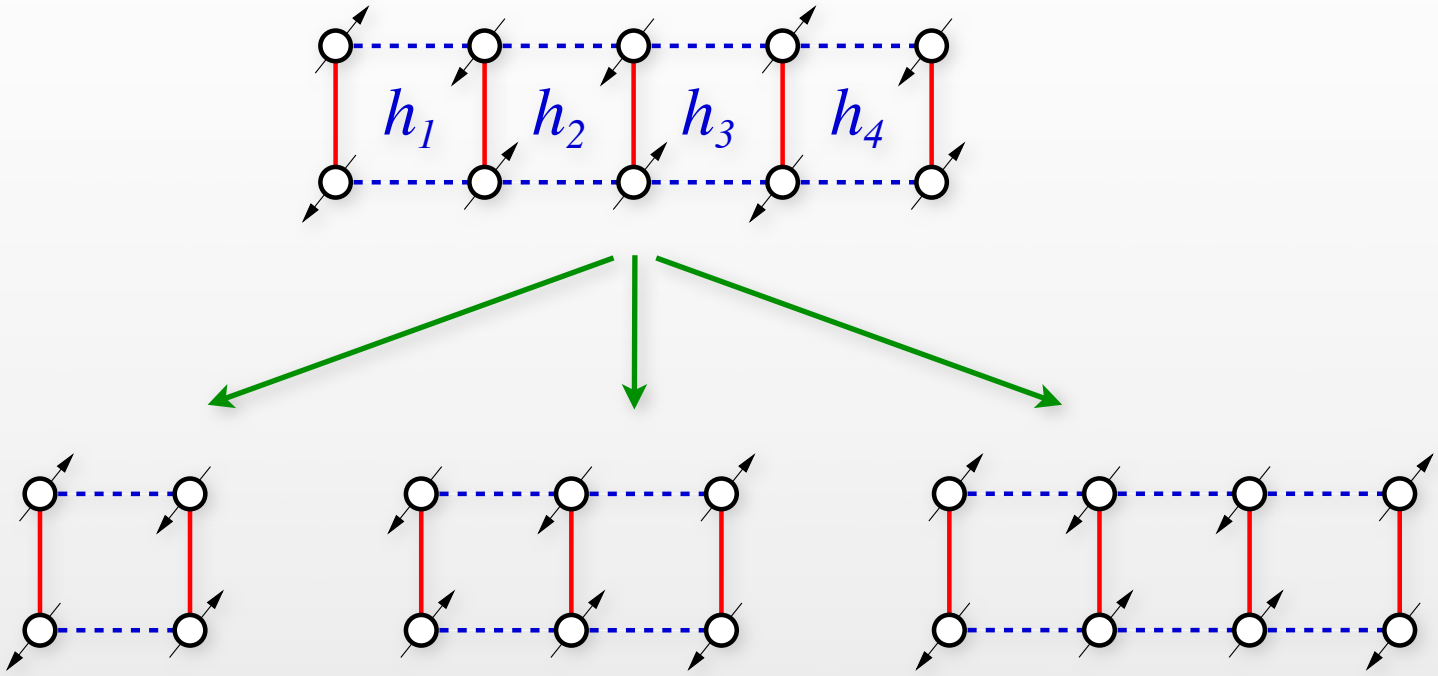
cluster weight



Linked-cluster expansions

Simplify multivariable expansion by setting all λ_k equal to λ.

Topologically equivalent clusters then give identical contributions.



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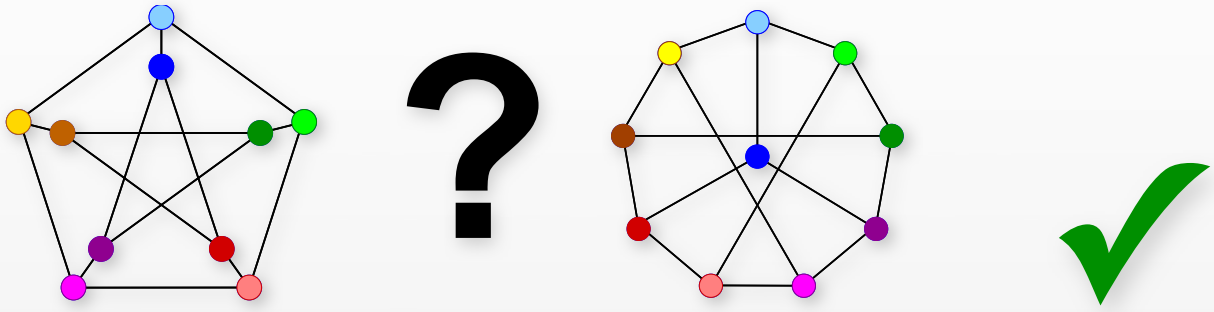


Two clusters G and H are called topologically equivalent, if there is a mapping M of the vertices of G to the vertices of H such that $M(G) = H$.

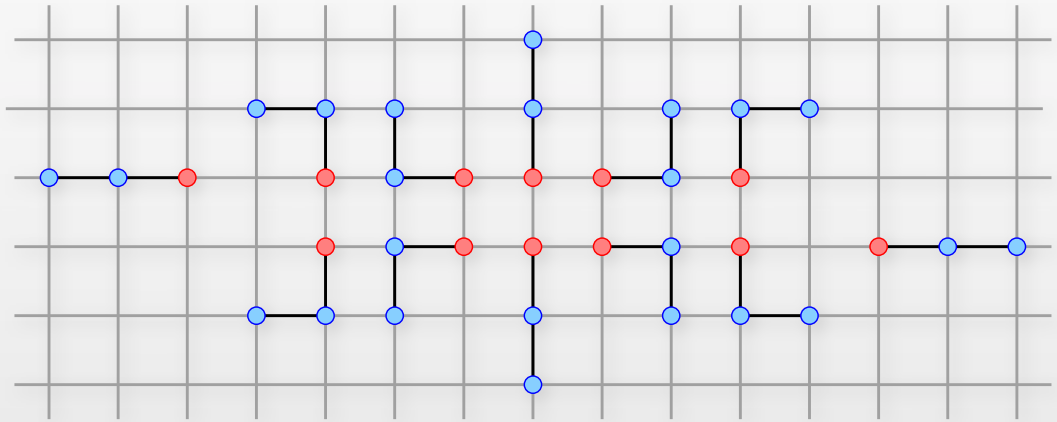
Linked-cluster expansions

Simplify multivariable expansion by setting all λ_k equal to λ.

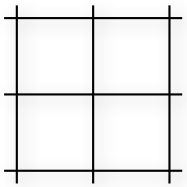
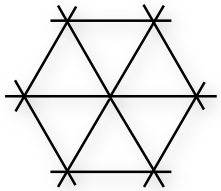
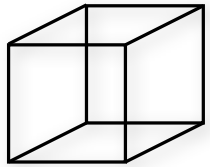
Topologically equivalent clusters then give identical contributions.

$$P(\lambda)/N = \sum_{\tilde{C}} L(\tilde{C}) \cdot W_{[P]}(\tilde{C})$$

"lattice constant"
counts the # of embeddings



Efficiency gain of a linked-cluster expansion

N	*Square lattice* Cluster	*Square lattice* Embeddings	*Triangular lattice* Cluster	*Triangular lattice* Embeddings	*Cubic lattice* Cluster	*Cubic lattice* Embeddings
1	1	4	1	6	1	6
2	2	16	2	36	2	36
3	4	76	5	306	4	306
4	8	280	10	1.860	8	2.016
5	14	1.180	22	13.278	15	16.278
6	28	4.856	50	89.988	31	126.036
7	56	21.060	122	656.862	64	1.071.954
8	124	90.568	320	4.756.596	147	9.008.808
9	280	419.468	910	37.095.654	353	82.540.686
10	679	1.911.352	2.727	284.221.236	908	742.248.348

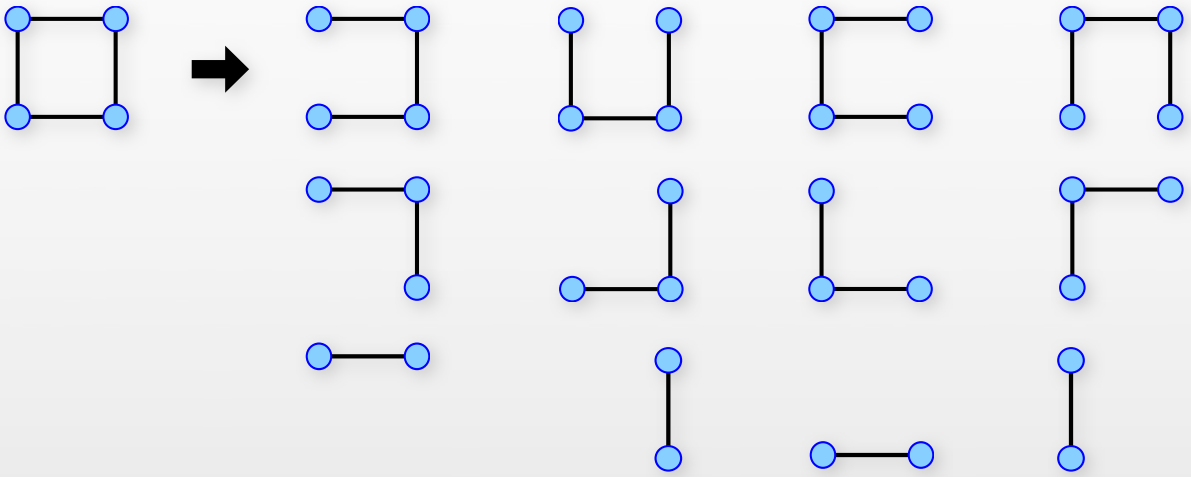
We can reduce the number of calculations
by many orders of magnitude!

The thermodynamic limit

Reconsider the cluster weight

$$W_{[P]}(C) = P_C - \sum_{C' \subset C} W_{[P]}(C')$$

The **subcluster subtraction** eliminates
all (low-order) contributions of subclusters.



The thermodynamic limit

Reconsider the cluster weight

$$W_{[P]}(C) = P_C - \sum_{C' \subset C} W_{[P]}(C')$$

The **subcluster subtraction** eliminates
all (low-order) contributions of subclusters.

Each cluster contributes **only the additional high-order terms**,
which can be evaluated first for the respective cluster size.

We obtain results directly for the **thermodynamic limit**.

However, we trade **finite-size scaling** with **series extrapolation**.

The linked-cluster theorem

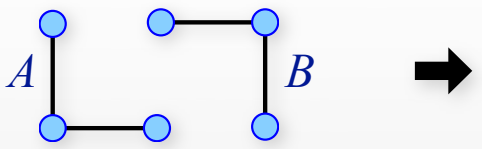
Disconnected clusters have vanishing weight

$$P_C = P_A + P_B \quad \Rightarrow \quad W_{[P]}(C) = 0$$

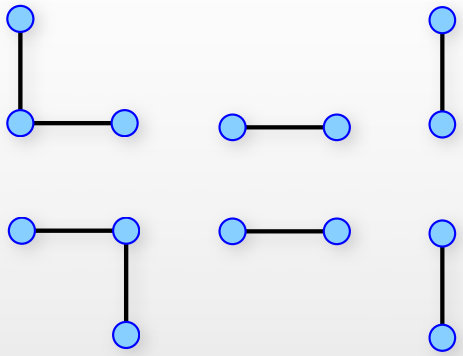
because

$$W_{[P]}(C) = P_C - \sum_{C' \subset C} W_{[P]}(C')$$

$$= P_A - \sum_{C' \subseteq A} W_{[P]}(C') + P_B - \sum_{C' \subseteq B} W_{[P]}(C') \; = 0$$

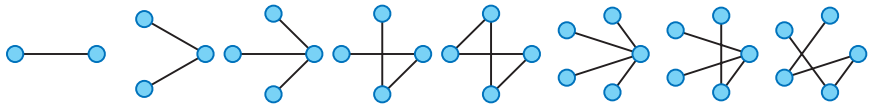


disconnected cluster C



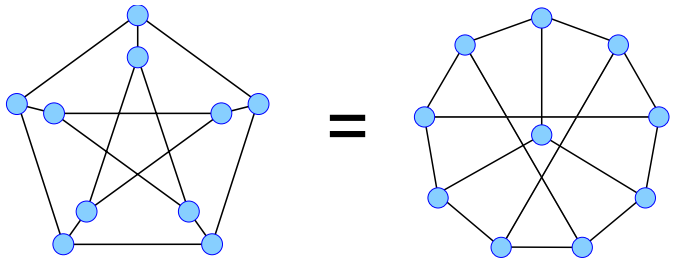
Graph theory

- Generation of clusters



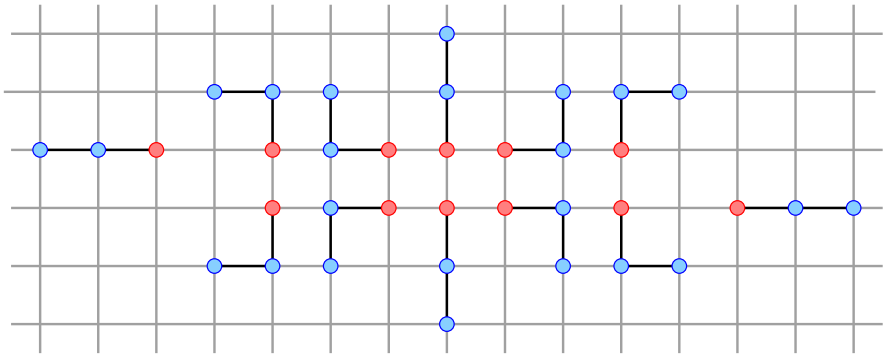
- Isomorphism of clusters

→ identify topologically equivalent clusters



- Embedding of clusters onto given lattices

→ topologically equivalent clusters have identical weights

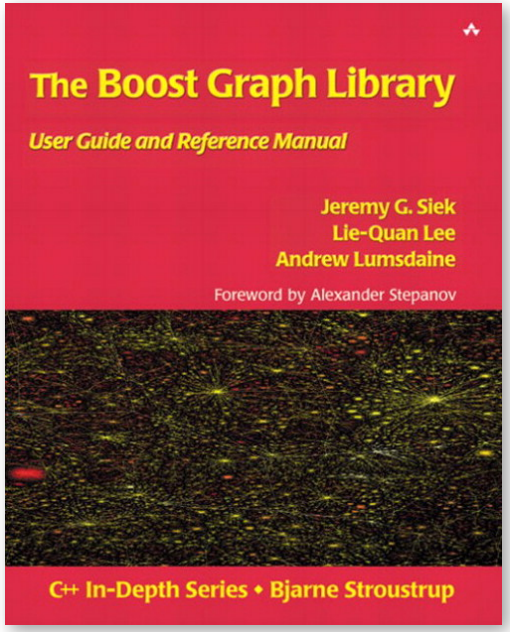


Efficient graph handling

- Graphs and and their general properties (vertices, edges, labels, …)

  Boost graph library

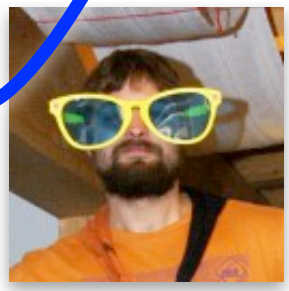
  `http://www.boost.org`



- Graph isomorphisms (automorphism group, canonical labeling, sorting, …)

  The **nauty** algorithm by Brendan McKay

  `http://cs.anu.edu.au/people/bdm/nauty/`



Lukas Gamper

Calculating cluster observables

- Perturbation theory for T=0
  - Rayleigh-Schrödinger perturbation theory

ground-state energy

$$E(C) = \sum_n \lambda^n e_n$$

$$e_n = \langle \psi_0 | H_1 | \psi_{n-1} \rangle$$

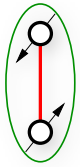
ground-state wavefunction

$$|\psi\rangle = \sum_n \lambda^n \psi_n$$

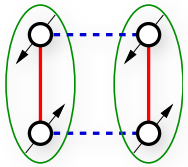
$$\langle k|\psi_n\rangle = \frac{\langle k|H_1|\psi_{n-1}\rangle - \sum_{m=1}^{n-1} e_m \langle k|\psi_{n-m}\rangle}{\langle 0|H_0|0\rangle - \langle k|H_0|k\rangle}$$

  - High-temperature expansion for finite T.
  - A cluster with n edges will contribute first in order n.

Ground-state expansion for spin ladder

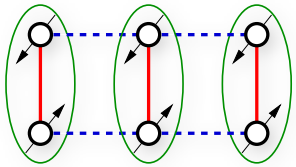


$$E(C_0) = W_{[E]}(C_0) = -\frac{3}{4}$$



$$E(C_1) = -\frac{3}{2} - \frac{3}{8}x^2 - \frac{3}{16}x^3 - \frac{3}{128}x^4 = W_{[E]}(\quad) + 2 \bullet W_{[E]}(\quad)$$

$$W_{[E]}(C_1) = \frac{3}{8}x^2 - \frac{3}{16}x^3 - \frac{3}{128}x^4$$

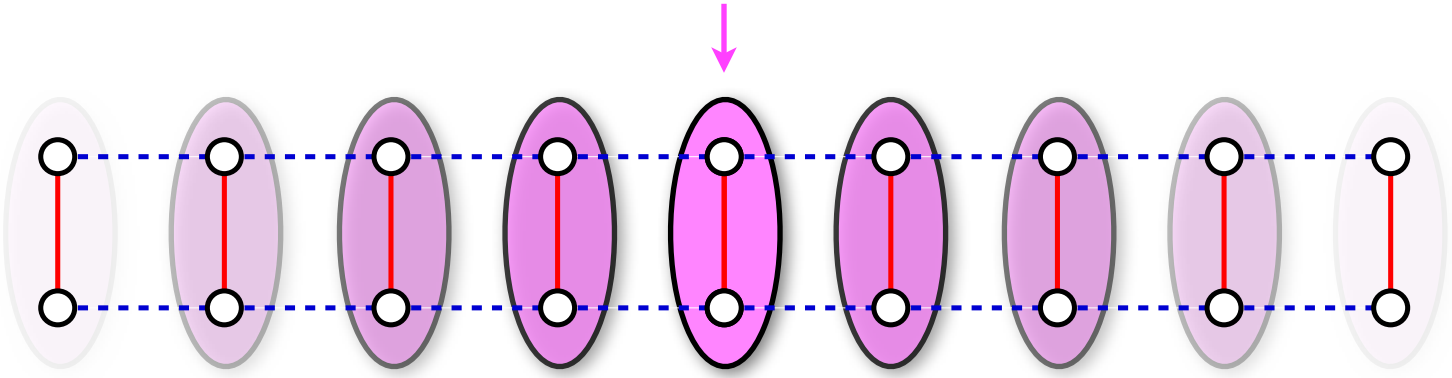


$$E(C_2) = -\frac{9}{4} - \frac{3}{4}x^2 - \frac{3}{8}x^4 = W_{[E]}(\quad) + 2 \bullet W_{[E]}(\quad) + 3 \bullet W_{[E]}(\quad)$$

$$W_{[E]}(C_2) = \frac{3}{64}x^4$$

$$E / J_\perp = W_{[E]}(C_0) + W_{[E]}(C_1) + W_{[E]}(C_2) = -\frac{3}{4} - \frac{3}{8}x^2 - \frac{3}{16}x^3 + \frac{3}{128}x^4 + O(x^5)$$

Quasiparticle dynamics: Excitation spectrum



What is the **elementary excitation** of the coupled system?

What is the **excitation spectrum**?

What can be calculated using (high-order) cluster expansions?

One-particle excited states

Calculate effective Hamiltonians in the degenerate manifold of excited one-particle states for each cluster.

$$S^{-1}HS = \begin{pmatrix} \boxed{H^{\text{eff}}(1)} & 0 \\ 0 & \boxed{\cdots} \end{pmatrix}$$

However, there is no cluster expansion

$$H_C^{\text{eff}} = \left[H^{\text{eff}} + e_B I\right]_A \oplus \left[H^{\text{eff}} + e_A I\right]_B \neq H_A^{\text{eff}} \oplus H_B^{\text{eff}}$$

Calculate **irreducible matrix elements** instead

$$H^{\text{eff}} - e_C I \qquad \Delta(i,j) = \langle j|H^{\text{eff}}|i\rangle - E_0\delta_{i,j}$$

Calculation of eigenvalues

For a translationally invariant system we have

$$\Delta(i,j) = \Delta(\delta)$$

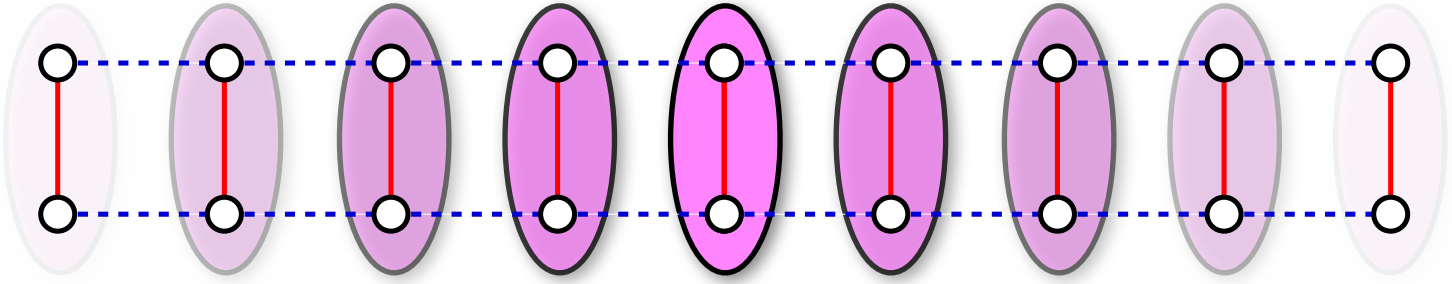
and the momentum K is a good quantum number.

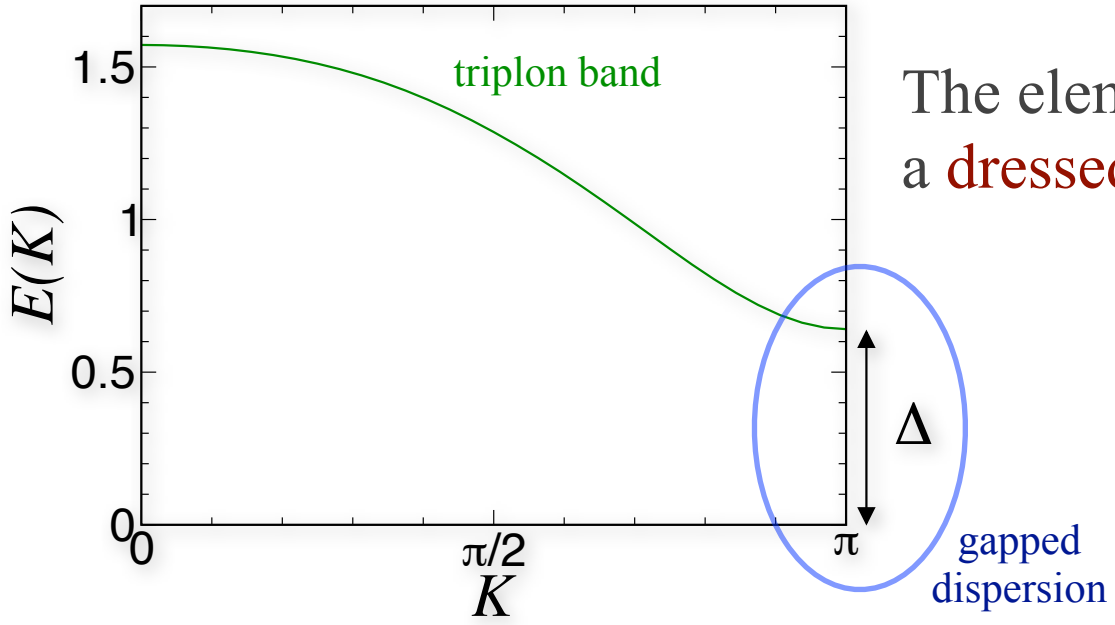
The effective one-particle Hamiltonian can then easily be diagonalized by a Fourier transformation.

The energy eigenvalues are

$$E(K) = \sum_{\delta} \Delta(\delta) \cos(K \cdot \delta)$$

Spectrum for spin-1/2 ladder





The elementary excitation becomes a dressed triplet state, the **triplon**.

Two-particle excitations

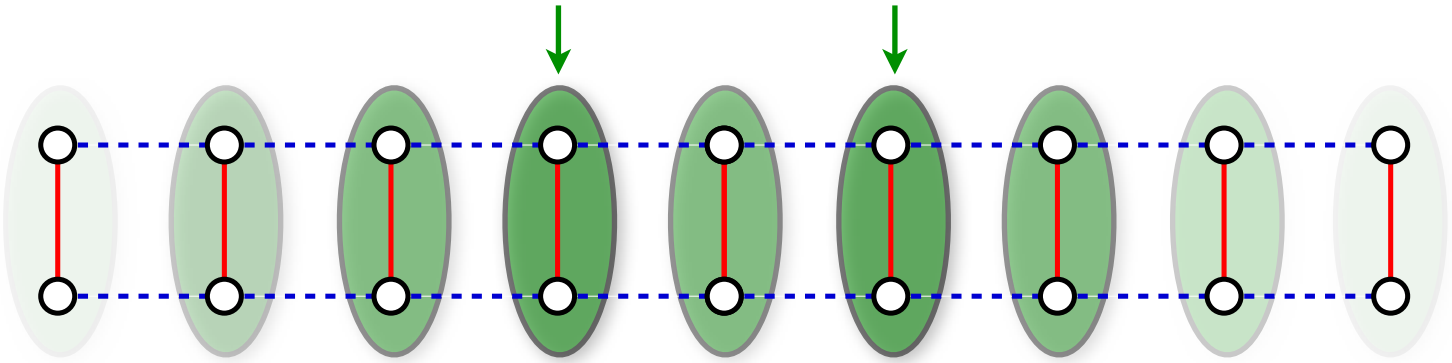
Generalize single-particle approach to block diagonalize Hamiltonian

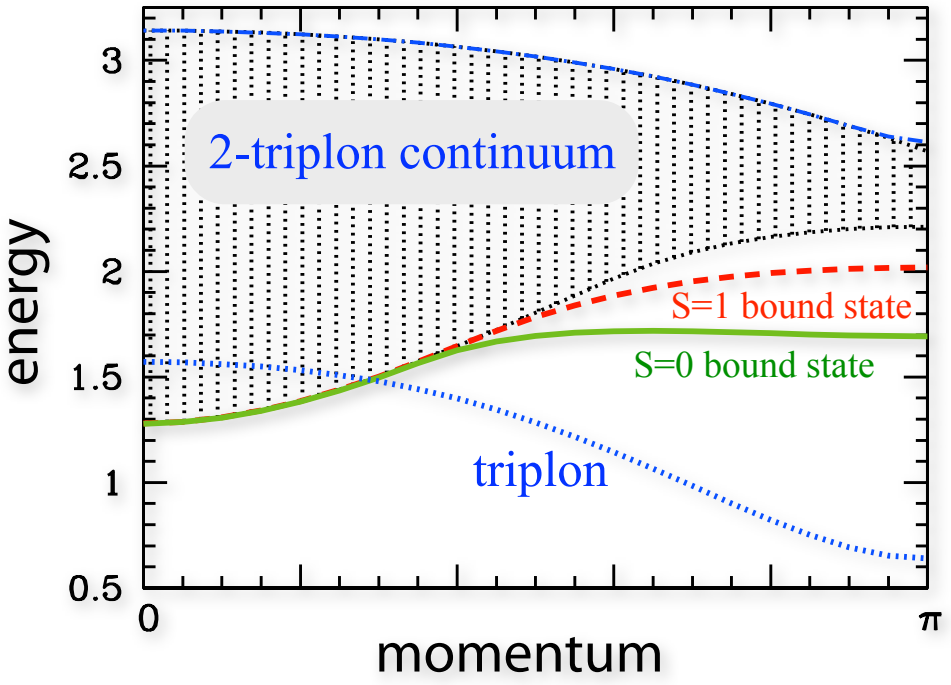
$$O^T H O = \begin{pmatrix} \boxed{H^{eff}(0)} & 0 & 0 & 0 \\ 0 & \boxed{H^{eff}(1)} & 0 & 0 \\ 0 & 0 & \boxed{H^{eff}(2)} & 0 \\ 0 & 0 & 0 & \boxed{\ldots} \end{pmatrix}$$

Cluster expansion for effective Hamiltonians,
more precisely their irreducible matrix elements.

This gives the exact 2-particle Schrödinger equation,
which can be (numerically) solved.

Spin-1/2 ladder





- The **2-triplon states** form
  - a continuum of states,
  - bound states (S = 0,1),
  - antibound states (S = 2).
- Typical ladder materials $(La,Ca)_{14}Cu_{24}O_{41}$

Further extensions

- multiparticle excitation spectra
- spectral weights
- ...

$$O^T H O = \begin{pmatrix} \boxed{H^{eff}(0)} & 0 & 0 & 0 \\ 0 & \boxed{H^{eff}(1)} & 0 & 0 \\ 0 & 0 & \boxed{H^{eff}(2)} & 0 \\ 0 & 0 & 0 & \boxed{\ldots} \end{pmatrix}$$

Does the calculated series (always) converge?

Sometimes, we do get **convergent** series.

Quantum spin-S models

e.g. ground state energy of the spin-1/2 Heisenberg ladder

$$E/J_\perp = -\frac{3}{4} - \frac{3}{8}\lambda^2 - \frac{3}{16}\lambda^3 + \frac{3}{128}\lambda^4 + O(\lambda^5)$$

But sometimes, we also obtain **asymptotic** series.

Bose-Hubbard model

e.g. ground state energy of chain of bosons

$$E/U = -\frac{1}{2} - 4\lambda^2 + 4\lambda^4 + 30.22\lambda^6 - 62.57\lambda^8 + 121.18\lambda^{10} + O(\lambda^{12})$$

Series extrapolation: Padé approximants

A Padé approximant to some finite series is a rational function

$$f_{\mathrm{Pade}}(\lambda) = \frac{p_N(\lambda)}{q_M(\lambda)}$$

where the Taylor expansion of f matches the approximated series.

$$E/J_\perp = -\frac{3}{4} - \frac{3}{8}x^2 - \frac{3}{16}x^3 + \frac{3}{128}x^4 + O(x^5)$$

$$\begin{aligned}
\mathrm{Pade}[2,2] &= \left(-\frac{3}{4} + \frac{3}{8}x - \frac{39}{64}x^2\right) / \left(1 - \frac{1}{2}x + \frac{5}{16}x^2\right) \\
&= -\frac{3}{4} - \frac{3}{8}x^2 - \frac{3}{16}x^3 + \frac{3}{128}x^4 \\
&\quad + \frac{9}{128}x^5 + \frac{57}{2048}x^6 - \frac{33}{4096}x^7 - \frac{417}{32768}x^8 + \ldots
\end{aligned}$$

Series extrapolation: Padé approximants

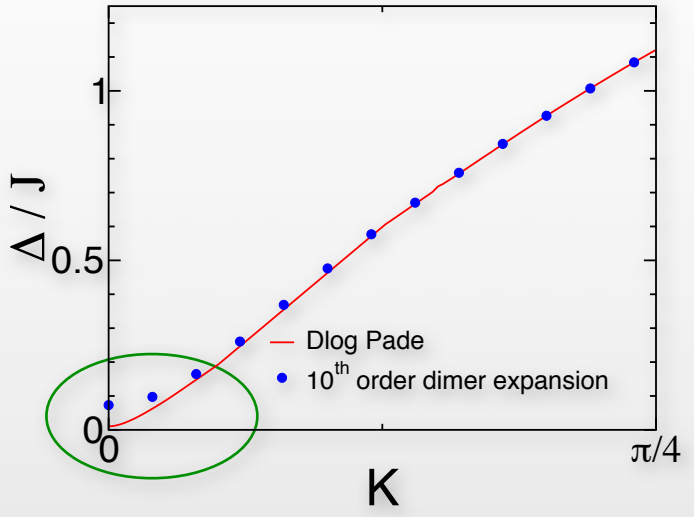
A Padé approximant to some finite series is a rational function

$$f_{\mathrm{Pade}}(\lambda) = \frac{p_N(\lambda)}{q_M(\lambda)}$$

where the Taylor expansion of f matches the approximated series.

Well-suited to estimate small gaps.

dimer expansion for
AFM Heisenberg chain



Dlog Padés: Critical points and exponent

Assume a series obeys a power-law dependency

$$s(\lambda) = f(\lambda) \cdot (\lambda - \lambda_c)^{\nu}$$

ν: critical exponent

λ_c: critical point

Let's differentiate the logarithm of $s(\lambda)$

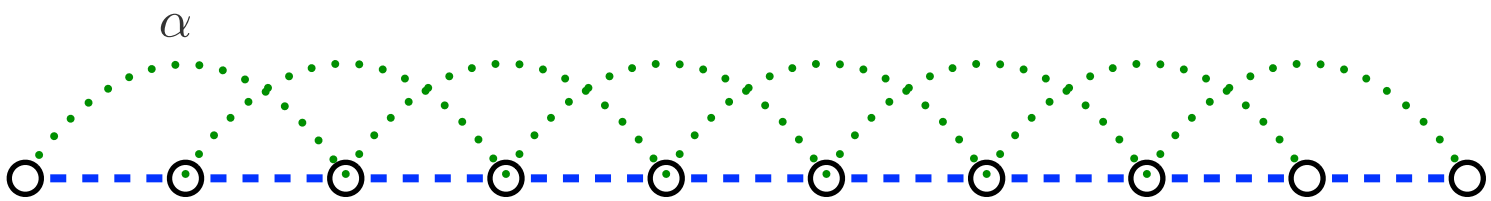
$$D \log\, s(\lambda) = \frac{f'(\lambda)}{f(\lambda)} + \frac{\nu}{\lambda - \lambda_c} = \frac{p_N(\lambda)}{q_M(\lambda)}$$

The critical point λ_c is a root of the denominator $q_M(\lambda)$.

The critical exponent ν can be evaluated by

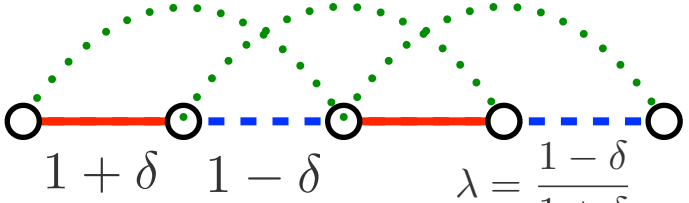
$$\nu = res_{\lambda_c} \left(\frac{f'(\lambda)}{f(\lambda)} + \frac{\nu}{\lambda - \lambda_c} \right) = \frac{p_N(\lambda_c)}{q'_M(\lambda_c)}$$

Example: J1-J2 Heisenberg chain

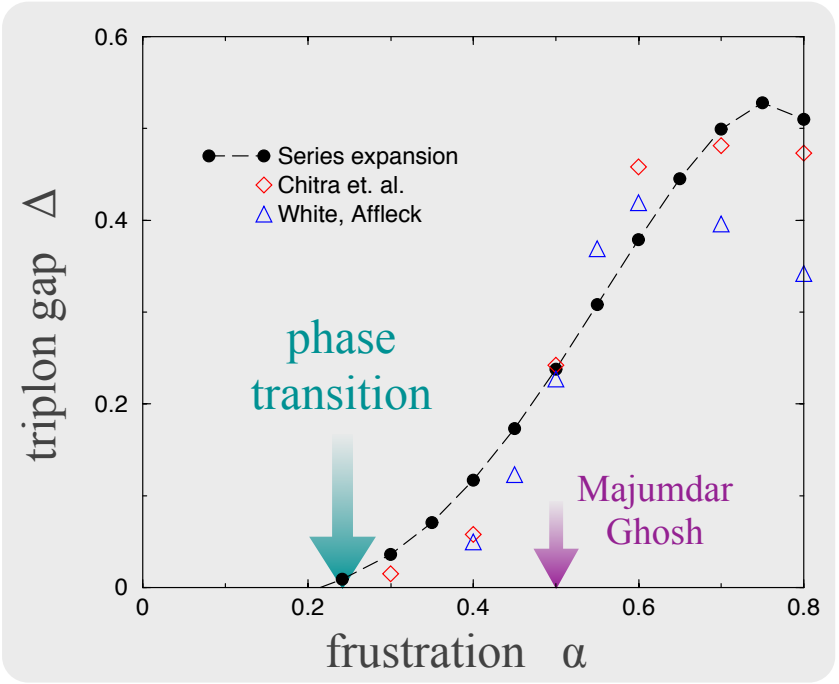


$$\mathcal{H} = \sum_i \left[\vec{S}_i \cdot \vec{S}_{i+1} + \alpha \vec{S}_i \cdot \vec{S}_{i+2} \right]$$

Dimer series expansion



$$\mathcal{H} = \sum_i \vec{S}_{2i} \cdot \vec{S}_{2i+1} + \lambda \sum_i \left[\vec{S}_{2i} \cdot \vec{S}_{2i-1} + \alpha \vec{S}_i \cdot \vec{S}_{i+2} \right]$$



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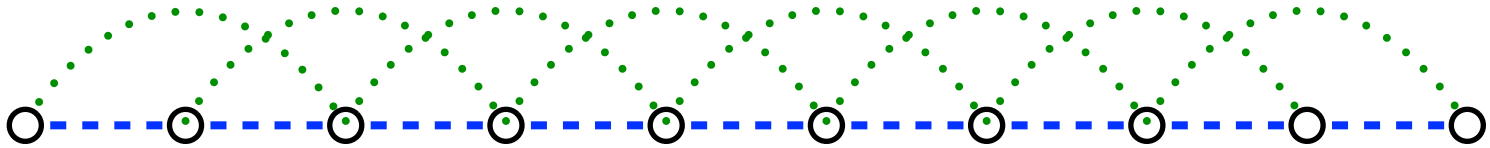
Rajiv Singh and Zhengh Weihong, Phys. Rev. B **59**, 9911 (1999).



Dlog Padé approximants

n	$[(n-2)/n]$	$[(n-1)/n]$	$[n/n]$	$[(n+1)/n]$	$[(n+2)/n]$
			$\alpha = 0$		
n= 3	0.9531(0.621)	0.9906(0.711)	1.0158(0.793)	0.9982(0.724)	
n= 4	1.0495(0.986)	1.0047(0.751)	1.0016(0.738)	1.0018(0.740)	$\nu = 0.74(3)$
n= 5	1.0021(0.741)	1.0018(0.739)			
			$\alpha = 0.2411$		
n= 3	1.0587(0.737)	0.7755(0.191)*	1.1038(1.021)	0.9923(0.620)	
n= 4	0.9563(0.531)	1.0082(0.680)	1.0002(0.649)	0.9960(0.632)	$\nu = 0.65(3)$
n= 5	1.0017(0.656)	1.0517(0.670)*			
			$\alpha = 0.5$		
n= 4	0.6425(0.049)	1.0901(0.586)	1.1669(0.787)	1.1641(0.777)	
n= 5	1.2006(0.920)	1.1642(0.777)			

Applications / frustrated magnetism

Series expansion techniques can be used to calculate **effective Hamiltonians** for the highly **degenerate manifold** of ground states characteristic of a frustrated magnet.

Two types of effective Hamiltonians

- those which act only in the **degenerate subspace** of an unperturbed Hamiltonian.
  → systematic calculation by a linked-cluster expansion
  → isolates effective degrees of freedom
  → solving effective Hamiltonian allows to study degeneracy splitting
- those which act on the **full Hilbert space**.
  → non-trivial, as one needs suitable generator (see CUTs below)

F. Mila and K.P. Schmidt, arXiv:1005.2495

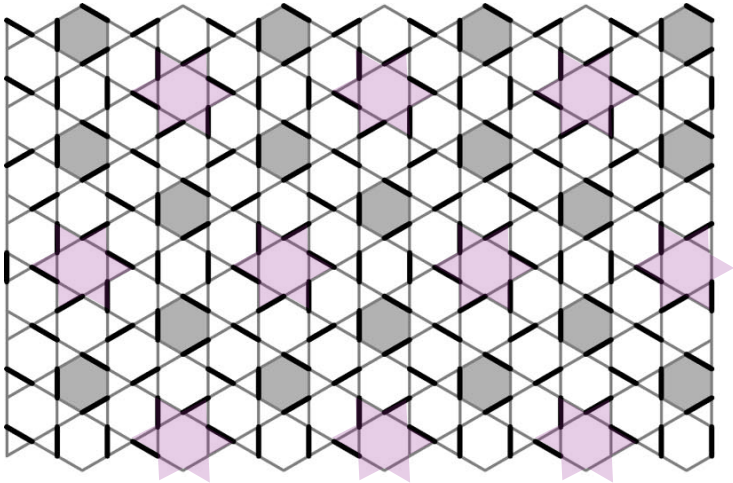
Example: kagome Heisenberg model

Rajiv Singh and David Huse, Phys. Rev. B **76**, 180407 (2007); Phys. Rev. B **77**, 144415 (2008)

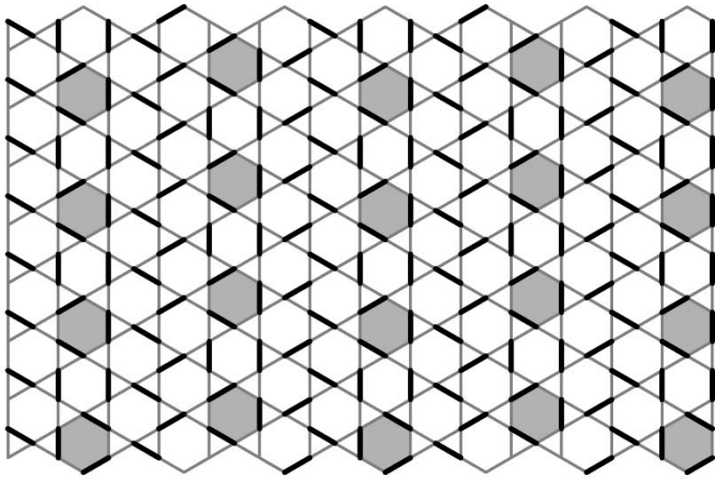
series expansions for
various dimer coverings

candidate dimer coverings
honeycomb VBC of perfect hexagons
stripe VBC of perfect hexagons

honeycomb VBC



stripe VBC



Example: kagome Heisenberg model

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series expansions for
various dimer coverings

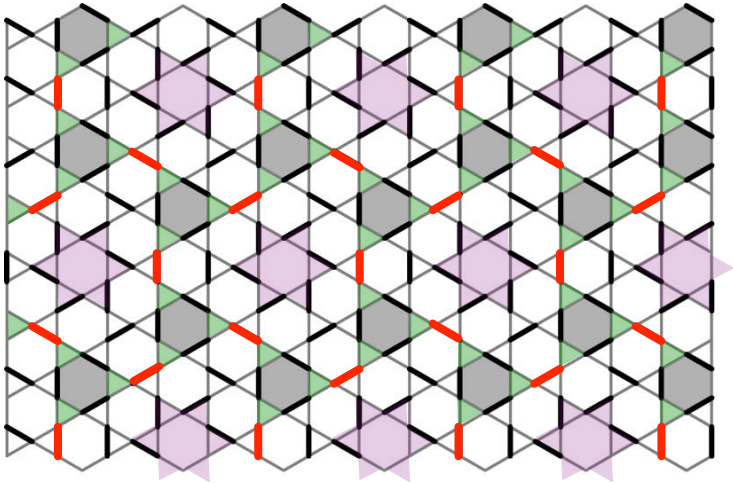
candidate dimer coverings
honeycomb VBC of perfect hexagons
stripe VBC of perfect hexagons

2nd order
dimers resonate across empty triangles

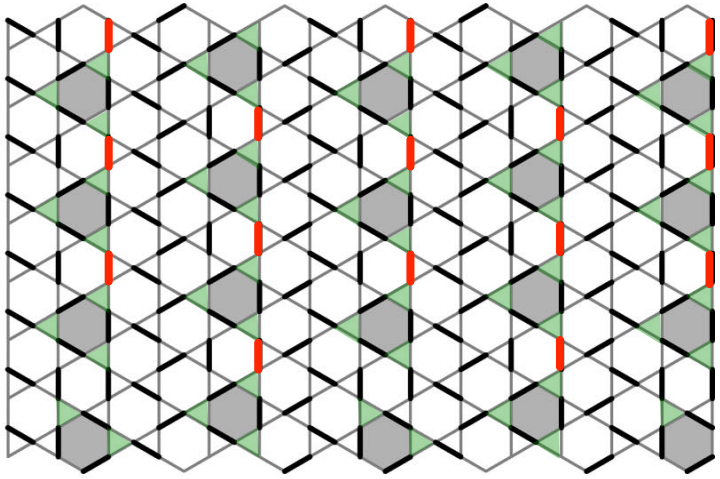
3rd order
formation of perfect hexagons
(binding of 3 empty triangles)
lifts the degeneracy of all dimer coverings

4th order
lifts degeneracy of stripe vs. pinwheel states

honeycomb VBC



stripe VBC



Example: kagome Heisenberg model

Rajiv Singh and David Huse, Phys. Rev. B **76**, 180407 (2007); Phys. Rev. B **77**, 144415 (2008)

order	honeycomb VBC	stripe VBC	36-site cluster
0	-0.375	-0.375	-0.375
1	-0.375	-0.375	-0.375
2	-0.421875	-0.421875	-0.421875
3	-0.42578125	-0.42578125	-0.42578125
4	-0.431559245	-0.43101671	-0.43400065
5	**-0.432088216**	-0.43153212	**-0.43624539**

Exact diagonalization, DMRG for honeycomb-VBC
extrapolated: -0.433(1) 36-site cluster: -0.43837653

Multiscale entanglement renormalization ansatz (MERA)
-0.43221 (exact upper bound)

Gutzwiller projected wavefunction study (variational) → U(1) spin liquid
-0.429

Future prospects

- Experience has shown that adding **5 more terms** in the expansion can lead to **qualitatively new insights** upon series extrapolation.
- Series expansions can be **highly parallelized**, and potentials benefit substantially from peta-flop computing.

	Square lattice		***Triangular lattice***		***Cubic lattice***	
N	Cluster	Embeddings	Cluster	Embeddings	Cluster	Embeddings
1	1	4	1	6	1	6
2	2	16	2	36	2	36
3	4	76	5	306	4	306
4	8	280	10	1.860	8	2.016
5	14	1.180	22	13.278	15	16.278
6	28	4.856	50	89.988	31	126.036
7	56	21.060	122	656.862	64	1.071.954
8	124	90.568	320	4.756.596	147	9.008.808
9	280	419.468	910	37.095.654	353	82.540.686
10	679	1.911.352	2.727	284.221.236	908	742.248.348

Future prospects

- Experience has shown that adding **5 more terms** in the expansion can lead to **qualitatively new insights** upon series extrapolation.
- Series expansions can be **highly parallelized**, and potentials benefit substantially from peta-flop computing.
- **Estimates** (Rajiv Singh):
  - 2D t-J model: superconducting susceptibilities up to order β^{15}
  - triangular lattice Heisenberg model: susceptibilities and correlations length up to order β^{18}

Related / alternative approaches

- **Numerical linked-cluster expansions**

  For every cluster keep complete spectrum, e.g. contributions from all powers of β (or other expansion parameter). Allows to go to (slightly) lower temperatures (without extrapolation techniques), but no symbolic series anymore.

  M. Rigol, T. Bryant, R.R.P. Singh, Phys. Rev. Lett. **97**, 187202 (2006).

- **Continuous unitary transformations (CUTs)**

  Unitary transformation to block-diagonalize Hamiltonian is constructed as an infinite product of infinitesimal transformations. High-energy processes are integrated out first, before treating those at lower energies (similar to renormalization-group approach).

  F.J. Wegner, Ann. Physik **3**, 77 (1994).
  S.D. Glazek and K.G. Wilson, Phys. Rev. D **48**, 5863 (1993).
  C. Knetter and G.S. Uhrig, Eur. Phys. J. B **13**, 209 (2000).

Related / alternative approaches

- **Contractor renormalization (CORE)**

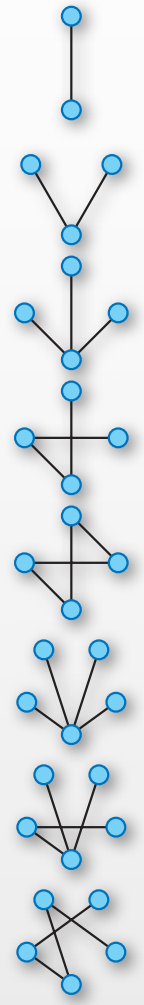
  Related non-perturbative approach to construct an effective Hamiltonian in a real-space block-decimation procedure that can fully capture the low-energy physics of a given system. Construction works via exact diagonalization of subunits (in real space), keeping a set of low-energy states, and then combining results similar to a cluster expansion. Non-perturbative character allows to study systems across a quantum phase transition (in contrast to the previous perturbative techniques).

  C.J. Morningstar and M. Weinstein, Phys. Rev. Lett. **73**, 1873 (1994).

Summary

Linked-cluster expansions

- **controlled** numerical framework
  - for strongly correlated systems, particularly **gapped** quantum states,
  - static and dynamic properties calculated in **thermodynamic limit**,
  - close connection to graph theory.
- advantages / disadvantages
  - no sign problem.
  - works for (1,2,3)-dimensional quantum systems.
  - perturbative approach (T=0, finite T).
  - 'clever' series extrapolation tools needed.



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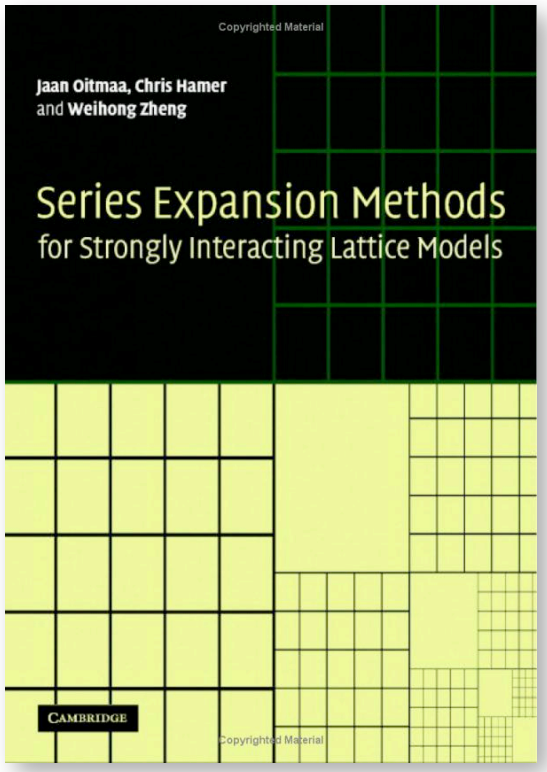

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