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**1855-20**

# School and Workshop on Highly Frustrated Magnets and Strongly Correlated Systems: From Non-Perturbative Approaches to Experiments

***30 July - 17 August, 2007***

## Numerical Simulations of Frustrated Systems

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# Numerical Simulations of Frustrated Systems

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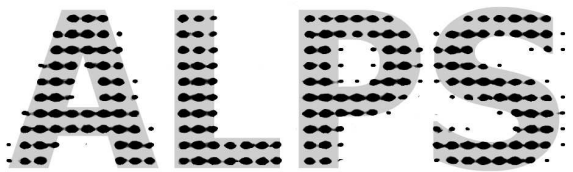
HFM-ESF-ICTP School on Highly Frustrated Magnetism, 4/8/07, Trieste

# Outline

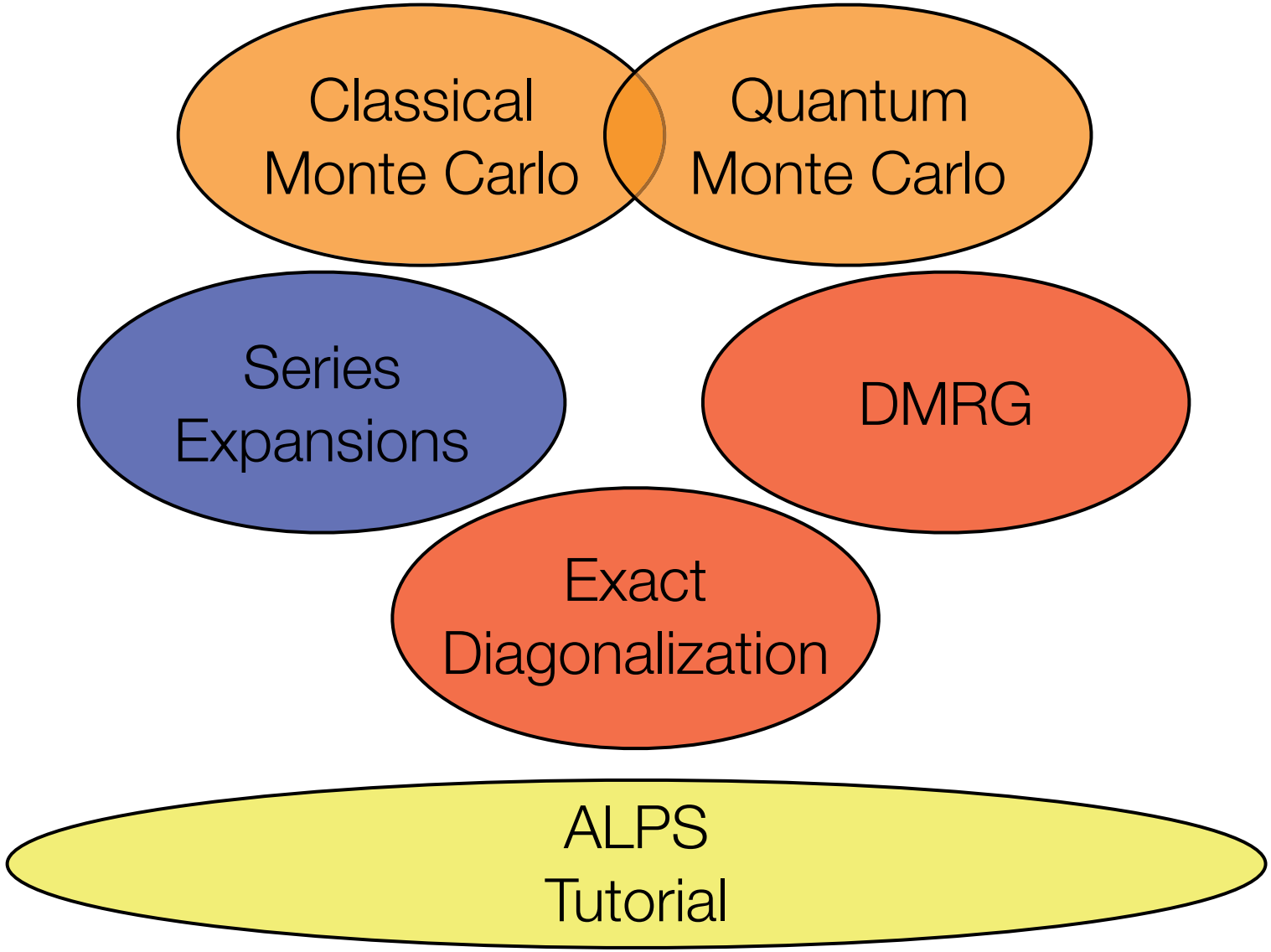
- Introduction
- Overview of numerical methods for frustrated systems
  - Principle and main idea of the method
  - advantages / disadvantages
  - illustration of applications of the method

- Introduction to ALPS
- Tutorial: ALPS hands-on session




http://alps.comp-phys.org

# Overview of the methods covered



# Monte Carlo for Classical Systems

# Monte Carlo for classical systems

- In classical statistical mechanics the canonical partition function reads:

$$Z(T) = \sum_i e^{-E_i/T}$$

  where $E_i$ is the energy of the state i

- The weight of an individual state is given as:

$$p_i = \frac{e^{-E_i/T}}{Z(T)}$$

- How can we calculate efficiently expectation values ?

$$\langle \mathcal{O} \rangle = \sum_i p_i \mathcal{O}_i$$

# Monte Carlo for classical systems

- Problem: direct sampling of the distribution $p_i$ is difficult for two reasons:
  - the number of states is exponentially large with system size
  - the partition function $Z$ is therefore not known !
- A breakthrough came with the invention of the Metropolis algorithm more than 50 years ago (in the really early days of scientific computing!)

$$W(i \to j) = \min\{1, \exp(-(E_j - E_i)/T)\}$$

no need to know $Z$ anymore.

# Metropolis Algorithm I

- Main idea: Random walk in the space of configurations (Markov chain)

$$c_1 \longrightarrow c_2 \longrightarrow \ldots \longrightarrow c_N$$

- Given a configuration i , propose a new configuration j and accept the new configuration with probability: (otherwise keep the old as current)

$$W(i \to j) = \min\{1, \exp(-(E_j - E_i)/T)\}$$

- Observables are calculated as a simple arithmetic mean over the visited states:

$$\langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_n \mathcal{O}_{c_n}$$

- One has to care about THERMALIZATION and ERROR ANALYSIS !! You might use the MC observables of the ALPS project if you write your own MC code. Binning / Jackknife / Timeseries etc available.

# Metropolis Algorithm II

- This is therefore a very general algorithm which works in principle for all classical statistical physics problems.

- However there are a few challenges in an application to a specific model
  - The algorithm does not yet specify which state j to propose given state i. But this is a crucial point. First, the proposed moves need to be ergodic, and they commonly satisfy detailed balance.
  - For classical spin models on a lattice a simple algorithm is given by choosing a site, choosing a new orientation for that spin and accepting or discarding the new state according to the Metropolis formula.
  - While this prescription gives a working algorithm, these local updates generically have problems being efficient at low temperature or close to phase transitions (critical slowing down). Local updates can not cope with the diverging correlation length at the transitions.

# Monte Carlo for classical frustrated systems

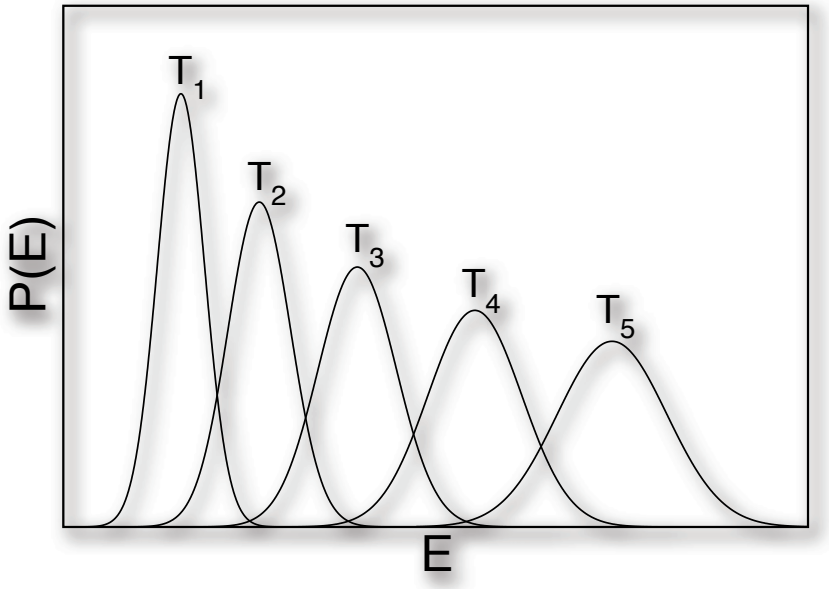
- In the context of unfrustrated classical spin models very powerful cluster updates have been found (Swendsen-Wang, Wolff) which were again break-throughs and enabled the detailed study of critical phenomena (Ising, Potts, XY, Heisenberg models).

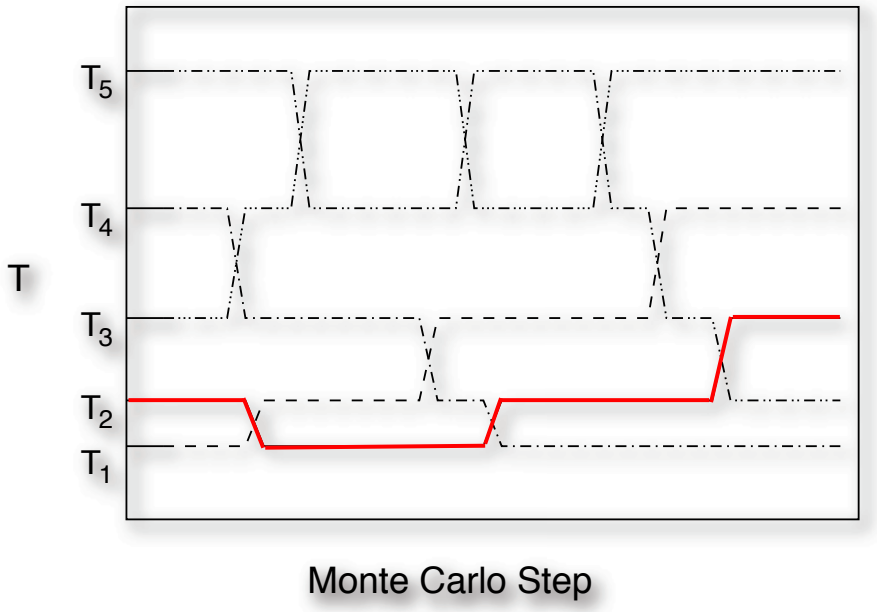
- While these algorithms can formally also be applied to frustrated systems, their performance is seldom better than the simple single spin updates.

- There is a generic lack of efficient updates for classical frustrated systems. In individual cases a good physical intuition can be helpful for devising efficient updates, but these are rather the exception than the rule.

- New “extended ensemble” techniques, such as “(optimized) parallel tempering” can help to better equilibrate the system and to yield shorter autocorrelation times.

# Monte Carlo: Parallel Tempering




Observation: Systems at close temperatures have overlapping energy distributions. MC configurations at a given T can be valid configurations also at slightly higher / lower T.

⇒ propose moves in temperature!

$$W(\beta_i \rightarrow \beta_j) = \min\{1, \exp[+(\beta_i - \beta_j)(E_i - E_j)]\}$$

Measurements at constant T are averaged over samples which are much more decorrelated than in a poorly equilibrating simulation at the same T.

# Applications of Classical Monte Carlo
# I) Order by disorder in the $J_1$-$J_2$ Square Lattice

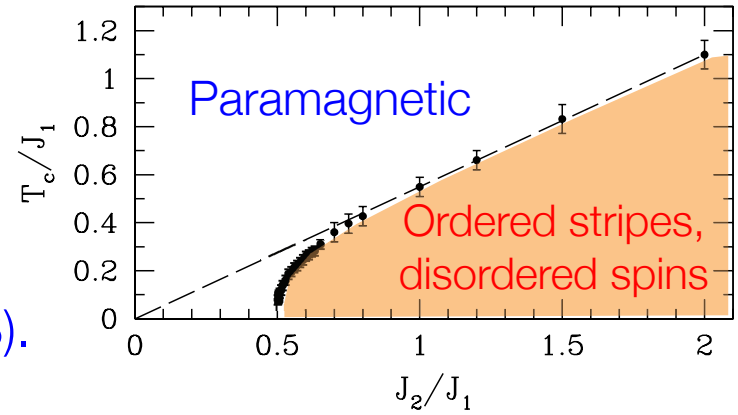
- Heisenberg model with competing nearest and next-nearest AF couplings and $J_2/J_1 > 1/2$

$$\hat{\mathcal{H}} = J_1 \sum_{n.n.} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + J_2 \sum_{n.n.n.} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \ ,$$

- At finite but low T two collinear structures are locally selected (order by disorder), but without long-range order in the spin variables (Mermin-Wagner forbidden).

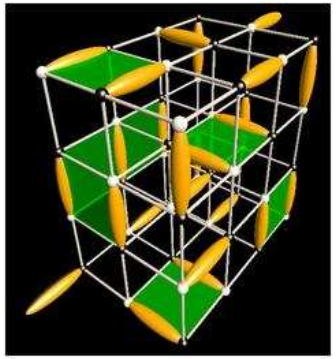
$$\sigma = (\mathbf{S}_1 - \mathbf{S}_3) \cdot (\mathbf{S}_2 - \mathbf{S}_4)$$


- Large scale Monte Carlo simulations reveal Ising transition to ordered state of emerging $\sigma$ degrees of freedom, while the individual spins remain disordered!



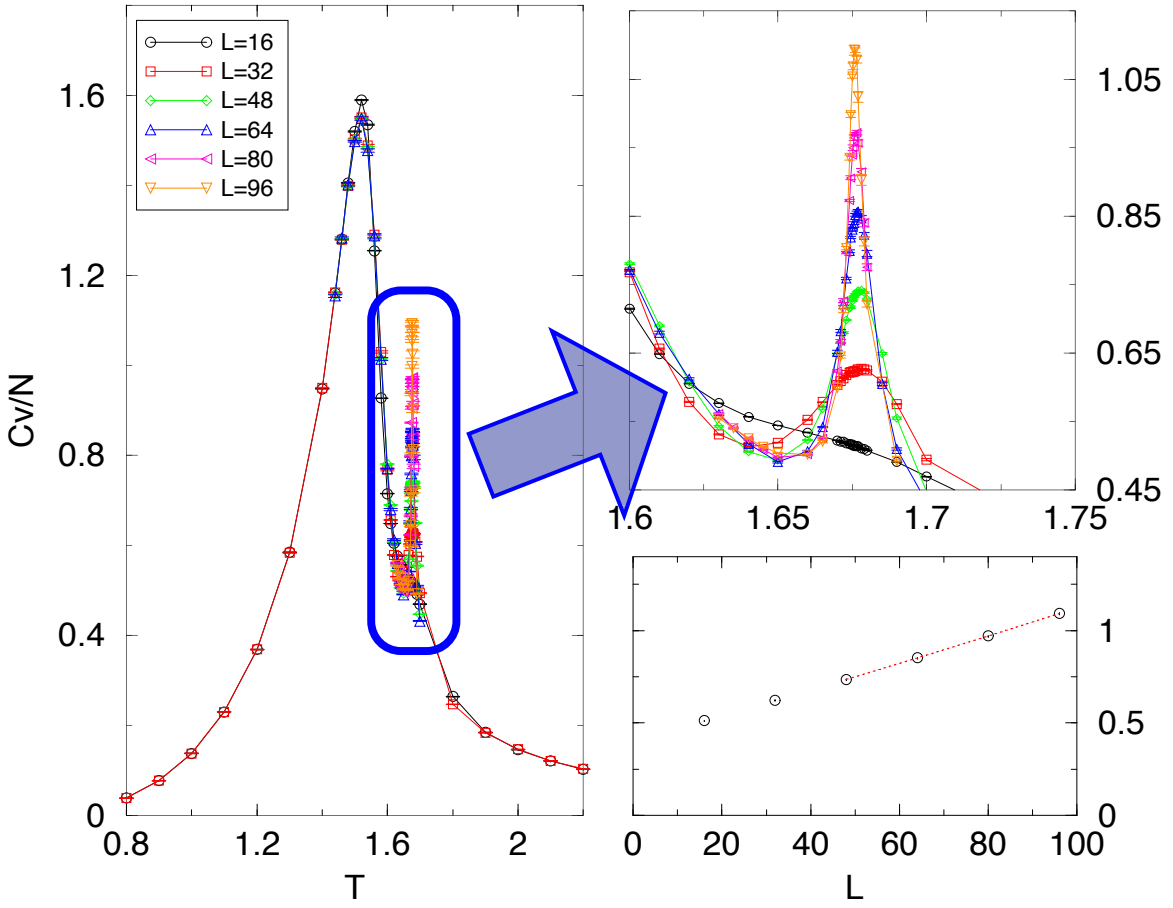

C. Weber et al, Phys. Rev. Lett. **91**, 177202 (2003).

# Applications of Classical Monte Carlo
# II) interacting classical dimer models



Alet / Misguich

- Classical closed packed dimers on a 3D simple cubic lattice
- Interaction prefers parallel dimers.
- Highly efficient non-local worm updates !
  $N=L^3$ with $L \sim 100$
- Unconventional transition between dimer crystal and Coulomb phase.

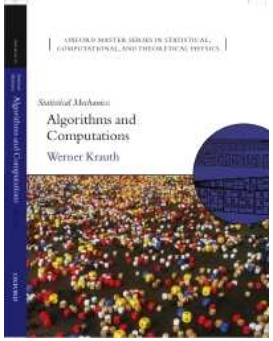



F. Alet et al, Phys. Rev. Lett. **97**, 030403 (2006).

# Monte Carlo for classical systems: Literature

- A very pedagogical introduction to Monte Carlo methods in statistical physics by Werner Krauth:

  There are also lecture notes available on his website
  http://www.lps.ens.fr/~krauth/




- Fabien Alet (http://www.lpt.ups-tlse.fr/alet) has detailed lecture notes on MC and QMC methods available on his webpage.
  The first lecture discusses classical Monte Carlo for unfrustrated spin models in depth http://www-spht.cea.fr/articles/T05/022/lecture1.pdf.

- Introduction to parallel tempering and optimized ensembles can be found in: David J. Earl and Michael W. Deem,
  "*Parallel tempering: Theory, applications, and new perspectives*",
  Phys. Chem. Chem. Phys., **7** 3910 (2005).

# Quantum Monte Carlo

# Quantum Monte Carlo

- In quantum statistical mechanics the canonical partition function now reads:

$$Z(T) = \mathrm{Tr}\ e^{-H/T}$$

- Expectation values:

$$\langle \mathcal{O} \rangle = \frac{1}{Z(T)} \mathrm{Tr}[\mathcal{O} e^{-H/T}] \equiv \mathrm{Tr}[\mathcal{O}\rho(T)]$$

- We need to find a mapping onto a “classical” problem in order to perform MC
  - World-line methods (Suzuki-Trotter, Worm algorithm, ...)
  - Stochastic Series Expansions (discussed in this lecture)

- Potential Problem: The mapping can give “probabilities” which are negative ⇒ infamous sign problem. Common cause is frustration or fermionic statistics.

# Stochastic Series Expansion (SSE)

- Quantum to Classical mapping is done based on a Taylor series expansion of the partition function (Sandvik 1991, 1999, 2003)

$$Z(\beta) = \mathrm{Tr}\ e^{-\beta H} = \sum_{\alpha} \sum_{n} \frac{(-\beta)^n}{n!} \langle \alpha | H^n | \alpha \rangle$$

- Split the Hamiltonian into (off-)diagonal bond pieces: $H = \sum_b h_b$

- One gets the following form

$$Z(\beta) = \sum_{n} \frac{\beta^n}{n!} \sum_{\alpha} \sum_{(b_1,\ldots,b_n)} \langle \alpha | \prod_{i=1}^{n} (-h_{b_i}) | \alpha \rangle$$

$$\propto P[n, \alpha, (b_1, \ldots, b_n)] \geq 0$$

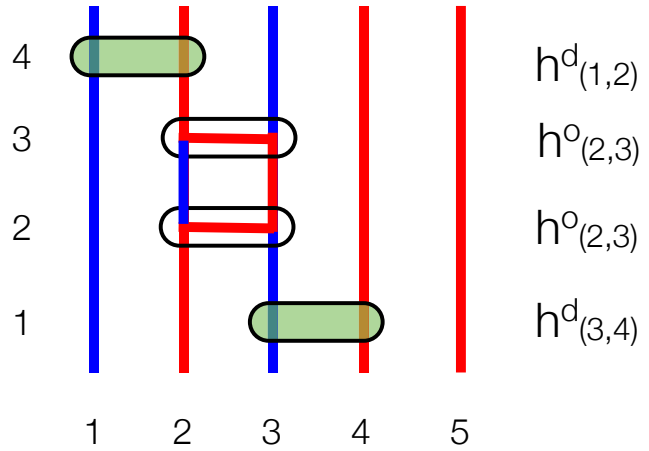
- In this form one can come up with a random walk in the space of the discrete indices $n, \alpha, (b_1, \ldots, b_n)$

# Stochastic Series Expansion (SSE)

$$Z(\beta) = \sum_n \frac{\beta^n}{n!} \sum_\alpha \sum_{(b_1,\ldots,b_n)} \langle\alpha| \prod_{i=1}^{n} (-h_{b_i}) |\alpha\rangle$$

- A configuration looks like this:

$$n = 4 \qquad |\alpha\rangle = |01011\rangle$$




- Updates:

  Insertion or Removal of diagonal bonds (changes n)
  Loop or Worm updates change diagonal into offdiagonal and vice-versa (n unchanged) and modify $\alpha$

- Measurements:

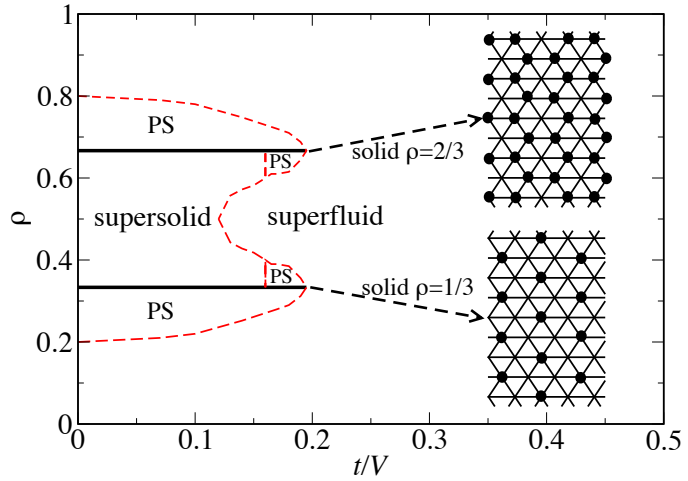
$$\langle H \rangle = -\frac{1}{\beta} \langle n \rangle \qquad \chi = \beta \left\langle \langle\alpha| \sum_i S_i^z |\alpha\rangle^2 \right\rangle$$

# Applications of Quantum Monte Carlo
# Supersolids on the triangular lattice

- Antiferromagnetic Ising Model on the triangular lattice augmented by a ferromagnetic transverse exchange
  SSE QMC is possible without a sign problem !

- AF Ising model has a macroscopic degeneracy at T=0 (Wannier, Houtappel).

- In a whole region of magnetizations $-1/3 < m/m_{\rm sat} < 1/3$
  the system becomes supersolid upon switching on the ferromagnetic transverse exchange




In a bosonic language a supersolid is a state which shows charge order and superfluidity at the same time


G. Murthy et al, Phys. Rev. B **55**, 3104 (1997).
S. Wessel & M. Troyer, Phys. Rev. Lett. **95** 127205 (2005).
D. Heidarian & K. Damle, Rev. Lett. **95** 127206 (2005).
R. Melko et al, Phys. Rev. Lett. **95** 127207 (2005).

# Quantum Monte Carlo: Literature

- Sandvik's original papers:
  A. Sandvik, Phys. Rev. B **59**, 14157 (1999).
  O.F. Syljuåsen and A.W. Sandvik, Phys. Rev. E **66**, 046701 (2002).

  F. Alet, S. Wessel, and M. Troyer, Phys. Rev. E **71**, 036706 (2005).

- Many reviews: Evertz, Troyer et al, Kawashima & Harada

- Fabien Alet (http://www.lpt.ups-tlse.fr/alet) has lecture notes on MC and QMC methods available on his webpage.
  The second and third lecture are devoted to Quantum Monte Carlo
  http://www-spht.cea.fr/articles/T05/022/QMC.Lecture2.pdf
  http://www-spht.cea.fr/articles/T05/022/QMC.Lecture3.pdf

# Series Expansions

# Series Expansions

- High-Temperature Expansions for quantum lattice models

  Taylor Expansion of the partition function around $\beta = 0$ :

$$Z(\beta) = \mathrm{Tr}\ e^{-\beta H} = \sum_n \mathrm{Tr} \frac{(-\beta H)^n}{n!} = \sum_n \mathrm{Tr} \frac{(-\beta \sum_k h_k)^n}{n!}$$

- In the discussion of SSE before, we were performing a stochastic evaluation of Z. Here in contrast we aim at an exact expression for each order $\beta$. Lowest order terms are often very easy to obtain.

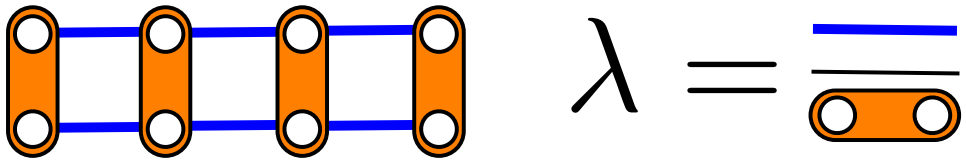
- Higher orders require a computer assisted enumeration and identification of lattice animals, and the calculation of the trace for those graphs. Typical orders are up to n ~ 20 for quantum lattice models, but this depends a lot on the problem.

# Series Expansions

- Perturbative Expansions for Quantum Lattice Models

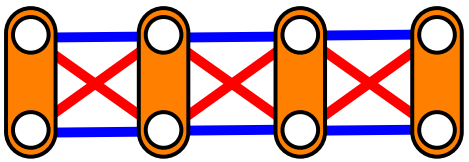
  Taylor Expansion of the Energy around a non-degenerate starting state

$$E(\lambda) = E_0 + \lambda E_1 + \lambda^2 E_2 + \lambda^3 E_3 + \ldots + \lambda^n E_n + O(\lambda^{n+1})$$



$$\frac{E_{GS}}{L} = -J_\perp[\frac{3}{4} + \frac{3}{8}\left(\frac{J}{J_\perp}\right)^2 + \frac{3}{16}\left(\frac{J}{J_\perp}\right)^3 + \ldots]$$

- Multivariable expansions are also possible



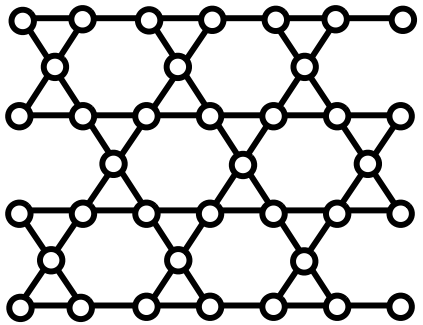
- The lowest orders are simple to obtain, but high orders in complex geometries require a fully developed graph manipulation machinery. Typical orders: 10 - 20

# Series Expansions for frustrated systems

- Series expansion have no intrinsic difficulty with frustrated systems.
- Symbolic expressions for thermodynamic quantities allow a rapid fit of model parameters to experimental data.
- High-temperature series tend to not to converge at low temperatures. Series extrapolations, biased series extrapolations, numerical linked cluster techniques, combination with exact diagonalization etc, can help to get somewhat lower in temperature than the bare series.
- Perturbative series expansions are also very useful in deriving dispersion relations for elementary excitations. Collapse of excitation energies can indicate a quantum phase transition.
- Useful also to derive effective Hamiltonians in degenerate perturbation theory, which is a common theme in frustrated systems → talk of F. Mila this morning

# Applications of Series Expansions: High Temperature Series for the S=1/2 Kagome

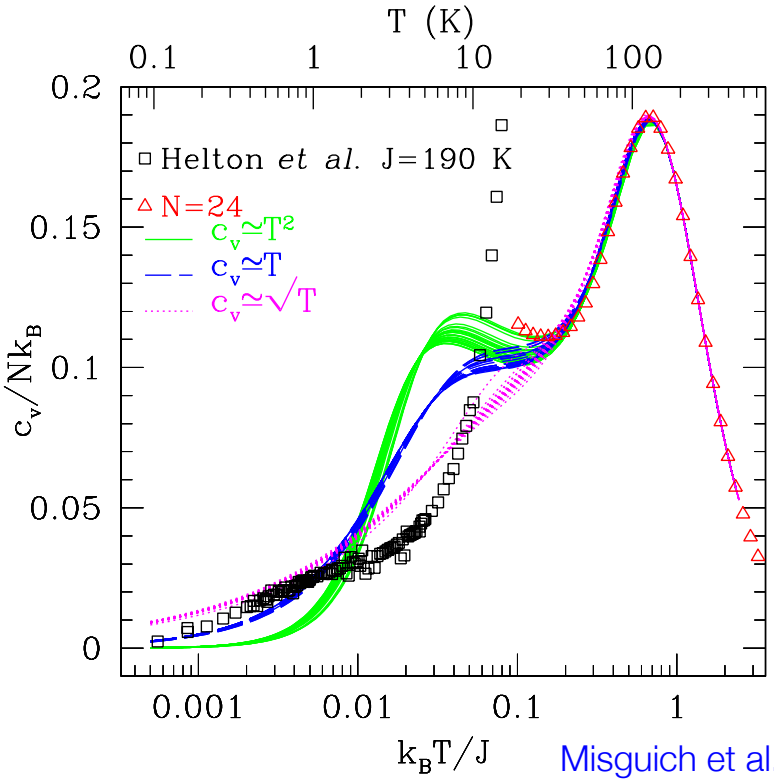
- Heisenberg S=1/2 model on the kagome lattice



- Series for the specific heat:

TABLE I. For each quantity $A$ we define the coefficients $a_n$ by $A = \sum_{n=0} \frac{a_n}{n!} \left(\frac{\beta}{4}\right)^n$. The table shows the values of $a_n$ for the specific heat $C$ and the uniform susceptibility $\chi$.

| $N$ | $4C$ | $4\chi$ |
|---|---|---|
| 0 | 0 | 0 |
| 1 | 0 | 4 |
| 2 | 48 | −32 |
| 3 | 0 | 192 |
| 4 | −9792 | −384 |
| 5 | 0 | −1280 |
| 6 | 4106880 | −155136 |
| 7 | −5193216 | 2711184 |
| 8 | −2927834112 | 56705024 |
| 9 | 11470159872 | −1716811776 |
| 10 | 3193027983360 | −47711784960 |
| 11 | −26121748561920 | 2004747075584 |
| 12 | −4944246830899200 | 55843726884864 |
| 13 | 70892246893658112 | −3367208347123712 |
| 14 | 10284867640404983808 | −88720801213743104 |
| 15 | −234226245436710912000 | 7723917022263705600 |
| 16 | −2753852369728747732992 0 | |

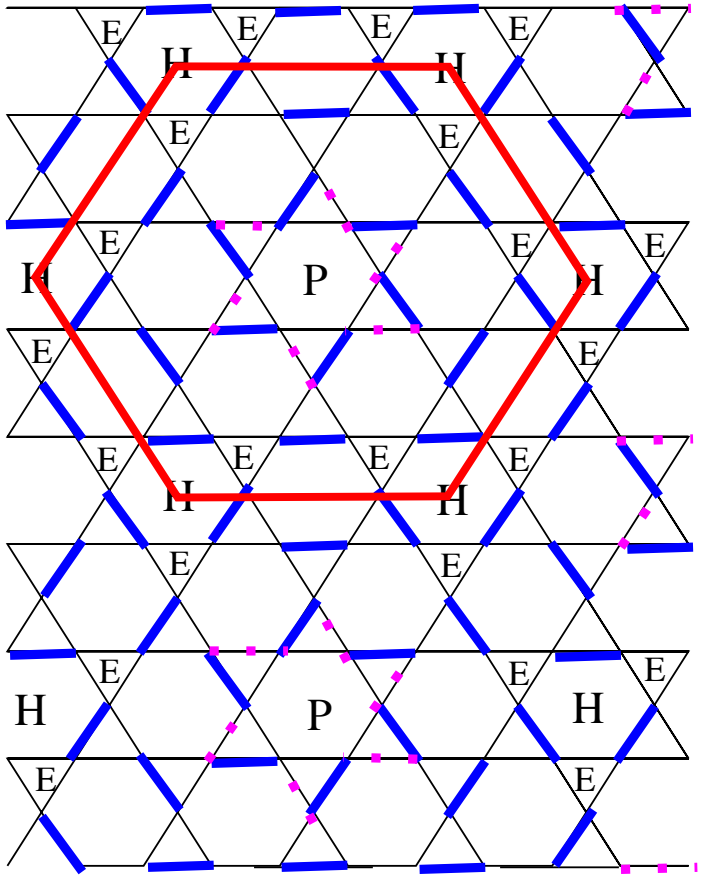



Elstner & Young PRB 94

Misguich et al. arXiv 07

# Applications of Series Expansions: Dimerized Groundstate of the S=1/2 Kagome ?

- Expansion in the interdimer coupling, extrapolation to equal couplings on all bonds
- large unit cell of the unperturbed state (36 spins / 18 dimers)
- this specific dimer pattern is selected among others, according to their analysis
- obtained also series for triplet excitations, however less conclusive




R.R.P. Singh & D. Huse, arXiv:0707.0892

# Series Expansions: Literature


- J. Oitmaa , C. Hamer and W. Zheng
  "*Series expansion method for strongly interacting lattice models*"
  Cambridge University Press, 2006.

- M.P. Gelfand & R.R.P. Singh,
  "*High-order convergent expansions for quantum many-particle systems*"
  Advances in Physics **49**, 93 (2000).

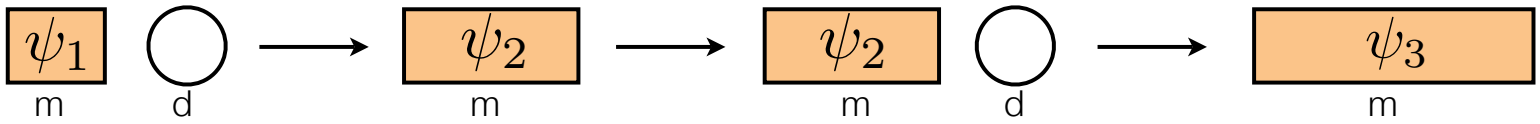
- C. Domb & M.S. Green
  "*Phase Transitions and Critical Phenomena:*
  *Series Expansion for Lattice Models*",
  Elsevier, 1974.

- Talk by S. Trebst on "*Cluster Expansions*"
  http://www.kitp.ucsb.edu/~trebst/Talks/ClusterExpansions.pdf

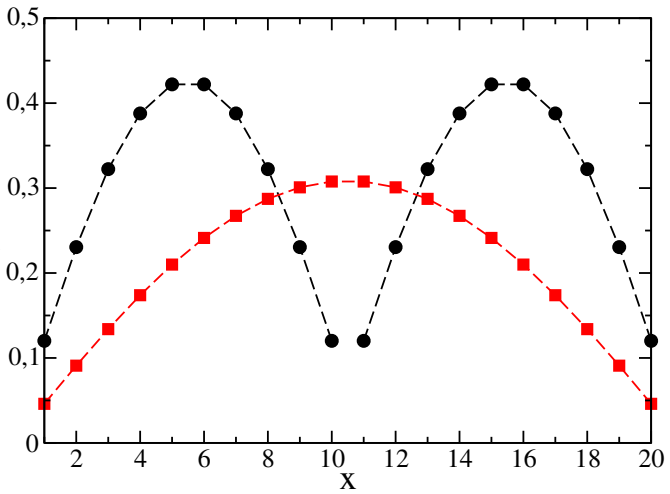
# Density Matrix Renormalization Group

# Density Matrix Renormalization Group

- K. Wilson introduced the numerical renormalization group as a powerful numerical tool to solve the Kondo problem (Wilson RMP 75).




- Many people tried to apply this idea in a straightforward way to quantum many body problems and failed. The reason for this failure was understood in a study of the tight-binding problem on a chain (White & Noack PRL 92):

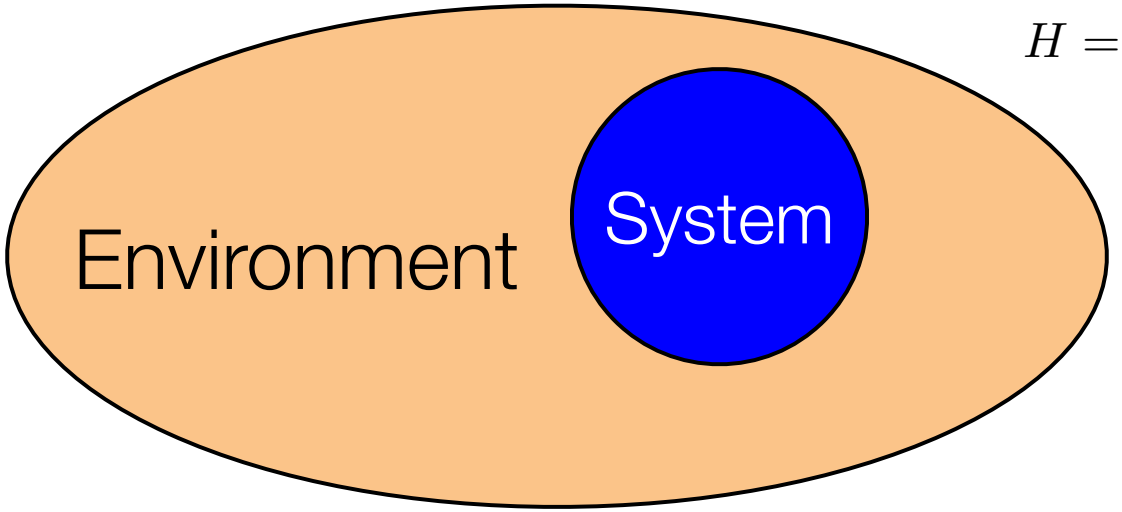



$$\psi[2L] \neq \psi[L] \otimes \psi[L]$$

The groundstate of the large system is not at all well approximated by the tensor product of the groundstates of the smaller systems

# Density Matrix Renormalization Group

- The next crucial step was to realize how one has to choose the states to be kept in a partition of the universe:




$$H = H_S + H_E + H_{SE}$$

groundstate $|\psi\rangle$

- System description with *m* states:

$$|\tilde{\psi}\rangle = \sum_{n}^{m} \sum_{\alpha} \tilde{\psi}_{n,\alpha} |\phi_n\rangle_S \otimes |\alpha\rangle_E$$

- How to choose the *m* states in order to approximate $|\psi\rangle$ best ?

# Density Matrix Renormalization Group

- The answer is given by the subsystem density matrix

$$\rho_{i,j} = \mathrm{Tr}_E |\psi\rangle\langle\psi|$$

- With the help of the Schmidt decomposition one can show that the *m* eigenfunctions of $\rho$ associated with the largest eigenvalues $w_n$ give the best approximation of $|\psi\rangle$ . (and not the lowest eigenstates of $H_S$)

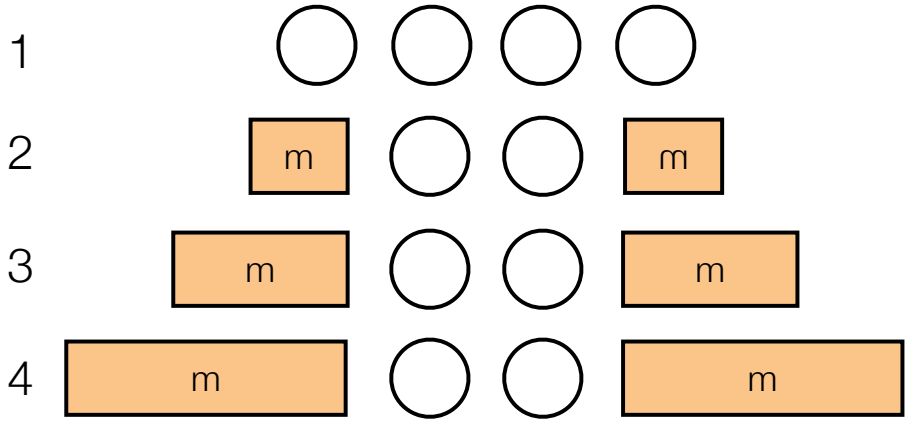
- The error can be estimated to be

$$\left| |\tilde{\psi}\rangle - |\psi\rangle \right|^2 \approx 1 - \sum_n^m w_n = P_m$$

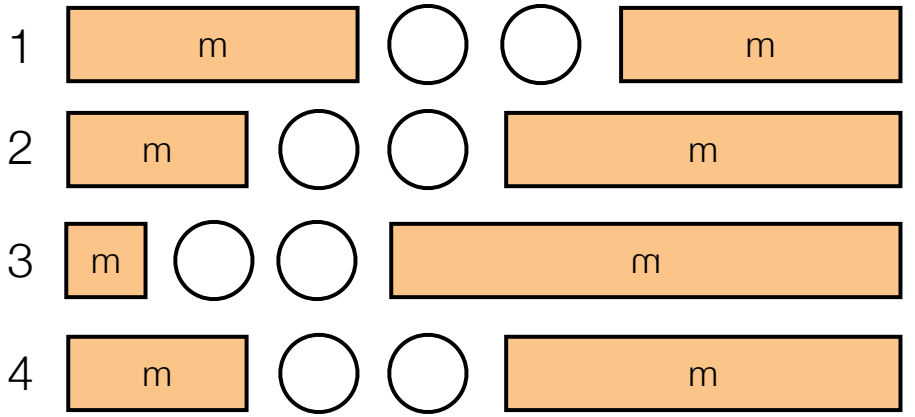
# Density Matrix Renormalization Group

- Based on these condsiderations, S.R. White came up with the DMRG
  S.R. White, PRL **69**, 2863 (1992); PRB **48**,10345 (1993).

- Infinite System Algorithm




- Finite System Algorithm



# DMRG for frustrated systems

- Very efficient groundstate simulations for many 1D systems.
  Frustration or fermions pose no particular problem.

- Typical system sizes and number of states:
  unfrustrated spin systems: 100-1000 sites, lower hundred states
  frustrated spin systems: hundred sites, larger hundred to thousand states
  fermionic systems, wide systems, many low energy states, they all increase $m$

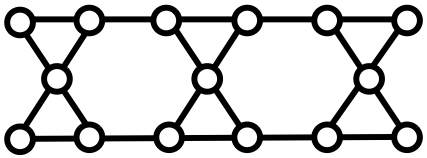
- Variational, quasi-exact method.

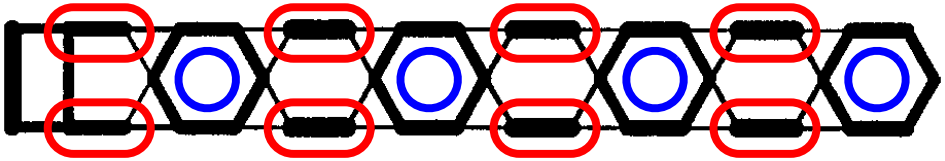
- Wavefunction method, therefore many observables are easily available.

- Drawbacks: it is not yet possible to simulate large 2D systems,
  open boundaries might not always be what we desire, especially
  because of the lack of spatial quantum numbers.

# DMRG Applications
# The S=1/2 Kagome Strips

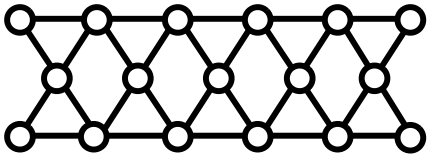
1st Kagome Strip (Azaria et al, 1998)



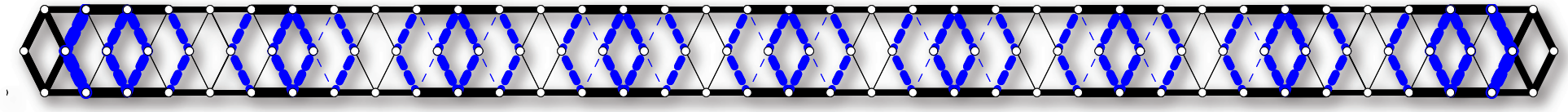



S.R. White & R.R.P. Singh PRL (2000)

2nd Kagome Strip (Waldtmann, Everts et al, 2000)

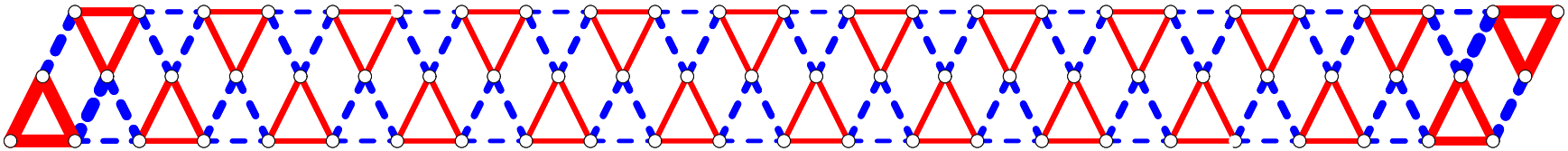


undoped, Heisenberg model



AML, unpublished

doped <n>=2/3 → 3 site singlets



M. Indergand, AML, S. Capponi, M.Sigrist, PRB (2006)

# DMRG Further Developments

- TMRG
  Finite temperature properties based on the transfer matrix

- DDMRG
  Calculation of dynamical response functions

- t-DMRG
  Real-time evolution of quantum many body systems
  Imaginary-time evolution for finite temperature properties

- PEPS / MERA
  new ideas coming from the Quantum Information community might strengthen our understanding on how to simulate D>1 quantum many body systems efficiently.

# DMRG Literature

- Original papers:

  S.R. White, "*Density matrix formulation for quantum renormalization groups*", Phys. Rev. Lett. **69**, 2863 (1992).

  S.R. White, "*Density-matrix algorithms for quantum renormalization groups*", Phys. Rev. B **48**, 10345 (1993).

- U. Schollwöck, "*The density-matrix renormalization group*",
  Rev. Mod. Phys. **77**, 259 (2005).

- K. Hallberg, "*New Trends in Density Matrix Renormalization*"
  Adv. Phys. **55**, 477 (2006).

- R.M. Noack & S. Manmana, "*Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems*",
  AIP Conf. Proc. **789**, 93 (2005).

- Talk by E. Jeckelmann at http://heraeus2006.physik.uni-greifswald.de/invited.html

## Exact Diagonalization

$$H|\psi\rangle = E|\psi\rangle$$

The Quantum Mechanics Toolbox

# Exact Diagonalization

- Solve the time-independent Schrödinger equation for a many body Hamiltonian on a finite (lattice) system ⇒ (Sparse) Matrix Eigenvalue problem:

$$H|\psi\rangle = E|\psi\rangle$$

- Within this approach we can basically simulate any model.

- However due to the exponentially growth of the computational cost the method is most useful where more powerful methods fail:

  - Fermionic Models in 1D and 2D (no sign problem)
  - Frustrated Quantum Magnets in 1D/2D/(3D)
  - Well suited for detection of (exotic) ordered phases, somewhat less useful for critical points in d>1
  - Quantum number resolved quantities
  - Calculation of basically any observable possible, also time dynamics
  - Benchmark for all other methods

# Exact Diagonalization : Present Day Limits

- Spin S=1/2 models:
  40 spins square lattice, 39 sites triangular, 42 sites star lattice
  Dimension: up to 1.5 billion basis states

- t-J models:
  32 sites checkerboard with 2 holes
  32 sites square lattice with 4 holes
  Dimension: up to 2.8 billion basis states

- Holstein models
  14 sites on a chain + phonon pseudo-sites
  Dimension: up to 30 billion basis states

- Hubbard models
  20 sites square lattice at half filling, 20 sites quantum dot structure
  22-25 sites in ultracold atoms setting
  Dimension: up to 80 billion basis states (on the earth simulator @ TFlop speed !)

# Exact Diagonalization : Not just “Lanczos”

- Hilbert space
  - Symmetries
  - Site-Basis represention, Lookup techniques
- Hamiltonian Matrix
  - Sparse Matrix representation (memory/disk)
  - Matrix recalculation on the fly (matrix-free)
- Linear Algebra : Eigensolver / Time propagation
  - LAPACK full diagonalization
  - Lanczos type diagonalization (needs only $|v\rangle = H|u\rangle$ operations)
  - More exotic techniques, time propagation
- Observables
  - Static quantities (multipoint correlation functions, correlation density matrices,...)
  - Dynamic observables (spectral functions, density of states,...)
  - Real-time evolution

# Exact Diagonalization: Symmetries

- Symmetries in ED are useful for two reasons:
  1) They reduce the dimension of the linear algebra problem to be solved.
  2) The symmetry classification of eigenstates is the foundation of further, more sophisticated analyses, such as the “Tower of States” technique (later in this talk).

- Consider a XXZ spin model on a lattice.
  What are the symmetries of the problem ?

$$H = \sum_{i,j} J^{xy}_{i,j}(S^x_i S^x_j + S^y_i S^y_j) + J^z_{i,j} S^z_i S^z_j$$

  - The Hamiltonian conserves $S^z$, we can therefore work within a given $S^z$ sector
  - The Hamiltonian is invariant under the space group (SG=Translations x Pointgroup) Usually 1 dimensional irreducible representations are used only, but larger irreps are possible too (somewhat more complicated). Bookkeeping of norms and phases of individual states.
  - At the Heisenberg point, the total spin is conserved. It is however very difficult to combine the SU(2) symmetry with the lattice symmetries in a computationally useful way (non-sparse and computationally expensive matrices). At $S^z$=0 one can however use the spin-flip symmetry which seperates even and odd spin sectors.

# Exact Diagonalization: State representation

- States of the Hilbert space (Fock space) need to be represented in the computer.

- Choose a representation which makes it simple to act with the Hamiltonian or other operators on the states

- Simple example: ensemble of S=1/2 sites in binary coding

$$|\uparrow\uparrow\downarrow\uparrow\rangle \rightarrow [1\ 1\ 0\ 1]_2 = 13$$

  detection of up or down spin can be done with bit-test.
  transverse exchange $S^+S^- + S^-S^+$ can be performed by an XOR operation:

$$[1\ 1\ 0\ 1]_2\ \mathrm{XOR}\ [0\ 1\ 1\ 0]_2 = [1\ 0\ 1\ 1]_2$$

  initial config  bit 1 at the two sites coupled  final config

- One of the key problems for a fast ED code is to find the index of the new configuration in the list of all configurations (index f in $H_{i,f}$). Lookup / Hashing / ...

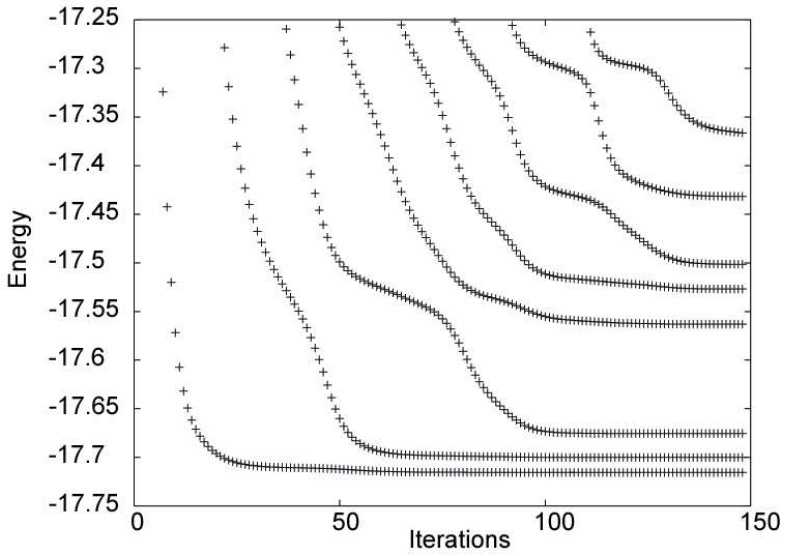
# Exact Diagonalization: Linear Algebra

- Lanczos Algorithm (C. Lanczos, 1950), but others are possible too (Davidson,...)

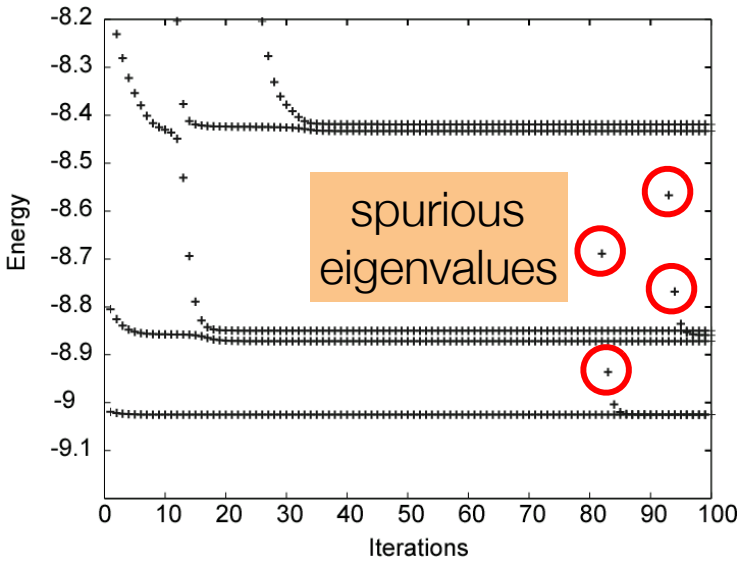
Three vector recursion

$$
\begin{aligned}
|\phi'\rangle &= H|\phi_n\rangle - \beta_n|\phi_{n-1}\rangle\,, \\
\alpha_n &= \langle\phi_n|\phi'\rangle\,, \\
|\phi''\rangle &= |\phi'\rangle - \alpha_n|\phi_n\rangle\,, \\
\beta_{n+1} &= ||\phi''|| = \sqrt{\langle\phi''|\phi''\rangle}\,, \\
|\phi_{n+1}\rangle &= |\phi''\rangle/\beta_{n+1}\,,
\end{aligned}
$$

$$
\tilde{H}_N = \begin{bmatrix}
\alpha_0 & \beta_1 & 0 & \cdots & \cdots & 0 \\
\beta_1 & \alpha_1 & \beta_2 & 0 & \cdots & 0 \\
0 & \beta_2 & \alpha_2 & \beta_3 & 0 & 0 \\
 & & \ddots & \ddots & \ddots & \\
0 & \cdot\cdot & 0 & \beta_{N-2} & \alpha_{N-2} & \beta_{N-1} \\
0 & \cdots & \cdots & 0 & \beta_{N-1} & \alpha_{N-1}
\end{bmatrix}
$$



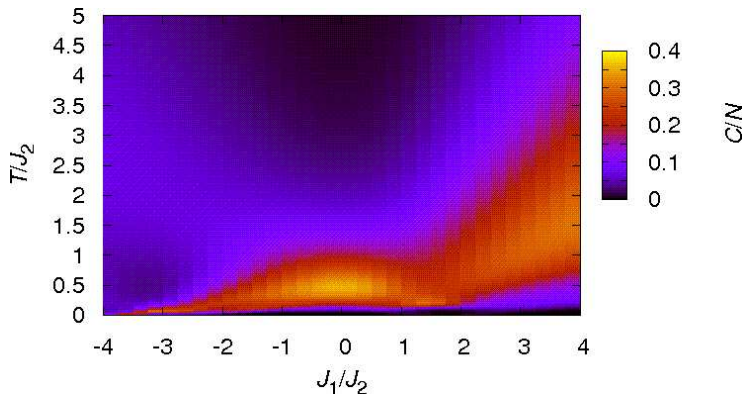

very rapid convergence !




care is needed for excited states

# Full Diagonalization: Thermodynamics

- Lapack / Householder complete diagonalization of the spectrum.
- Calculate partition function and all the thermodynamic quantities you want, often the only pedestrian method available for frustrated systems.
- Symmetries are also very important, because the computational requirements scale as $O(D^3)$, where D is the dimension of the block Hilbert space. Typical D's for a workstation are a few 1'000, up to a few 100'000 on supercomputers.



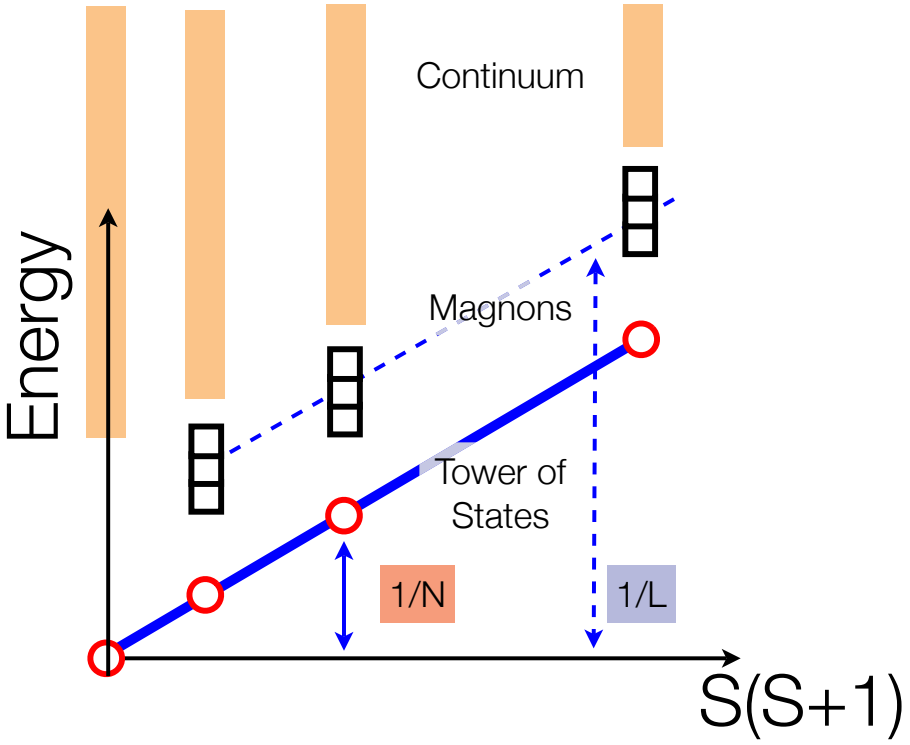

F. Heidrich-Meisner, A. Honecker, T. Vekua, Phys. Rev. B **74**, 020403(R) (2006).

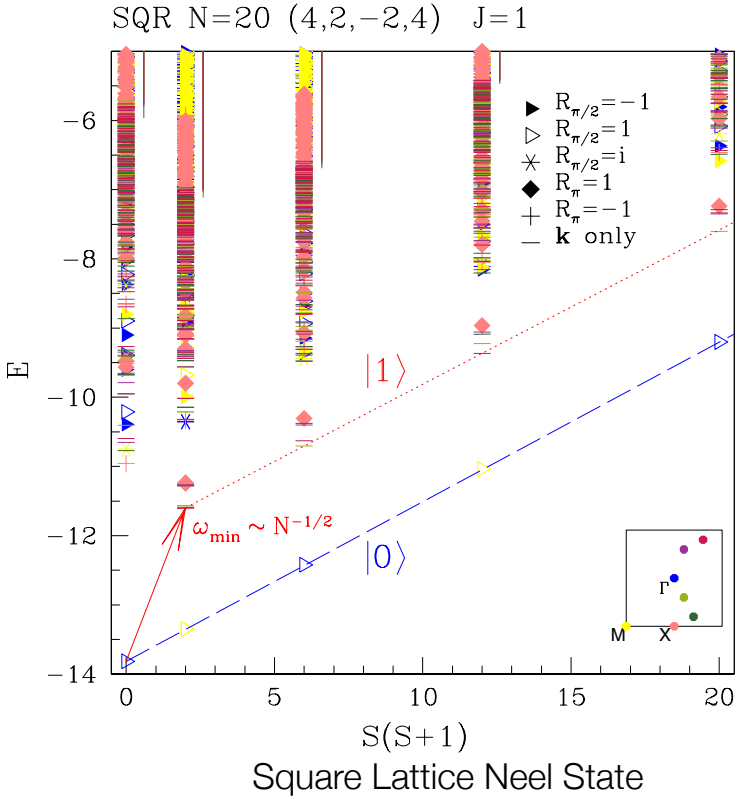
- You are going to use this method in the tutorial

# Exact Diagonalization
# "Tower of States" spectroscopy

- What are the finite size manifestations of a continuous symmetry breaking ?

- Low-energy dynamics of the order parameter
  Theory: P.W. Anderson 1952, Numerical tool: Bernu, Lhuillier and others, 1992 -



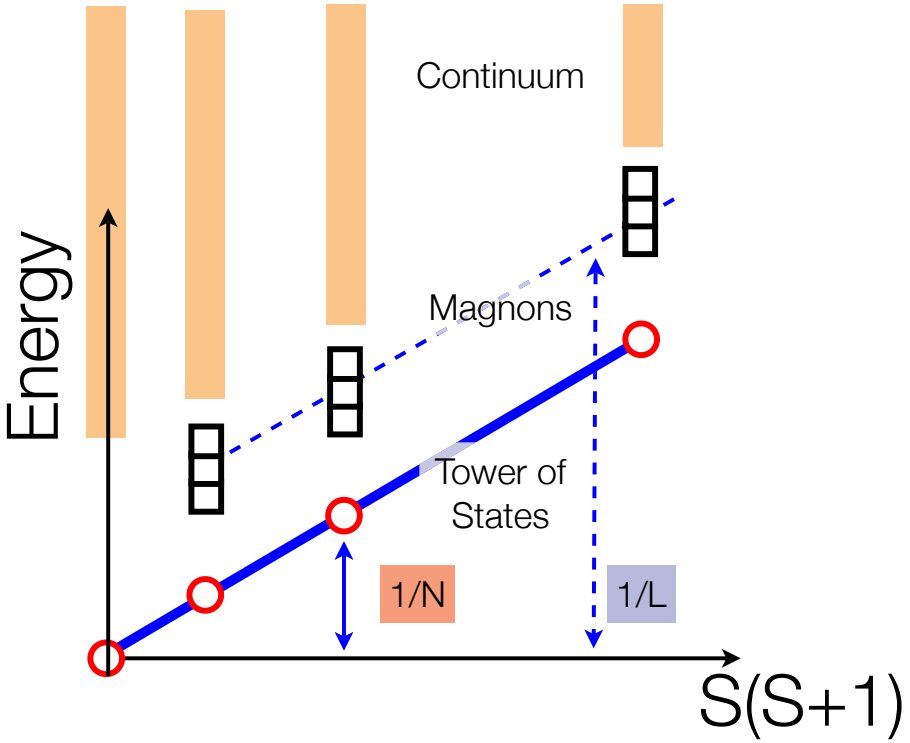



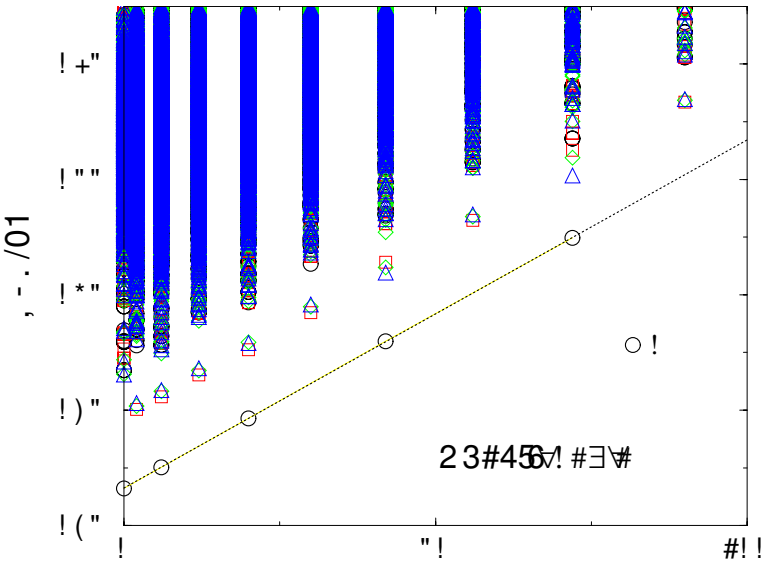

Square Lattice Neel State

# Exact Diagonalization
# “Tower of States” spectroscopy

- What are the finite size manifestations of a continuous symmetry breaking ?

- Low-energy dynamics of the order parameter
  Theory: P.W. Anderson 1952, Numerical tool: Bernu, Lhuillier and others, 1992 -



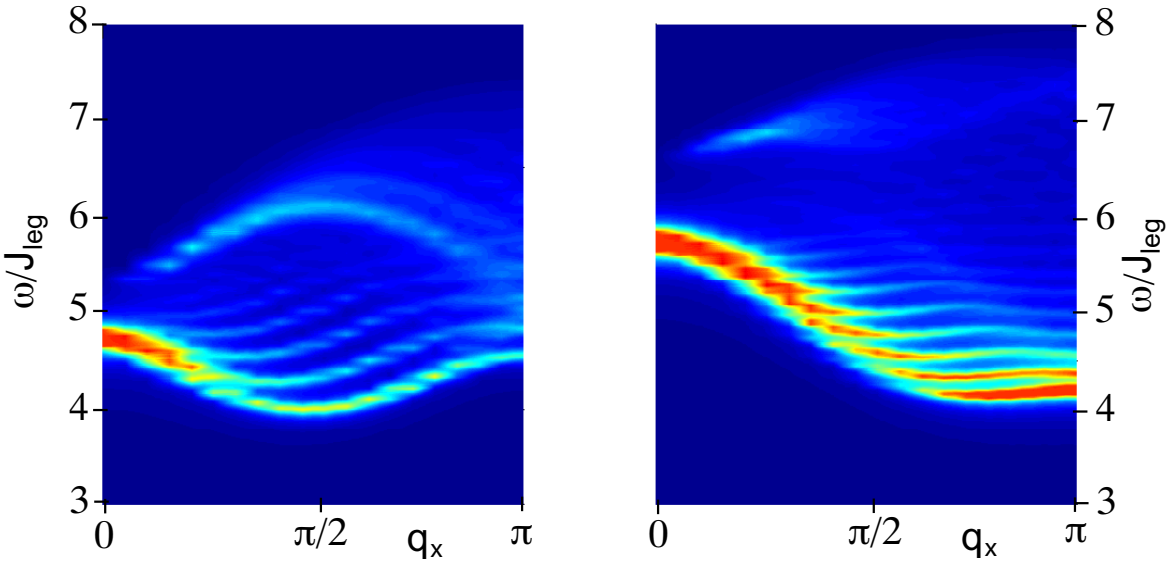
Ferroquadrupolar state

# Exact Diagonalization
# Frequency Dynamics

- $$G_A(\omega + i\eta) = \langle\psi|A^\dagger \frac{1}{E_0 + \omega + i\eta - H} A|\psi\rangle \quad A = S^\alpha(\mathbf{q}), c_\mathbf{k}, \ldots$$

- Generate Krylov space of $A|\psi\rangle$
  Use continued fraction used to invert $(E_0 + \omega + i\eta - H)$
  More information in talk by D. Poilblanc on monday!

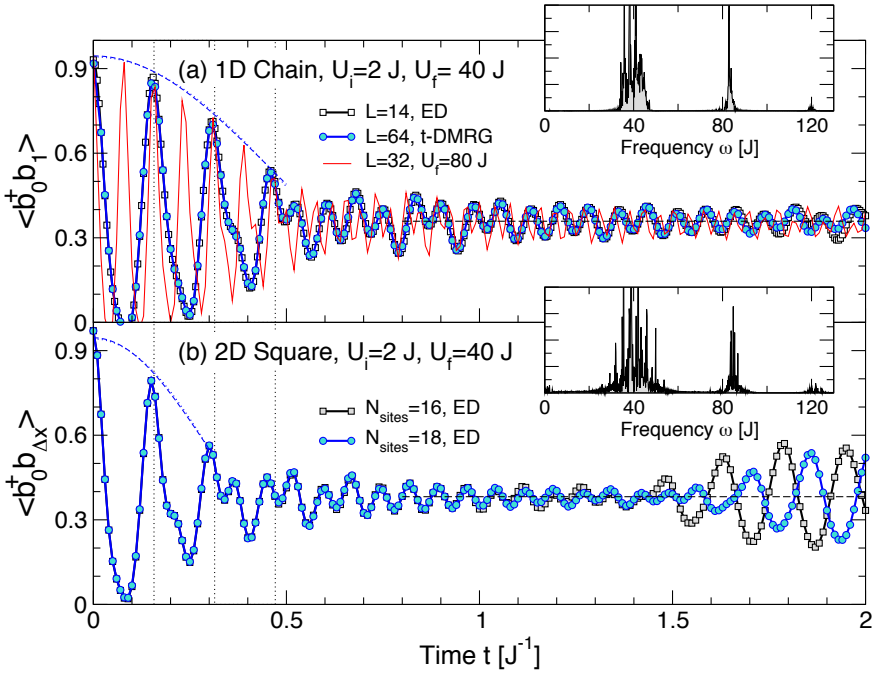
- Example:
  Spin dynamics of a spin ladder in a uniform magnetic field:




AML, unpublished

# Exact Diagonalization
# Real-Time Dynamics

- It is expensive to obtain the full propagator $\exp[-itH]$
- Krylov methods exist to approximate the propagator for a given state $|\psi(0)\rangle$
  One can get the time propagated state $|\psi(t)\rangle$ with only $|v\rangle = H|u\rangle$ operations.
- Example: time evolution of a strongly correlated quantum systems after an abrupt change in the parameters in the Hamiltonian. Revivals and Relaxation.
- Real-time evolution of spin excitations in frustrated quantum magnets ?




C. Kollath, AML, E. Altman, PRL 2007

S. Manmana et al. PRL 2007

# Exact Diagonalization Literature

- N. Laflorencie & D. Poilblanc,
  Lecture Notes in Physics **645**, 227 (2004).

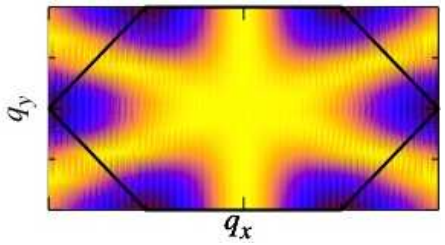
- R.M. Noack & S. Manmana,
  "*Diagonalization- and Numerical Renormalization-Group-Based Methods for Interacting Quantum Systems*",
  AIP Conf. Proc. **789**, 93 (2005).

- G. Misguich, P. Sindzingre
  "Detecting spontaneous symmetry breaking in finite-size spectra of frustrated quantum antiferromagnets"
  J. Phys.: Condens. Matter **19**, 145202 (2007).

- Talk by A. Weisse at http://heraeus2006.physik.uni-greifswald.de/invited.html

# Miscellanea

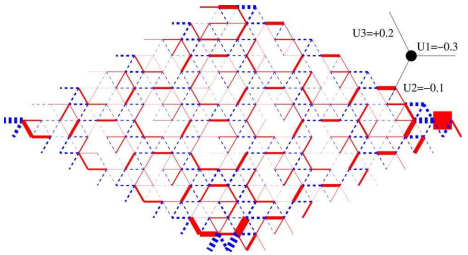
- Dynamical Mean-Field Theory
  Ohashi et al

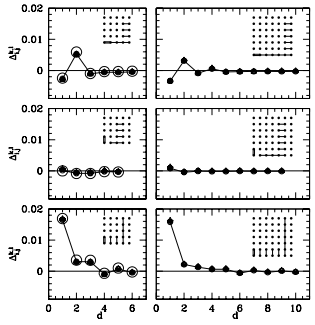



- Classical Spin Dynamics Simulations
  (Spin Molecular Dynamics)
  Shastry, Keren, D. Landau, Moessner & Chalker

$$\frac{\mathrm{d}\mathbf{S}_i}{\mathrm{d}t} = \mathbf{S}_i \times \mathbf{H}_i(t)$$

- Green's function / Diffusion Monte Carlo (T=0 methods)
  rather popular these days for Quantum Dimer Models
  Ralko et al, Syljuasen ...

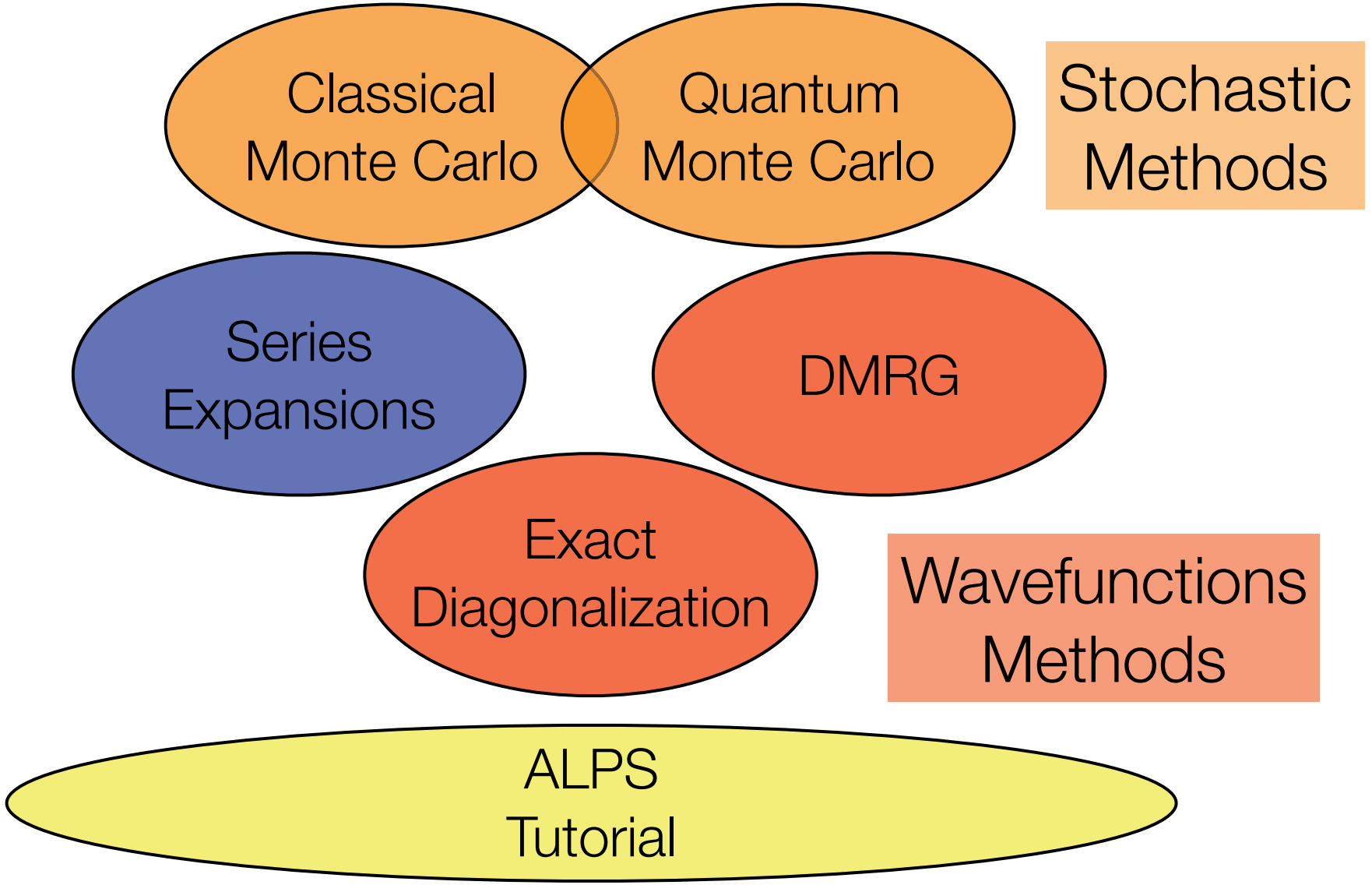


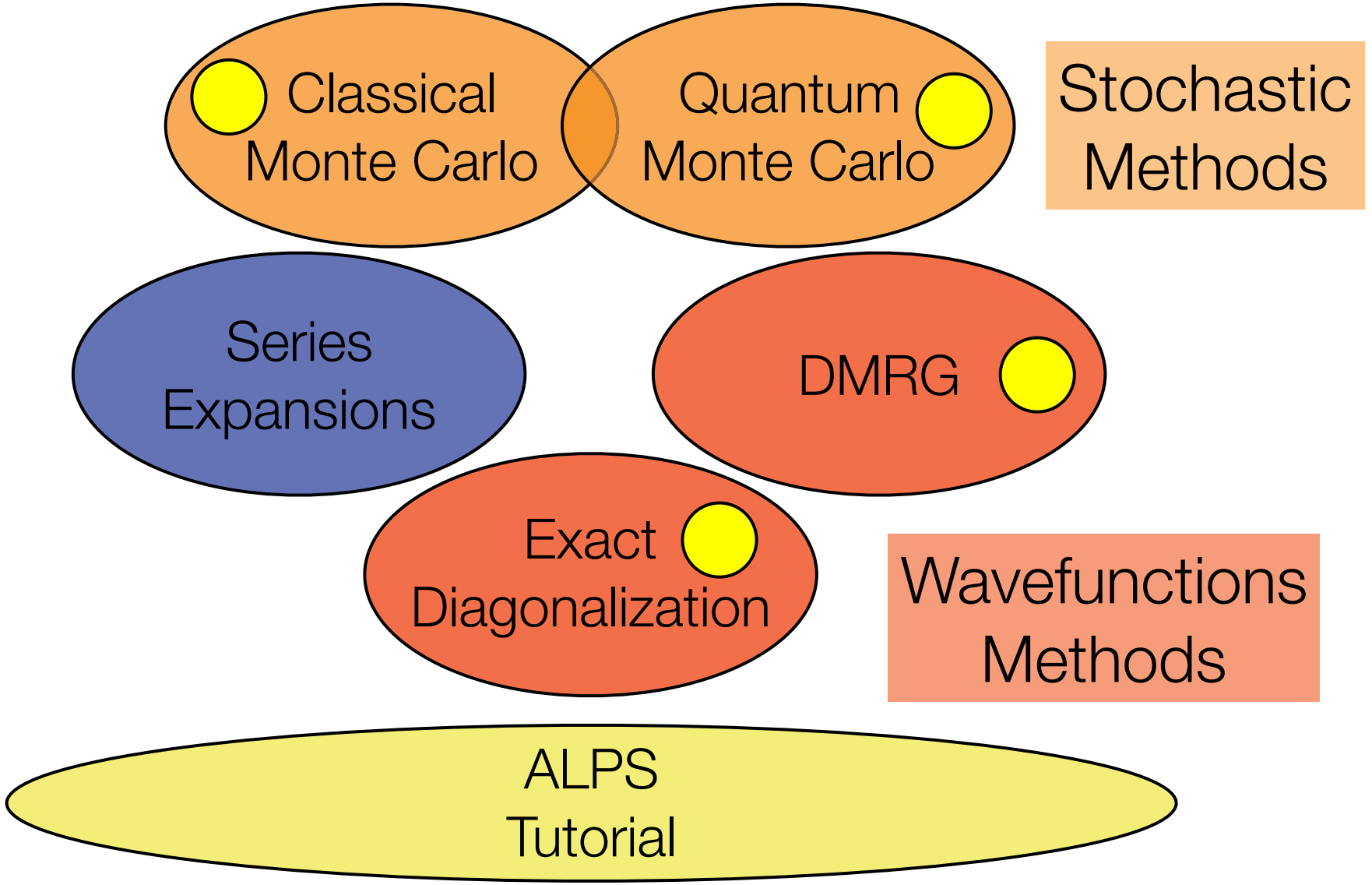
- Variational Monte Carlo, Fixed node ...
  talk on tuesday by S. Sorella

- Valence Bond basis Monte Carlo
  Sandvik, talk on thursday by F. Alet

# Overview of the methods covered



# Overview of the methods covered



Thank you !