Computational Studies of Quantum Criticality

Examples of quantum Monte Carlo studies of critical quantum magnets

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Related review articles

Thermal (classical) phase transition
- Fluctuations regulated by temperature $T>0$

Quantum (ground state, $T=0$) phase transition
- Fluctuations regulated by parameter $g$ in Hamiltonian

Lecture outline
Part I
- classical spin models
- Monte Carlo simulations
- finite-size scaling to study critical points

Part II
- quantum spin models
- quantum Monte Carlo methods ($S=1/2$ quantum spins)
- criticality in dimerized systems on 2 and 3 dimensions
  [- valence-bond solids and “deconfined” quantum criticality in 2D]
Classical spin models

Lattice models with “spin” degrees of freedom at the vertices

Classified by type of spin:

- **Ising model**: discrete spins, normally two-state $\sigma_i = -1, +1$
- **XY model**: planar vector spins (fixed length)
- **Heisenberg model**: 3-dimensional vector spins.

Statistical mechanics

- spin configurations $C$
- energy $E(C)$
- some quantity $Q(C)$
- temperature $T$ ($k_B=1$)

\[
\langle Q \rangle = \frac{1}{Z} \sum_C Q(C) e^{-E(C)/T}
\]

\[
Z = \sum_C e^{-E(C)/T}
\]

\[
E = \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \quad \text{(Ising)}
\]

\[
E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} \cos(\Theta_i - \Theta_j) \quad \text{(XY)}
\]

\[
E = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \quad \text{(Heisenberg)}
\]
Phase transition in the Ising model

For 2D square lattice with nearest-neighbor couplings

\[ \frac{T_c}{J} = \frac{2}{\ln(1 + \sqrt{2})} \approx 2.269 \]

- first-order transition versus \( h \) (at \( h=0 \)) for \( T<T_c \)
- continuous transition at \( h=0 \)

Mean-field solution:

\[ J = J_i = \sum_j J_{ij} \quad m = \tanh[(Jm + h)/T], \quad (m = \langle \sigma_i \rangle) \]

- Here \( J \) is the sum of local couplings

\[ J = \sum_j J_{ij} \]
Monte Carlo simulation of the Ising model

The Metropolis algorithm

Generate a series of configurations (Markov chain); $C_1 \rightarrow C_2 \rightarrow C_3 \rightarrow C_4 \rightarrow \ldots$
- $C_{n+1}$ obtained by modifying (updating) $C_n$
- changes satisfy the detailed-balance principle

\[
\frac{P_{\text{change}}(A \rightarrow B)}{P_{\text{change}}(B \rightarrow A)} = \frac{W(B)}{W(A)}
\]

\[
W(A) = e^{-E(A)/T}
\]

\[
P_{\text{change}}(A \rightarrow B) = P_{\text{select}}(B|A)P_{\text{accept}}(B|A)
\]

\[
P_{\text{select}} = 1/N, \quad P_{\text{accept}} = \min[W(B)/W(A), 1]
\]

\[
\frac{W(B)}{W(A)} = e^{-\Delta E/T} = e^{[E(A)-E(B)]/T}
\]

is easy to calculate (only depends on spins interacting with lipped spin)

Starting from any configuration, such a repeated stochastic process leads to configurations distributed according to $W$
- the process has to be **ergodic**
  - any configuration reachable in principle
- it takes some time to reach equilibrium
  (typical configurations of the Boltzmann distribution)
Metropolis algorithm for the Ising model. For each update perform:

- select a spin $i$ at random; consider flipping it $\sigma_i \rightarrow -\sigma_i$
- compute the ratio $R = \frac{W(\sigma_1, \ldots, -\sigma_i, \ldots, \sigma_N)}{W(\sigma_1, \ldots, \sigma_i, \ldots, \sigma_N)}$
  - for this we need only the neighbor spins of $i$
- generate random number $0 < r \leq 1$; accept flip if $r < R$ (stay with old config else)
- repeat (many times...)

Simulation time unit
(Monte Carlo step or sweep)
- $N$ spin flip attempts

“Measure” physical observables
(averaged over time) on the generated configurations
- begin after equilibration
  (when configurations are typical representatives of the Boltzmann distribution)

Example
- $128 \times 128$ lattice
  ($N=16384$) at $T/J=4$
  ($> T_c/J \approx 2.27$)
Going closer to $T_c$
Going below $T_c$....
Staying at same T, speeding up time by factor 10
Time series of simulation data; magnetization vs simulation time for $T<T_c$

![Time series of simulation data](image)

<table>
<thead>
<tr>
<th>L</th>
<th>M/N</th>
<th>Time scale of m reversals diverges when $L \to \infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td><img src="image" alt="Graph" /></td>
<td>- symmetry breaking</td>
</tr>
<tr>
<td>16</td>
<td><img src="image" alt="Graph" /></td>
<td></td>
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</tbody>
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Order parameter (magnetization)

$$
\frac{M}{N} = m = \frac{1}{N} \sum_{i=1}^{N} \sigma_i
$$

Compute time-average of $<m^2>$ to carry out finite-size scaling

Squared magnetization for $L \times L$ Ising lattices

Order (size independent)

Critical scaling (non-trivial power-law)

Disordered (trivial power-law $1/N = 1/L^2$)
Finite-size scaling hypothesis

In general there are two relevant length scales
- system length $L$, physical correlation length $\xi(T)$ (defined on infinite lattice)

In general physical quantities depend on both

$$\langle A \rangle = f(T, L) = g(\xi, L)$$

For $\xi << L$ or $\xi >> L$ one argument becomes irrelevant:

$$g \rightarrow g(L) \quad \text{or} \quad g \rightarrow g(\xi) = f(T)$$

Close to critical point: $\xi(T) \sim |T-T_c|^{-\nu}$ ($\nu$ is a critical exponent) and when $L \sim \xi(T)$:

$$g \rightarrow L^\kappa g(\xi/L) \sim L^\kappa g(|T-T_c|^{-\nu} L^{-1}) = L^\kappa g^*(|T-T_c| L^{1/\nu})$$

Use in “data collapse”. Example: susceptibility $\chi = (\langle m^2 \rangle - \langle |m| \rangle^2) / T$

$$t = |T - T_c|$$

$$T_c = 2 / \ln(1 + \sqrt{2})$$

$$\nu = 1, \gamma = 7/4$$
Binder ratios and cumulants

Consider the dimensionless ratio

\[ R_2 = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} \]

We know \( R_2 \) exactly for \( N \to \infty \)

- **For \( T<T_c \):** \( P(m) \to \delta(m-m^*)+\delta(m+m^*) \)
  \( m^* = |\text{peak m-value}|. \ R_2 \to 1 \)

  The **Binder cumulant** is defined as (n-component order parameter; \( n=1 \) for Ising)

\[
U_2 = \frac{3}{2} \left( \frac{n+1}{3} - \frac{n}{3} R_2 \right) \to \begin{cases} 
1, & T < T_c \\
0, & T > T_c 
\end{cases}
\]

- **For \( T>T_c \):** \( P(m) \to \exp[-m^2/a(N)] \)
  \( a(N) \sim N^{-1} \ R_2 \to 3 \) (Gaussian integrals)

2D Ising model; MC results

Curves for different \( L \) asymptotically cross each other at \( T_c \)

Extrapolate crossing for sizes \( L \) and \( 2L \) to infinite size

- converges faster than single-size \( T_c \) defs.
Quantum spin models

- the spins have three \((x, y, z)\) components, satisfy commutation relations
- interactions may contain 1 (Ising), 2 (XY), or 3 (Heisenberg) components

\[
H = \sum_{\langle ij \rangle} J_{ij} S_i^z S_j^z = \frac{1}{4} \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j \quad \text{(Ising)}
\]

\[
H = \sum_{\langle ij \rangle} J_{ij} [S_i^x S_j^x + S_i^y S_j^y] = \frac{1}{2} \sum_{\langle ij \rangle} J_{ij} [S_i^+ S_j^- + S_i^- S_j^+] \quad \text{(XY)}
\]

\[
H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} [S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)] \quad \text{(Heisenberg)}
\]

+ many modifications and extensions... and local spin \(S=1/2, 1, 3/2, \ldots\)

Quantum statistical mechanics

\[
\langle Q \rangle = \frac{1}{Z} \text{Tr} \left\{ Q e^{-H/T} \right\} \quad Z = \text{Tr} \left\{ e^{-H/T} \right\} = \sum_{n=0}^{M-1} e^{-E_n/T}
\]

Large size \(M\) of the Hilbert space; \(M=2^N\) for \(S=1/2\)
- difficult problem to find the eigenstates and energies
- we may be especially interested in the ground state \((T \to 0)\)
  (for classical systems the ground state is often trivial)
**Quantum antiferromagnets**

Nearest-neighbor $\langle i,j \rangle$ interactions (Heisenberg) on some lattice

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \quad J > 0$$

**Lattices can be classified as**

**Bipartite**
- nearest-neighbors $i,j$ always on different sublattices
- compatible with Neel order
- but other states possible

**Non-bipartite**
- no bipartition is possible
- frustrated antiferromagnetic interactions
- different kinds of order or no long-range order (spin liquid)

**Fully ordered Neel state** (ground state of $H$ for classical spins)

is not an eigenstate of $H$ even on a bipartite lattice
- if there is order at $T=0$ it is reduced by quantum fluctuations

**Mermin-Wagner theorem** (on breaking a continuous symmetry) implies:
- No Neel order in 1D Heisenberg model
- Neel order possible only at $T=0$ in 2D system
- Order possible also at $T>0$ in 3D
Quantum Monte Carlo

Rewrite the quantum-mechanical expectation value into a classical form

\[ \langle A \rangle = \frac{\text{Tr}\{ A e^{-\beta H} \}}{\text{Tr}\{ e^{-\beta H} \}} \to \frac{\sum_c A_c W_c}{\sum W_c} \]

Monte Carlo sampling in the space \( \{c\} \) with weights \( W_c \) (if positive-definite...)

**Different ways of doing it**

- World-line methods for spins and bosons
- Stochastic series expansion for spins and bosons
- Fermion determinant methods

For ground state calculations we can also do projection from a “trial state”

\[ |\Psi_m\rangle \sim H^m |\Psi_0\rangle \quad |\Psi_m\rangle \to |0\rangle \text{ when } m \to \infty \]

\[ |\Psi_\beta\rangle \sim e^{-\beta H} |\Psi_0\rangle \quad |\Psi_\beta\rangle \to |0\rangle \text{ when } \beta \to \infty \]

Particularly simple and efficient schemes exist for S=1/2 models

\[ H = -J \sum_{b=1}^{N_b} \left( \frac{1}{4} - \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)} \right) \quad (+ \text{ certain multi-spin terms}) \]

No sign problem on **bipartite lattices**
Finite-temperature QMC
(Stochastic series expansion, SSE)

$$\text{tr}\{e^{-\beta H}\} = \sum_n \frac{\beta^n}{n!} \langle \alpha | (-H)^n | \alpha \rangle$$

periodic “time” boundary conditions

Sampling of operator sequences and boundary states using efficient loop updates

Ground state projection

$$\sum_{\alpha \beta} f_\beta f_\alpha \langle \beta | (-H)^m | \alpha \rangle$$

open boundaries capped by valence bonds (2-spin singlets) [AWS, HG Evertz, PRB 2010]

Trial state can conserve relevant ground state quantum numbers (S=0, k=0,...)
Does it work?  
Compare with exact results
- $4 \times 4$ exact diagonalization
- Bethe Ansatz; long chains

Susceptibility of the $4 \times 4$ lattice $\Rightarrow$
- SSE results from $10^{10}$ sweeps
- improved estimator gives smaller error bars at high $T$ (where the number of loops is larger)

$E/N$ versus $T/J$
- SSE results for $10^6$ sweeps
- Bethe Ansatz ground state $E/N$
- SSE can achieve the ground state limit ($T \to 0$)
Spin correlation function of the Heisenberg chain (T=0)

\[ C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \]

If there is long-range Neel order \( C(r) \rightarrow (-1)^r \langle m^2 \rangle \)
- but not possible in 1D
- exact results and low-energy field theory predict critical state

\[ C(r) \rightarrow \frac{\ln^{1/2}(r/r_0)}{r} (-1)^r \]  
SSE \( T \rightarrow 0 \) results agree with this form

![Graph showing the spin correlation function for chains of length 1024 and 4096 at distances \( r = 2^m \). The error bars are smaller than the symbols. The solid curve is expected form \( \propto r^{-1} \ln^{1/2}(r/r_0) \), with \( A = 0 \). The dashed curve shows the pure \( 1/r \) form for comparison. These results were obtained using inverse temperatures \( \beta = 2^{13} \) and 2^{14} for \( N = 1024 \) and 4096, respectively, which is sufficient for \( T \rightarrow 0 \) convergence.]

5.3.1. The Heisenberg chain

Spin correlations at \( T = 0 \).

In Sec. 4.3.1 we discussed Lanczos results for the spin correlation function of the Heisenberg chain and saw some hints of the expected logarithmic correction to the \( \sim 1/r \) critical behavior (Fig. 34). The system sizes accessible with the Lanczos method are not sufficient for studying these scaling corrections quantitatively, however. As we saw above, with the SSE method unbiased studies of the ground state is possible for chains of several thousand spins (with careful checks of the convergence to the \( T \rightarrow 0 \) limit). Fig. 66 shows the spin correlations for \( N = 1024 \) and 4096 at distances \( r = 2^m \), graphed on a log-log scale. To save time, only the correlations at these distances were computed [for a scaling \( N \log(N) \) of the time to carry out spatially averaged measurements]. The results for the two system size coincide closely for \( r \) up to \( 2^7 \), indicating convergence to the infinite value at this distance for \( N = 1024 \) (and therefore up to \( r \approx 2^9 \) for \( N = 4096 \), since the convergence behavior should scale approximately linearly with \( N \)).

The expected form

\[ |C(r)| = A \ln^{1/2}(r/r_0) r^{-1} \]

[57, 58, 59] is very well reproduced up to \( r = 2^9 \) for \( N = 4096 \). The parameters \( A \) and \( r_0 \) obtained from a fit are listed in the figure caption. If one leaves the exponent \( \sigma = 1/2 \) of the logarithmic correction as a parameter to be obtained from the data based on a fit, the exponent indeed comes out close to \( 0 \), but with a rather large error bar of, roughly, \( \pm 0.1 \). To really investigate the exponent carefully, one should further increase the chain length (which is possible in principle).

If one did not know about the existence of a log correction and tried to extract the form of the spin correlations on the basis of numerical calculations alone, one might at first sight conclude that the decay is \( \propto 1/r \) with \( \alpha \approx 0.85 \), based on the data in Fig. 66. There are, however, small but significant deviations from a pure power-law, which can be detected only if the relative statistical errors are sufficiently small. In the data shown...
2D S=1/2 antiferromagnetic Heisenberg model

\[ H = J \sum_{\langle i,j \rangle} S_i \cdot S_j \]

Sublattice magnetization

\[ \vec{m}_s = \frac{1}{N} \sum_{i=1}^{N} \phi_i \vec{S}_i, \quad \phi_i = (-1)^{x_i+y_i} \]

(2D square lattice)

Long-range order: \( <m_s^2> > 0 \) for \( N \to \infty \)

Quantum Monte Carlo
- finite-size calculations
- no approximations
- extrapolation to infinite size

Reger & Young 1988

\[ m_s = 0.30(2) \]

\( \approx 60 \% \) of classical value

AWS & HG Evertz 2010

\[ m_s = 0.30743(1) \]
T=0 Néel-paramagnetic quantum phase transition

Example: Dimerized S=1/2 Heisenberg models
• every spin belongs to a dimer (strongly-coupled pair)
• many possibilities, e.g., bilayer, dimerized single layer

Singlet formation on strong bonds $\Rightarrow$ Néel - disordered transition

Ground state (T=0) phases

$\Rightarrow$ 3D classical Heisenberg (O3) universality class; QMC confirmed

Experimental realization (3D coupled-dimer system): TlCuCl₃
SSE calculations to locate the critical point

**Figure 4:** (a) The Binder cumulant and (b) the spin stiffness as functions of the coupling ratio $g$ for different system sizes $L$. The data show a crossover behavior at finite system sizes, with the Binder cumulant decreasing and the spin stiffness increasing as $g$ is increased.

**Figure 5:** The finite-size scaling hypothesis: the Binder cumulant (left) and the spin stiffness (right) as functions of inverse system size $1/L$. The data are shown for different system sizes $L$. The scaling function $\xi(\beta, g)$ is defined according to (77), with the number of components $n = 3$. Note, however, that (77) is defined with the full scalar product $\langle m^2 \rangle$.

**Figure 6:** Curve crossing analysis: dimensionless quantities $\beta_L$ and $\rho_L$ as functions of $g$. The data are shown for different system sizes $L$. The quantities of interest. This approach is discussed for various cases (87, 88) and is in good agreement with the expectations of the single-argument limit.

**Figure 7:** Additional data showing the size dependence for several values of the renormalization-group treatments of one such field theory.

**Figure 8:** Being a consequence of the Mermin-Wagner theorem, there is now compelling evidence already that $z$ is a critical exponent consistent with $z = 1$ in the 3D Ising model. There would then expect the Ising model to transition to the RVB spin-liquid state at inverse temperature $\beta = 0$, and there is again only one argument for each $g$. There is plenty of evidence already that the three-sublattice Néel order actually surviving the quantum Heisenberg model, and (b) shows the size dependence for several values of the renormalization-group treatments of one such field theory.
Crossing points drift as the system size is increased
- extrapolations necessary
- can use \((L, 2L)\) crossing points

\[ g_c(L) = g_c(\infty) + aL^{-b} \]

Different quantities give consistent results: \(g_c = 1.90948(4)\)

**What’s special with quantum-criticality?**
- large \(T > 0\) quantum-critical fan where \(T\) is the only relevant energy scale
- physical quantities expect power laws governed by the \(T=0\) critical point

2D Neel-paramagnet
“cross-over diagram”
[Chakravarty, Halperin, Nelson, PRB 1988]
Making connections with quantum field theory

Low-energy properties described by the (2+1)-dimensional nonlinear σ-model - Chakravarty, Halperin, Nelson (1989), Chubukov, Sachdev, Ye (1994)

Expand O(3) order-parameter symmetry to O(N), large-N calculations

T>0 properties at quantum-critical coupling (N=3):

\[ \chi(T) = \frac{1.0760}{\pi c^2} T \]

\[ E(T) = E_0 + \frac{12 \cdot 1.20206}{5\pi c^2} T^3 \]

QMC results for bilayer model: \( g_c = 2.5220(1) \), \( c(g_c) = 1.9001(2) \)
- L×L lattices with L up to 512 (no size-effects for \( T/J_1 \geq 0.03 \))

T and \( T^3 \) prefactors agree with theory to within 3%
Quantum and classical criticality in a dimerized quantum antiferromagnet

P. Merchant, B. Normand, K. W. Krämer, M. Boehm, D. F. McMorrow and Ch. Rüegg

3D Network of dimers - couplings can be changed by pressure

Universality of the Neel temperature in 3D dimerized systems?
[S. Jin, AWS, PRB2012]

Determine the Neel ordering temperature $T_N$ and the $T=0$ ordered moment $m_s$ for 3 different dimerization patterns

Example: Columnar dimers

\[
\langle m_{z}^2 \rangle = \begin{cases} 
  \bullet g=1.0 \\
  \circ g=2.5, 3.6, 4.5 \\
  \square g=4.7717 
\end{cases}
\]

\[
\begin{align*} 
T_N & = \begin{cases} 
  \bullet \rho_s^x L \text{ crossing} \\
  \circ \rho_s^y L \text{ crossing} \\
  \square R_2 \text{ crossing} 
\end{cases} \\
& = 3.4
\end{align*}
\]
**Couplings vs pressure not known experimentally**
- plot $T_N$ vs $m_s$ to avoid this issue and study universality
- but how to normalize $T_N$?

**Three normalizations**
- weaker coupling $J_1$
- sum $J_s$ of couplings per spin
- peak $T^*$ of magnetic susceptibility

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**Figure 3.** Extrapolation of the sublattice magnetization for the three different dimerized models and with because it comes out very close to zero in fits including it. (a) $T_m$ normalized in three different ways.

**Figure 4.** The $N$ Couplings vs pressure not known experimentally. (b) The peak temperature vs the coupling ratio for the $L$ average coupling. In Fig. 8 we note that in Fig. 5(b), where an interdimer coupling $\delta$ stays nonzero at the quantum-critical point. (c) $T_m$ versus $1/L$ for all three models. Normalizing with a physical quantity that measures the effective lattice-scale energy. One can do even better when normalizing with a physical way up to $g=2.0, 3.0, 3.5$.

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**Figure 5.** (Color online) (a) Susceptibility vs temperature of the Double Cube. (b) The peak temperature vs the coupling ratio for the Columnar Dimer and 6. (c) $T_m$ close to its peak, and in Fig. 4(a) we can do even better when normalizing with a physical quantity that measures the effective lattice-scale energy. One can do even better when normalizing with a physical way up to $g=2.0, 3.0, 3.5$.

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**References.**
**T* normalization is in principle accessible experimentally**
- some experimental susc. results available
- neutron data analyzed with this normalization

![Graph](Jin and Sandvik (2012))

**Universality is not a feature of quantum-criticality**
- extends far from the quantum critical point
- linear behavior is expected from semiclassical theory
  (decoupling of quantum and thermal fluctuations)
- deviations show coupling of quantum and thermal fluctuations
  (high \( T_N \), high density of excited spin waves)

**Same features observed in models and experiment**
- experimental slope about 25% lower of g-factor 2 assumed
  (what exactly is the g-factor?)