Quantum Phase Transitions in Low Dimensional Magnets

Synge Todo (藤堂真治)

Department of Applied Physics, University of Tokyo
<wistaria@ap.t.u-tokyo.ac.jp>
Low-Dimensional Magnets

- Spin-$S$ Heisenberg antiferromagnets
  \[ H = J \sum_{\langle i,j \rangle} \left[ S_i^z S_j^z - \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) \right] \]
  (non-frustrated, no external field)
- 3D or higher: thermal phase transitions at finite $T$
- 2D: Néel long-range order at ground state
- 1D: Haldane conjecture
  - $S=1/2, 3/2,...$ : critical (i.e. quasi-LRO) GS
  - $S=1,2,...$ : singlet GS with finite gap
2D Heisenberg Antiferromagnet

\[ \mathcal{H} = \sum_{i,j} S_{2i,j} \cdot S_{2i+1,j} + \alpha \sum_{i,j} S_{2i+1,j} \cdot S_{2i+2,j} + J' \sum_{i,j} S_{i,j} \cdot S_{i,j+1} \]

Spatial structure

Agenda

- (Very brief) review on loop cluster quantum Monte Carlo
- Gap estimation by using loop cluster QMC
  - extended moment method
- Topological order in 1D magnets
  - twist order parameter and its improved estimator
- Quantum surface transition in 2D
  - perturbation by using QMC
Path-Integral Representation

- $H = H_0$ (diagonal part) + $V$ (off-diagonal part)

  \[ Z = \text{tr}\ e^{-\beta H_0} U(\beta) \text{ with } e^{-\beta(H_0+V)} \equiv e^{-\beta H_0} U(\beta) \]

- Time-dependent perturbation expansion

  \[
  dU(\tau)/d\tau = -V(\tau)U(\tau) \quad V(\tau) \equiv e^{\tau H_0} V e^{-\tau H_0}
  \]

  \[
  U(\beta) = 1 - \int_0^\beta V(\tau)U(\tau) \, d\tau \\
  = 1 - \int_0^\beta V(\tau_1) \, d\tau_1 + \int_0^\beta \int_0^{\tau_1} V(\tau_1)V(\tau_2) \, d\tau_1 \, d\tau_2 + \cdots
  \]

\[
Z = \text{tr}\ e^{-\beta H_0} \left[ 1 + \sum_{n=1}^\infty (-1)^n \int_0^\beta \int_0^{\tau_1} \cdots \int_0^{\tau_{n-1}} \prod_{i=1}^n V(\tau_i) \prod_{i=1}^n \, d\tau_i \right]
\]
World-Line Configuration

• Each term is specified by \((\alpha, n, \{b_i, \tau_i\})\)

\[ w(\alpha, n, \{b_i, \tau_i\}) \equiv (-1)^n \langle \alpha | e^{-\beta H_0} V_{b_1}(\tau_1) V_{b_2}(\tau_2) \cdots V_{b_n}(\tau_n) | \alpha \rangle \]

\Rightarrow \text{“world-line configuration”}

\[ n=8 \]

\[ |\alpha\rangle = | \uparrow \downarrow \downarrow \uparrow \downarrow \uparrow \rangle \]

• Weight of each configuration can be calculated easily
Path Integral Representation

• A d-dimensional quantum system is mapped to a \((d+1)\)-dimensional classical system. Additional dimension = imaginary time

• Up (down) spins form world lines due to \(S_z\) conservation.

• Weight of mapped configuration (world lines) is expressed as a product of local weights.

• Local updates or cluster updates (loop update) can be performed on world lines.
High Temperature Series Representation (SSE)

• Break up the Hamiltonian into diagonal and off-diagonal bond terms

\[-H = \sum_{k=1,2} \sum_{b} H_{k,b}\]

diagonal

\[H_{1,b} = -J s_i^z s_j^z + \frac{h}{\hbar} (s_i^z + s_j^z)\]

off-diagonal

\[H_{2,b} = \frac{J}{2} (s_i^+ s_j^- + s_i^- s_j^+)\]

• Taylor expansion of density matrix (ip={k,b})

\[Z = \sum_\alpha \langle \alpha | e^{-\beta H} | \alpha \rangle = \sum_\alpha \sum_{n=0}^{\infty} \sum S_n \frac{\beta^n}{n!} \langle \alpha | H_{i_1} H_{i_2} \cdots H_{i_n} | \alpha \rangle\]

Sandvik and Kurkijarvi (1991)
World-Line Configuration in HTSR

• Each term is specified by \((\alpha, \{H_{i_p}\})\)

\[
Z = \sum_\alpha \langle \alpha | e^{-\beta H} | \alpha \rangle = \sum_\alpha \sum_{n=0}^{\infty} \sum {S_n} \frac{\beta^n}{n!} \langle \alpha | H_{i_1} H_{i_2} \cdots H_{i_n} | \alpha \rangle
\]

\(\Rightarrow \) “operator string”
High Temperature Series Representation (SSE)

- High temperature series always converges due to the finiteness of the system (cf. HT series in thermodynamic limit)

- Similarity to path-integral representation

- Integer index instead of continuous variable in imaginary time direction
Non-Local Updates

• **Non-local updates** are necessary for simulating in grand canonical ensemble (different winding number of world lines)

• **Strong restriction** in world-line configuration: All possible changes of world lines form “loops” due to local Sz conservation. (Finding allowed local update is also very tough task!)

• Non-local updates may reduce auto-correlation time

  ⇒ loop cluster update
One MCS of Loop Algorithm

PT breakup ⇒ loop flip

HTS diagonal update ⇒ loop flip
Loop Cluster Update

- Changes shape of world lines as well as their winding number
- Does not change expansion order \( n \) in HTSR
  Not ergodic by itself (used with diagonal update)
- Loop cluster update for spin-\( S \) XYZ models
- No loop solution in the presence of (longitudinal) external field (need to introduce global weight to loops)
- Both in PI and HTS representations
C++ implementation for S=1/2 Heisenberg antiferromagnet path integral

for (unsigned int mcs = 0; mcs < therm + sweeps; ++mcs) {
    std::swap(operators, operators_p); operators.clear();
    fragments.resize(nsites);
    std::fill(fragments.begin(), fragments.end(), fragment_t());
    std::copy(boost::counting_iterator<int>(0),
              boost::counting_iterator<int>(nsites), current.begin());
    double t = r_time();
    for (std::vector<local_operator_t>::iterator opi = operators_p.begin();
           t < 1
         || opi != operators_p.end();) {
        if (opi == operators_p.end() || t < opi->time) {
            unsigned int b = nbonds * random();
            if (spins[left(nbonds, b)] != spins[right(nbonds, b)]) {
                operators.push_back(local_operator_t(b, t));
                t += r_time()
            } else {
                t += r_time(); continue;
            }
        } else {
            if (opi->type == diagonal) {
                ++opi; continue;
            } else {
                operators.push_back(*opi); ++opi;
                try_gap = true;
            }
        }
    }
    std::vector<local_operator_t>::iterator oi = operators.end() - 1;
    unsigned int s0 = left(nbonds, oi->bond);
    unsigned int s1 = right(nbonds, oi->bond);
    oi->lower_loop = unify(fragments, current[s0], current[s1]);
    oi->upper_loop = current[s0] = current[s1] = add(fragments);
    if (oi->type == offdiagonal) { spins[s0] ^= 1; spins[s1] ^= 1; }
    for (int s = 0; s < nsites; ++s) unify(fragments, s, current[s]);
    int nc = 0;
    for (std::vector<fragment_t>::iterator ci = fragments.begin();
             ci != fragments.end(); ++ci) if (ci->is_root()) ci->id = nc++;
    clusters.resize(nc);
    for (std::vector<cluster_t>::iterator pi = clusters.begin();
             pi != clusters.end(); ++pi) *pi = cluster_t(random() < 0.5);
    for (std::vector<local_operator_t>::iterator oi = operators.begin();
             oi != operators.end(); ++oi)
        if (clusters[fragments[oi->lower_loop].id].to_flip ^
            clusters[fragments[oi->upper_loop].id].to_flip) oi->flip();
    for (unsigned int s = 0; s < nsites; ++s)
        if (clusters[fragments[s].id].to_flip) spins[s] ^= 1;
}

for (unsigned int mcs = 0; mcs < therm + sweeps; ++mcs) {
    int nop = operators.size();
    std::swap(operators, operators_p); operators.clear();
    fragments.resize(nsites);
    std::fill(fragments.begin(), fragments.end(), fragment_t());
    std::copy(boost::counting_iterator<int>(0),
              boost::counting_iterator<int>(nsites), current.begin());
    bool try_gap = true;
    for (std::vector<local_operator_t>::iterator opi = operators_p.begin();
              try_gap
           || opi != operators_p.end();) {
        if (try_gap) {
            unsigned int b = nbonds * random();
            if (spins[left(nbonds, b)] != spins[right(nbonds, b)] &&
                (nop + 1) * random() < lb2) {
                operators.push_back(local_operator_t(b)); ++nop;
            } else {
                try_gap = false; continue;
            }
        } else {
            if (opi->type == diagonal &&
                lb2 * random() < nop) {
                --nop; ++opi; continue;
            } else {
                operators.push_back(*opi); ++opi;
            }
        }
    }
    std::vector<local_operator_t>::iterator oi = operators.end() - 1;
    unsigned int s0 = left(nbonds, oi->bond);
    unsigned int s1 = right(nbonds, oi->bond);
    oi->lower_loop = unify(fragments, current[s0], current[s1]);
    oi->upper_loop = current[s0] = current[s1] = add(fragments);
    if (oi->type == offdiagonal) { spins[s0] ^= 1; spins[s1] ^= 1; }
    for (int s = 0; s < nsites; ++s) unify(fragments, s, current[s]);
    int nc = 0;
    for (std::vector<fragment_t>::iterator ci = fragments.begin();
             ci != fragments.end(); ++ci) if (ci->is_root()) ci->id = nc++;
    clusters.resize(nc);
    for (std::vector<fragment_t>::iterator ci = fragments.begin();
             ci != fragments.end(); ++ci) ci->id = cluster_id(fragments, *ci);
    for (std::vector<cluster_t>::iterator pi = clusters.begin();
             pi != clusters.end(); ++pi) *pi = cluster_t(random() < 0.5);
    for (std::vector<local_operator_t>::iterator oi = operators.begin();
             oi != operators.end(); ++oi)
        if (clusters[fragments[oi->lower_loop].id].to_flip ^
            clusters[fragments[oi->upper_loop].id].to_flip) oi->flip();
    for (unsigned int s = 0; s < nsites; ++s)
        if (clusters[fragments[s].id].to_flip) spins[s] ^= 1;
Improved Estimator

- Fortuin-Kasteleyn Representation

$$Z = \sum_c W(c) = \sum_{c,g} W(c, g) = \sum_{c,g} \Delta(c, g) f(g)$$

- In loop algorithm, graphs are generated according to

$$W(g) \equiv \sum_c W(c, g) = 2^{N_c} f(g)$$

- Expected value of a quantity: $A(c)$

$$\langle A(c) \rangle = Z^{-1} \sum_c A(c) W(c)$$

$$= Z^{-1} \sum_c A(c) \sum_g \Delta(c, g) f(g)$$

$$= Z^{-1} \sum_g A(g) W(g) \quad A(g) \equiv \sum_c A(c) \Delta(c, g)$$
Improved Estimator

\[ \langle A(c) \rangle \approx N_{\text{MC}}^{-1} \sum A(g) \]

- e.g.) spin correlation function \( C_{i,j}(c) = S_i^z S_j^z \)

- spin correlation represented in “graph language”
  \[
  |C_{i,j}(g)| = \begin{cases} 
    1/4 & \text{if } i \text{ and } j \text{ are on the same loop} \\
    0 & \text{otherwise}
  \end{cases}
  \]

- improved statistics (i.e. small statistical errors)

- “loops” (or “graphs”) themselves have a physical meaning
Gap Estimation by using loop cluster QMC
How to Calculate Gap by QMC

- “gap” is easily calculated in exact diagonalization

\[ \Delta = E_1 - E_0 \]

but not in world-line QMC

- fitting temperature dependence of susceptibility, etc

\[ \chi \sim \exp(-\Delta/T) \]

- temperature range?
- error estimation?

spin-1 ladder
A Tiny Gap in a Huge Gap

- frequency distribution at $T \ll \Delta_1$

$$P_0 = \frac{d_0}{d_0 + d_1 \exp(-\Delta_0/T)}$$

- ex) edge state in open $S=1$ chain

$\Delta_0 \ll \Delta_1$ = singlet-triplet gap $\ll$ bulk gap $\sim 0.41J$
Imaginary-Time Correlation Function

- We want a generic and systematic way of measuring gap
- Correlation function in imaginary-time direction

\[ C(\tau) = \sum_{i,j} \langle (-1)^{|i-j|} S_i^z(0) S_j^z(\tau) \rangle \]
\[ = \sum a_i \cosh[(\tau - \beta/2)/\xi_i] \quad \xi_0 = \Delta^{-1} > \xi_1 > \cdots \]

- However, numerical inverse Laplace transformation is ill-posed problem (c.f. MaxEnt)
- Systematic improvement of moment method
Moment Method

- Fourier transform of correlation function

\[ \tilde{C}(\omega) = \int_{0}^{\beta} C(\tau) e^{i\omega \tau} d\tau \]

- Effectively measured by using improved estimator

\[
\hat{\xi}^{(0)} = \frac{\beta}{2\pi} \sqrt{\frac{\tilde{C}(0)}{\tilde{C}(2\pi/\beta)}} - 1 \rightarrow \xi_0 \left[ 1 - \sum_{i=1}^{\infty} \frac{a_i}{2a_0} \frac{\xi_i}{\xi_0} \right]
\]

- Second-moment method (0-th order approximation)
Higher-Order Approximations

- **Second-order estimator**

\[
\hat{\xi}^{(2)} = \frac{\beta}{4\pi} \sqrt{3 \frac{\tilde{C}(0) - \tilde{C}(2\pi/\beta)}{\tilde{C}'(2\pi/\beta) - \tilde{C}'(4\pi/\beta)}} - 1 \rightarrow \xi_0 \left[ 1 - \sum_{i=1} a_i \left( \frac{\xi_i}{\xi_0} \right)^3 \right]
\]

- **Fourth-order estimator**

\[
\hat{\xi}^{(4)} = \frac{\beta}{6\pi} \sqrt{10 \frac{3\tilde{C}(0) - 4\tilde{C}(2\pi/\beta) + 4\tilde{C}(4\pi/\beta)}{5\tilde{C}'(2\pi/\beta) - 8\tilde{C}'(4\pi/\beta) + 3\tilde{C}'(6\pi/\beta)}} - 1
\]

\[
\rightarrow \xi_0 \left[ 1 - \sum_{i=1} a_i \left( \frac{xi_i}{\xi_0} \right)^5 \right]
\]

- **convergence test**

\[ S=1, \ L=128, \ T=1/64 \]

| \(1/\hat{\xi}^{(0)}\) | 0.41127(2) |
| \(1/\hat{\xi}^{(2)}\) | 0.41048(6) |
| \(1/\hat{\xi}^{(4)}\) | 0.4104(1) |
| ED | 0.41048(2) |
Haldane Gap of $S=3$ Chain

- Estimation of extremely large correlation length and small gap

$S=3$ Chain Results

$\xi = 637(1)$

$\Delta = 0.01002(3) J$

Simulation

$L = 5792$

$T = 0.001$
Haldane gap of $S=1,2,3$ chains

<table>
<thead>
<tr>
<th>$S$</th>
<th>$\Delta$</th>
<th>$\xi_x$</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.413(7)</td>
<td></td>
<td>MCPM (Nightingale-Blöte 1986)</td>
</tr>
<tr>
<td></td>
<td>0.4150(2)</td>
<td>6.03(2)</td>
<td>DMRG (White-Huse 1992)</td>
</tr>
<tr>
<td></td>
<td>0.41049(2)</td>
<td>6.2</td>
<td>ED (Golinelli et al 1994)</td>
</tr>
<tr>
<td></td>
<td>0.408(12)</td>
<td></td>
<td>QMC (Yamamoto 1995)</td>
</tr>
<tr>
<td></td>
<td>0.41048(6)</td>
<td>6.0164(2)</td>
<td>QMC+loop (Todo-Kato 2001)</td>
</tr>
<tr>
<td>2</td>
<td>0.074(16)</td>
<td></td>
<td>QMC (Yamamoto 1995)</td>
</tr>
<tr>
<td></td>
<td>0.055(15)</td>
<td></td>
<td>DMRG (Nishiyama et al 1995)</td>
</tr>
<tr>
<td></td>
<td>0.085(5)</td>
<td>49(1)</td>
<td>DMRG (Schollwöck-Jolicœur 1995)</td>
</tr>
<tr>
<td></td>
<td>0.090(5)</td>
<td>50(1)</td>
<td>QMC+loop (Kim et al 1997)</td>
</tr>
<tr>
<td></td>
<td>0.0876(13)</td>
<td></td>
<td>DMRG (Wang et al 1999)</td>
</tr>
<tr>
<td></td>
<td>0.08916(5)</td>
<td>49.49(1)</td>
<td>QMC+loop (Todo-Kato 2001)</td>
</tr>
<tr>
<td>3</td>
<td>0.01002(3)</td>
<td>637(1)</td>
<td>QMC+loop (Todo-Kato 2001)</td>
</tr>
</tbody>
</table>
Full Dispersion Curve

• (In principle) moment method can be extended to any k-values
• But (in practice) suffers from large systematic and statistical errors
Topological Order in 1D Magnets
Topological order in 1D magnets

- S=1 antiferromagnetic Heisenberg ladder

- no QPT between two limits

Haldane state

dimer state

ST, M. Matsumoto, C. Yasuda, and H. Takayama (2001)
Lieb-Schultz-Mattis Theorem

- Lieb-Schultz-Mattis overlap function

\[ z_L \equiv \langle \Psi_0 | \exp[i \frac{2\pi}{L} \sum_{j=1}^{L} j S_j^z] | \Psi_0 \rangle \]

- \( |\Psi_0\rangle \): ground state

- \( \exp[i \frac{2\pi}{L} \sum_{j=1}^{L} j S_j^z] |\Psi_0\rangle \): “twisted” state with

\[ E \approx E_0 + O(L^{-1}) \]

\[ z_L \to 0 \ (L \to \infty) \]

gapless or degenerating ground state

E.Lieb, T. Schultz, D.Mattis 1961
**Twist Order Parameter**

- QPT in spin-$S$ bond-alternating chain as a rearrangement of VBS pattern

\[
S=1/2 \\
\begin{array}{cccc}
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
\end{array} \\
S=1 \\
\begin{array}{cccc}
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
\end{array} \\
S=3/2 \\
\begin{array}{cccc}
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
\end{array}
\]

- Expected value of LSM twist-operator

\[
S=1/2 \\
\text{Expected value of LSM twist-operator} = \text{twist order parameter}
\]

\[
z_L \equiv \langle \Psi_0 | \exp[i \frac{2 \pi}{L} \sum_{j=1}^{L} j S_j^z] | \Psi_0 \rangle
\]

M. Nakamura and ST (2002)
Sign of Twist Order Parameter

- contribution from a dimer

\[ \cos \left[ \frac{\pi}{L} |i - j| \right] \]

- S=1 dimer phase: (2,0) VBS state

\[
\begin{array}{cccc}
1 & 2 & 3 & 4 \\
\end{array}
\] \[ \rightarrow +1 \]

\[
\begin{array}{cccc}
1 & 2 & 3 & 4 \\
\end{array}
\] \[ \rightarrow -1 \]

- Haldane phase: (1,1) VBS state

\[
\begin{array}{cccc}
\cos \left[ \frac{\pi}{L} \right] \to +1 \\
\end{array}
\]
Effects of Randomness on $z_L$

- weak bond randomness
  rearrangement of local VBS pattern

$z_L$ could be a good topological order parameter also for random systems

T. Arakawa, ST, and H. Takayama (2005)
Twist Order Parameter in Loop Algorithm

- **Split-spin representation** of $S=1$ chain

- **Twist order parameter**

$$z_L = \left\langle \exp \left( \frac{2\pi i}{L} \sum_{j=1}^{L} \sum_{k=1,2} j \hat{s}^z_{j,k} \right) \right\rangle_{\text{MCS}}$$

- **Decomposing into contributions from each loop**

$$\exp \left( \frac{2\pi i}{L} \sum_{j=1}^{L} \sum_{k=1,2} j \hat{s}^z_{j,k} \right) = \exp \left( \frac{\pi i}{L} \sum_{\ell=1}^{N_c} X_\ell \right) = \prod_{\ell=1}^{N_c} \exp \left( \frac{\pi i}{L} X_\ell \right)$$

$$X_\ell \equiv \sum_{(j,k) \in C_\ell} 2 j \hat{s}^z_{j,k}$$
Improved Estimator

• Averaging over $2^{N_c}$ configurations to obtain “A(g)"

$$\frac{1}{2^{N_c}} \sum_{d_1=\pm 1} \cdots \sum_{d_N=\pm 1} \prod_{\ell=1}^{N_c} \exp \left( \frac{\pi i}{L} d_\ell X_\ell \right)$$

$$= \prod_{\ell=1}^{N_c} \frac{1}{2} \left[ \exp \left( \frac{\pi i}{L} X_\ell \right) + \exp \left( - \frac{\pi i}{L} X_\ell \right) \right] = \prod_{\ell=1}^{N_c} \cos \left( \frac{\pi}{L} |X_\ell| \right)$$

• Contribution from a loop

$$\cos \left( \frac{\pi}{L} |X_\ell| \right)$$

• for 2-site loop

$$\cos \left( \frac{\pi}{L} |X_\ell| \right) = \cos \left( \frac{\pi}{L} |i - j| \right)$$

= contribution from a dimer
Loops vs VBS picture

- loop defines a singlet pair (or group) of spins in the VBS picture
- loop across the periodic boundary $4n$ ($4n+2$) times contributes +1 (-1) to twist-order parameter
- local fluctuation of loop structure can not change the sign (as seen in the VBS picture for random system): well-defined (topologically protected) sign in each VBS phase.
- $zL = 0$ means the existence of global loop(s), i.e. correlation length $\sim$ system size
Spin-1 ladder

- Plaquette singlet solid (PSS) state in $S=1$ ladder

Haldane state

PSS state

dimer state

ST, M.Matsumoto, C.Yasuda, and H.Takayama (2001)
Quantum Surface Transition
Edge State of Open $S=1$ chain

- Open $S=1$ chain with odd $L$

$$\begin{align*}
S_z &= \theta \\
S_z &= \pm 1
\end{align*}$$

$J_{\text{eff}} \approx 0.754 \exp(-L/6.01)$

0-dim surface of 1-dim system $\Rightarrow$

generalization to higher-dimensions?
Spin-1 Strips with Finite Width

\[ \mathcal{H} = \sum_{i,j} S_{2i,j} \cdot S_{2i+1,j} + \alpha \sum_{i,j} S_{2i+1,j} \cdot S_{2i+2,j} + J' \sum_{i,j} S_{i,j} \cdot S_{i,j+1} \]

Periodic boundary conditions in y-direction and \( L \rightarrow \infty \)

What happens for open boundaries?

Open S=1 Strips

\[ H = \sum_{i,j} S_{2i,j} \cdot S_{2i+1,j} + \alpha \sum_{i,j} S_{2i+1,j} \cdot S_{2i+2,j} + J' \sum_{i,j} S_{i,j} \cdot S_{i,j+1} \]

- **Open boundaries** in y-direction (multi-leg ladder)
- Consider **odd L** and **\( J' \gg 1, \alpha \) limit**
- Edge spins form **triplet** \(|\uparrow\rangle, |0\rangle, |\downarrow\rangle\) on each rung if

\[ T \ll 0.754J' \exp(-L/6.01) \]

- Take first two terms (leg interaction) into account as **weak perturbation**
Effective Hamiltonian

- **9x9** Effective Hamiltonian between two rungs

\[
\mathcal{H}_{\text{eff}} = \begin{pmatrix}
\langle \uparrow \uparrow | \mathcal{H}' | \uparrow \uparrow \rangle & \langle \uparrow \uparrow | \mathcal{H}' | \uparrow 0 \rangle & \langle \uparrow \uparrow | \mathcal{H}' | \uparrow \downarrow \rangle & \cdots & \langle \uparrow \uparrow | \mathcal{H}' | \downarrow \downarrow \rangle \\
\langle \uparrow 0 | \mathcal{H}' | \uparrow \uparrow \rangle & \langle \uparrow 0 | \mathcal{H}' | \uparrow 0 \rangle & \langle \uparrow 0 | \mathcal{H}' | \uparrow \downarrow \rangle & \cdots & \langle \uparrow 0 | \mathcal{H}' | \downarrow \downarrow \rangle \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\langle \down \down | \mathcal{H}' | \uparrow \uparrow \rangle & \langle \down \down | \mathcal{H}' | \uparrow 0 \rangle & \langle \down \down | \mathcal{H}' | \uparrow \downarrow \rangle & \cdots & \langle \down \down | \mathcal{H}' | \down \down \rangle 
\end{pmatrix}
\]

12 non-zero elements among 81

\[
\mathcal{H}' = K \sum_j S_{1,j} \cdot S_{2,j} \quad K = 1 \text{ or } \alpha
\]

- comparing with Hamiltonian of spin-1 dimer \( \tilde{J} S_1 \cdot S_2 \)

\[
\tilde{J} = \langle \uparrow \uparrow | \mathcal{H}' | \uparrow \uparrow \rangle
\]

\[
= K \sum_j \langle \uparrow \uparrow | S_{1,j} \cdot S_{2,j} | \uparrow \uparrow \rangle = K \sum_j \langle \uparrow_1 | S_{1,j}^z | \uparrow_1 \rangle \langle \uparrow_2 | S_{2,j}^z | \uparrow_2 \rangle
\]

\[
\langle \uparrow_1 | S_{1,j}^z | \uparrow_1 \rangle : \text{z-component of } j\text{-th spin in total } S_z=1 \text{ sector}
\]
QMC Results

\[ C = \sum_{j} \langle \uparrow | S_{j}^{z} | \uparrow \rangle^{2} \]

No temperature dependence at \( T < 0.1 \)

cconverges to a finite value for large \( L \)
Effective S=1 Chain

• Effective S=1 bond alternating chain for $J' \gg 1, \alpha$

\[ \mathcal{H}_{\text{eff}} = \sum \tilde{J}_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} \quad \tilde{J} = C \text{ or } C\alpha \]

• Quantum phase transition at $\alpha_c \approx 0.587$

• Only spins near surfaces participate

Quantum Surface Transition

• Phase transitions at finite $J'$

• No quantum phase transition in semi-infinite system (i.e. system with only one surface)
Summary

- (Very brief) review on loop cluster quantum Monte Carlo
- **Gap estimation** by using loop cluster QMC
  - extended moment method
- **Topological order** in 1D magnets
  - twist order parameter and its improved estimator
- **Quantum surface transition** in 2D
  - perturbation by using QMC
• Randomness effects to spin gapped state
  ⇒ Poster presentations in symposium
    by C. Yasuda and M. Matsumoto

• Finite-temperature phase transition in quasi-1D magnets ⇔ quantum critical point
  ⇒ Oral presentation in symposium by ST