Quantum Phase Transitions in Low Dimensional Magnets

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Low-Dimensional Magnets

- Spin-S Heisenberg antiferromagnets

$$H = J \sum_{\langle i,j \rangle} \left[S_i^z S_j^z - \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \right]$$

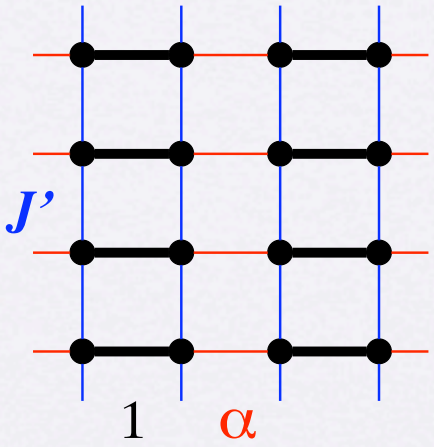
(non-frustrated, no external field)

  - 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

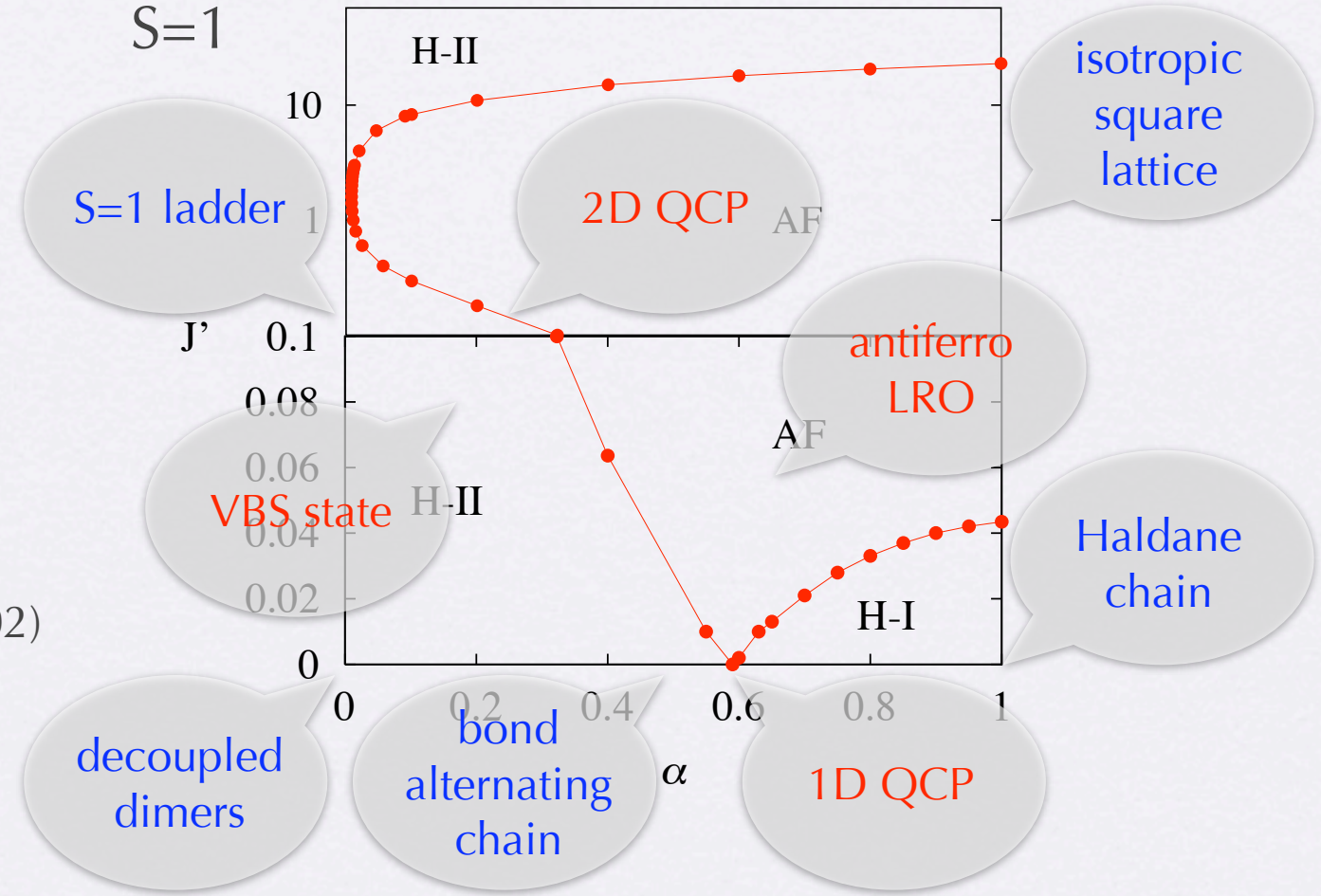
$$\mathcal{H} = \sum_{i,j} \mathbf{S}_{2i,j} \cdot \mathbf{S}_{2i+1,j} + \alpha \sum_{i,j} \mathbf{S}_{2i+1,j} \cdot \mathbf{S}_{2i+2,j} + J' \sum_{i,j} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1}$$

spatial structure



M.Matsumoto, et al (2002)

ground state phase diagram



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)

$$Z = \mathrm{tr}\, e^{-\beta H_0} U(\beta) \text{ with } e^{-\beta(H_0+V)} \equiv e^{-\beta H_0} U(\beta)$$

- Time-dependent perturbation expansion

$$dU(\tau)/d\tau = -V(\tau)U(\tau) \qquad V(\tau) \equiv e^{\tau \mathcal{H}_0} V e^{-\tau \mathcal{H}_0}$$

$$U(\beta) = 1 - \int_0^\beta V(\tau)U(\tau)\, d\tau$$

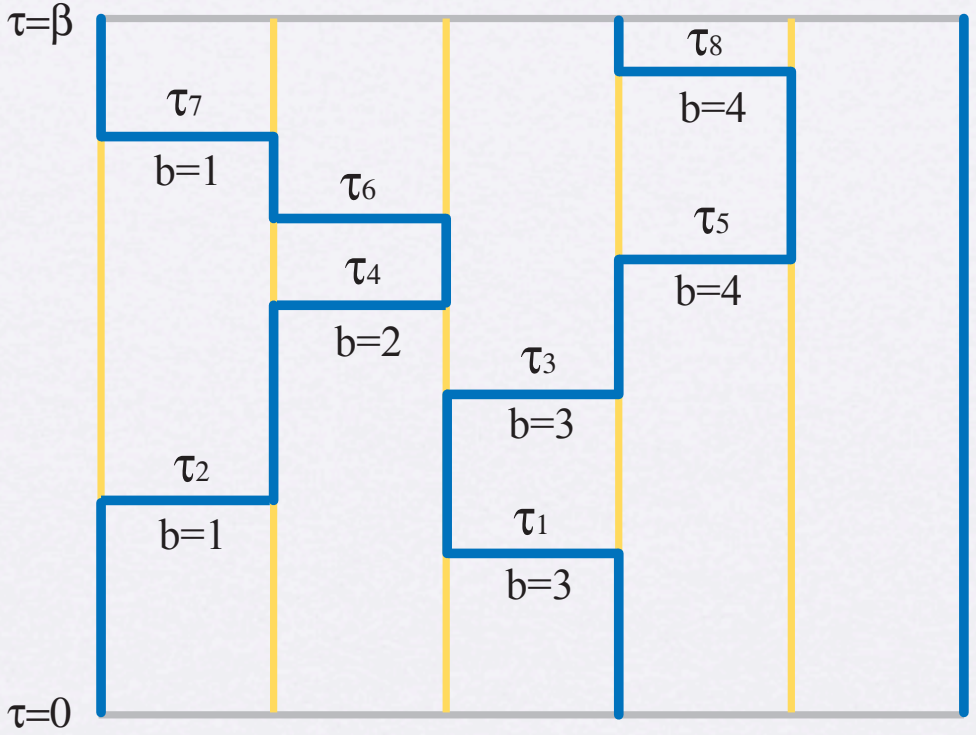
$$= 1 - \int_0^\beta V(\tau_1)\, d\tau_1 + \int_0^\beta \int_0^{\tau_1} V(\tau_1)V(\tau_2)\, d\tau_1\, d\tau_2 + \cdots$$

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

World-Line Configuration

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

$\Rightarrow$ "world-line configuration"



n=8

$$|\alpha\rangle = |\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\rangle$$

- Weight of each configuration can be calculated easily

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

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 Sz 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 $$H_{1,b} = -J s_i^z s_j^z + \frac{h}{z}(s_i^z + s_j^z)$$

off-diagonal $$H_{2,b} = \frac{J}{2}(s_i^+ s_j^- + s_i^- s_j^+)$$

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

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

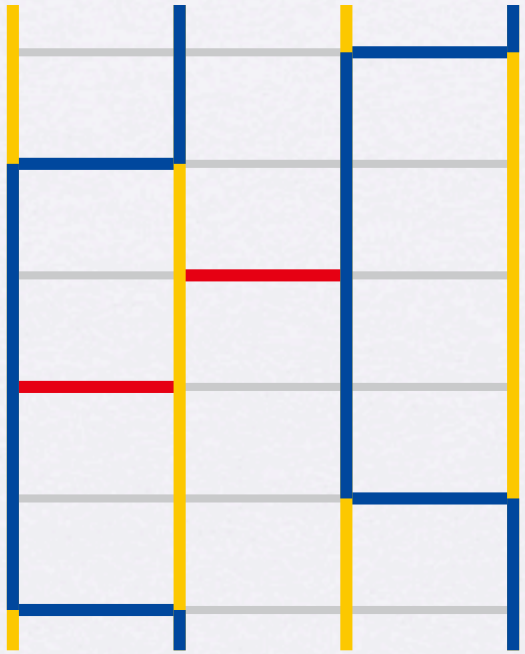
Sandvik and Kurkijarvi (1991)

World-Line Configuration in HTSR

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

$\Rightarrow$ "operator string"

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



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

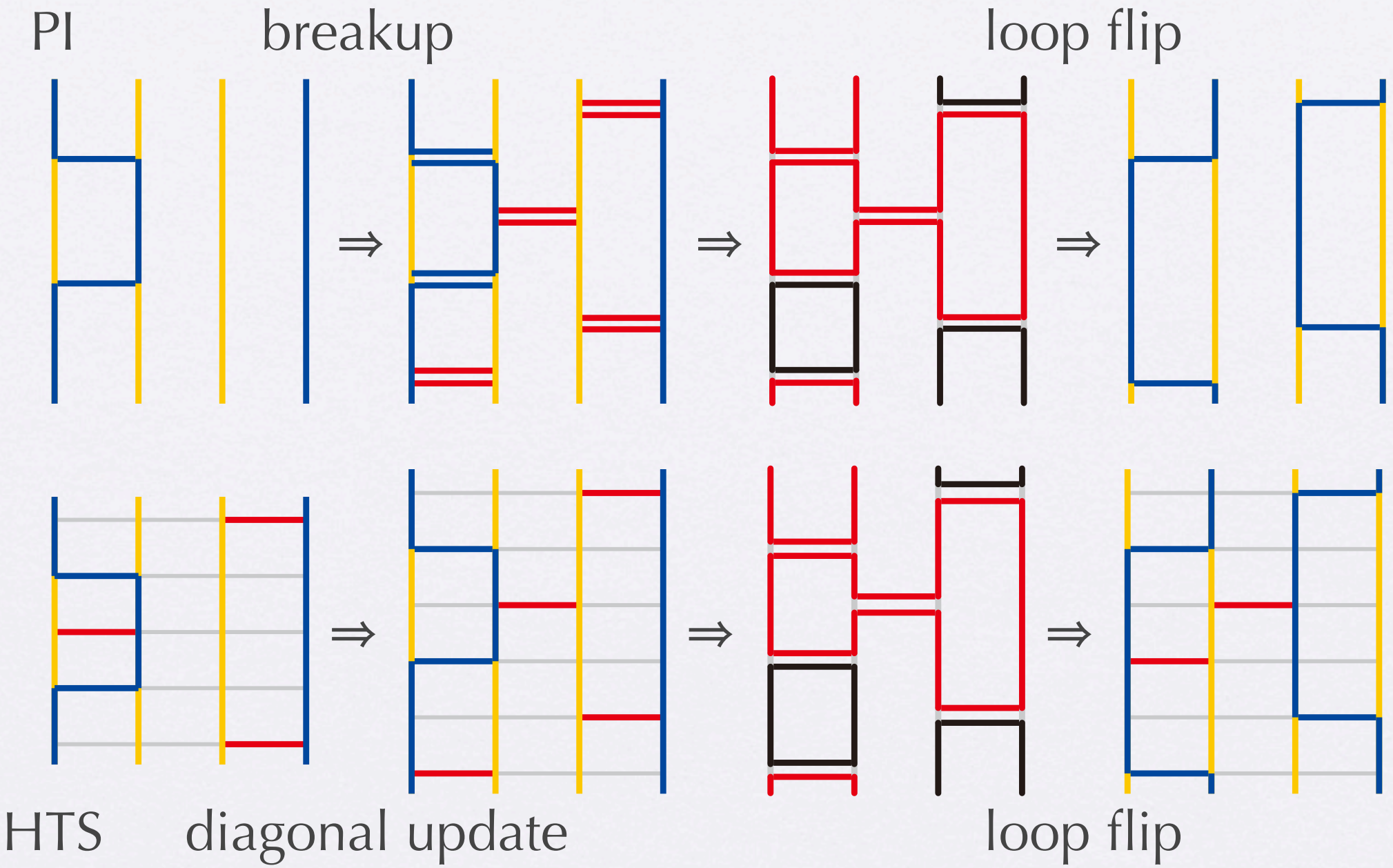
Non-Local Updates

- 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



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;
      }
    }


    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;
  }
}
```

high temperature series

```
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; 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<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 Representaion

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

- 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: $A(c)$

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

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

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

Improved Estimator

$$\langle A(c) \rangle \approx N_{\mathrm{MC}}^{-1} \sum A(g)$$

- e.g.) spin correlation function $C_{i,j}(c) = S_i^z S_j^z$
- spin correlation represented in "graph language"

$$|C_{i,j}(g)| = \begin{cases} 1/4 & \text{if i and j are on the same loop} \\ 0 & \text{otherwise} \end{cases}$$

- 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

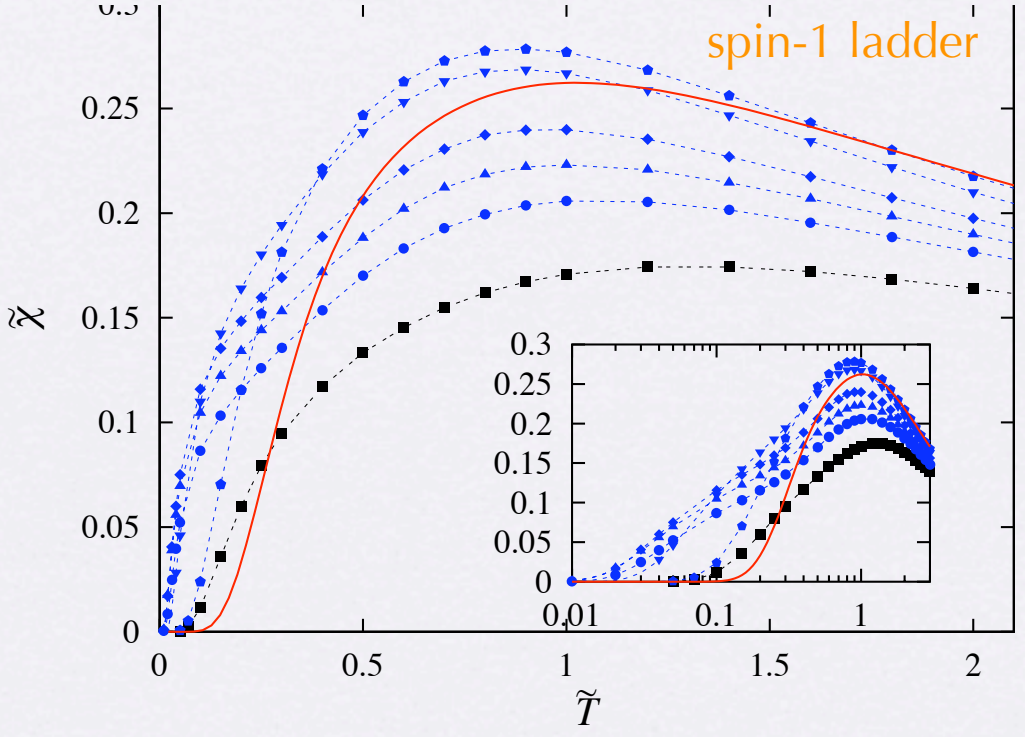
$$\Delta = E_1 - E_0$$

  but not in world-line QMC

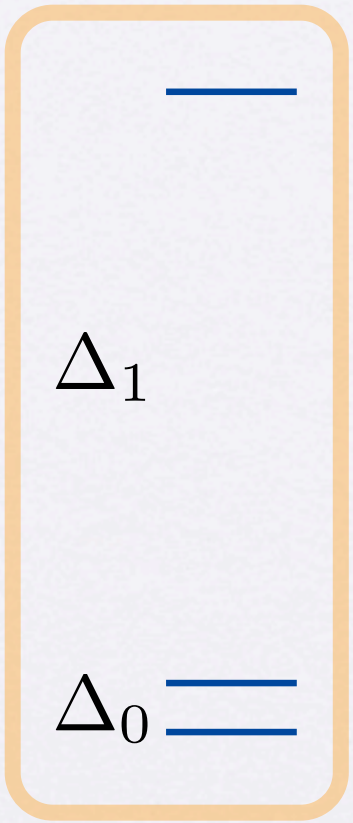
- fitting temperature dependence of susceptibility, etc

$$\chi \sim \exp(-\Delta/T)$$

  - temperature range?
  - error estimation?



A Tiny Gap in a Huge Gap

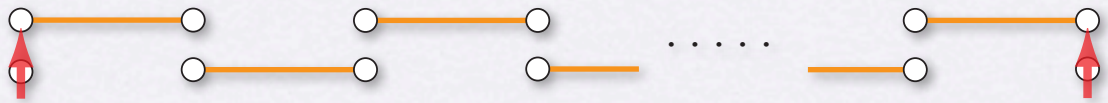


$\Delta_0 \ll \Delta_1$

- 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



effective interaction

= singlet-triplet gap << bulk gap ~ 0.41J

Imaginary-Time Correlation Function

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

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

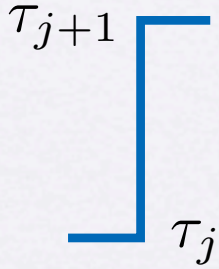
- However, numerical inverse Laplace transformation is ill-posed problem (c.f. MaxEnt)
- Systematic improvement of moment method

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



$$= \left\langle \sum_\ell \left| \oint S_i(\tau) e^{i\omega\tau} d\tau \right|^2 \right\rangle$$

$$= \left\langle \sum_\ell \left| \sum_j S_i(\tau_j) e^{i\omega(\tau_{j+1}-\tau_j)}/\omega \right|^2 \right\rangle$$

- Second-moment method (0-th order approximation)

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

Higher-Order Approximations

- Second-order estimator

$$\hat{\xi}^{(2)} = \frac{\beta}{4\pi}\sqrt{3\frac{\tilde{C}(0)-\tilde{C}(2\pi/\beta)}{\tilde{C}(2\pi/\beta)-\tilde{C}(4\pi/\beta)}-1} \rightarrow \xi_0\left[1-\sum_{i=1}\frac{a_i}{2a_0}\left(\frac{\xi_i}{\xi_0}\right)^3\right]$$

- Fourth-order estimator

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

$$\rightarrow \xi_0\left[1-\sum_{i=1}\frac{a_i}{2a_0}\left(\frac{xi_i}{\xi_0}\right)^5\right]$$

- 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

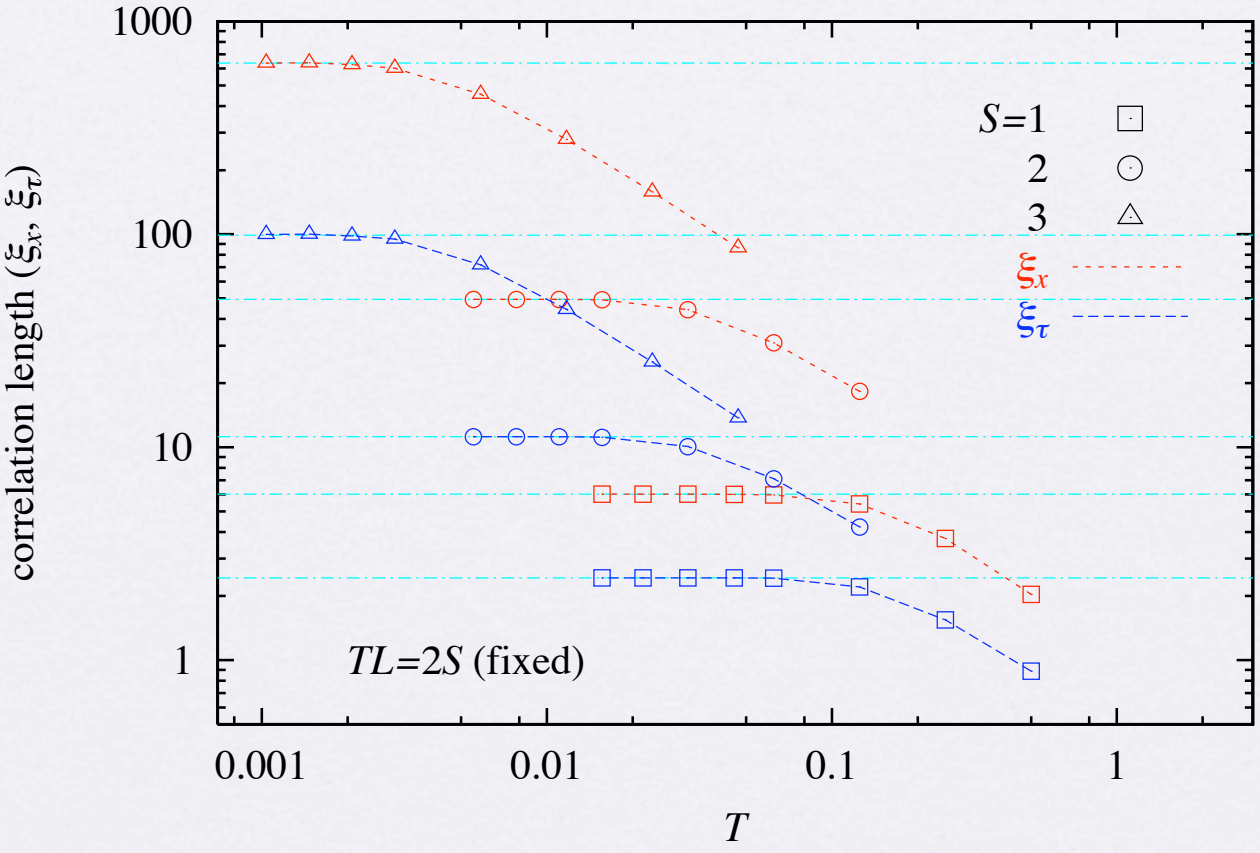
$$\xi = 637(1)$$

$$\Delta = 0.01002(3)J$$

Simulation

$$L = 5792$$

$$T = 0.001$$

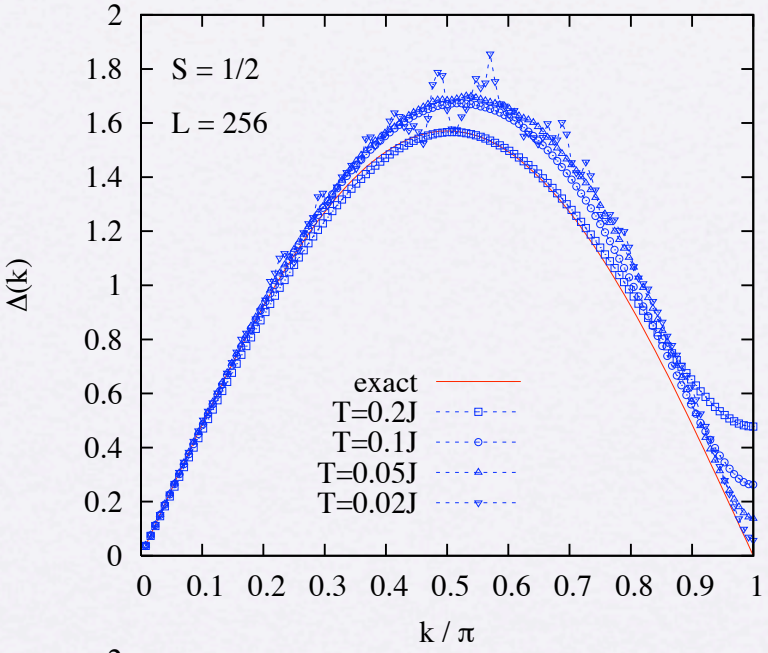


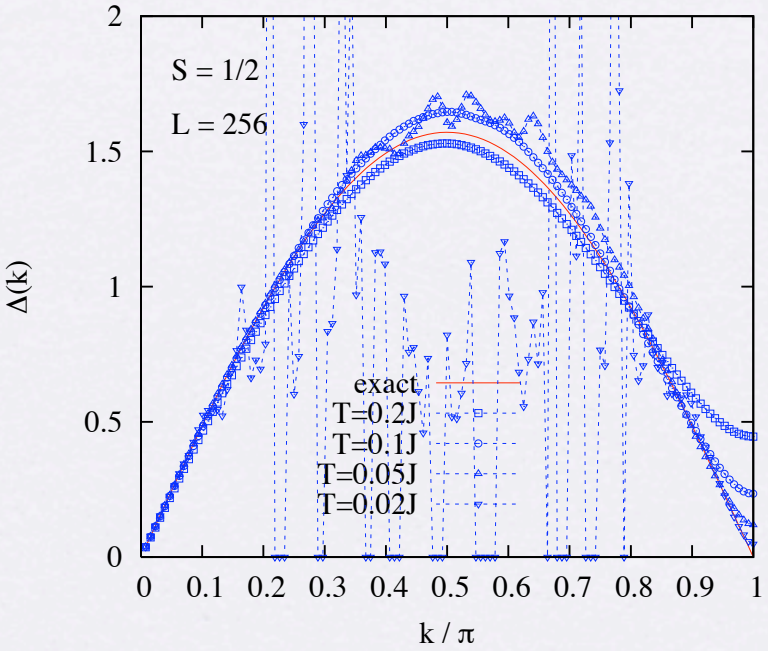
Todo and Kato (2001)

Haldane gap of S=1,2,3 chains

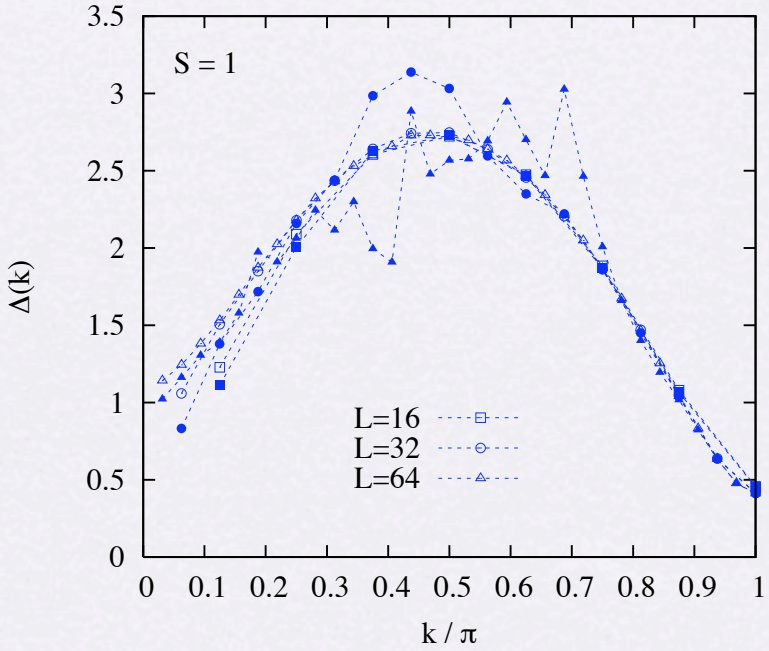
	Δ	ξ_x	method
S=1	0.413(7)		MCPM (Nightingale-Blöte 1986)
	0.4150(2)	6.03(2)	DMRG (White-Huse 1992)
	0.41049(2)	6.2	ED (Golinelli et al 1994)
	0.408(12)		QMC (Yamamoto 1995)
	0.41048(6)	6.0164(2)	QMC+loop (Todo-Kato 2001)
S=2	0.074(16)		QMC (Yamamoto 1995)
	0.055(15)		DMRG (Nishiyama et al 1995)
	0.085(5)	49(1)	DMRG (Schollwöck-Jolicœur 1995)
	0.090(5)	50(1)	QMC+loop (Kim et al 1997)
	0.0876(13)		DMRG (Wang et al 1999)
	0.08916(5)	49.49(1)	QMC+loop (Todo-Kato 2001)
S=3	0.01002(3)	637(1)	QMC+loop (Todo-Kato 2001)

Full Dispersion Curve





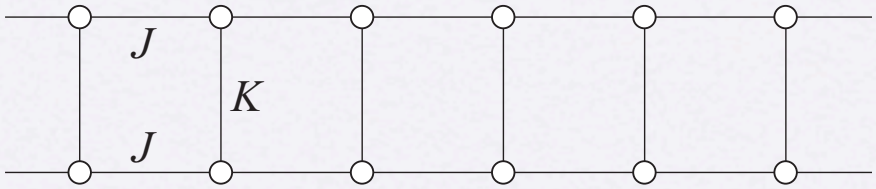
- (In principle) moment method can be extended to any k-values
- But (in practice) suffers from large systematic and statistical errors



Topological Order in 1D Magnets

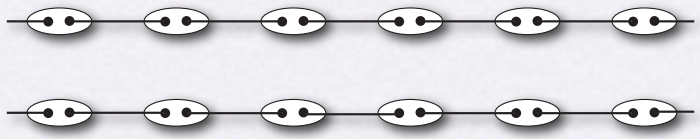
Topological order in 1D magnets

- S=1 antiferromagnetic Heisenberg ladder

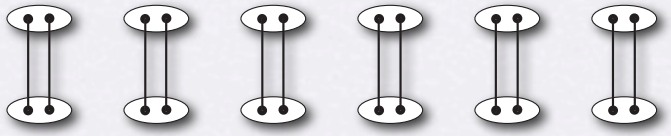


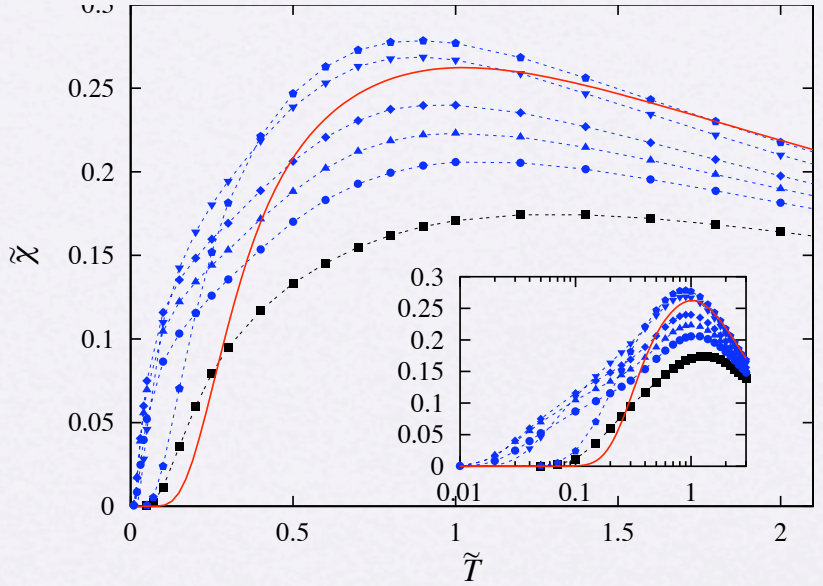
- no QPT between two limits

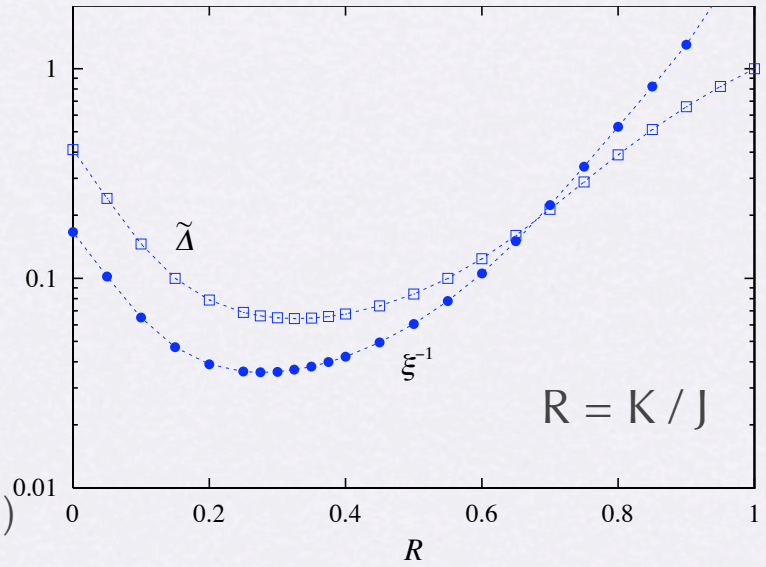
Haldane state



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

$$E \simeq E_0 + O(L^{-1})$$

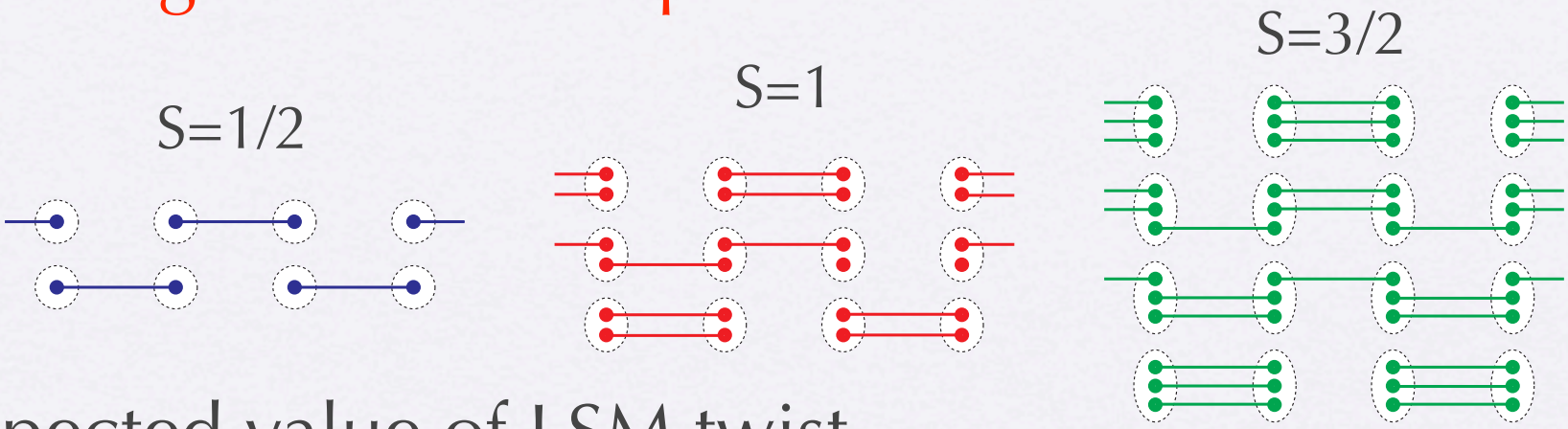
$z_L \to 0 \quad (L \to \infty)$

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

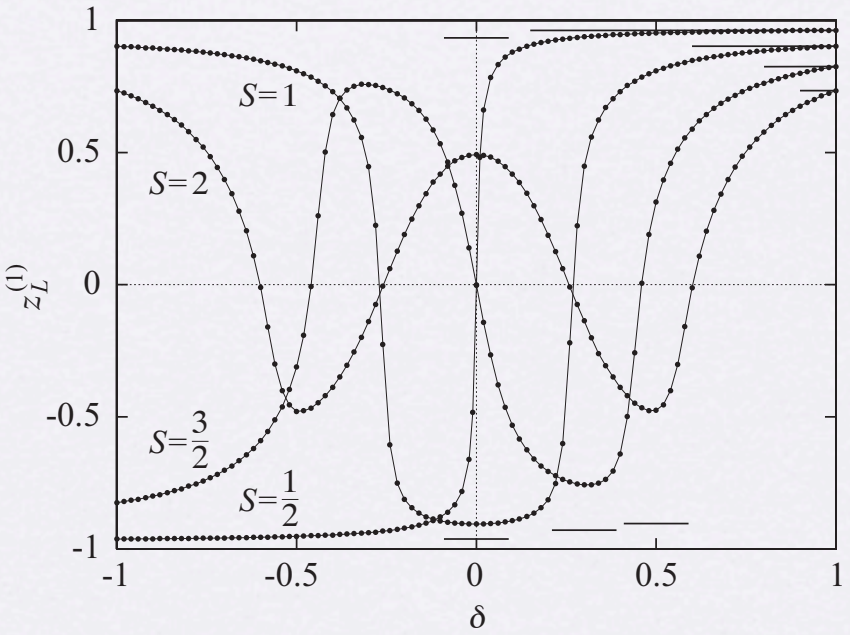


- Expected value of LSM twist-operator

  = twist order parameter

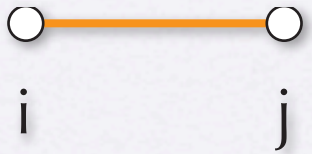
$$z_L \equiv \langle \Psi_0 | \exp[i \frac{2\pi}{L} \sum_{j=1}^{L} j S_j^z] | \Psi_0 \rangle$$

M.Nakamura and ST (2002)



Sign of Twist Order Parameter

- contribution from a dimer



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

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

$$[\cos\frac{\pi}{L}]^L \to +1$$

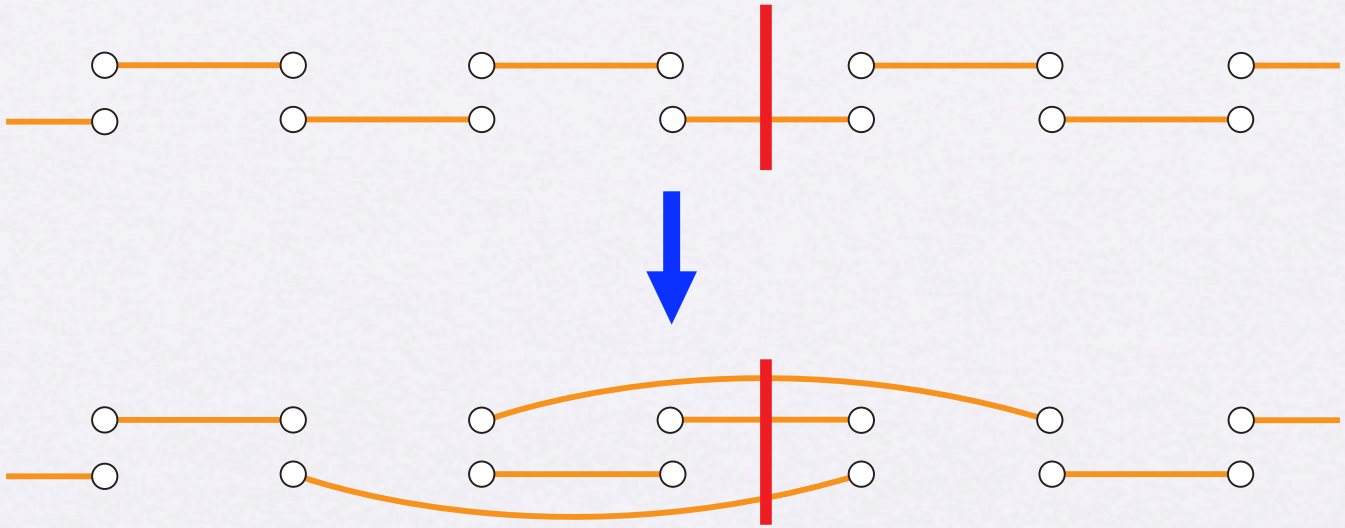
- Haldane phase: (1,1) VBS state

$$z_L \to (-1)^b$$

$$[\cos\frac{\pi}{L}]^{L-1}[\cos\frac{\pi}{L}(L-1)] \to -1$$

Effects of Randomness on z_L

- weak bond randomness
  rearrangement of local VBS pattern



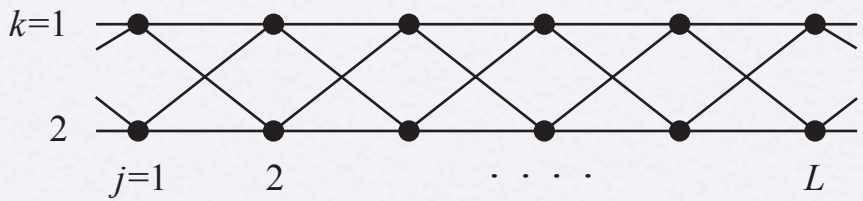
local rearrangement of VBS pattern can not change the parity at boundary

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

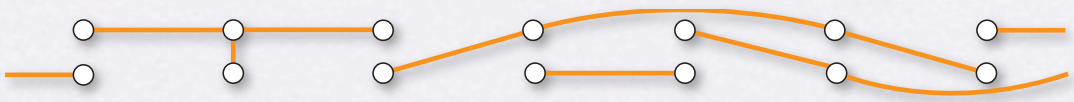


- Twist order parameter

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

- 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)"

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

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

- Contribution from a loop

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

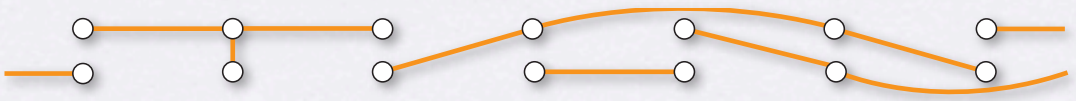
- for 2-site loop

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

= contribution from a dimer

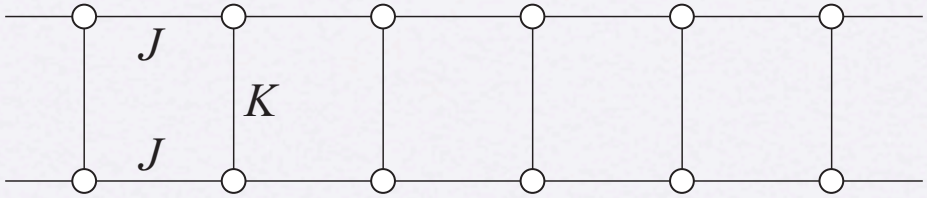
Loops vs VBS picture

- 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 ~ system size

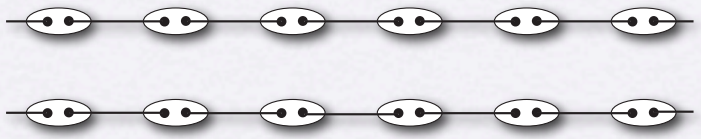


Spin-1 ladder

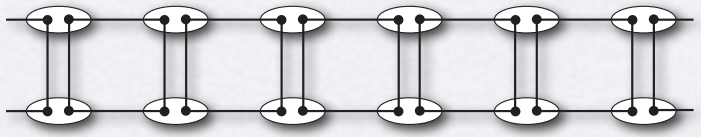
- Plaquette singlet solid (PSS) state in S=1 ladder



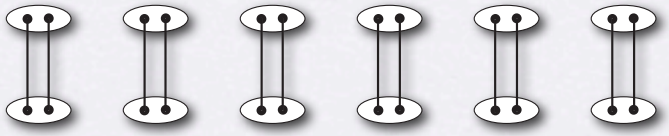
Haldane state



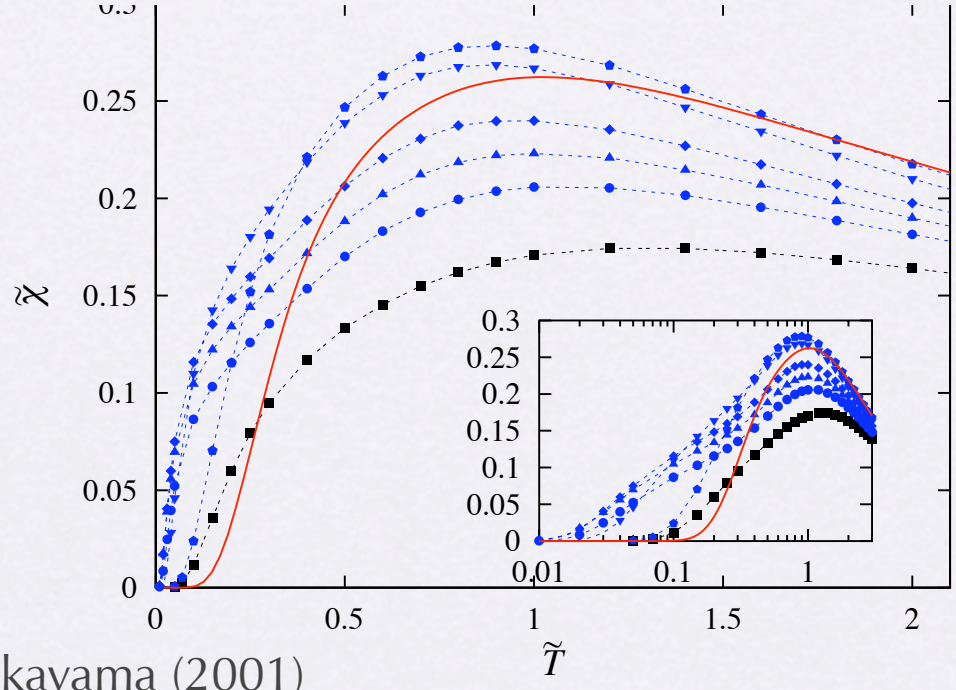
PSS state



dimer state



uniform susceptibility

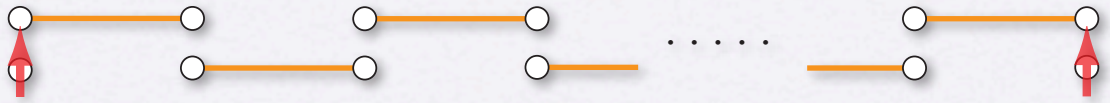


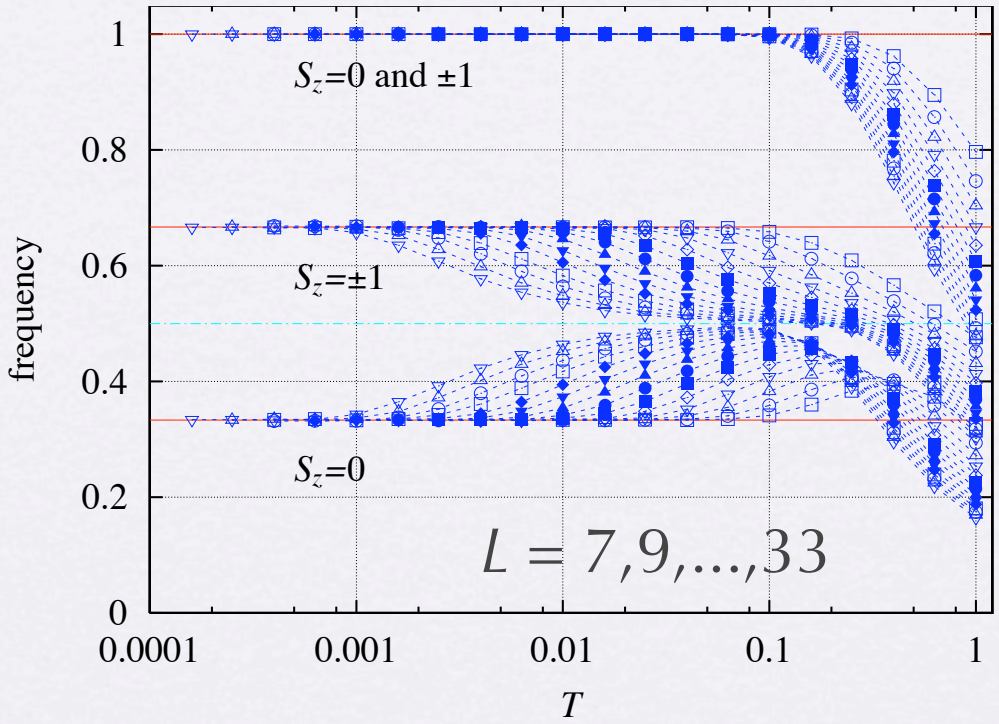
ST, M.Matsumoto, C.Yasuda, and H.Takayama (2001)

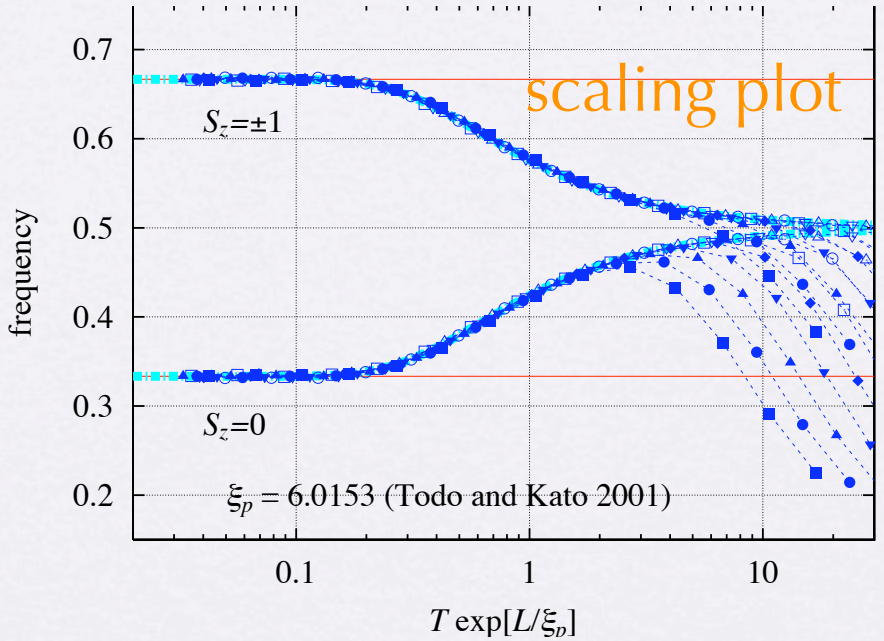
Quantum Surface Transition

Edge State of Open S=1 chain

- Open S=1 chain with odd L







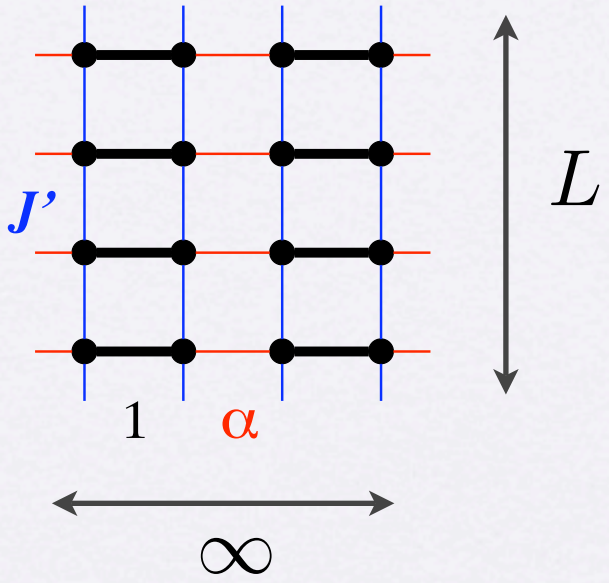
$J_{\mathrm{eff}} \approx 0.754 \exp(-L/6.01)$

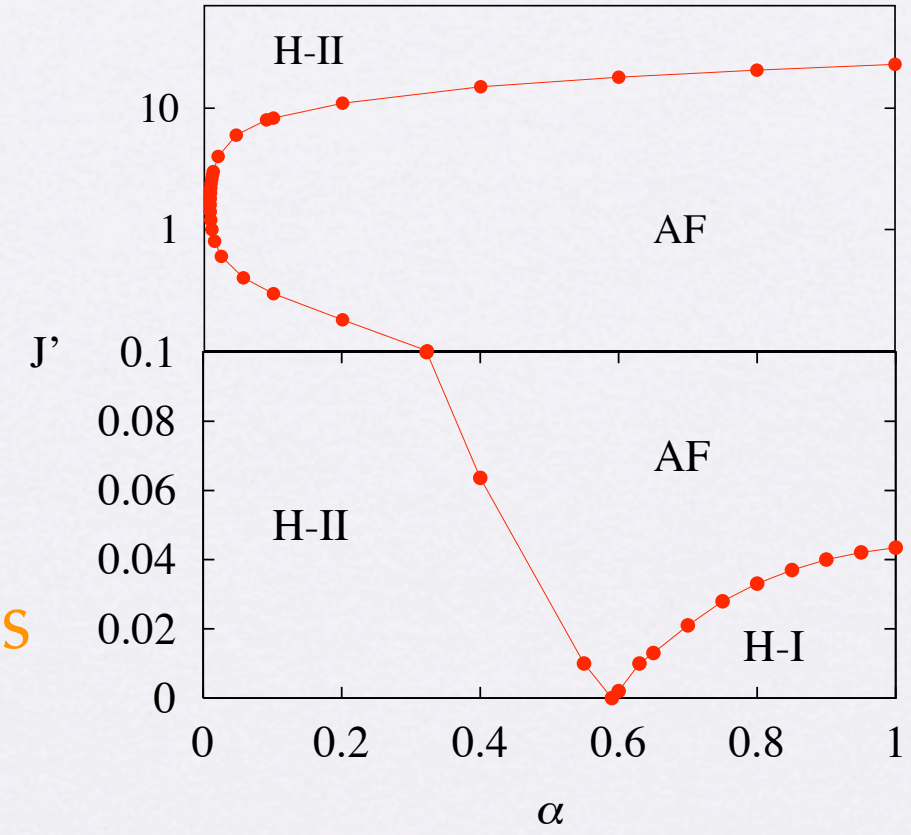
0-dim surface of 1-dim system ⇒

generalization to higher-dimensions?

Spin-1 Strips with Finite Width

$$\mathcal{H} = \sum_{i,j} \mathbf{S}_{2i,j} \cdot \mathbf{S}_{2i+1,j} + \alpha \sum_{i,j} \mathbf{S}_{2i+1,j} \cdot \mathbf{S}_{2i+2,j} + J' \sum_{i,j} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1}$$





Periodic boundary conditions
in y-direction and $L \to \infty$

What happens for open boundaries?

M.Matsumoto, et al (2002)

Open S=1 Strips

$$\mathcal{H} = \sum_{i,j} \mathbf{S}_{2i,j} \cdot \mathbf{S}_{2i+1,j} + \alpha \sum_{i,j} \mathbf{S}_{2i+1,j} \cdot \mathbf{S}_{2i+2,j} + J' \sum_{i,j} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1}$$

- 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

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

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

Effective Hamiltonian

- 9x9 Effective Hamiltonian between two rungs

$$\mathcal{H}_{\text{eff}} = \begin{pmatrix} \langle\uparrow\uparrow|\mathcal{H}'|\uparrow\uparrow\rangle & \langle\uparrow\uparrow|\mathcal{H}'|\uparrow 0\rangle & \langle\uparrow\uparrow|\mathcal{H}'|\uparrow\downarrow\rangle & \cdots & \langle\uparrow\uparrow|\mathcal{H}'|\downarrow\downarrow\rangle \\ \langle\uparrow 0|\mathcal{H}'|\uparrow\uparrow\rangle & & & & \langle\uparrow 0|\mathcal{H}'|\downarrow\downarrow\rangle \\ \cdots & & & & \cdots \\ \langle\downarrow\downarrow|\mathcal{H}'|\uparrow\uparrow\rangle & \langle\downarrow\downarrow|\mathcal{H}'|\uparrow 0\rangle & \langle\downarrow\downarrow|\mathcal{H}'|\uparrow\downarrow\rangle & \cdots & \langle\downarrow\downarrow|\mathcal{H}'|\downarrow\downarrow\rangle \end{pmatrix}$$

12 non-zero elements among 81 $\quad \mathcal{H}' = K\sum_j \mathbf{S}_{1,j}\cdot\mathbf{S}_{2,j} \quad K = 1 \text{ or } \alpha$

- comparing with Hamiltonian of spin-1 dimer $\tilde{J}\,\mathbf{S}_1\cdot\mathbf{S}_2$

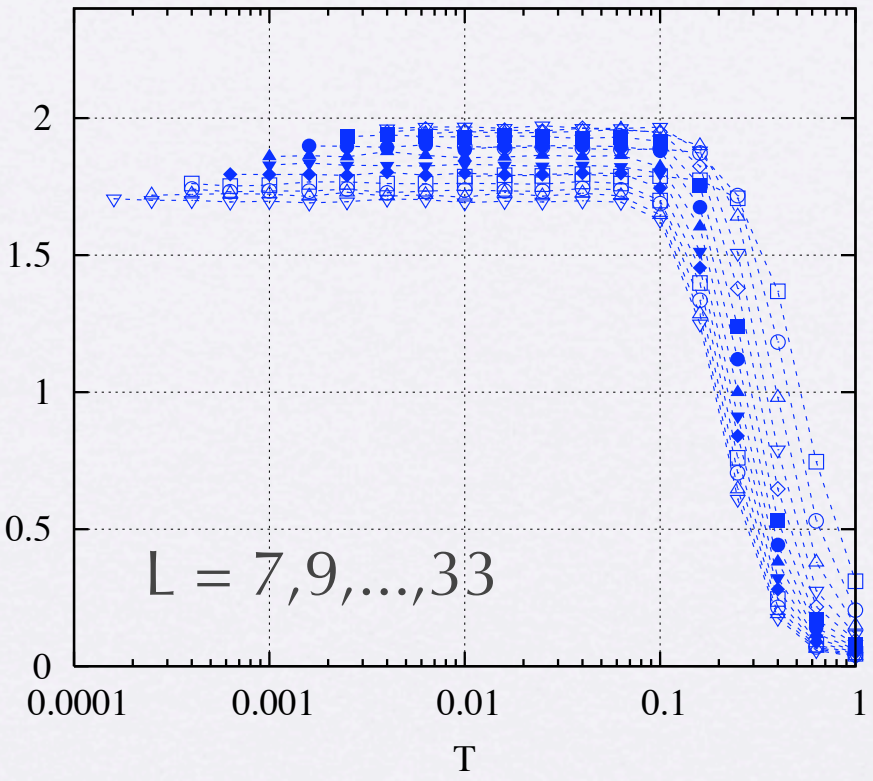
$$\tilde{J} = \langle\uparrow\uparrow|\mathcal{H}'|\uparrow\uparrow\rangle$$

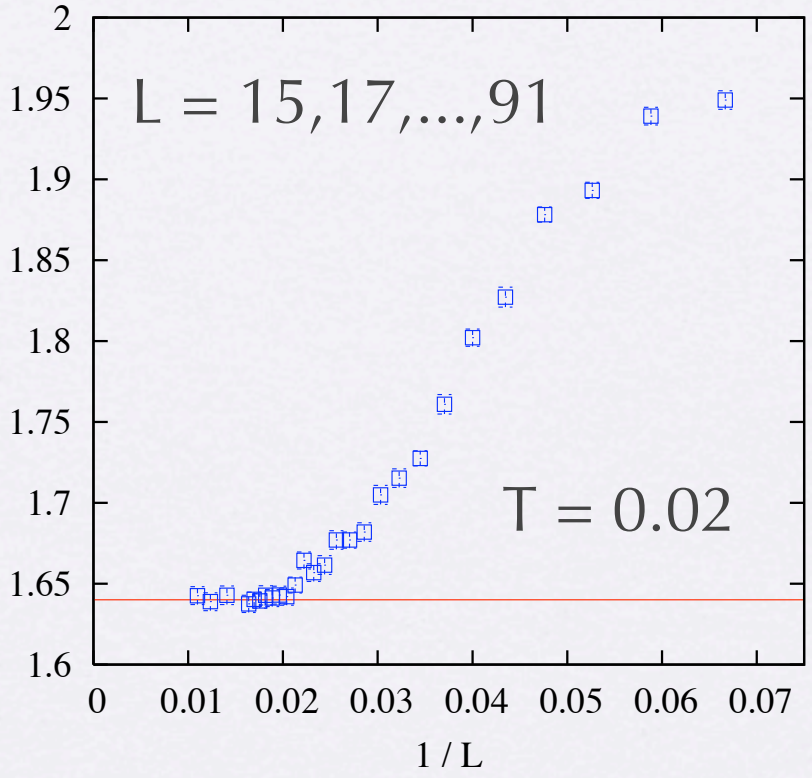
$$= K\sum_j \langle\uparrow\uparrow|\mathbf{S}_{1,j}\cdot\mathbf{S}_{2,j}|\uparrow\uparrow\rangle = K\sum_j \langle\uparrow_1|S^z_{1,j}|\uparrow_1\rangle\langle\uparrow_2|S^z_{2,j}|\uparrow_2\rangle$$

$\langle\uparrow_1|S^z_{1,j}|\uparrow_1\rangle$: z-component of j-th spin in total Sz=1 sector

QMC Results

$$C = \sum_j \langle \uparrow | S_j^z | \uparrow \rangle^2$$





No temperature dependence
at T < 0.1

converges to a finite value
for large L

Effective S=1 Chain

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

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

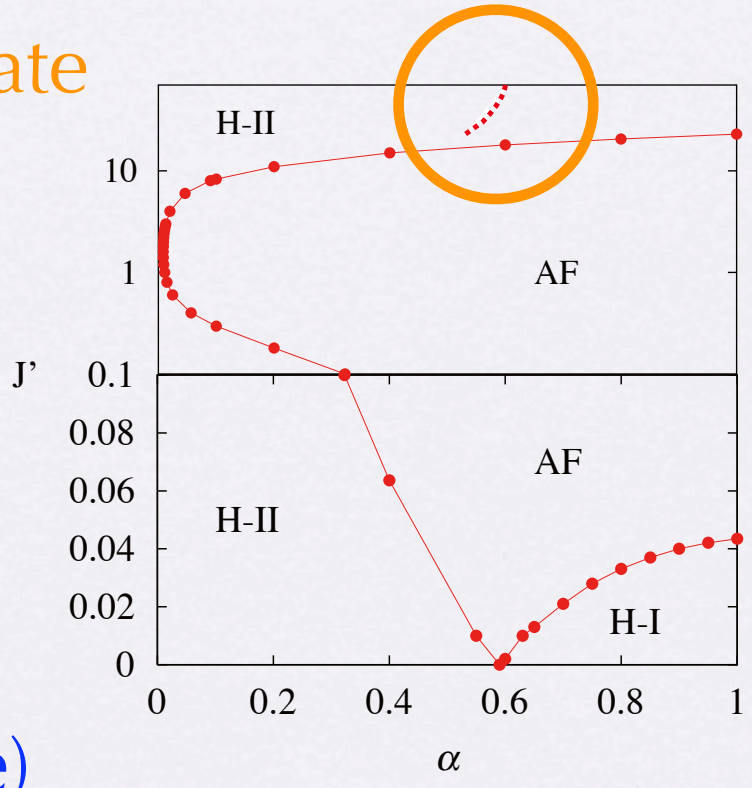
- Quantum phase transition at $\alpha_c \approx 0.587$
- Only spins near surfaces participate

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