Valence bonds and Ground-State Projection in the valence-bond basis

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Loop updates for variational and projector quantum Monte Carlo simulations in the valence-bond basis

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systems with up to 256"256 spins. Extrapolating the results to the thermodynamic limit gives *Ms*

Common bases for quantum spin systems

Lattice of S=1/2 spins, e.g., Heisenberg antiferromagnet

$$
H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_{\langle i,j \rangle} \left[S_i^z S_j^z + (S_i^+ S_j^- + S_i^- S_j^+) / 2 \right]
$$

The most common basis is that of 'up' and 'down' spins

$$
\bullet = | \uparrow \rangle = |S^z = +1/2\rangle
$$

$$
\bullet = | \downarrow \rangle = |S^z = -1/2\rangle
$$

One can also use eigenstates of two or more spins

• dimer singlet-triplet basis

The hamiltonian is more complicated in this basis - but some times can be used to solve sign problems [S. Wessel et al. Phys. Rev. B 98, 174432 (2018)]

Marshall's sign rule for bipartite antiferromagnets or bipart σ Warshall's sign rule for bipartite antiferromagnets

Consider a bipartite S=1/2 Heisenberg model

 \overline{P} , and the sign rule si

the valence-bond basis.

7.2.1 Marshall's sign rule

$$
H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_{\langle i,j \rangle} \left[S_i^z S_j^z + (S_i^+ S_j^- + S_i^- S_j^+) / 2 \right] = H_{\text{dia}} + H_{\text{off}}
$$

n E wave function to describe its ground state
 $E(\lambda | \lambda)$ and a proposed wave function to describe its ground state
and a proposed wave function to describe its ground state $\frac{1}{2}$ matrix elements are of the form ⟨τ|S⁺ ⁱ S[−] $\frac{1}{2}$ and a proposed wave function to describe its ground state

$$
|\Psi\rangle = \sum_{\sigma} \Psi(\sigma) |\sigma\rangle \qquad \sigma = \{S^z_1, \ldots, S^z_N\}
$$

In a variational calculation we minimize the energy wrt some parameters $\frac{1}{2}$ In a variational calculation we minimize the energy wrt some parameters $\sum_{n=0}^{\infty}$ the off-diagonal part depends strongly on it, through the ratio Ψ∗(τ)/Ψ∗(σ), lation we minimize the energy wrt some parameters In a variational calculation we minimize the energy wrt some parameters

$$
E = \langle \Psi | H | \Psi \rangle = \sum_{\sigma} \sum_{\tau} \Psi^*(\tau) \Psi(\sigma) \langle \tau | H | \sigma \rangle \qquad \langle \tau | S_i^- S_j^+ | \sigma \rangle \ge 0
$$

=
$$
\sum_{\sigma} |\Psi(\sigma)|^2 \langle \sigma | H_{\text{dia}} | \sigma \rangle + \sum_{\sigma} |\Psi(\sigma)|^2 \sum_{\tau} \frac{\Psi^*(\tau)}{\Psi^*(\sigma)} \langle \tau | H_{\text{off}} | \sigma \rangle
$$

of the can write which we can write the extreme variational annoach is to construct the extreme variational annoach is to construct the extreme variational annoach is to construct the extreme variation of α $\psi(\sigma)$ as an individually adjustable parameter An extreme variational approach is to consider each wave function coefficient lead to the lowest energy (i.e., for any choice of the magnitude of the wavefunction coefficients, a lower bound on the energy is obtained by assuming $\mathcal{L} = \mathcal{L} \mathcal{L}$ a approach is to consider each wave function coefficient An extreme variational approach is to consider each wave function coefficient

 \mathbf{E} et's focus on the signs (or phases) or Let's focus on the signs (or phases) of the coefficients: Let's focus on the signs (or phases) of the coefficients: Let's focus on the signs (or phases) of the coefficients:

- $-$ diagonal energy contributions independent of the signs \sim contributions independent of the signs - diagonal energy contributions independent of the sign
- $\overline{\text{or}}$ οπ-diagonal matrix e lemen $\frac{1}{\sigma}$ ($\frac{1}{\sigma}$). F must be required - off-diagonal matrix elements positive; optimal E if wave-function signs change addition the original the original terms of the change of the substitution of the wave function phase, when as $\frac{1}{2}$ taken to be just a sign superiorment is real (since the model of the model is real), is chosen as $\frac{1}{2}$ - off-diagonal matrix elements positive; optimal E if wave-function signs change

$$
\Psi^*(\tau)/\Psi^*(\sigma) = e^{i\delta} |\Psi(\tau)|/|\Psi(\sigma)|
$$

 $\frac{\psi(\tau)}{\psi(\tau)}$ matshall s sight tule Marshall's sign rule

 $\Psi^*(\tau)/\Psi^*(\sigma) = e^{i\delta} |\Psi(\tau)|/|\Psi(\sigma)|$ E must be real (*w* can also be real)

Internationally choice the magnitude of the hamiltonian is real in the magnitude of the hamiltonian is real in the hamiltonian is real in the magnitude of $Marshall's cion rule$ minimum for all negative signs

corresponding matrix element is non-zero. Thus, the ground-state wave-function α is non-zero. Thus, the ground-state wave-function α

$$
\frac{\text{sign rule}}{S(z)} = (-1)^{n_{A\uparrow}} \quad \text{sign always} \quad \Psi(\tau)/\Psi(\sigma) \le 0
$$

where nA↑ is the number of α spins on substitute α spins on substitute α spins on spins α spins fli

sign always

 $\{sign[\Psi(S_1^2,\ldots, S_N^2)] = (-1)^{n_A}\}$ changes when two spins flinned fact possible to choose phases such that this condition is always fulfilled. Per $\text{sign}[\Psi(S_1^z,\ldots,S_N^z)] = (-1)^{n_{A\uparrow}}$ Sign always
changes when two spins flipped elements are positive. It is the wave function phases could be wave function phases could be wave function phases could be wave function of the wave function $\mathcal{L}_\mathbf{p}$ $\mathcal{L}(\mathcal{L}_{\mathcal{D}})$ is a sign changes when two spins flipped changes when two spins flipped changes when two spi

rule (7.6), which is named after Marshall $\mathcal{P}(\mathcal{S})$ and hand $\mathcal{P}(\mathcal{S})$ and hamiltonian conserves $\mathcal{P}(\mathcal{S})$

 \mathcal{L}_A CHAPTER 7. VALENCE BOND METHODS \mathcal{L}_A CHAPTER 7. VALENCE BOND METHODS \mathcal{L}_A

The valence bond basis for S=1/2 spins

 $(i, j) = (|\uparrow_i \downarrow_j \rangle - |\downarrow_i \uparrow_j \rangle)/$ Valence-bonds between sublattice A, B sites $(i, j) = (|\uparrow_i \downarrow_j \rangle - |\downarrow_i \uparrow_j \rangle)/\sqrt{2}$ Basis states; singlet products (obey Marshall's sign rule)

$$
|V_r\rangle = \prod_{b=1}^{N/2} (i_{rb}, j_{rb}), \quad r = 1, \dots (N/2)!
$$

The valence bond basis is overcomplete and non-orthogonal • expansion of arbitrary singlet state is not unique

 $|\Psi\rangle = \sum f_r |V_r\rangle$ (all f_r positive for non-frustrated system) *r*

All valence bond states overlap with each other

 $\langle V_l | V_r \rangle = 2^{N_o - N/2}$ $N_o =$ number of loops in overlap graph

Spin correlations from loop structure

$$
\frac{\langle V_l | \vec{S}_i \cdot \vec{S}_j | V_r \rangle}{\langle V_l | V_r \rangle} = \begin{cases} \frac{3}{4}(-1)^{x_i - x_j + y_i - y_j} & (i, j \text{ in same loop})\\ 0 & (i, j \text{ in different loops}) \end{cases}
$$

More complicated matrix elements (e.g., dimer correlations) are also related to the loop structure

K.S.D. Beach and A.W.S., Nucl. Phys. B 750, 142 (2006)

Projector Monte Carlo in the valence-bond basis

Liang, 1991; AWS, Phys. Rev. Lett 95, 207203 (2005)

*(-H)*n projects out the ground state from an arbitrary state

$$
(-H)^n |\Psi\rangle = (-H)^n \sum_i c_i |i\rangle \to c_0 (-E_0)^n |0\rangle
$$

S=1/2 Heisenberg model

$$
H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = -\sum_{\langle i,j \rangle} H_{ij}, \quad H_{ij} = (\frac{1}{4} - \vec{S}_i \cdot \vec{S}_j)
$$

Project with string of bond operators

$$
\sum_{\{H_{ij}\}} \prod_{p=1}^n H_{i(p)j(p)} |\Psi\rangle \to r |0\rangle \qquad (\text{r} = \text{irrelevant})
$$

Action of bond operators

$$
H_{ab}|...(a, b)...(c, d)... \rangle = |...(a, b)...(c, d)... \rangle
$$

\n
$$
H_{bc}|...(a, b)...(c, d)... \rangle = \frac{1}{2}|...(c, b)...(a, d)... \rangle
$$

Simple reconfiguration of bonds (or no change; diagonal)

- no minus signs for A→B bond 'direction' convention
- sign problem does appear for frustrated systems

Sampling the wave function

Simplified notation for operator strings

$$
\sum_{\{H_{ij}\}} \prod_{p=1}^n H_{i(p)j(p)} = \sum_k P_k, \quad k = 1, \dots N_b^n
$$

Simplest trial wave function: a basis state *[|]Vr*

 $P_k|V_r\rangle = W_{kr}|V_r(k)\rangle$

2

The weight *Wkr* of a path is given by the number of off-diagonal operations ('bond flips') nflip

$$
W_{kr} = \left(\frac{1}{2}\right)^{n_{\text{flip}}} \quad n = n_{\text{dia}} + n_{\text{flip}}
$$

6-site chain $|\Psi\rangle$ P_{ν}

$$
H_{ab}|...(a,b)...(c,d)... \rangle = |...(a,b)...(c,d)... \rangle
$$

$$
H_{bc}|...(a,b)...(c,d)... \rangle = \frac{1}{2}|...(c,b)...(a,d)... \rangle
$$

Note: all paths contribute - no 'dead' (W=0) paths **Sampling:** Trivial way: Replace m (m ≈ 2-4) operators at random $P_{\text{accept}} =$ $\sqrt{1}$ $\gamma^{n_{\text{flip}}-n_{\text{flip}}^{\text{old}}}$

The state has to be re-propagated with the full operator string

• More efficient updating scheme exists (later....)

Expectation values: $\langle A \rangle = \langle 0 | A | 0 \rangle$

Strings of singlet projectors

$$
P_k = \prod_{p=1}^n H_{i_k(p)j_k(p)}, \quad k = 1, \dots, N_b^n \quad (N_b = \text{ number of interaction bonds})
$$

We have to project bra and ket states

$$
\sum_{k} P_{k} |V_{r}\rangle = \sum_{k} W_{kr} |V_{r}(k)\rangle \rightarrow (-E_{0})^{n} c_{0} |0\rangle
$$

$$
\sum_{g} \langle V_{l} | P_{g}^{*} = \sum_{g} \langle V_{l}(g) | W_{gl} \rightarrow \langle 0 | c_{0} (-E_{0})^{n} \rangle
$$

6-spin chain example:

$$
\langle A \rangle = \frac{\sum_{g,k} \langle V_l | P_g^* A P_k | V_r \rangle}{\sum_{g,k} \langle V_l | P_g^* P_k | V_r \rangle}
$$

=
$$
\frac{\sum_{g,k} W_{gl} W_{kr} \langle V_l(g) | A | V_r(k) \rangle}{\sum_{g,k} W_{gl} W_{kr} \langle V_l(g) | V_r(k) \rangle}
$$

- Monte Carlo sampling of operator strings
- Estimators based on transition graphs

Sampling an amplitude-product state

- A better trial state leads to faster n convergence
- bond-amplitude product state [Liang, Doucot, Anderson, 1990]

 $|\Psi_0\rangle = \sum \prod$ *k b*=1 *N /*2 $h(x_{rb}, y_{rb}) | V_k \rangle$

Update state by reconfiguring two bonds

If reconfiguration accepted

- calculate change in projection weight
- used for final accept/reject prob.
- S. Liang [PRB 42, 6555 (1990)]
- used parametrized state amplitudes
- determined parameters variationally
- improved state by projection

$$
\sum_{\substack{\text{X} \text{accept} \\ \text{Y}_l \mid \text{Y}_l}}^{h(x_a, y_a)h(x_b, y_b)}
$$

 $P_{\text{accept}} =$

Variational wave function (2D Heisenberg)

All amplitudes h(x,y) can be optimized

[J. Lou and A.W.S., PRB 2007, AWS and H.-G. Evertz, PRB 2010]

- variational energy error 50% smaller than previously best (<0.1%)
	- spin correlations deviate by less than 1% from exact values
- amplitudes decay as ∼1/r3 $\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1-\frac{1}{\sqrt{1+\frac{1}{\sqrt{1+\frac{1}{\sqrt{1+\frac{1}{\sqrt{1+\frac{1}{\sqrt{1+\frac{1$

Variational energy can be further improved by including optimized bond correlations; Lin et al. PRB 2012 (posted on course web site) sible and would require other rules for the boundary loops%.

Loop updates in the valence-bond basis More efficient ground state QMC algorithm → larger lattices

AWS and H. G. Evertz, PRB 2010

Put the spins back in a way compatible with the valence bonds

 $(a_i, b_i)=(\uparrow_i\downarrow_j-\downarrow_i\uparrow_j)/$ √ 2

and sample in a combined space of spins and bonds

Loop updates similar to those in finite-T methods (world-line and stochastic series expansion methods)

- good valence-bond trial wave functions can be used
- larger systems accessible
- sample spins, but measure using the valence bonds

Improved Valence-bond Estimators

The transition graphs give us improved estimators automatically $|V_r\rangle$ $\langle V_l|V_r\rangle$

Put the spins back in:

- staggered spin configurations on each loop
- two 'orientations' (loop flips)

Average over all the two orientations of all the loops

- 2^{No} configurations -> determines overlap $\langle V_l | V_r \rangle = 2^{N_{\circ} - N/2}$

$$
\langle M_{z,\rm stagg}^2 \rangle = \frac{1}{4} \sum_{C=1}^{N_{\rm clus}} \langle n_C^2 \rangle
$$

Some off-diagonal operators can also be considered

$$
\frac{\langle V_l | \vec{S}_i \cdot \vec{S}_j | V_r \rangle}{\langle V_l | V_r \rangle} = \begin{cases} \frac{3}{4}(-1)^{x_i - x_j + y_i - y_j} & \text{(i,j in same loop)} \\ 0 & \text{(i,j in different loops)} \end{cases}
$$

4-spin correlations depend on 2 loops, etc

T>0 and T=0 algorithms side-by-side by
 c
 c \mathbf{S} id
id patible spin states %*Zj* ces " are also indicated. There are three loops, part of which consistent which consis

Finite-temperature QMC (world lines, SSE,...)

periodic time boundary conditions

• Computer implementations similar

columna of and open circles represent and open circles represent A and ↓ spins of com-

of VBs. Expectation values are evaluated at the midpoint indicated

are enormous (as in the classical case, leading to a much reduced dynamic exponent)

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

tive world line system for the system of the system for the system for the system for the system for the syste in the SSE method in performance relative to \mathbf{r} . Trial state can conserve relevant ground state quantum numbers $(S=0, k=0,...)$

Convergence

 32×32 Heisenberg

ANDERS W. SANDVIK AND HANS GERD EVERTZ PHYSICAL REVIEW B **82**, 024407 !2010"

mined by minimizing the energy in two independent optimizations, which is two independent optimizations, which

- m/N $>> e_0/\Delta$
- in valence-bond basis Δ is the singlet-singlet gap \mathcal{F}_1 , the energy \mathcal{F}_2 is the energy \mathcal{F}_2 . The energy interpretation of the energy \mathcal{F}_1 and subject-subjected panel **subject**
- \bullet trial state also can have fixed momentum k=0 (e.g., ampl. product state) - only k=0 excited states (gap) with amplitudes *h*!*r*"= 1/*r^p* !*p*=2,3,4" as well as with *h*!*x*, *y*" deter-

Results for 2D Heisenberg model

Sublattice magnetization

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

Long-range order: **<ms2> > 0 for N→∞**

Quantum Monte Carlo

- finite-size calculations
- no approximations
- extrapolation to infinite size

Reger & Young (world-line) 1988 $m_s = 0.30(2)$

 ≈ 60 % of classical value

AWS & HG Evertz 2010

 $m_s = 0.30743(1)$

 $H = J$

 $\sqrt{}$

 $S_i \cdot S_j$

 $\langle i,j \rangle$

Frustrated systems

Consider the full valence-bond basis, including

- normal bonds, connecting A,B spins (sublattices)
- frustrated bonds, connecting A, A or B, B

For a non-frustrated system

• projection eliminates frustarted bonds

For a frustrated system

- frustrated bonds remain and cause a sign problem
- frustrated bonds can be eliminated using over-completeness

In a simulation, one of the branches can be randomly chosen

• but there is a sign problem