The spin stiffness at criticality

For a quantum-critical point with dynamic exponent z:

$$\rho_s \sim L^{-(d+z-2)}$$

$d=2, z=1 \rightarrow$ plot $L\rho_s$ vs $g$ for different $L$

• curves should cross (size independence) at $g_c$
• x- and y-stiffness different in this model

Finite-size scaling in agreement with $z=1$, $g_c \approx 1.9094$
Valence-bond basis and resonating valence-bond states

As an alternative to single-spin $\uparrow$ and $\downarrow$ states, we can use singlets and triplet pairs

- **Static dimers** (complete basis)
- **Arbitrary singlets** (overcomplete in singlet subspace)
- **One triplet in the “singlet soup”** (overcomplete in triplet subspace)

In the valence-bond basis (b,c) one normally includes pairs connecting two groups of spins - sublattices A and B (bipartite system, no frustration)

$$ (a, b) = (\uparrow_a \downarrow_b - \downarrow_a \uparrow_b)/\sqrt{2} \quad a \in A, b \in B $$

Superpositions, “resonating valence-bond” (RVB) states

$$ |\Psi_s\rangle = \sum_\alpha f_\alpha |(a_1^\alpha, b_1^\alpha) \cdot \cdot \cdot (a_{N/2}^\alpha, b_{N/2}^\alpha)\rangle = \sum_\alpha f_\alpha |V_\alpha\rangle $$

Coefficients $f_\alpha > 0$ for bipartite (unfrustrated) Heisenberg systems

- corresponds to **Marshall’s sign rule**: $\text{sign}=(-1)^{N\uparrow(A)}$, $N\uparrow(a) = \# \text{ of spin-}\uparrow \text{ on sublattice } A$
Calculating with valence-bond states

All valence-bond basis states are non-orthogonal
- the overlaps are obtained using transposition graphs (loops)

Each loop has two compatible spin states \( \langle V_{\beta} | V_{\alpha} \rangle = 2^{N_{\text{loop}} - N/2} \)

This replaces the standard overlap for an orthogonal basis; \( \langle \beta | \alpha \rangle = \delta_{\alpha \beta} \)

Many matrix elements can also be expressed using the loops, e.g.,

\[
\frac{\langle V_{\beta} | S_i \cdot S_j | V_{\alpha} \rangle}{\langle V_{\beta} | V_{\alpha} \rangle} = \begin{cases} 
0, & \text{for } \lambda_i \neq \lambda_j \\
\frac{3}{4} \phi_{ij}, & \text{for } \lambda_i = \lambda_j
\end{cases}
\]

\( \lambda_i \) is the loop index (each loop has a label), staggered phase factor

\[
\phi_{ij} = \begin{cases} 
-1, & \text{for } i, j \text{ on different sublattices} \\
+1, & \text{for } i, j \text{ on the same sublattice}
\end{cases}
\]

Solution of the frustrated chain at the Majumdar-Ghosh point

\[ H = \sum_{i=1}^{N} \left[ J_1 S_i \cdot S_{i+1} + J_2 S_i \cdot S_{i+2} \right] \]

We will show that these are eigenstates when \( J_2/J_1 = 1/2 \)

Write \( H \) in terms of singlet projectors

\[ H = -\sum_{i=1}^{N} (C_{i,i+1} + gC_{i,i+2}) + N \frac{1+g}{4}, \quad C_{ij} = -(S_i \cdot S_j - \frac{1}{4}) \]

Useful valence-bond results
(easy to prove, just write as \( \uparrow \) and \( \downarrow \) spins)

Act with one “segment” of the terms of \( H \) on a VB state (\( J_1 = 1, J_2 = g \)) :

\[ \begin{align*}
|\Psi_A\rangle &= |(1,2)(3,4)(5,6)\cdots\rangle \\
|\Psi_B\rangle &= |(N,1)(2,3)(4,5)\cdots\rangle
\end{align*} \]

Eigenstate for \( g = 1/2 \); one can also show that it’s the lowest eigenstate (more difficult)
Amplitude-product states

Good variational ground state for bipartite models can be constructed

$$|\Psi_s\rangle = \sum_\alpha f_\alpha |(a_1^\alpha, b_1^\alpha) \cdots (a_{N/2}^\alpha, b_{N/2}^\alpha)\rangle = \sum_\alpha f_\alpha |V_\alpha\rangle$$

Let the wave-function coefficients be products of “amplitudes” (real positive numbers)

$$f_\alpha = \prod_r h(r)^{n_\alpha(r)},$$

Liang, Doucot, Anderson (PRL, 1990)

$\mathbf{r}$ is the bond length ($n(r) =$ number of length $\mathbf{r}$ bonds)

The amplitudes $h(\mathbf{r})$ are adjustable parameters

• use some optimization method to minimize $E=\langle H \rangle$

Variational QMC method

Given $h(\mathbf{r})$, one can study the state using Monte Carlo sampling of bonds

• elementary two-bond moves
  • Metropolis accept/reject
• loop updates when spins are included
  • more efficient

2D Heisenberg results

• $h(\mathbf{r}) = 1/r^3$

• good ground state properties
  • error in $E < 0.1\%$, error in $m_s < 1\%$
**Projector Monte Carlo in the valence-bond basis**


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

\[ (-H)^n |\Psi\rangle = (-H)^n \sum_i c_i |i\rangle \rightarrow c_0 (-E_0)^n |0\rangle \]

**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

\[ \sum \prod_{\{H_{ij}\}} H_{i(p)j(p)} |\Psi\rangle \rightarrow r |0\rangle \quad (r \text{ irrelevant}) \]

**Action of bond operators**

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

\[ H_{bc} |...(a, b)...(c, d)...\rangle = \frac{1}{2} |...(c, b)...(a, d)...\rangle \quad (i, j) = (|\uparrow_i \downarrow_j\rangle - |\downarrow_i \uparrow_j\rangle) / \sqrt{2} \]

Simple reconfiguration of bonds (or no change; diagonal)

- no minus signs for A→B bond ‘direction’ convention
- sign problem does appear for frustrated systems
Expectation values: $\langle A \rangle = \langle 0 | A | 0 \rangle$

Strings of singlet projectors

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

We have to project bra and ket states

$$\sum_k P_k |V_r\rangle = \sum_k W_{kr} |V_r(k)\rangle \rightarrow (-E_0)^n c_0 |0\rangle$$

$$\sum_g \langle V_l | P^*_g = \sum_g \langle V_l(g) | W_{gl} \rightarrow \langle 0 | c_0 (-E_0)^n$$

6-spin chain example:

Monte Carlo sampling of operator strings
More efficient ground state QMC algorithm → larger lattices

Loop updates in the valence-bond basis

AWS and H. G. Evertz, ArXiv:0807.0682

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

\[(a_i, b_i) = (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j) / \sqrt{2}\]

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

Friday, April 23, 2010
J-Q model: T=0 results obtained with valence-bond QMC

Two different models: J-Q$_2$ and J-Q$_3$

\[ H_1 = -J \sum_{\langle ij \rangle} C_{ij} \]
\[ H_2 = -Q_2 \sum_{\langle ijk \rangle} C_{kl} C_{ij} \]
\[ H_3 = -Q_3 \sum_{\langle ijklmn \rangle} C_{mn} C_{kl} C_{ij} \]

Studies of J-Q$_2$ model and J-Q$_3$ model on L×L lattices with L up to 64

Exponents \( \eta_s, \eta_d, \) and \( \nu \) from the squared order parameters

\[ D^2 = \langle D_x^2 + D_y^2 \rangle, \quad D_x = \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+x}, \quad D_y = \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+y} \]

\[ M^2 = \langle \mathbf{M} \cdot \mathbf{M} \rangle, \quad M = \frac{1}{N} \sum_{i} (-1)^{x_i+y_i} \mathbf{S}_i \]
Using coupling ratio
\[ q = \frac{Q_p}{Q_p + J}, \quad p = 2, 3 \]

- AF order for \( q \to 0 \)
- VBS order for \( q \to 1 \)

**J-Q\(_2\) model; \( q_c = 0.961(1) \)**

\[ \eta_s = 0.35(2) \]
\[ \eta_d = 0.20(2) \]
\[ \nu = 0.67(1) \]

**J-Q\(_3\) model; \( q_c = 0.600(3) \)**

\[ \eta_s = 0.33(2) \]
\[ \eta_d = 0.20(2) \]
\[ \nu = 0.69(2) \]

**Exponents universal (within error bars)**

- still higher accuracy desired (in progress)
- there may be log-corrections (see arXiv:1001.4296)
Columnar or plaquette VBS?

QMC sampled state in the valence-bond basis

\[ |0\rangle = \sum_{k} c_k |V_k\rangle \]

Joint probability distribution \( P(D_x, D_y) \) of x and y columnar VBS order parameters

\[
D_x = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{x_i} \mathbf{S}_i \cdot \mathbf{S}_{i+x} | \mathbf{V}_p \rangle}{\langle V_k | \mathbf{V}_p \rangle} 
\]

\[
D_y = \frac{\langle V_k | \frac{1}{N} \sum_{i=1}^{N} (-1)^{y_i} \mathbf{S}_i \cdot \mathbf{S}_{i+y} | \mathbf{V}_p \rangle}{\langle V_k | \mathbf{V}_p \rangle} 
\]

4 peaks expected in VBS phase
- \( Z_4 \)-symmetry unbroken in finite system

Friday, April 23, 2010
**VBS fluctuations** in the theory of deconfined quantum-critical points

- plaquette and columnar VBS “degenerate” at criticality
- $\mathbb{Z}_4$ “lattice perturbation” irrelevant at critical point
  - and in the VBS phase for $L<\Lambda\sim\xi^a$, $a>1$ (spinon confinement length)
- emergent $U(1)$ symmetry
- ring-shaped distribution expected for $L<\Lambda$

No sign of cross-over to $\mathbb{Z}_4$ symmetric order parameter seen in the $J-Q_2$ model
- length $\Lambda > 32$

Order parameter histograms $P(D_x, D_y)$, J-Q$_3$ model


This model has a more robust VBS phase

• can the symmetry cross-over be detected?

$\int dr \int d\phi P(r, \phi) \cos(4\phi)$

VBS symmetry cross-over

• $Z_4$-sensitive order parameter

$D_4 = \int r dr \int d\phi P(r, \phi) \cos(4\phi)$

Finite-size scaling gives U(1) (deconfinement) length-scale

$\Lambda \sim \xi^a \sim q^{-a\nu}$

$\alpha \approx 1.20 \pm 0.05$

$L = 32$

$q = 0.635$

$q_c \approx 0.60$

$L = 32$

$q = 0.85$

$L = 32$

$q_c = 0.635$

$q = 0.85$

$L = 32$

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