6. PEPS - III: PEPS via finite-size MPS

**Goal:** reduce PEPS computations to familiar MPS computations (reduce core)

[Uwerstraete 2004] (spin 1/2 Heisenberg)

[Mug 2007] (2D XY model; uniform field)

**Strategy:**

(i) \( \langle \Psi_8 \rangle = e^{-\mathcal{H}_{ST}} \langle \Psi_A \rangle \quad (D \to D^3 d) \)

(ii) Variational ansatz:

\[
K = \sum_{\text{pairs}} \langle \Psi_A \mid \Psi_A \rangle \quad \text{should be minimized,}
\]

one term at a time:\n
\[
\langle \Psi_A \mid \Psi_A \rangle, \quad \langle \Psi_A \mid \Psi_A \rangle
\]

\[
\delta = \frac{\partial K}{\partial \Psi_{\text{in}}} \Rightarrow \text{Ni}; \quad \text{Ai} = \text{Wi}, \quad \text{yields}; \quad \text{Ai} = \text{Ai}
\]

Computation of \( \text{Ni} \), \( \text{Wi} \): repeated application of H0's to MPS.

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**6. PEPS - IV: PEPS - Torber - finite adiabatic** [Mug 2007]

\[
\mathcal{H} = \underline{\mathcal{H}_{el}} + \underline{\mathcal{H}_{sc}} + \underline{\mathcal{H}_{ex}} + \underline{\mathcal{H}_{int}}
\]

\[
e^{-\mathcal{H}_{ST}} = e^{-\mathcal{H}_{ex}} e^{-\mathcal{H}_{sc}} e^{-\mathcal{H}_{el}} e^{-\mathcal{H}_{int}} + O(\tau^2)
\]

\[
\langle \Psi_0 \rangle = e^{-\mathcal{H}_{ex} \mathcal{H}_{sc} \mathcal{H}_{el} \mathcal{H}_{int}} \langle \Psi_A \rangle
\]

\[
\text{Torber - finite adiabatic}
\]

\[
\begin{align*}
\text{SU2} & = D_2 = \frac{2D^2}{2D^2} = \frac{2D^2}{2D^2} \\
\text{linearized} & = \text{linearized}
\end{align*}
\]

\[
\text{near} \quad \text{vanishingly small}: \quad K = \sum \langle \Psi_0 \rangle - \langle \Psi_0 \rangle^2
\]
(ii) Variational compression

We need \( \langle \Psi_A | \Psi_A \rangle \)

\[
E = \sum_j A_j^\sigma \otimes A_j^\sigma
\]

Iteratively we use "\(\text{mps}\)" or "\(\text{mpo}\)"

\[
\begin{array}{cccc}
\downarrow & \downarrow & \downarrow & \\
D^0 & D^1 & D^2 & D^3
\end{array}
\]

\[
\text{Variational optimisation} \quad D^2
\]

\[
\text{Last step:} \quad \begin{array}{cccc}
\downarrow & \downarrow & \downarrow & \\
D^1 & D^2 & D^3 & D^4
\end{array} \Rightarrow \langle \Psi | \Psi \rangle \Rightarrow W_i, N_i
\]

\[\text{Note: } N_i A_i = W_i \Rightarrow A_i\]

Results for ground state energy

[Mar 2007]

FIG. 3. Energy as a function of time for the imaginary time evolution of the system of hard-core bosons on a \(4 \times 4\) lattice. The evolutions are performed sequentially with PEPS of virtual dimension \(D = 2, D = 3, D = 4,\) and \(D = 5\). The times at which \(D\) is increased are indicated by vertical lines. For comparison, the exact ground-state energy, the exact imaginary time evolution, and the energy of the optimal Gutzwiller ansatz are included.

Back dimension was increased at three discrete times \(\Rightarrow\) ground state energy decreases.

FIG. 4. Energy as a function of time for the imaginary time evolution of the system of hard-core bosons on a \(11 \times 11\) lattice. The evolutions are performed sequentially with PEPS of virtual dimension \(D = 2, D = 3, D = 4,\) and \(D = 5\). The times at which \(D\) is increased are indicated by vertical lines. For comparison, the energy of the optimal Gutzwiller ansatz is included.
Accuracy & Numerical performance

\[ K \leq 10^{-3} \quad \text{for } D = 2 \]
\[ 10^{-4} \quad \text{for } D = 3, 4 \]
\[ |\langle \tilde{n} \rangle - 14| \approx 10^{-5} \]

should be conserved

Main bottleneck: # multiplications = O(D^2), memory = O(D^8)

11x11 lattice with D = 5 took 55 hours for 1 time step,
and required 2 GB memory.

“going beyond D = 5 is difficult at the moment”
(2009)

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4. Infinite PEPS (iPEPS) via infinite PEPS methods

Jordan 2006] (2D quantum Ising)

Goal: exploit translational invariance, known holes from iTEBD

![Diagram of PEPS transformation](image)

(i) choose unit cell, adjacency A, B
(ii) construct zeroth environment \( \tilde{g} \), using iTEBD rules, transform
(iii) \( e^{-H_{SE}} = \tilde{A} \cdot \tilde{B} \)
(iv) construct \( \tilde{A}, \tilde{B} \) with “time-evolved environment” \( \tilde{g} \)
(v) minimal optimization to compress: \( A', B' \)

repeat to (iii).
(i) Identify active sites

Translational symmetry:

iPEPS obeys an $\mathcal{O}(d^2D^d)$ parafermion

\[ \mathcal{P} : \text{single-layer iPEPS} \]

\[ \mathcal{E} : \text{double-layer iPEPS} \]

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FIG. 1 (color online). Diagrammatic representations of (a) a PEPS tensor $A_{\text{indiff}}$ with one physical index $s$ and four inner indices $u$, $d$, $l$, and $s'$; (b) local detail of the tensor network $\mathcal{P}$ for an iPEPS. Copies of tensors $A$ and $B$ are connected through four types of links; (c) reduced tensor $a$ of Eq. (2); and (d) local detail of the tensor network $\mathcal{E}$. 

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(ii) Contract out environment

Approximate double-layer iPEPS by infinite strip

\[ \mathcal{P} = \mathcal{F}(a, b, c, d, c', d') \]

Then approximate strip $\mathcal{F}$ by 6-norm term

\[ \mathcal{P} = \mathcal{F}(E_1, \ldots, E_6) \]

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FIG. 2 (color online). The environment $\mathcal{G}[P_{\mathcal{F}}, P_{\mathcal{G}}]$ for a link of type $r$ is first approximated by an infinite strip $\mathcal{F}[P_{\mathcal{F}}, P_{\mathcal{G}}]$ and then by a six-tensor network $\mathcal{G}[P_{\mathcal{F}}, P_{\mathcal{G}}]$. These reductions can be performed according to either a vertical or horizontal scheme (b) or a diagonal scheme (c). Tensors $A$, $A^*$, $B$, and $B^*$ are not part of the environment.
(ii) Computing $\lambda$:

Compute $|\Phi\rangle = \begin{array}{cccc}
\cdot & \cdot & \cdot & \cdot \\
C & D & C & N
\end{array}$

as dominant eigenvalue of

transfer matrix $R$: $R|\Phi\rangle = \lambda|\Phi\rangle$

$|\Phi\rangle$ represents "upper half-plane".

In practice:

$|\Phi\rangle = \lim_{p \to \infty} \frac{R^p|\Phi\rangle}{\|R^p|\Phi\rangle\|}$

repeating application of

using $\mathcal{TEBD}$, with $R$ evolved $t = \frac{\pi}{2t}$ steps.

Similarly, define $\langle \Psi | \equiv \begin{array}{cccc}
\cdot & \cdot & \cdot & \cdot \\
C & D & C' & D'
\end{array}$

as dominant left eigenvector of $R$: $\langle \Psi | R = \lambda \langle \Psi |$

$(ii, \text{cat})$ Computing $\bar{\Omega}:

Compute $\langle \Omega | \equiv \begin{array}{c}
\cdot \\
B' \hspace{1cm} D
\end{array}$

as dominant left eigenvector of

transfer matrix $S$: $\langle \Omega | S = \lambda' \langle \Omega |$

$\langle \Omega |$ represents left part of strip.

Define $|\Omega\rangle = \begin{array}{c}
\cdot \\
B'
\end{array}$

as dominant right eigenvector: $S|\Omega\rangle = \lambda' |\Omega\rangle$.

$d(x, c, d, x', d', c')$

\[ g(x, c, d, x', d', c') \]

i-part: $A, B$
(ii) Imaginary time-evolution

$$H = H_0 + H_{\alpha} + H_{a} + H_{\alpha}$$

Time-evolution:

$$e^{-H_S t} = \left( e^{-H_S t} \right) \left( \begin{array}{c} \psi \\ \tilde{\psi} \end{array} \right)$$

$$\text{one would compress: } D_d \rightarrow D$$

recompute $$\mathcal{I}$$ using $$\tilde{A}, \tilde{B}, \tilde{D}$$ to get $$\tilde{\mathcal{I}}$$.

(iv) First updated $$A', B'$$: various compressions

maximizing:

$$\langle \langle \begin{array}{c} \tilde{E}_5 \\ \tilde{G}_{A51} \\ \tilde{E}_3 \\ \tilde{E}_5 \\ \tilde{G}_{A51} \\ \tilde{E}_3 \\ \tilde{E}_1 \\ \tilde{G}_{A51} \\ \tilde{E}_4 \\ \tilde{G}_{A51} \\ \tilde{E}_2 \\ \tilde{G}_{A51} \end{array} \rangle$$

$$\rightarrow A', B'$$, iterate:

• Expensive: recompute environment after each timestep: "full update"
• Cheap: use same environment for several time steps: "fast full update"
\[ H(t) = -\sum_i \sigma_i^x \sigma_j^x - J \sum_i \sigma_i^x \]

**FIG. 4** (color online). (a) Transverse magnetization \( m_y \) and energy per site \( e \) as a function of the transverse magnetic field \( b \). The continuous line shows series expansion results (to 26th and 16th order in perturbation theory) for \( b \) smaller and larger than \( h_c = 3.044 \) \cite{13}. Increasing \( D \) leads to a lower energy per site \( e \). For instance, at \( h = 3.1 \), \( e(D = 2) = -1.6417 \) and \( e(D = 3) = -1.6433 \). (b) Two-point correlator \( S_x(D) \) near the critical point, \( \lambda = 3.05 \). For nearest neighbors, the correlator quickly converges as a function of \( D \), whereas for long distances we expect to see convergence for larger values of \( D \).

**FIG. 5** (color online). Magnetization \( m_x(\lambda) \) as a function of the transverse magnetic field \( \lambda \). Dashed lines are a guide to the eye. We have used the diagonal scheme for \((D, \chi) = (2, 20), (3, 25) \) and \((4, 35) \) \cite{15} (the vertical or horizontal scheme leads to comparable results with slightly smaller \( \chi \)). The inset shows a log plot of \( m_x \) versus \(|\lambda - \lambda_c|\), including our estimate of \( \lambda_c \) and \( \beta \). The continuous line shows the linear fit.