Tensor networks and entanglement spectroscopy

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Entanglement spectrum (by momentum)

Spin-probability distribution in ES

MagLab Theory Winter School 2015

review of MPS and many of the figures in this talk: Kjäll, Zaletel, Mong, Bardarson & Pollmann 2012
Outline

- Day 1: Introduction to tensor network numerics
  - Entanglement and the Schmidt decomposition
  - 1D: the matrix product state ansatz
    - DMRG
  - 2D: the ‘tensor network’ ansatz
    - Dimer & RVB wavefunctions
    - Open problems
- Day 2: Entanglement spectroscopy: detecting emergent anyons in numerics
Goal:

Find an unbiased method for numerically calculating the low energy properties of any local (perhaps frustrated) quantum Hamiltonian in a time which is polynomial in the system size (or independent of system size with translation invariance).

Some amusing cold water first:

[David Pérez-Garcia, Toby Cubitt & Michael Wolf]

Our result (informal statement)

Problem (Spectral Gap):
Input: nearest-neighbor interaction \( h \)
Output: decide if \( H \) has a gap or not.

Theorem:
The Spectral Gap problem is undecidable.

There is no algorithm that on input \( h \) decides it

Corollary: There exist nearest neighbor interactions for which the existence or absence of gap cannot be proven within the axioms of mathematics.

[from David Pérez-Garcia]
The storage problem

Classical: 

\[
\begin{array}{c}
\begin{array}{c}
\uparrow \uparrow \downarrow \cdots \uparrow \\
110 \cdots 1
\end{array}
\end{array}
\Rightarrow \quad S = \log_2(2^L) = L
\]

Information **linear** in system size

Quantum:

\[
|\Psi\rangle = \Psi_0 |\uparrow \uparrow \cdots \rangle + \Psi_1 |\downarrow \uparrow \cdots \rangle + \Psi_2 |\uparrow \downarrow \cdots \rangle + \cdots
\]

(floating points) 

\[
\{\Psi_i\} \quad \Rightarrow \quad S \sim 4 \cdot 8 \cdot 2^L
\]

Information **exponential** in system size (limits exact-diagonalization)
Quantum compression?

My thesis actually contains surprisingly little information...

We are interested in states which have low energy for local Hamiltonians.

How big is the important space?
Parameterize space of ground states via space of local Hamiltonians:

\[ \hat{H} = \sum_{i=1}^{L} \hat{H}_i \]

Finite info for each \( \hat{H}_i \), so

\[ S \propto L \]
Estimate II: the ‘convenient illusion of Hilbert space’

from Poulin, et al., 2011

The Setup:

Start in a product state: \( |t = 0\rangle = \bigotimes_{n=1}^{L} |\uparrow\rangle \)

Time evolve under an arbitrary k-body Hamiltonian: \( \hat{H}(t) \)

After any time \( t \sim \text{poly}(L) \) we can only access a fraction

\[
\frac{\text{Vol}(\{|t\}\})}{\text{Vol}(\mathcal{H})} < L^L \epsilon^{2L}, \epsilon < 1
\]

of the many-body Hilbert space
Schmidt decomposition

\[ |\Psi\rangle = \sum_{i,j=1}^{D_L,D_R} \Psi_{ij} |i\rangle_L |j\rangle_R \]

If A & B are uncorrelated (not-entangled), there is a special basis in which

\[ |\Psi\rangle = |\alpha\rangle_L |\alpha\rangle_R \]

More generally, there is a special basis - the **Schmidt basis** in which

\[ |\Psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_L |\alpha\rangle_R \]

\[ \chi \times (D_L + D_R) \]
Schmidt compression

\[ \mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_R \]

\[ |\Psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_L |\alpha\rangle_R \]

\[ \chi \times (D_L + D_R) \#s \]

The “entanglement entropy:”

\[ \sum_{\alpha} \lambda_\alpha^2 = 1, \quad S_E = -\sum_{\alpha} \lambda_\alpha^2 \log(\lambda_\alpha^2) \]

When

\[ e^{S_E} \ll D_L \]

we can keep only important contributions and compress the state!
A qubit of entanglement

$$|\psi\rangle = \frac{1}{2} (|\uparrow\rangle_A + |\downarrow\rangle_A) (|\uparrow\rangle_B + |\downarrow\rangle_B) \quad \Rightarrow S = 0$$

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_A |\downarrow\rangle_B + |\downarrow\rangle_A |\uparrow\rangle_B) \quad \Rightarrow S = \log 2$$

$$S = -\sum \lambda^2 \gamma \log \lambda^2 \gamma$$
Example: 1D transverse field Ising model

Slightly perturbed from QCP

Cut length 2L chain in half:
The Area Law

[Preinedicki]

Proven in 1D for gapped states  [Hastings 2005]
Mild violations for certain critical systems (1+1 CFT, Fermi surfaces…)
*Volume law expected at finite energy density (eigenstate thermalization)*
The Area Law: $S_E(\ell) \sim \ell^{D-1}$ for $D = 1$ spin chain.
The MPS Ansatz

Step 1:
Cut state in half

\[ \Psi_{ij} = \sum_{\alpha} A^i_{\alpha} \lambda_{\alpha} B^j_{\alpha} \]

Penrose graphical notation:

Still giant Hilbert space: half the chain

Step 2:
Split off 1 site from the right

\[ B^j_{\alpha} = \sum_{\beta=1}^{\chi} \Gamma^p_{\alpha\beta} \chi'_{\beta} B'^{j'}_{\beta} \]

Schmidt coefficients 1 bond to right

[Fannes et al. 1992; Östlund & Rommer 1995]
The MPS Ansatz

Step 3: \( \Psi_{i_1 i_2 \cdots} = \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \cdots \)

is equal to

\[
\sum_{\alpha_1, \alpha_2, \ldots, \alpha_N} \Gamma^{[1]}_{\alpha_1} \lambda^{[1]}_{\alpha_1} \Gamma^{[2]}_{\alpha_1 \alpha_2} \lambda^{[2]}_{\alpha_2} \cdots \lambda^{[N-1]}_{\alpha_{N-1}} \Gamma^{[N]}_{\alpha_N} i_N
\]

Compressed L-site wavefunction into \( L \cdot d \cdot \chi \cdot \chi \) tensors
MPS: Computing observables

Exact diagonalization: $\sim O(e^{\alpha L})$

$\langle \psi | O | \psi \rangle = \begin{array}{c}
\langle \psi | \\
\text{O} \\
| \psi \rangle
\end{array}$

MPS: $\sim O(\chi^3)$

$\langle \psi | O | \psi \rangle = \begin{array}{c}
\Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \\
\Gamma^* \Lambda \Gamma^* \Lambda \Gamma^* \Lambda \Gamma^* \Lambda \\
\Gamma^* \Lambda \Gamma^* \Lambda \Gamma^* \Lambda \Gamma^* \Lambda
\end{array}$
MPS: Computing observables

\[ \langle \psi | O | \psi \rangle = \]

• Local expectation values

\[ \langle \psi | O^{[r]} | \psi \rangle = \]

• Correlation functions

\[ \langle \psi | O^{[r]} O^{[l]} | \psi \rangle = \]

• Correlation length: Second largest eigenvalue of the transfer matrix

Simplification Rule:

[Vidal 2007]
DMRG: Density Matrix Renormalization Group

Given $\hat{H}$, how do we find good a MPS approximations to the g.s.?

MPS: $\{\Gamma^{[j]} \lambda^{[j]}\} \rightarrow |\Psi\rangle$

Minimize $E(\Gamma^{[j]} \lambda^{[j]}) = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$

Non-linear minimization problem

Strategy:

1. Hold all tensors fixed but those at site $j$
2. Solve quadratic problem at site $j$
3. Move on to site $j + 1$; repeat

[White 1992; McCullough 2008]

Review of algorithm: Kjäll, Zaletel, Bardarson, Mong & Pollmann 2012, 1212.6255
For local-ish Hamiltonians, generalize MPS to Matrix Product Operator (MPO):

Transverse Field Ising: \( M = \begin{pmatrix} 1 & 0 & 0 \\ \sigma_z & 0 & 0 \\ g\sigma_x & \sigma_z & 1 \end{pmatrix} \)

Review of algorithm: Kjäll, Zaletel, Bardarson, Mong & Pollmann 2012, 1212.6255

[Verstraete, Porras & Cirac 2004; Murg 2008]
$$\langle \Psi | \hat{H} | \Psi \rangle$$

$$\hat{H}$$

$$\hat{H} | \Psi \rangle$$

$$\langle \Psi | \hat{H} | \Psi \rangle$$

Review of algorithm: Kjäll, Zaletel, Bardarson, Mong & Pollmann 2012, 1212.6255
Focus on two sites

\[ E = \langle \Theta | H_{\text{eff}} | \Theta \rangle = \]

Variational Wavefunction:

Orthonormal basis for 2 sites + L / R Schmidt states

Review of algorithm: Kjäll, Zaletel, Bardarson, Mong & Pollmann 2012, 1212.6255
Lower the energy by finding the ground state of effective Hamiltonian (Lanczos, etc.):

\[
H_{eff} \left| \tilde{\Theta} \right\rangle = E_0 \left| \tilde{\Theta} \right\rangle
\]

This is where you burn CPU hours:

Review of algorithm: Kjäll, Zaletel, Bardarson, Mong & Pollmann 2012, 1212.6255
Bring ansatz back to MPS form

\[ |\tilde{\Theta}\rangle = \sum_{\alpha=1}^{\chi} |\alpha\rangle_A \tilde{\Lambda}_\alpha |\alpha\rangle_B \]

Review of algorithm: Kjäll, Zaletel, Bardarson, Mong & Pollmann 2012, 1212.6255
Update L / R environments

Review of algorithm: Kjäll, Zaletel, Bardarson, Mong & Pollmann 2012, 1212.6255
“Sweep” until convergence

Review of algorithm: Kjäll, Zaletel, Bardarson, Mong & Pollmann 2012, 1212.6255
Algorithm works *unchanged* on an infinitely long system with periodic unit cell: “iDMRG” 

[McCullough 2008]

Comments

Complexity: length / unit cell = $L$  

(holding Hamiltonian fixed)

CPU: $L \chi^3$

RAM: $L \chi^2$

$\chi \sim e^{S_E}$

1D gapped: $S_E \sim \text{const}$

1D CFT: $S_E \sim \frac{c}{6} \log(\xi/a)$

2D: $S_E \sim L_y$
Time evolution

Trotter-decompose $U(dt)$ into 2-site gates:

TEBD [Vidal 03]

Dynamical structure factor: $S(k, \omega)$

$$C(x, t) = \langle \psi_0 | S_x^{-}(t)S_0^{+}(0) | \psi_0 \rangle$$

$$S(k, \omega) = \sum_x \int_{-\infty}^{\infty} dt e^{-i(kx+\omega t)} C(x, t)$$
Time evolution

Experiments of Coldea, et al.: 1D TFI perturbed by order parameter

\[ H = -J' \sum_n S_n^z S_{n+1}^z - h \sum_n S_n^x - h^z \sum_n S_n^z \]
\[ - J_p \sum_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + J_B \sum_n S_n^z S_{n+2}^z. \]

Near QCP: masses of emergent excitations root lattice of E_8

[from Kjäll 2011]
2D DMRG: The Kludge (alias - snake)

Order the 2D lattice into 1D chain with longer-range interactions

Entanglement scales with circumference: \( S_E \sim L_y \)

Complexity:

- \( L_x L_y e^{\alpha L_y} \)\( \quad \)DMRG
- \( e^{\alpha L_x L_y} \)\( \quad \)Exact Diagonalization

[from Stoudenmire 2011]
2D DMRG

Works if you are lucky
(i.e., near thermodynamic limit on small cylinders)

Frustrated magnetism & Spin-liquids on cylinders

Fractional quasiparticles in the fractional quantum hall effect

More on measuring topological order in these studies tomorrow

[Zaletel, Mong, Pollmann 2012]

[Yan, Huse, White 2010]
2D Tensor network: The Hope

[Verstraete & Cirac, 2004]

(a) MPS

(b) PEPS

[from Roman Orus, 1306.2164
Great review!]

\[ A_{\alpha\beta\gamma\delta}^p = \]

\[ \beta \]

\[ \alpha \]

\[ p \]

\[ \gamma \]

\[ \delta \]
Example: dimer model

Kagome NN dimer covering:

\[ | \Psi \rangle = \sum_{\text{dimer coverings}} | \text{hardcore-dimers} \rangle \]

[from Yejin Huh, 2011]

[RVB PEPs examples: Schuch, et al. 2012]
TN for dimers $|\Psi\rangle = \sum_{\text{dimer coverings}} |\text{hardcore-dimers}\rangle$

Using different topology than square TN: but you can always regroup things to turn it into “standard” form

$\chi = 2 : \alpha \in \{0, 1\}$

$p = 0$: no dimer
$p = 1$: dimer

$A_{\alpha\beta}^p = \begin{cases} 1 & \text{if } p = \alpha = \beta \\ 0 & \text{if else} \end{cases}$

$B_{\alpha\beta\gamma\delta} = \begin{cases} 1 & \text{if } \alpha + \beta + \gamma + \delta = 1 \\ 0 & \text{if else} \end{cases}$

Glue presence of dimer to “virtual” index

The constraint (no physical index)
Why is Kagome still being studied with snakes?

Finding the 2D TN is hard!

Square-lattice
J1

[from Stoudenmire 2011]
Why is Kagome still being studied with snakes?

*** Unsolved problem 0: which phases of matter can be represented by finite dimensional 2D TN? ***
1D MPS: represents gapped states of local H
2D TN: not known (certain things can’t be: fermi surface)

*** Unsolved problem 1: what is the right way to approximately calculate observables in a 2D TN? ***
Calculating expectation value in MPS exactly: linear complexity in size
Calculating expectation value in 2d TN exactly: exponential complexity in size

*** Unsolved problem 2: what is the right way to find a 2D TN given H? ***
DMRG: it works. complexity $\chi^3$
2D TN: algorithms proposed, but not fully understood what the nature of the approximations is. complexity $\chi^8 - \chi^{10}$
Thanks!

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Entanglement spectrum (by momentum)

Spin-probability distribution in ES

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