The Density Matrix Renormalization Group: Introduction and Overview

• Introduction to DMRG as a low entanglement approximation
  – Entanglement
  – Matrix Product States
  – Minimizing the energy and DMRG sweeping
• The low entanglement viewpoint versus the historical RG viewpoint
• Methods for 2D
  – applications to t-J model and stripes
  – Frustrated magnets and spin liquids
• Time evolution for spectral functions
• Some generalizations and extensions of DMRG

Software: ALPS (well developed); itensor.org (new, very flexible)
Energy levels of $S=1/2$ Heisenberg chains

$N=8$

$N=12$

Bulk eigenstates are “super-entangled”

Von Neumann Entanglement entropy $S$ for every eigenstate (system divided in center)
What is entanglement?

• Intuitive idea: general correlation between two parts of a system (think two separate spins: a Bell pair)

• Not always obvious: Which is more entangled?
  – 1) $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$ or
  – 2) $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$
SVD/Schmidt Decomposition

• Let the system have two parts: left and right
  
  \[ |\Psi> = \sum \Psi_{lr} \, |l> \, |r> \]

• Treat \( \Psi_{lr} \) as a matrix: perform the simple matrix factorization “singular value decomposition” (SVD): \( \Psi = U \, D \, V \), with \( U \) and \( V \) unitary, \( D \) diagonal.

• The diagonal elements \( \lambda \) of \( D \) are the singular values or Schmidt coefficients. In quantum information this is called the Schmidt decomposition. The Schmidt basis vectors are given as
  
  \[ |\alpha> = \sum_r V_{\alpha r} \, |r> , \quad |\bar{\alpha}> = \sum_l U_{\alpha l} \, |l> \]; the wavefunction is
  
  \[ |\Psi> = \sum_\alpha \lambda_\alpha \, |\bar{\alpha}> \, |\alpha> \quad (\text{diagonal}) \]

• The reduced density matrix for the left side is:
  
  \[ \rho_{ll'} = \sum_r \Psi_{lr} \Psi_{l'r} \]

• If you insert the SVD, you find that \( U \) contains the eigenvectors of \( \rho \), and the eigenvalues are \( (\lambda_\alpha)^2 \). Note \( \sum_\alpha (\lambda_\alpha)^2 = 1 \) (normalization).
Von Neumann entanglement entropy

If we think of \((\lambda_\alpha)^2\) as the probability of the state \(|\tilde{\alpha}\rangle |\alpha\rangle\), then we can plug in the standard probability formula to get the von Neumann entropy

\[
S = -\sum \alpha (\lambda_\alpha)^2 \ln (\lambda_\alpha)^2
\]

There are several other entropies (different formulas)

Low entanglement = small \(S\) occurs when the \(\lambda_\alpha\) fall off fast as the index \(\alpha\) increases.

Thus we have a natural low entanglement approximation: approximate the wavefunction by keeping a small number of \(\alpha\) (the largest).

In DMRG we imagine we do this Schmidt decomp for all positions of the dividing line between left and right.
Matrix Product States

• Insert a truncated set of density matrix/Schmidt eigenstates at every nn link (1D) (total error = sum of probabilities you’ve thrown away)

• The Schmidt basis states for position \( l + 1 \) must be linear combinations of those at \( l \)

\[
|\alpha_{l+1}\rangle = \sum_{\alpha_l, s_l} A[s_l] \alpha_{l+1} \alpha_l |s_l\rangle |\alpha_l\rangle
\]

• This produces a Matrix Product State (MPS) formula for the wavefunction:

\[
\Psi(s_1, s_2, .. s_N) \approx A^1[s_1] A^2[s_2] ... A^N[s_N]
\]

• A function is just a rule for giving a number from the inputs--here the \{s\} tell which matrices to multiply (first and last A’s are vectors).
Diagrams for Matrix Product States

Vertices are matrices or tensors. All internal lines are summed over. External lines are external indices, usually associated with states.

Ordinary Matrix Multiplication: $ABC = \begin{array}{ccc} & & \\ & & \\ i & j & s \\ A & & B \\ & & \\ \\ & & \\ \end{array}$

In an MPS, the basic unit has an extra index, like a Pauli spin matrix; or you can call it a tensor.

$A_{ij}^s = \begin{array}{ccc} & & \\ & & \\ i & j & s \\ A & & B \\ & & \\ \\ & & \\ \end{array}$

Simple diagram: $\text{Tr}[A^sB^t] = g(s,t)$

Dimensions: $i, j: m$ or $D \quad s: d$

Matrix Product State: $\Psi(s_1, s_2, .. s_N) \approx A_1^{s_1} A_2^{s_2} ... A_N^{s_N}$

$2^N \approx \begin{array}{ccc} & & \\ & & \\ s_1 & s_2 & s_N \\ A & & B \\ & & \\ \\ & & \\ \end{array}$

$N m^2$ for $m \times m$ matrices
MPS as Variational states

• Two things needed:
  – Evaluate energy and observables efficiently
  – Optimize parameters efficiently to minimize energy

• Observables:

Operators:

\[ \sum_{-} S_{\sigma} \left( J/2 \right) = H_{\text{block}} \]

– Working left to right, just matrix multiplies, \( N \times m^3 \)

• Optimization:
  – General-purpose nonlinear optimization is hard
  – Lanczos solution to eigenvalue problem is one of the most efficient optimization methods (also Davidson method). Can we use that? Yes!
DMRG algorithm: one step

1. Use exact diagonalization to get the lowest energy $\Psi(\alpha_{l-1}, s_l, s_{l+1}, \beta_{l+2})$ within the basis of fixed block approximate Schmidt vectors $\alpha_{l-1}$, $\beta_{l+2}$ and two sites $s_l$, $s_{l+1}$.

Do an SVD on the 4 parameter wavefunction to split it up into new $A[s_l]$ and $A[s_{l+1}]$. 
DMRG Sweeping Algorithm

• The optimization sweeps back and forth through the system.

DMRG sweeps

• At each step, diagonalize approximate representation of entire system (in reduced basis)
• Construct density matrix for block, diagonalize it, keep most probable eigenstates (or SVD version)
• Transform / update operators to construct H
• Sweep back and forth, increase m
Convergence in 1D

Comparison with Bethe Ansatz
DMRG: two ways of thinking about it

- What I explained here: the MPS variational state point of view.
- The original view: Numerical RG; “Blocks” which have renormalized Hamiltonians (reduced bases) and operator-matrices in that basis
  - What is a block?
    - A block is a collection of sites (I ... j), a matrix product basis for those sites, and the matrix representation of necessary operators in that basis.
    - We can think of a block as a renormalized system (doesn’t have all its original d.o.f.) and the whole DMRG sweeping algorithm as a renormalization of the whole system (Wilson’s original numerical RG).
    - Some things are easier to think about in each picture. DMRG practitioners should know both pictures!
DMRG: overview of extensions, generalizations, etc

• Original two papers covered ground state energies and properties of 1D spin systems.
  – Applications to fermions and targeting several excited states was understood from the beginning and was quickly implemented.

• Application to ladder systems was also done very soon--the first steps towards 2D. Later I will cover recent 2D methods.

• Another area of strong development: dynamics. First work produced spectral functions (frequency, not time); later, work showed how to do real and imaginary time dynamics (Vidal).

• Classical Stat mech systems: developed early on; related to transfer matrices.

• Quantum chemistry: solving small molecules in a Gaussian basis. First work: White & Martin; now, most well known practitioner is Garnet Chan (Cornell --> Princeton).

• Lots of connections to quantum information--a major development I don’t have time to do justice to.
2D algorithms

• Traditional DMRG method (MPS state)

Calc time: $L_x L_y^2 m^3$; allows $m \sim 10000, L_y \sim 10-12$

$S \sim L_y$ ("area law")

$m \sim \exp(a L_y)$

Long range bonds

Cut
Stripes forming from a blob of 8 holes

12x8
Cylindrical BCs
t=1, J=0.35
t’=t”=0
8 holes
No pinning fields

E = -31.7287
m = 70
Stripes forming from a blob of 8 holes

12x8
Cylindrical BCs
\( t=1, \; J=0.35 \)
\( t'=t''=0 \)
8 holes
AF edge
pinning fields
applied for two sweeps to favor one stripe

\[ E = -30.7350 \] \[ m = 40 \]
Stripes not forming from a bad initial

Cylindrical BCs
\( t=1, J=0.35 \)
\( t'=t''=0 \)
8 holes
No pinning fields.
Initial state has holes spread out so favored striped state is hard to find. Energy higher by \( \sim 0.3 \) t.
Curved Stripe forms due to open BCs

12x8 Open BCs
t=1, J=0.35
t'=t''=0
8 holes
No pinning fields

E = -30.8532
m = 40
Projected entangled pair states

- Generalize the 1D MPS ansatz to 2D:
  - Much more natural representation!
  - Key issues: optimization, contraction
  - V&C approach: \( \text{CPU} \sim L_x L_y m^{10} \) \textbf{No exponentials!!}

- MERA is another tensor network approach to 2D with similar properties

- Fermionic PEPS: simple treatment of fermionic exchange

(Nishio, Maeshima, Gendiar, and Nishino, cond-mat/0401115; Verstraete and Cirac, condmat 0407066)
Some Practical aspects of DMRG for hard systems and Applications to 2D

• Extrapolation in truncation error for energy and observables
• Tips for very efficient calculations
• Some results for 2D Heisenberg models:
  – Square lattice
  – Triangular lattice
  – Kagome lattice
Square lattice: benchmark against

- Cylindrical BCs: periodic in y, open in x
- Strong AF pinning fields on left and right edges
- 21 sweeps, up to $m=3200$ states, 80 hours
Extrapolation of the energy

Extrapolation improves the energy by a factor of 5-10 and provides an error estimate.
Energy extrapolation

12x6 square lattice Heisenberg

Fit based on circles

Probability of states thrown away = truncation error (function of m)

Assign error bars to result: if the fit is this good, assign (extrapolation from last point)/5

(no derivation, just experience that this works on lots of systems)

If the fit looks worse, increase the error bar (substantially) or don’t use that run/keep more states or smaller size system.
Extrapolation of local observables (ref: White and Chernyshev, PRL 99, 127004 (2007))

• Standard result for a variational state

\[ |\psi\rangle = |G\rangle + |\delta\rangle, \quad \langle G|\delta \rangle = 0, \]

\[ A = (1 + \langle \delta|\delta \rangle)^{-1}(A_G + 2\langle G|\hat{A}|\delta \rangle + \langle \delta|\hat{A}|\delta \rangle) \]

\[ E = (1 + \langle \delta|\delta \rangle)^{-1}(E_G + \langle \delta|\hat{H}|\delta \rangle) \]

• Consequences:

− Variational calculations can have excellent energies but poor properties
− Since DMRG truncation error \( \varepsilon \sim \langle \delta|\delta \rangle \), \( E \sim \varepsilon \), but otherwise extrapolations vary as \( A \sim \varepsilon^{1/2} \)

• These \( \varepsilon^{1/2} \) extrapolations have never worked well.
Typical extrapolation of magnetization

Pinning AF fields applied to edges, cylindrical BCs

Now we understand why the local measurements converge fast; see White & Chernyshev
Cubic fit to well-converged measurements

\[ \langle S_z(6,1) \rangle \]

\[ \Delta E \]

12 x 6
Result: central $M = 0.3032(9)$
Improved finite size scaling: choosing aspect ratios to reduce finite size effects

“Standard” measurements in QMC estimate $M^2$ using correlation functions and have large finite size effects $O(1/L_y)$

Can one choose a special aspect ratio to eliminate $O(1/L_y)$ term?

What is behavior at large length scales? Use finite system spin wave theory as a guide.

Long: 1D makes $M$ small

Short: proximity to strong pinning makes $M$ large
Square lattice

\[ M(\pi,\pi), \quad C(L/2,L/2) \]

\[ \alpha = \frac{L_x}{L_y} \]

\[ QMC \]
Finite size spin wave theory

- Optimal choice $\alpha = 1.764$ eliminates linear term
- Even $\alpha = 1$ has much smaller finite size effects
• Tilted lattice has smaller DMRG errors for its width
• For this “16 $\sqrt{2} \times 8 \sqrt{2}$” obtain $M = 0.3052(4)$
Tilted square lattice

Results are consistent with and with comparable accuracy to QMC! (of 1997, at least)

Latest QMC (Sandvik&Evertz) -0.30743(1) (No new E)

Sandvik, QMC

Energy, extrapolated to thermo limit:
-0.669444(5)

Sandvik (1997):
-0.669437(5)
Traditional DMRG for triangular lattice Heisenberg model

See White & Chernyshev, PRL 99, 127004 (2007)

\[ \Delta E \sim 0.3\%, \quad \Delta \langle S_z \rangle \sim 0.01 \]

Extrap order param to thermodynamic limit: \( M = 0.205(15) \)
Spin Liquid Ground state of the $S=1/2$ Heisenberg model on the Kagome lattice

Collaborators: Simeng Yan and David Huse
Quantum Spin Liquids: what are they?

- Starting ingredient: a lattice of localized spins.
- Then (at least) three classes of possible ground states.

Magnetic order
\[ \langle \psi | \vec{S}_i | \psi \rangle \neq 0 \]

Valence bond order
\[ \langle \psi | \vec{S}_i \cdot \vec{S}_j | \psi \rangle \neq \text{const} \]

Spin liquid
No broken symmetries

A spin liquid has no order at T=0 because quantum fluctuations overcome all tendencies for order.
Kagome systems: funny names

**Kagome:** Is it the name of a Japanese physicist?

No! It’s a Japanese basket!

**ZnCu₃(OH)₆Cl₂:** the most interesting current Kagome material. Is it named after a person?

Yes, with both first and last names! **Herbertsmithite!**

- No magnetic order down to fractions of 1K; it appears to be a spin liquid
- Complications: high concentration of impurities? What is the right model?
Kagome Basics

- The Heisenberg model on the kagome lattice is one of the most frustrated systems
  - Without frustration, magnetic order
  - Much more frustrated than the triangular lattice

- The kagome lattice has a small coordination \( z=4 \)

\[
\begin{align*}
E/N &= -zJ/8 \\
\text{Valence Bond state}
\end{align*}
\]

- It has an exponentially large number of degenerate VB configurations

All these features make the kagome Heisenberg model an excellent candidate for an RVB ground state, a \textit{spin liquid}. But, it could also be a \textit{valence bond crystal}. 
Valence bond crystal versus spin liquid

- Early field theory treatments gave a $Z_2$ spin liquid as a possible ground state (Sachdev, ...)

- Other approximate treatments pointed to a complicated 36 site unit cell VBC, the honeycomb VBC. Why?
  - Resonance only occurs in loops
  - Shortest loop is 6 site hexagon
  - Close pack the hexagons w/o touching
  - Use higher order flucs to break ties
  - The resulting HVBC appears (meta)stable: it doesn’t melt into a spin liquid!
Practical Issues for Kagome

1. Metastability: getting stuck in a higher energy state (usually an issue only on wider cylinders)
   • Need to understand system and find a simple state close to the ground state to initialize DMRG

2. Strong dependence on width (and shift) of cylinders
   • Need to do many cylinders and understand patterns of behavior

3. Open edges--obtaining bulk cylinder behavior
   • This is a minor problem for this system
   • Open ends useful for pinning, selecting different topological sectors...
Ground state energies per site

-0.431
-0.432
-0.433
-0.434
-0.435
-0.436
-0.437
-0.438

E/N

0 1000 2000 3000
m

YC10-4

150 sites - 90 sites
270 sites - 150 sites

-0.431
-0.432
-0.433
-0.434
-0.435
-0.436
-0.437
-0.438

E/N

0 0.01 0.02 0.03 0.04
Total Truncation Error

m=2000
m=3200
m=4400
m=6000

Lanczos 36, 42 sites
(HVBC
2D
Series
MERA
(Andreas L.)

270 - 150 sites
225 - 150 sites

m=1000
m=2000
m=3000

-0.6
-0.438
-0.437
-0.436
-0.435
-0.434
-0.433
-0.432
-0.431

E/N

m=6000

-0.6
-0.438
-0.437
-0.436
-0.435
-0.434
-0.433
-0.432
-0.431

Exchange Energy

Total Truncation Error
Smaller widths are nearly exact

- YC10-4
  - 270 - 150 sites
  - width = 10.6

- YC8, up to m=2400

Smaller widths are nearly exact
Energies of various cylinders and methods

-0.44 -0.43 -0.435 -0.43

-0.44 -0.435 -0.43

E/site

1/c

Upper Bound

MERA

DMRG

Cylinder

Torus

2D (est.)

Series (HVBC)

DMRG, Cyl, Odd

DMRG, Cyl, Even

DMRG, Torus (Jiang...)

Lanczos, Torus
Direct comparison of HVBC and SL

• Given metastability, and possible biases, how can you rule out the HVBC?
  — Make all the biases favor the HVBC. Then, if it’s unstable, you have strong evidence.
  — To make a strong bias: make the DMRG mapping to 1D follow the HVBC state!

• Nonresonating HVBC stable at m=2
  — Other ways to promote HVBC: initial state (pinning “fields” = strong J’s); edge shaped to match HVBC
XC8 cylinder, biased to HVBC

\[ \text{swp}=3, \ m=120, \ E=-89.7836 \]
Ruling out an HVBC on a width 12 cylinder

![Graph showing energy levels with labels for HVBC and Random/Spin Liquid.](image)

- HVBC
- Random/Spin Liquid

400 sites, YC12

Pinning
How can we understand the nature of the spin liquid?

• Is it closely connected to a nearby VBC? (a “melted” VBC)

• In an RVB description, what are the key resonances?

• What do we measure to answer these questions?
Response to small bond perturbations

Response to 1% increase in J on one diamond

Response to 1% increase in J on one hexagon

Response to 0.5% increase/decrease in J on fat vertical bonds: the “diamond pattern”, which fits only on the even cylinders
Singlet and Triplet Gaps

Singlet excitation before delocalization

Graph showing the relation between Gap and $1/c$ for different categories and symbols.

- Solid symbols for different categories:
  - YCn-2
  - YC6, YC10
  - Even

Graph indicates the triplet and singlet gaps with corresponding symbols and categories.
Varying $J_2$ with $x$ coordinate
36 site exact diagonalization: Sindzingre and Lhuillier

The finite size shift of the phase boundary explains the many low lying states in ED.

Note: no sign of 4-fold degeneracy for torus
Generalizations of MPS

- Periodic BCs: long a weakness of DMRG \((m \rightarrow m^2)\)
  - New variational state:
  - key issue is computational: optimization to minimize \(E\)
    - Ostlund and Rommer (‘95) \(m = 12\)
    - Verstraete, Porras, Cirac (PRL 93, 227205 ‘04) calc time \(\sim Nm^5\)
    - Pippan, White, Evertz (PRB 82, 024407 (2010)) calc time \(\sim Nm^3\)
    - Pirvu, Verstraete, Vidal \(m^3\)

- Infinite systems
  - Natural state:
    - But: very hard to optimize \(A\)
  - Much better:
    - Trotter imaginary time evolution: odd links, then even, repeat
      - iTEBD (infinite time evolving block decimation)

Vidal, PRL 98, 070201 (2007)
Critical 1D systems

1) $S \sim \ln(L)$, so MPS eventually fails
2) MPS does not exhibit scale invariance naturally

Still fails due to $S \sim \ln(L)$ !!
Tensor networks for 1D critical systems

Multiscale entanglement renormalization ansatz (MERA)

- Entanglement gets organized at different length scales at different layers: RG
- At criticality, expect translational/scale invariance in both directions!
  Compression: superb
- Computation time: $m^9 L \ln L$, or $m^9 \ln L$ for translational inv. systems, but $m=6$ has energy errors $\sim 10^{-7}$ (Critical transverse field Ising model)
- State directly yields CFT central charge, scaling dims of primary fields
- Accurate correlations at large distance, e.g. $r = 10^9$ !!

Vidal, PRL 99, 220405 (2007)
Rizzi, Montagero, Vidal PRA 77, 052328 (2008) (tMERA)
Evenbly & Vidal, arxiv:0707.1454
Pfeifer, Evenbly,&Vidal, arxiv: 0810.0580
Time Evolution \textit{(Vidal,...)}

Suzuki Trotter decomposition:
\[ \exp(-iH\tau) \approx \exp(-iH_{12}\tau) \exp(-iH_{34}\tau) \cdots \exp(-iH_{23}\tau) \cdots \]

In DMRG, the bond operator for the current middle two sites is trivial to apply:

\[ \exp(-iH_{ij}\tau) = \]

\[ s'_i \quad s'_j \]

\[ s_i \quad s_j \]
DMRG Sweeps

• Finite system method:

• During each step, instead of finding the ground state, we can apply $T_{ij} = \exp(-i H_{ij} \tau)$ (or leave $\psi$ alone).

• When to apply T’s: several versions:
  – Standard even/odd breakup:
    • 1 --- 2 --- 3 --- 4   do odd bonds in left-to-right half sweep
    • ---7 --- 6 ---5 --- do evens in right to left half sweep
  – White-Feiguin version:
    • 1 2 3 4 5 6 7   do all bonds in each half sweep
    • 14 13 12 11 10 9 8   reverse order each half sweep
Calculation of Spectral functions

- Start with standard ground state DMRG, get $\varphi$
- Apply operator to center site
  $$|\psi(t = 0)\rangle = S_0^+|\phi_0\rangle$$
- Time evolve:
  $$|\psi(t)\rangle = e^{-i(\mathcal{H}-E_0)t}|\psi(0)\rangle$$
- Measure time dependent correlation function
  $$G(x, t) = \langle \phi_0 | S_x^- | \psi(t) \rangle = \langle \phi_0 | S_x^-(t) S_0^+ (0) | \phi_0 \rangle$$
- Fourier transform with $x = 0$ to get $N(\omega)$ or in $x$ and $t$ to get $S(k, \omega)$
  - But what about finite size effects, finite time, broadening, etc??
Finite size effects: gapped systems

S=1 Heis chain

Real and Imag parts

For $t < L/(2v)$, finite size effects are negligible.
Growth of entanglement with time

• Lots of work on growth of entanglement with time—sounds very discouraging at first
  – For “macro” changes to the wavefunction, S grows linearly (e.g. suddenly change the Hamiltonian). Then matrix dimension m must grow exponentially (and effort $\sim m^3$)

• Fortunately, for what we need here, one local change, growth is only logarithmic!
  – Still limited in total time we can simulate—still the key issue

• Example: for spin chains, we can go out to $t_{\max} \sim 30$.

• It appears that one should be limited in frequency resolution to $\sim 1/t_{\max}$

• But: the long time behavior is determined almost completely be the singularities in $A(\omega)$, and if there are just a few, we can fit them and get extremely high resolution (SRW, Affleck, Pereira)
Extrapolation to large time: linear prediction

S=1 chain

Windows for time FT

\[ y_i = \sum_{j=1}^{n} d_j y_{i-j} \]

See *Numerical Recipes*

Parameters \(d_j\) determined from correlation functions of available data.
Example where singularities were fit to and used to extrapolate (less automatic than linear prediction)

$S=1/2$ Chain, XXZ model

$J_z = 0.125$

$J_z = 0.25$

$J_z = 0.375$

$J_z = 0.5$
How accurate are the spectra?

\[ J_z = 0.5 \]

\[ N(\omega) \]

- L=200
- L=400
Summary

• DMRG and related low entanglement approximations have been the most powerful and diverse techniques for 1D systems known.

• Recently, many 2D models with either frustration or fermions can be treated on cylinders large enough to extrapolate to 2D.

• Lots of fascinating connections to quantum information and entanglement.
Questions raised by Sandvik, arxiv:1202.3118: Could a weak VBC look like a SL on the modest size cylinders used by DMRG? Addressed on J-Q_2 model by QMC

Correlation function based

Direct measurement with pinning

Note: we find all correlation lengths of order 1 lattice spacing

Conclusion: our kagome SL data does not look at all like a weak VBC