Update on DMRG Implementation and Use

Includes Dynamics at Finite Temperature

October 11, 2019

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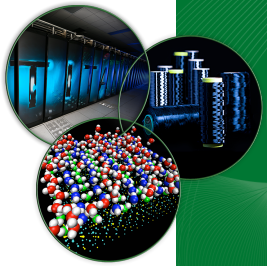
With FWP Collaborators.



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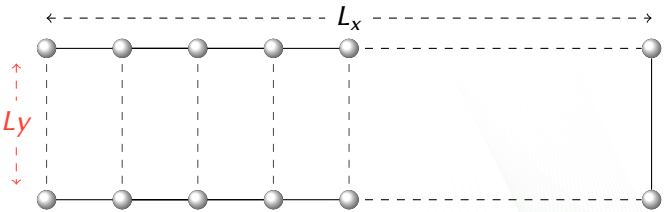
Why the Density Matrix Renormalization Group?

Because it is an accurate method for 1D and quasi-1D.[1] The DMRG is a method to obtain ground state and *beyond-ground-state* properties of quantum Hamiltonians.

The DMRG is systematically exact, and its error is controlled by the parameter m, the number of kept states. To achieve constant error, on a $L_x \times L_y$ ladder, ...

...the number of kept states m must increase linearly in L_x, and exponentially in L_y



[1] White, 1992, White and Noack, 1992

Why DMRG beyond ground state?

In the FWP, we proposed to go beyond ground state with the DMRG, in order to calculate static observables at finite temperature, real frequency observables at zero temperature, and ...

...real frequency observables at finite temperature,...

..., which is arguably a frontier in DMRG. This overview today thus focuses on beyond ground state properties.

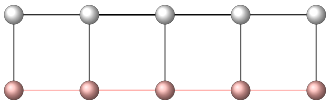
Finite Temperature: Duplicate Sites

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}(e^{-\beta H}\hat{O})}{\mathrm{Tr}(e^{-\beta H})} \qquad \boxed{\beta = 1/T} \tag{1}$$

Replace the trace Tr by a single state $|\phi\rangle \equiv |\psi(T=\infty)\rangle$

$$\langle \hat{O} \rangle = \frac{\langle \phi | e^{-\beta H/2} \hat{O} e^{-\beta H/2} | \phi \rangle}{Z} \quad \text{where} \quad Z = \mathrm{Tr}(e^{-\beta H}) \tag{2}$$

Eq. (2) is *exact* but in larger space



- Physical site or orbital
- Ancilla site or orbital

Statics at Finite Temperature: Ancilla Sites

The infinite temperature state on two composite sites is

$$|\psi_{2\text{ spins}}(\infty)\rangle = \frac{1}{2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \otimes (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \tag{3}$$

The first entry of the ket refers to the state of the physical site and the second entry in red to its ancilla.

$$|\psi(T)\rangle = e^{-\beta H/2}|\psi(\infty)\rangle \qquad \boxed{\beta/2 \longleftrightarrow \sqrt{-1}\, t}. \tag{4}$$

$$\langle O\rangle = \langle\psi(T)|O|\psi(T)\rangle / \langle\psi(T)|\psi(T)\rangle, \tag{5}$$

Verstraete et al., 2004, Zwolak and Vidal, 2004, Feiguin and White, 2005, Takahashi and Umezawa, 1975, Nocera and Alvarez, 2016b

Statics at Finite Temperature: Canonical Space

Consider the Heisenberg model without a magnetic field. The canonical state should then have $S^z_{tot}|\phi\rangle = 0$, $S^z_{\text{ph.}}|\phi\rangle = 0$, $S^z_{\text{an.}}|\phi\rangle = 0$; it conserves the spin of the physical and ancilla chains separately, leading to

$$|\phi_{2\text{ spins}}(\infty)\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle \otimes |\downarrow\uparrow\rangle + |\downarrow\uparrow\rangle \otimes |\uparrow\downarrow\rangle\right). \tag{6}$$

This state is exponentially large.

So, how do we represent it in DMRG?

Statics at Finite Temperature: Entangler Hamiltonian

How do we represent the infinite temperature $|\psi(\infty)\rangle$ state in DMRG?

We find a Hamiltonian whose ground state is $|\psi(\infty)\rangle$.

For the Heisenberg model, this entangler Hamiltonian is

$$H_C^{spin} = -\sum_{i\neq j} \Gamma_i^\dagger \Gamma_j + \text{h. c.}, \quad \text{where } \Gamma_i^\dagger = S_i^+ S_{a(i)}^-. \tag{7}$$

Connects all points

Acts on physical and ancilla sites

$$|\psi(\infty)\rangle_C = \frac{1}{\sqrt{\mathcal{N}'}} P_{(S^z_{\text{ph.}}=0)} \left[\prod_{i=0}^{L-1} \sum_{\sigma=\uparrow,\downarrow} |\sigma\bar{\sigma}\rangle \right],$$

where $\mathcal{N}'$ is a normalization constant, $P_{(S^z_{\text{ph.}}=0)}$ is the projector operator such that the z-component of the *total* spin of the physical (ancilla) chain is conserved and equal to zero: $S^z_{\text{ph.}}|\psi(\infty)\rangle_C = S^z_{\text{an.}}|\psi(\infty)\rangle_C = 0$.

Statics at Finite Temperature: Two Steps

Step 1 (Fast): Find the ground state $|\psi(\infty)\rangle_C$ of Entangler Hamiltonian. This is the infinite temperature state of the composite physical and ancilla Hamiltonian.

Step 2 (Slow and Serial): Reach finite temperatures $\beta > 0$ by time evolving with $\hat{H} = \hat{H}_{ph.} \otimes \mathbf{1}_{an.}$ acting on physical Hilbert space only: $|\psi(T)\rangle = e^{-\beta H/2}|\psi(\infty)\rangle$. Observables are computed with $\langle O\rangle = \langle\psi(T)|O|\psi(T)\rangle / \langle\psi(T)|\psi(T)\rangle$,

Remark I: There is one state at each finite temperature T.

Remark II: Excited states are not directly computed.

Methods for Dynamics at Zero Temperature with the DMRG[2]

- Time evolution, and then Fourier transform into ω
  White and Affleck, 2008 Preferred method of Steve White.
- Correction vector Kühner and White, 1999 Pati et al., 1999 Kühner et al., 2000. Scalable. Discussed in the next slides.

Please read our work.

Nocera and Alvarez, 2016a

[1] First method that is now superseded: continued fraction approach Hallberg, 1995. Other methods include Jeckelmann, 2002, Dargel et al., 2011, Dargel et al., 2012.

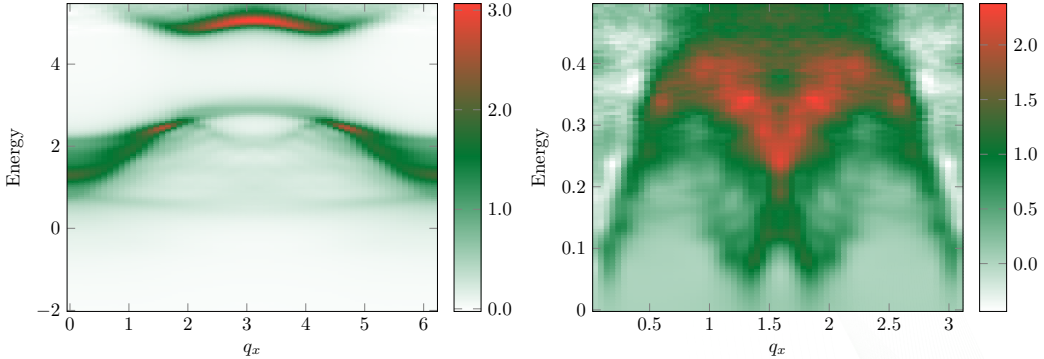
Dynamics at Zero Temperature

We are interested in the calculation of the Green's function

$$G(\omega) = -\frac{1}{\pi}\langle\psi_0|\hat{B}\frac{1}{\omega + i\eta + E_0 - \hat{H}}\hat{A}|\psi_0\rangle,$$

$|\psi_0\rangle$ is the ground state of some Hamiltonian $\hat{H}$ with ground-state energy E_0, $\hat{A}$ and $\hat{B}$ are operators associated with the dynamical correlation function to be calculated (ex. S^+, S^z, S^-, $c^\dagger$, c,), where ω is the real frequency and η is a positive constant (giving broadening of the peaks).

$A(k,\omega)$ and $S(k,\omega)$ at Zero Temperature



$A(q_x, q_y = 0, \omega)$ (left) and $S(q_x, q_y = 0, \omega)$ (right) for a 64×2 extended Hubbard ladder with $t_x = -0.42$, $t_y = -0.34$, $U = 3.72$, $V_{\text{offsite}} = 0.615387651996596$, and $4 + 4$ holes.

Correction Vector DMRG

We calculate $G(z)$ using $G(\omega) = -\frac{1}{\pi}\langle\psi_0|\hat{B}|x(\omega,\eta)\rangle$, where the *correction-vector* is defined by

$$|x(\omega,\eta)\rangle = \frac{1}{\omega + i\eta + E_0 - \hat{H}}|A\rangle, \quad \text{where } |A\rangle \equiv \hat{A}|\psi_0\rangle.$$

Assuming $|x(\omega,\eta)\rangle$ is *known*, how to compute $G(\omega)$ with DMRG? Answer: Use multi-target approach. At each step of the DMRG algorithm, target the ground state of the system $|\psi_0\rangle$, the vector $|A\rangle$ and the $|x(\omega,\eta)\rangle$ in the reduced density matrix, for each frequency value ω and broadening η.

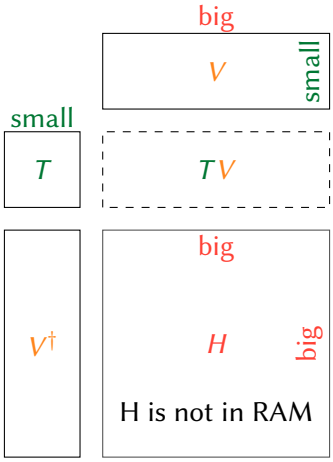
Correction Vector DMRG

How do we compute the correction-vector? Most used method is Conjugate Gradient. Kühner and White, 1999 But we use the Krylov-space method proposed by us Nocera and Alvarez, 2016a. The correction-vector $|x(\omega,\eta)\rangle$ is calculated *directly* as

$$|x(\omega,\eta)\rangle = V^\dagger S^\dagger \frac{1}{E_0+\omega-D+i\eta} SV|A\rangle,$$

where D is the diagonal form of the Hamiltonian operator $\hat{H}$, we assume $\hat{H}|A\rangle \simeq V^\dagger TV|A\rangle = V^\dagger S^\dagger DSV|A\rangle$, V is the matrix of the Lanczos vectors spanning the Krylov space, and T is the representation of the Hamiltonian in tridiagonal form.

Tridiagonal Decomposition of H



$H = V^\dagger T V$, where V are the Lanczos vectors, with small = hundreds, and big = millions.

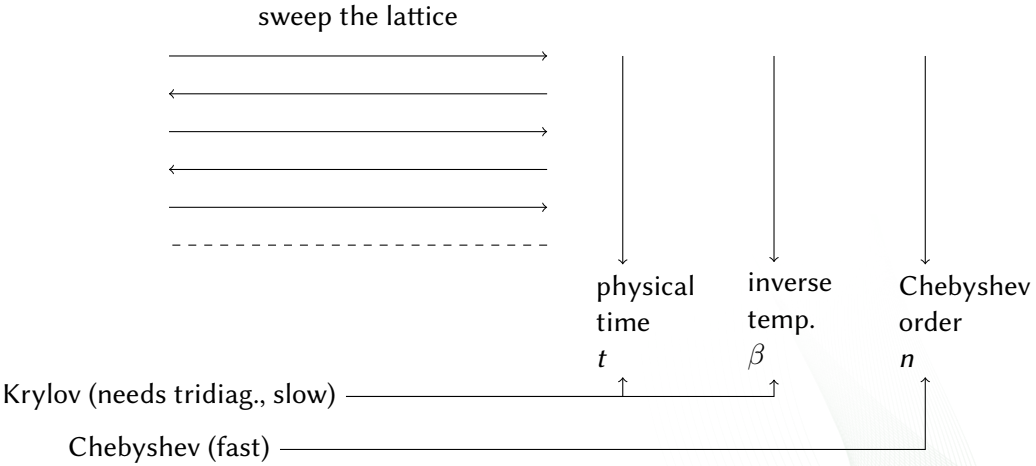
$$\exp(\alpha H) \to V^\dagger \exp(\alpha T) V$$

only for $\alpha \ll 1 \to$ needs evolution $\exp(\alpha H) \cdots \exp(\alpha H) = \exp(n\alpha H)$

$$\frac{1}{\omega + i\eta + H} \to V^\dagger \frac{1}{\omega + i\eta + T} V$$

(correction vector does *not* need evolution)

Evolving in DMRG



Evolving or Not. Tridiagonalizing or Not

Method	Tridiagonalize	Evolves in	Scales Trivially
Correction Vector	Yes	No	Yes[3]
Krylov Evolution	Yes	t or β	No
Chebyshev Evolution	No	n	No

[3] One frequency ω per node.

Dynamics at Finite Temperature

Definition. The finite temperature correlation between observables B and C, with at least one of them bosonic, at time $t \in \mathbb{R}$ and inverse temperature $\beta \geq 0$ is defined as

$$I(\beta, t) \equiv \mathrm{Tr}(e^{-\beta H} e^{-iHt} B e^{iHt} C)/Z. \tag{8}$$

Definition. The Liouvillian or Liouville operator $\mathcal{L} : \mathcal{H} \otimes \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$ associated with the Hamiltonian $\hat{H}$ is $\mathcal{L} \equiv \hat{H} \otimes 1 - 1 \otimes \hat{H}$.

Proposition Tiegel et al., 2014, Dalton, 1982, Barnett and Dalton, 1987, Takahashi and Umezawa, 1975

$$\boxed{I(\beta, \omega) = \langle \psi(\beta) | [B \otimes 1] \frac{1}{\omega + i\eta + \mathcal{L} - E_0} [C \otimes 1] | \psi(\beta) \rangle / Z} \tag{9}$$

Dynamics at Finite Temperature in Three Steps

Step 1 (Fast): Find the ground state $|\psi(\infty)\rangle_C$ of Entangler Hamiltonian. This is the infinite temperature state of the composite physical and ancilla Hamiltonian.

Step 2 (Slow and Serial): Reach finite temperatures $\beta > 0$ by time evolving with $\hat{H} = \hat{H}_{ph.} \otimes \mathbf{1}_{an.}$ acting on physical Hilbert space only: $|\psi(T)\rangle = e^{-\beta H/2}|\psi(\infty)\rangle$.

Step 3 (Fast): Do a correction vector given by

$$|cv(\omega,\eta)\rangle = \frac{1}{\omega + i\eta + \mathcal{L} - E_0}[C \otimes 1]|\psi(\beta)\rangle \tag{10}$$

DMRG Highlights of FY2018

paper81 is a computational and experimental study of telephone compounds, where we simulated the $S(k, \omega)$ of doped and undoped ladders with the DMRG, and compared with experimental results by Alan Tennant. Use of GPUS achieved over approximately 30%. Runs and restart done by Wael E. This work exemplifies a collaboration between ORNL SNS and ORNL HPC.

dmrgppPluginSc is the GPU support for DMRG++, done by Ed D'Azevedo in collaboration with Wael E.. More details in their talk. Crucial work to support GPUs!

DMRG Highlights of FY2019

paper84 *Targeting Multiple States in the DMRG with The Singular Value Decomposition* (by Ed, Wael, Nirav Patel and I) described how to use the SVD when multitargeting, which is nowhere to be found in the literature. But paper was rejected.

Krylov-time evolution has been implemented in DMRG++, for real and imaginary time, as well as for RIXS (Steve J.).

Chebyshev expansion has been implemented in DMRG++ by Alberto N.. This method is fast but needs careful consideration of the spectrum bounds, due to the Cheybshev functions having support in $[-1, 1]$, making the method somewhat brittle, and dependent on model and observable.

Highlights for the Next Two Years

GPU work moves beyond MAGMA library... Difficult area and we need to write guidelines for GPU use.

DMRG++ becomes capable of obtaining real frequency observables at finite temperature. Already coded, but needs testing.

Honeycomb lattice study of dynamical observables becomes possible, enabling simulation of Kitaev-like models; collaboration with Satoshi O. and Pontus L.

Diagonalization "impurity" solvers based on DMRG help Quantum Monte Carlo in the simulation of topological materials; collaboration with Thomas M.

Obstacles and Workarounds

Obstacle: NVIDIA is BAD for free and open source work.

> …Torvalds laid into Nvidia, calling it 'the single worst company' the Linux developer community has ever dealt with, …[4]

Workaround: AMD GPUs have free and open source drivers and should offer a much better option than NVIDIA.

Obstacle: GPUs in general aren't general purpose computers; its use is more limited than that of CPUs.
Workaround: None. We need GPU programming guidelines

[4] ["Linus Torvalds Gives Nvidia the Finger. Literally" `https://www.wired.com/2012/06/torvalds-nvidia-linux/`]

Computer Programming

Obstacle: Computer programming is not often taken seriously: people want to get things done quickly. But as corners are cut, "technical debt" accumulates and quality suffers.

Workaround: "Traditional programmers" should be hired to improve quality, and achieve better results long term. Collaboration with Jay Billings.

Workaround: Tooling: GDB, valgrind, git. Also need CI and CD, including in-house tools.

DMRG++ and related software is at `https://github.com/g1257/` and at `https://code.ornl.gov/gonzalo_3`

Summary as of October 14, 2019

1. Summit has been less helpful that we thought.[5]
2. Traditional Programmers might be helpful.
3. We'll do real ω at finite T, which is a DMRG frontier.

Please download this talk

`https://g1257.github.io/talks/`

DMRG++ and related software is at `https://github.com/g1257/` and at `https://code.ornl.gov/gonzalo_3`

[5] For example, we failed to reach ground state for 12×12.

Credits

Thanks to the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

Produced with LaTeX and the Beamer package
with a custom theme.
Tikz was used for some figures.

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