Multi-Configuration Time Dependent Hartree Theory

A Tensor Network Perspective

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Non-Relativistic Multi-Dimentional Problem

- TDSE:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi(\vec{q},t)\rangle = H|\Psi(\vec{q},t)\rangle$$

- TISE:

$$H|\Psi(\vec{q},t)\rangle = E|\Psi(\vec{q},t)\rangle$$

where

$$H = T + V$$

and $\vec{q} = (q_1, q_2, \ldots, q_d)$.

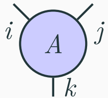
d-D Problem: $\vec{q} = (q_1, \ldots, q_d)$

Standard procedure:

1. Choose a set of d-D basis $\{|\Phi_I(\vec{q})\rangle\}_{I=1}^{N}$, where $|\Phi_I(\vec{q})\rangle = \prod_{\kappa=1}^{d} \left|\varphi_{i_\kappa}^{(\kappa)}(q_\kappa)\right\rangle$
2. Integrate $H_{IJ} = T_{IJ} + V_{IJ}$
3. Solve TDSE/TISE in matrix form
    - TDSE: $\mathrm{i}\hbar\dot{\mathbf{c}} = \mathbf{H}\mathbf{c}$
    - TISE: $\mathbf{H}\mathbf{c} = E\mathbf{c}$

Language: Tensor Network Notation

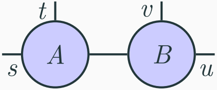
- Tensors



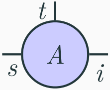
$:= \quad A_{ijk}$

$:= \quad H_{ij}$

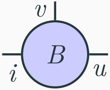
- Contraction



$:= \quad \sum_i$



$\times$

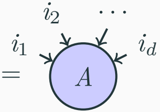


Bridgeman, J. C. & Chubb, C. T. J. Phys. A: Math. Theor. 50 223001 (2017). (arXiv:1603.03039)

Express the Standard Procedure in TNN

- Wavefunction

$\langle \Phi_I | \Psi \rangle \quad =$

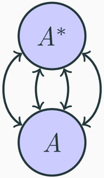


where $i_\kappa \in \{1, \ldots, n_\kappa\}, \kappa = 1, \ldots, d$.
Space for saving a wavefunction: $\prod_{\kappa=1}^{d} n_\kappa$ floats.

Express the Standard Procedure in TNN (Cont'd)

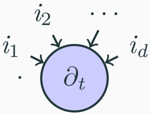
- Normalization condition

$$1 = \langle \Psi | \Psi \rangle \approx \langle \Psi | P | \Psi \rangle =$$

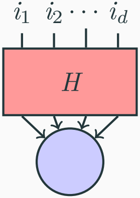


- TDSE

$$i\hbar \quad \cdot$$

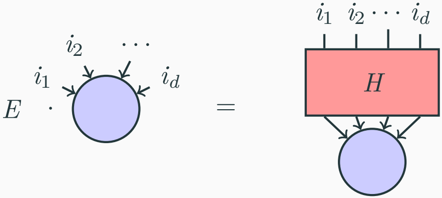


$$=$$



Express the Standard Procedure in TNN (Cont'd)

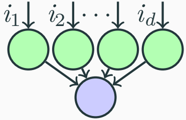
- TISE



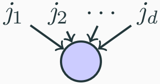
where $i_\kappa \in \{1, \dots, n_\kappa\}, \kappa = 1, \dots, d$.

Problem: $N = \prod_{\kappa=1}^{d} n_\kappa$ exponentially increase as d grows.

Structure of MCTDH Wavefunction

$\langle \Phi_I | \Psi \rangle \quad =$ 

where

$\left\langle \Phi_J^{(1)} \middle| \Psi \right\rangle \quad =$ 

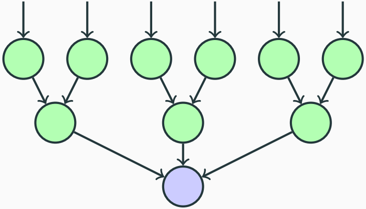
Idea: $j_\kappa \in \{1, \ldots, n_\kappa^{(1)}\}, \kappa = 1, \ldots, d$, and $n_\kappa^{(1)} < n_\kappa$.

Space for saving a wavefunction: $\prod_{\kappa=1}^{d} n_\kappa^{(1)} + \sum_{\kappa=1}^{d} n_\kappa^{(1)} n_\kappa$ floats.

Multi-Layer

More nodes, but smaller ranks.

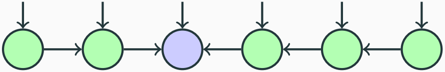
Example 1:

$\mathbf{c} =$ 

Wang, H & Thoss, M. J. Chem. Phys. 119, 1289 (2003)

Multi-Layer (Cont'd)

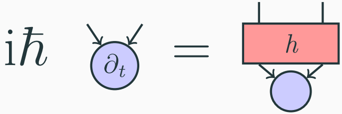
Example 2: matrix product states (MPSs) in DMRG

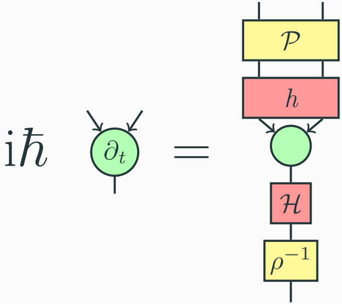
$\mathbf{c} =$ 

For a complete binary tree, the space for saving a wavefunction is $\mathcal{O}(dn^3)$ floats, if $n_\ell = \mathcal{O}(n)$ for all ℓ.

Generally, if $\mathrm{rank} \leqslant p$ for all nodes, the space for saving a wavefunction is of $\mathcal{O}(dn^p)$.

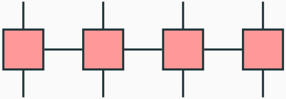
Equations of Motion



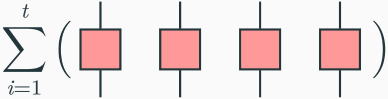


Structure of $\mathbb{H}$

- Matrix product operators (MPOs)

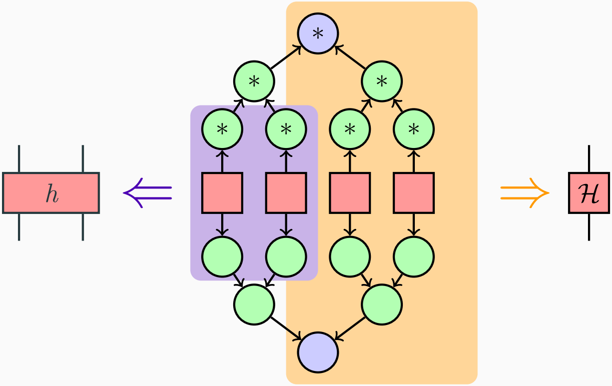


- Summation of products of operators

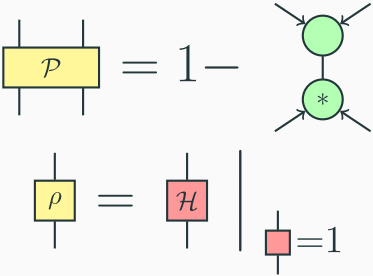


Equations of Motion (Cont'd)

where for all nodes, w. l. o. g., choose one term in $\mathbf{H}$ and one node as an example:



and



Time complexity: if $\mathrm{rank} \leqslant p$ for all nodes, then a step of multiplication is of $\mathcal{O}(tpdn^{p+1})$;

Space complexity: $\mathcal{O}(tpdn^2 + dn^p)$.

Example: 2-D harmonic oscillator

$V = \frac{1}{2}x^2 + \frac{1}{2}y^2 + \frac{1}{4}xy$ (all in a. u.).

Start from the ground state when $V = \frac{1}{2}x^2 + \frac{1}{2}y^2$. Use Sine-DVR as the (primitive) basis set and $n = 40$, $L = 10$.

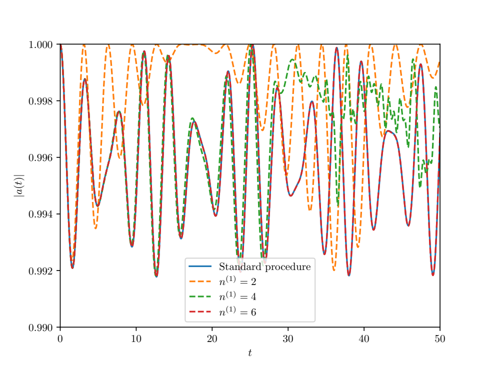
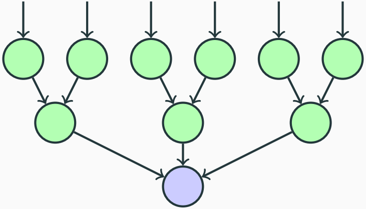


Figure 1: $|a(t)| - t$ (using RK45 as ODE solver, $\Delta t = 0.001$ a. u.)

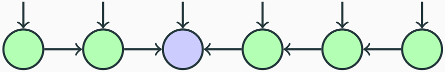
MCTDH vs. DMRG

Structure of Wavefunction: a TN perspective

- MCTDH

$\mathbf{c} =$ 

- DMRG

$\mathbf{c} =$ 

Algorithm: Differnet Choices

	TDSE	TISE
DMRG	Based on propergators	DMRG1, DMRG2
MCTDH	Based on DFVP	Self-consistent

- Other combinations?

Conclusions

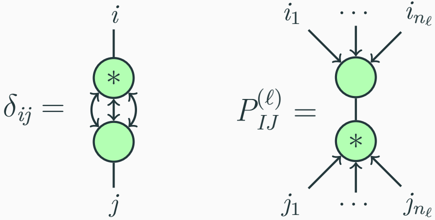
- The structure of wavefunctions in MCTDH and DMRG can be unified in tensor network theory;
- The algorithms used in traditional MCTDH and DMRG are interchangeable in principle;
- The proper structure of wavefunctions in a specific problem needs further studying.

Acknowledgments

Thank you for your listening!

Normalization

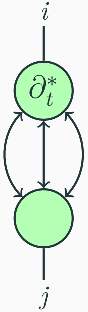
General normalization condition at the ℓ-th node:



Normalization (Cont'd)

In order to hold all general normalization conditions during the propergation, one must have

$$\mathrm{i}g_{ij} \quad =$$



where $\mathbf{g}$ is Hermitian. For simplicity, choose $\mathbf{g} = 0$.