

MULTI-CONFIGURATION TIME DEPENDENT HARTREE THEORY

A TENSOR NETWORK PERSPECTIVE

Xinxian Chen

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Department of Chemistry, Tsinghua University

Non-Relativistic Multi-Dimensional Problem

- TDSE:

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

- TISE:

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

where

$$H = T + V$$

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

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

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: $i\hbar\dot{\mathbf{c}} = \mathbf{H}\mathbf{c}$
 - TISE: $\mathbf{H}\mathbf{c} = E\mathbf{c}$

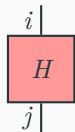
Language: Tensor Network Notation

- Tensors



A blue circle labeled A with three external legs: a diagonal line labeled i on the left, a diagonal line labeled j on the right, and a vertical line labeled k at the bottom.

$$:= A_{ijk}$$



A red square labeled H with two external legs: a vertical line labeled i at the top and a vertical line labeled j at the bottom.

$$:= H_{ij}$$

- Contraction



Diagram showing the contraction of two tensors A and B . On the left, tensor A (blue circle) has legs s (left), t (top), and i (bottom). Tensor B (blue circle) has legs v (top), u (right), and i (left). A horizontal line connects the bottom leg of A to the left leg of B , representing the contraction over index i . This is equated to a summation over i of the product of the two tensors with their respective legs.

$$:= \sum_i$$

Express the Standard Procedure in TNN

- Wavefunction

$$\langle \Phi_I | \Psi \rangle = \text{Diagram of a purple circle labeled } A \text{ with } d \text{ incoming arrows labeled } i_1, i_2, \dots, i_d$$

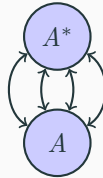
where $i_\kappa \in \{1, \dots, n_\kappa\}$, $\kappa = 1, \dots, d$.

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

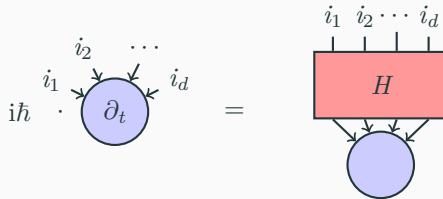
Express the Standard Procedure in TNN (Cont'd)

- Normalization condition

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

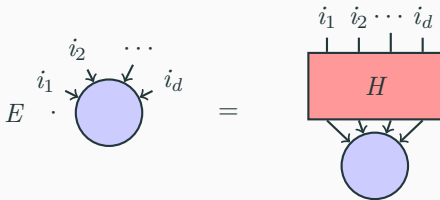


- TDSE



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

$$\langle \Phi_I | \Psi \rangle = \begin{array}{c} i_1 \downarrow \quad i_2 \downarrow \quad \cdots \downarrow \quad i_d \downarrow \\ \text{---} \circ \text{---} \circ \text{---} \circ \text{---} \circ \text{---} \\ \quad \quad \quad \swarrow \quad \downarrow \quad \searrow \\ \quad \quad \quad \circ \end{array}$$

where

$$\langle \Phi_J^{(1)} | \Psi \rangle = \begin{array}{c} j_1 \quad j_2 \quad \cdots \quad j_d \\ \quad \swarrow \quad \downarrow \quad \searrow \\ \quad \quad \quad \circ \end{array}$$

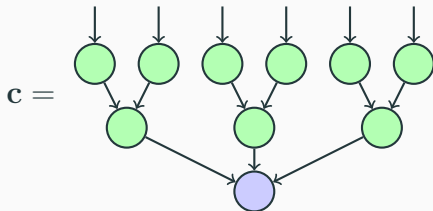
Idea: $j_\kappa \in \{1, \dots, n_\kappa^{(1)}\}$, $\kappa = 1, \dots, d$, and $n_\kappa^{(1)} < n_\kappa$.

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

Multi-Layer

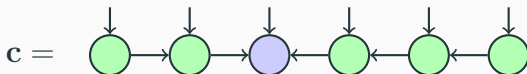
More nodes, but smaller ranks.

Example 1:



Multi-Layer (Cont'd)

Example 2: matrix product states (MPSs) in DMRG



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

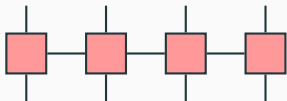
Equations of Motion

$$i\hbar \quad \text{[blue circle with } \partial_t \text{ and two incoming arrows]} = \text{[red box } h \text{ with one incoming and one outgoing line, and a blue circle below it]}$$

$$i\hbar \quad \text{[green circle with } \partial_t \text{ and two incoming arrows]} = \text{[stack of boxes: } \mathcal{P} \text{ (yellow), } h \text{ (red), } \mathcal{H} \text{ (red), } \rho^{-1} \text{ (yellow)]}$$

Structure of \mathbb{H}

- Matrix product operators (MPOs)



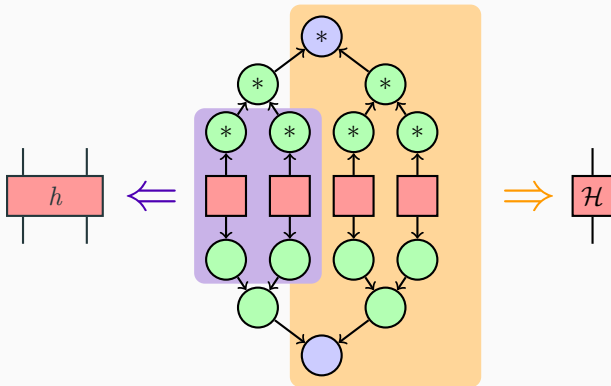
- Summation of products of operators

$$\sum_{i=1}^t \left(\begin{array}{c} \text{MPO}_1 \\ \text{MPO}_2 \\ \text{MPO}_3 \\ \text{MPO}_4 \end{array} \right)$$

The diagram shows a summation over t terms. Each term is a product of four MPOs, represented by red squares with vertical lines. The MPOs are arranged horizontally within the parentheses of the summation.

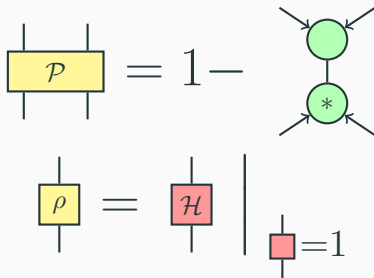
Equations of Motion (Cont'd)

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



Equations of Motion (Cont'd)

and



Time complexity: if $\text{rank} \leq p$ 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

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

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 $n = 40$, $L = 10$.

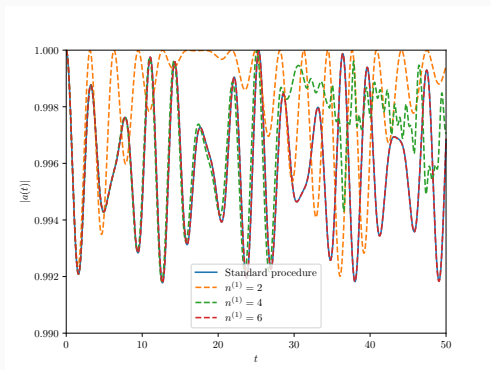
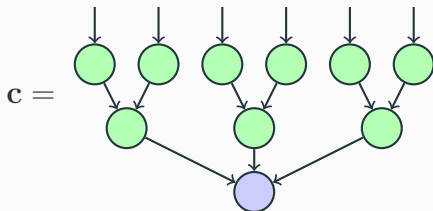


Figure 1: $|a(t)| - t$ (using RK45 as ODE solver, $\Delta t = 0.001$ a. u.)

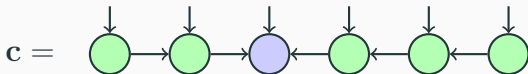
MCTDH vs. DMRG

Structure of Wavefunction: a TN perspective

- MCTDH



- DMRG



Algorithm: Different Choices

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

- Other combinations?

Conclusions

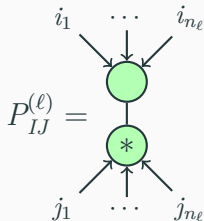
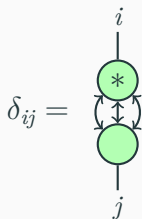
- The structure of wavefunctions in MCTDH and DMRG can be unified in tensor network theory;
- The algorithms used in traditional MCTDH and DMRG are interchangeable in principle;
- The proper structure of wavefunctions in a specific problem needs further studying.

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

$$ig_{ij} = \begin{array}{c} i \\ \downarrow \\ \textcircled{\partial_t^*} \\ \updownarrow \\ \textcircled{} \\ \downarrow \\ j \end{array}$$

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