Finite temperature 2D spin lattices solved using minimally entangled typically thermal states (METTS) algorithm

Computational Physics Project

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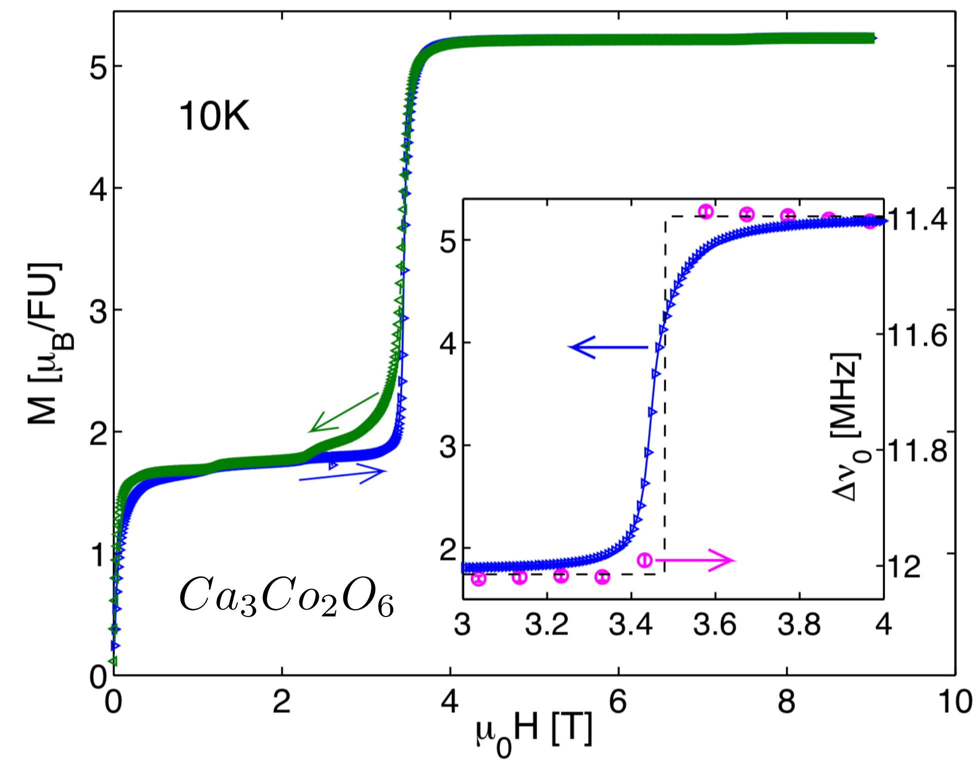
MOTIVATION AND GOAL

- Understanding magnetic ordering and phases shown in recent years experimental results.
- Highly ordered magnetic phases in antiferromagnets tend to give rise to high magneto caloric effect that can be useful for magnetic refrigeration.



G. Allodi, R. De Renzi, S. Agrestini, C. Mazzoli, and M. R. Lees PHYSICAL REVIEW B **83**, 104408 (2011)

- Goal is to find and study magnetisation plateaus (highly ordered magnetic phases) using METTS in 2D Heisenberg antiferromagnets for the first time.

$$H = \sum_{\langle i,j \rangle} J_{i,j} \vec{S}_i \cdot \vec{S}_j - h \sum_i S_i^z$$

METTS ALGORITHM (Idea)

- Goal is to measure physical quantities like expectation values: $\langle A \rangle = \frac{1}{Z} Tr\left[e^{-\beta H} A\right]$
- Possible ways of solving the problem:
  - -Exact diagonalization: Intractable! 2^N
  - -Quantum Monte Carlo: fermion sign Problem! (error bars grow exponentially)

- Possible solution:
  1. Rewrite expectation value:

$$\langle A \rangle = \frac{1}{Z} \sum P(i) \langle \phi(i) | A | \phi(i) \rangle \longrightarrow |\phi(i)\rangle = P(i)^{-1/2} \bar{e}^{\beta H/2} \, |i\rangle$$

  2. Sample states $|\phi(i)\rangle$ with probability $P(i)/Z$.

- Any basis of $|i\rangle$ could be used to carry out the calculation, however the computational cost increases the more entangled $|i\rangle$ is.

$\downarrow$

$\boxed{\text{Chose } |i\rangle \text{ to be a classical product state (CPS).}}$

$$|i\rangle = |i_1\rangle |i_2\rangle ... |i_N\rangle$$

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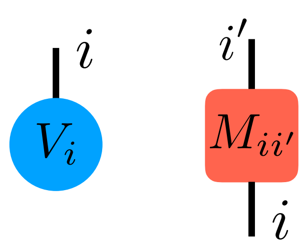
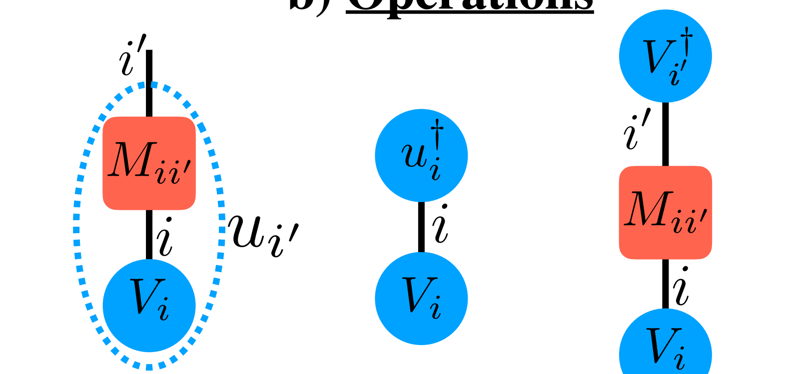
COMMENT (Basics on tensor networks)

a) Definitions



Vector **Matrix**

b) Operations

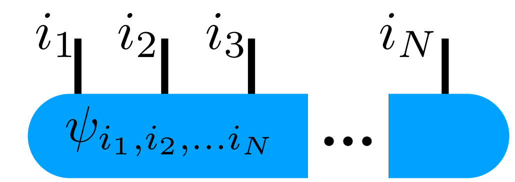


$u_{i'} = M_{ii'} V_i$ $E = u_i^\dagger V_i$ $\langle M \rangle = V_{i'}^\dagger M_{ii'} V_i$

Multiplication of vector by matrix **Scalar product** **Expectation value**

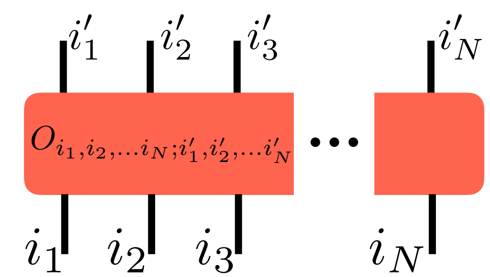
c) Many body wave function

$$|\psi\rangle = \sum_{i_1, i_2, \dots i_N} \psi_{i_1, i_2, \dots i_N} |i_1\rangle |i_2\rangle |i_3\rangle \dots |i_N\rangle$$

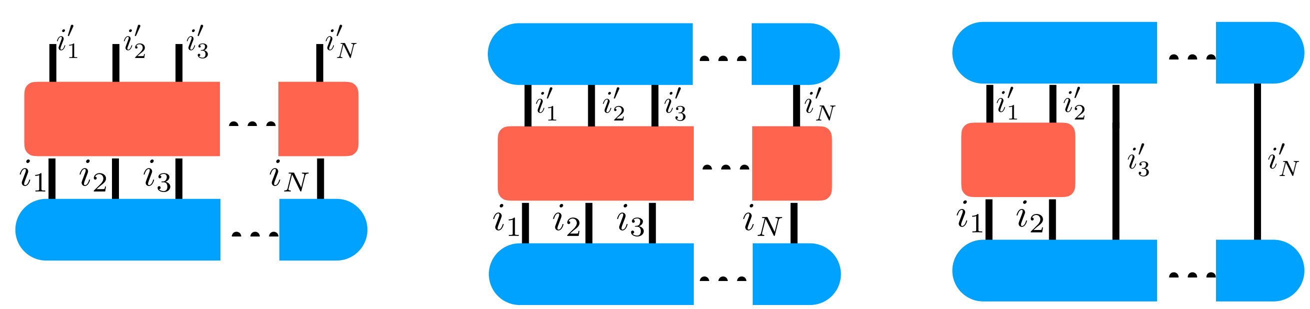


d) Non local many body operator

$$\hat{O} = \sum_{\substack{i_1, i_2, \dots i_N \\ i'_1, i'_2, \dots i'_N}} O_{i_1, i_2, \dots i_N; i'_1, i'_2, \dots i'_N} |i'_1\rangle |i'_2\rangle |i'_3\rangle \dots |i'_N\rangle \langle i_1 | \langle i_2 | \langle i_3 | \dots \langle i_N |$$



d) Some operations in a many body system



$|\psi'\rangle = \hat{O}|\psi'\rangle$ $\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi' \rangle$ $\langle \hat{O}(1,2) \rangle = \langle \psi | \hat{O}(1,2) | \psi' \rangle$

METTS ALGORITHM (Implementation)

Choose a random CPS: $|i\rangle$

↓

1 Write $|i\rangle$ as a MPS

↓

2 Construct the METTS using Trotter for the imaginary time evolution

$$|\phi(i)\rangle = p(i)^{-1/2} e^{-\beta H/2} |i\rangle$$

- Trotter-Suzuki decomposition for $e^{-\beta H/2}$

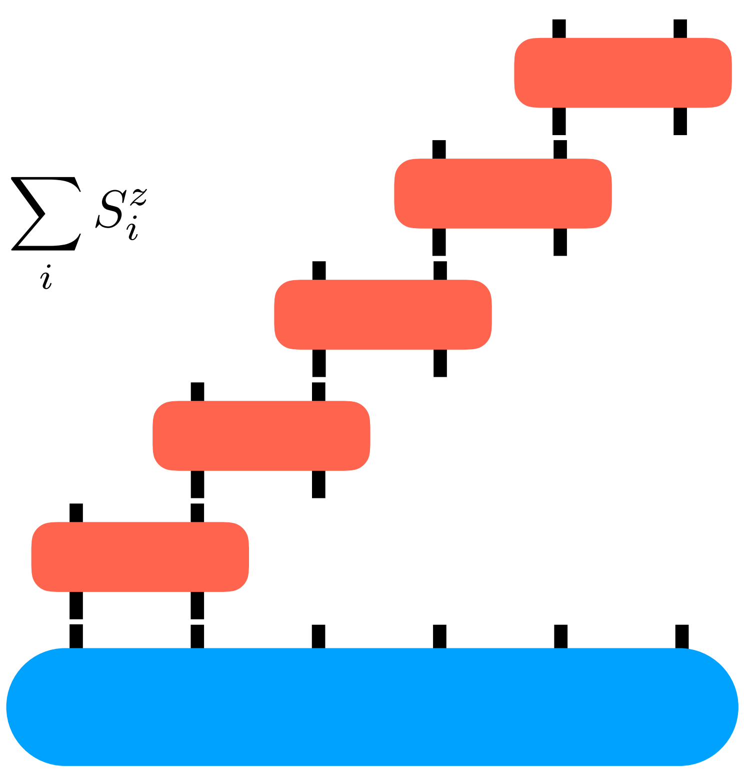
$$H = \sum_n H_n$$ Sum of terms acting on small subsystems.

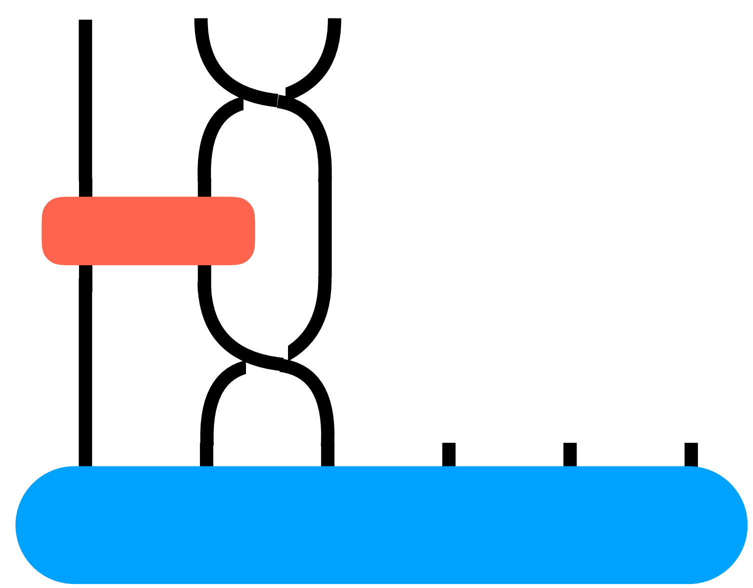
$$e^{-\beta H/2} = e^{-\beta H_1/4} e^{-\beta H_2/4} \ldots e^{-\beta H_N/2} \ldots e^{-\beta H_2/4} e^{-\beta H_1/4} + O\left(\left(\frac{\beta}{2}\right)^3\right)$$

- Low temperatures give rise to big errors!

$$\beta = m\tau \qquad e^{-\beta H/2} = \left(e^{-\tau H/2}\right)^m$$

$$H = \sum_{\langle i,j\rangle} J_{i,j} \vec{S}_i \cdot \vec{S}_j - h \sum_i S_i^z$$





METTS ALGORITHM (Implementation)

Choose a random CPS: $|i\rangle$

1 Write $|i\rangle$ as a MPS

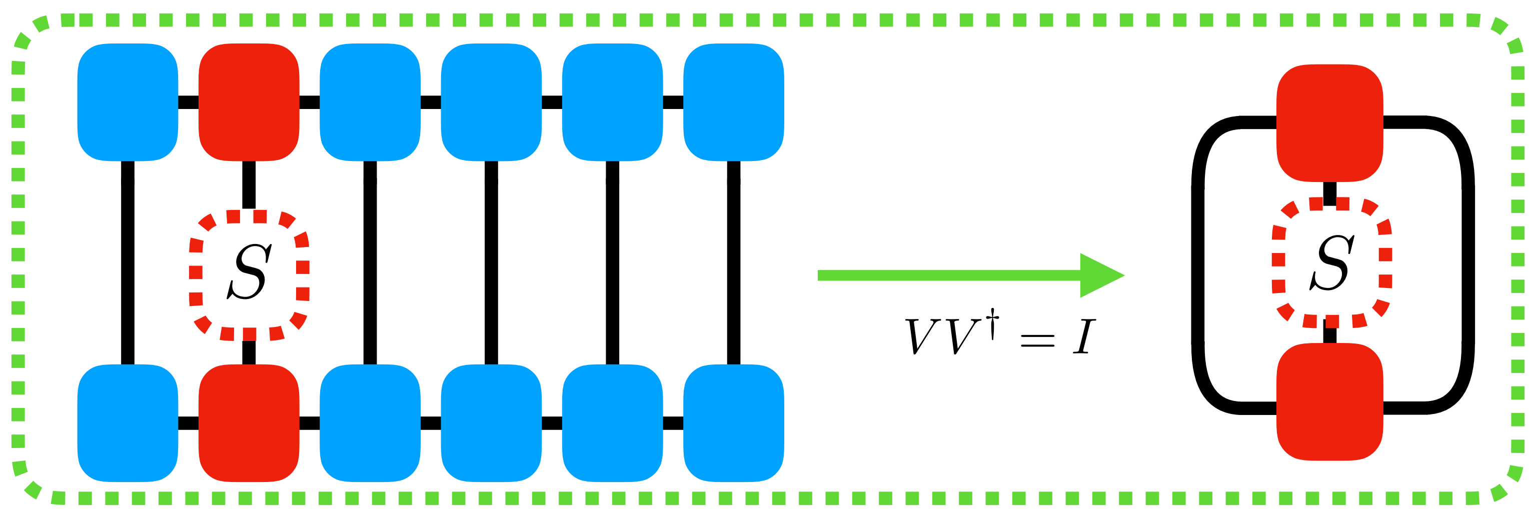
2 Construct the METTS using Trotter for the imaginary time evolution
$$|\phi(i)\rangle = p(i)^{-1/2} e^{-\beta H/2} |i\rangle$$

3 Measure physical observables of interest.
$$\langle A \rangle_i = \langle \phi(i) | A | \phi(i) \rangle$$

- In our case we just want to measure the magnetization:

$$\langle M \rangle = \frac{1}{SN} \sum_i \langle S_i^z \rangle$$

- Sum of local expectation values → exploit the notion of orthogonality center to make the measurement in polynomial time.



Polynomial time!

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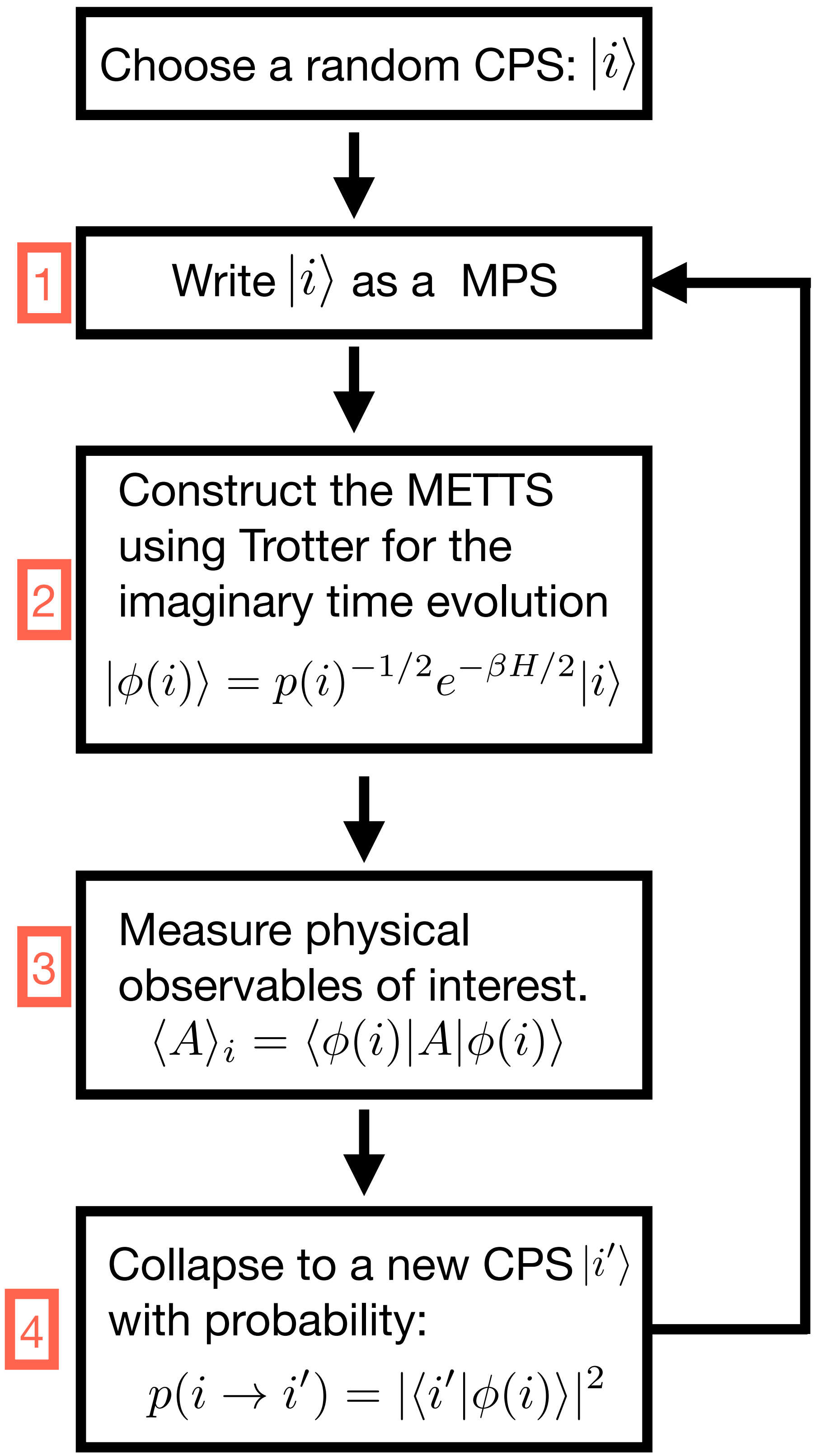
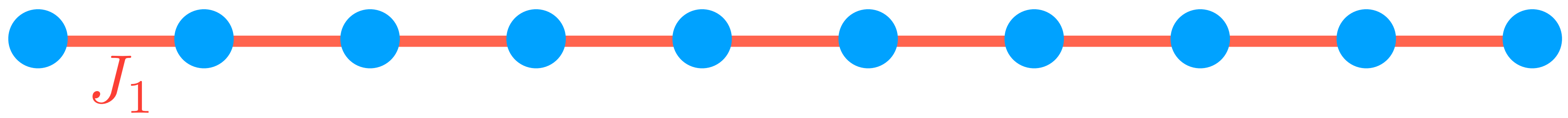
METTS ALGORITHM (Implementation)



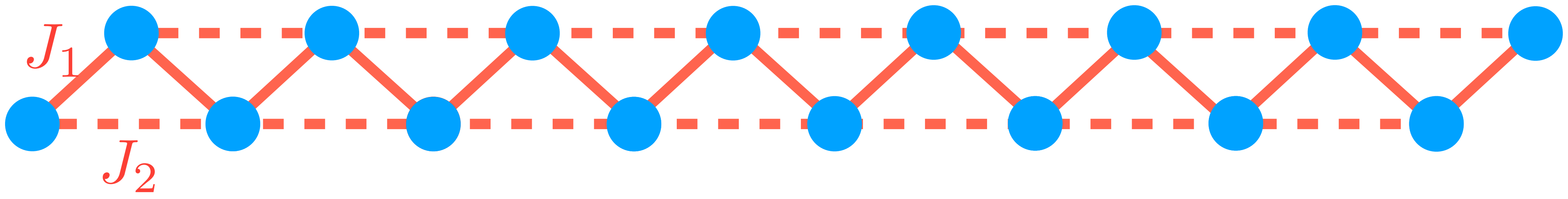
- This step ensures that $|\phi(i)\rangle$ are being sampled with probability $P(i)/Z$.
- Wave function can be collapsed site by site to use the notion of orthogonality centre to calculate the probability of projection in polynomial time.
- Algorithm is embarrassingly parallel.

PHYSICAL SYSTEMS STUDIED

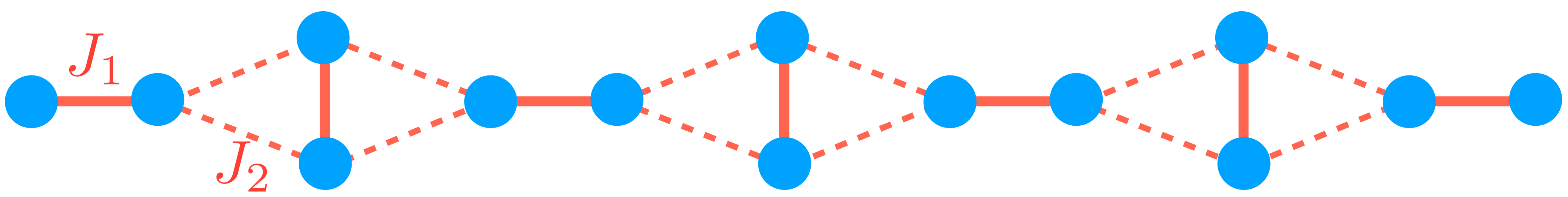
- 1D nearest neighbour chain.



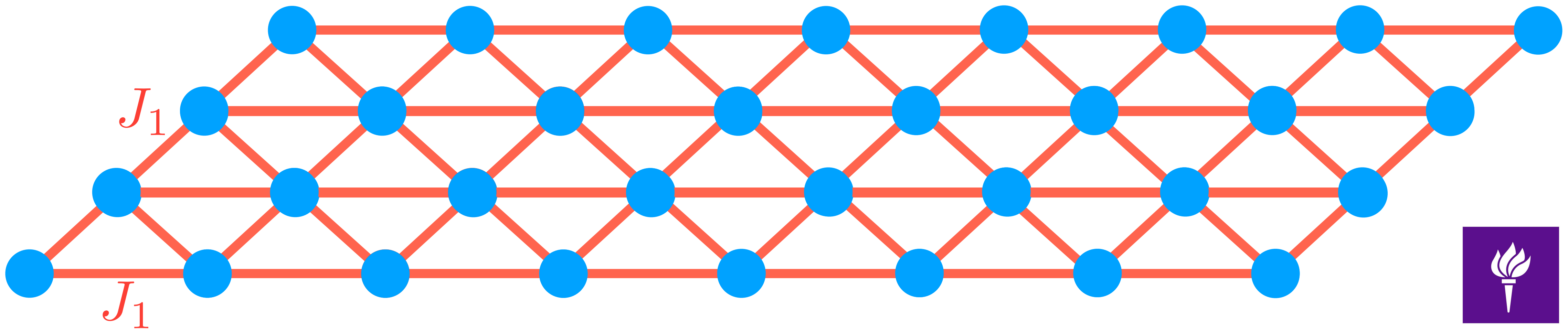
- 1D next-nearest neighbour chain.



- Dimer chain.



- Triangular lattice.



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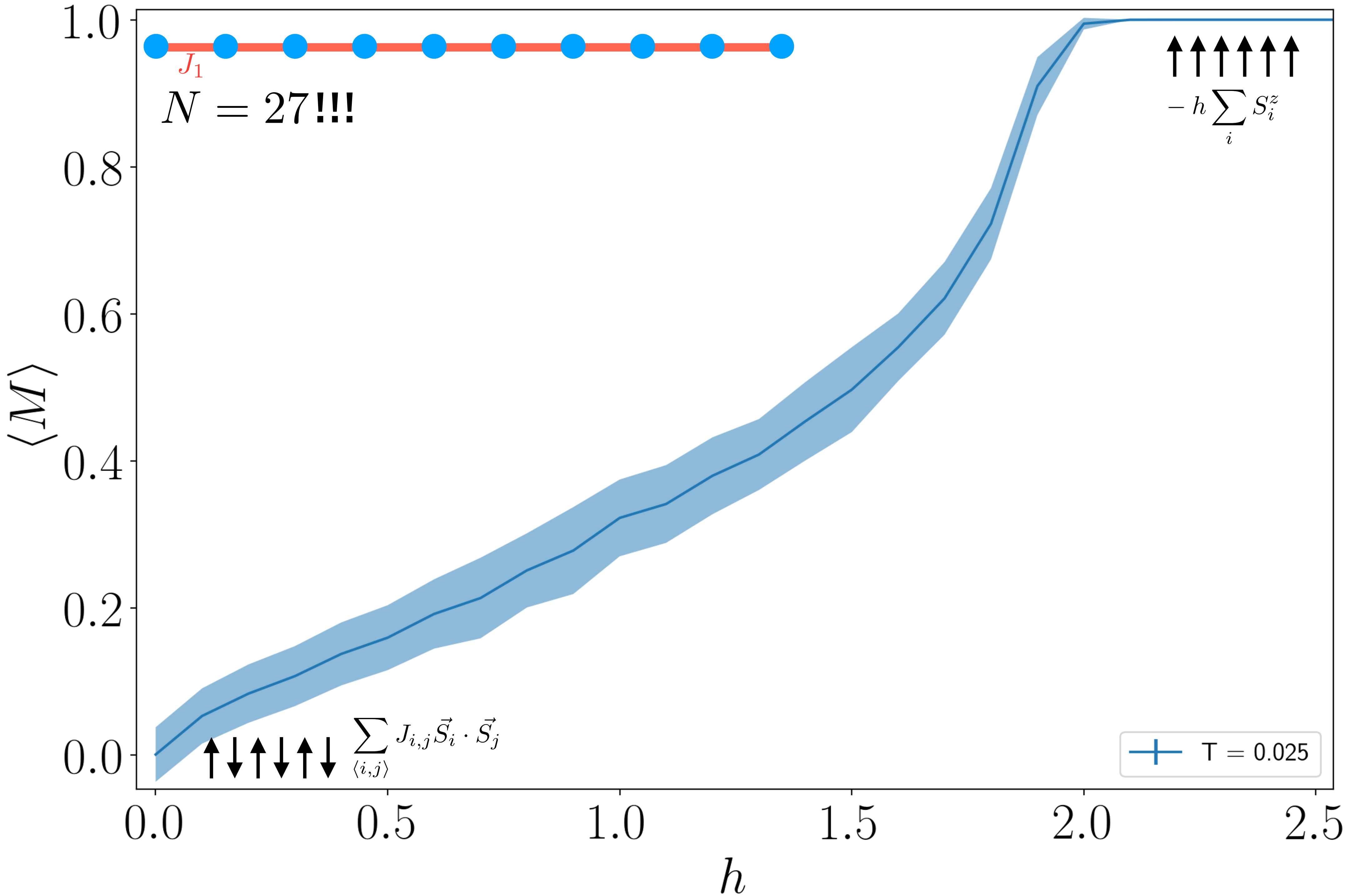
RESULTS: 1D NEAREST NEIGHBOUR

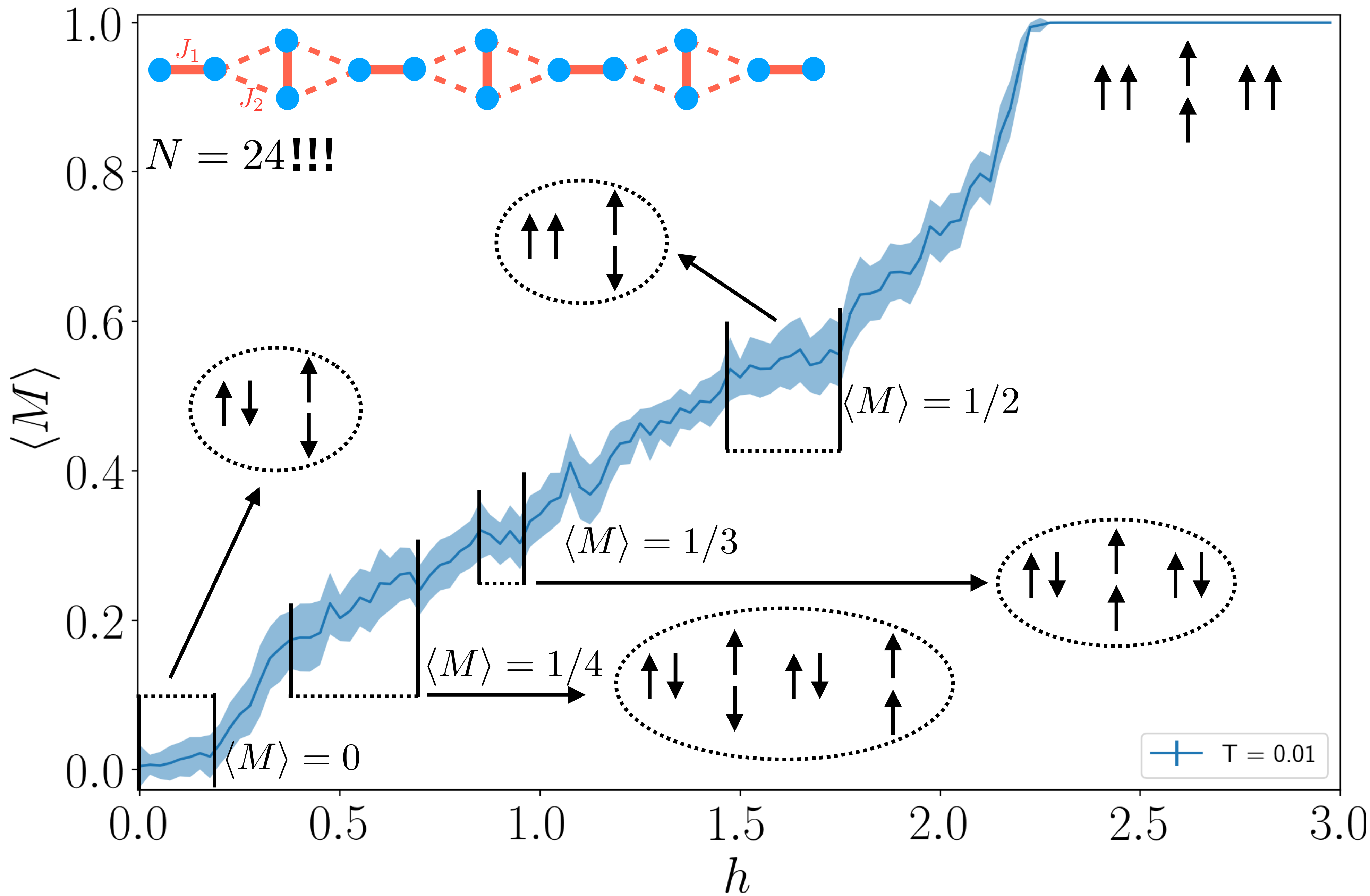


There is nothing very interesting going on in this case, but it serves as a test to show the algorithm works well.

RESULTS: 1D NEXT-NEAREST NEIGHBOUR

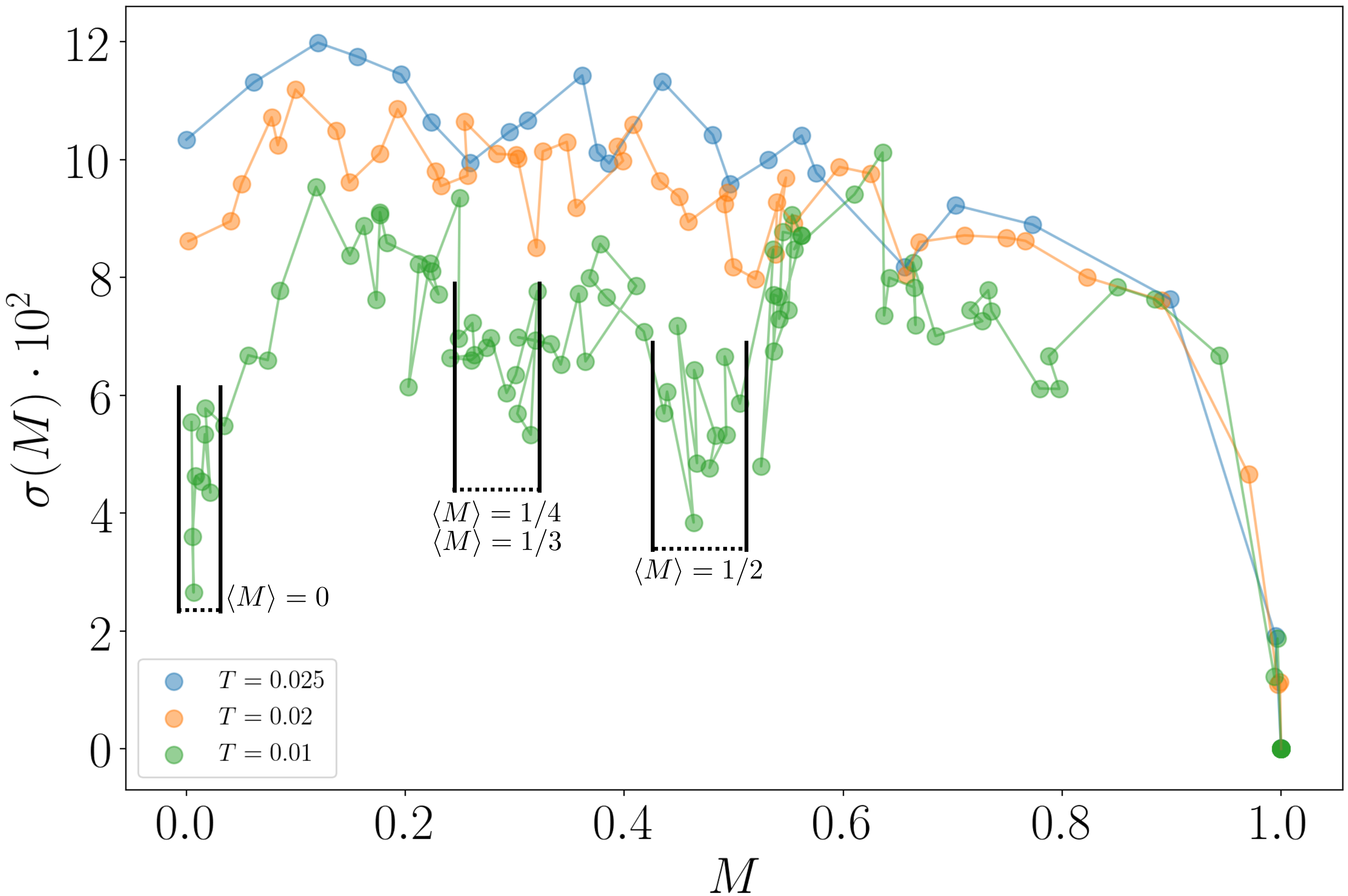
Calculations are running right now...

RESULTS: DIMER CHAIN



Magnetisation plateaus are observed due to highly ordered spin configurations.

RESULTS: DIMER CHAIN



- Plateaus show lower thermal fluctuations in the magnetization.
- Plateaus do not appear at higher temperatures.

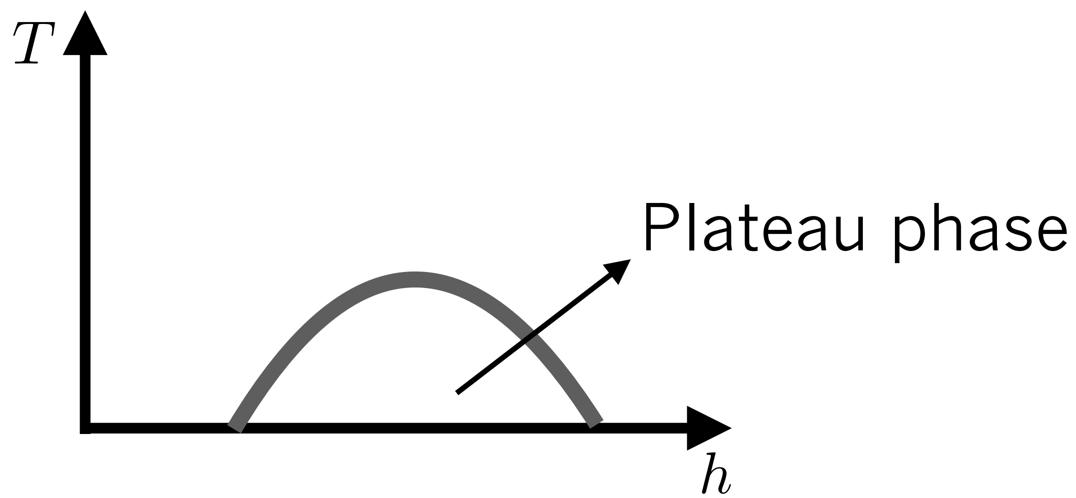
RESULTS: TRIANGULAR LATTICE

Calculations are running right now...

CONCLUSION

- METTS is a very powerful algorithm to simulate in polynomial time quantum many-body systems at finite temperature.
- Reached the goal of finding the magnetisation plateaus.
- Drawback is that it becomes slow when trying to simulate low temperatures.

- Future work:
    - Run simulations in the triangular lattice in a computer cluster.
    - Match simulated magnetisation with experimental data.
    - Construct plateau phase diagram.



Thank you very much for you attention.

Questions?

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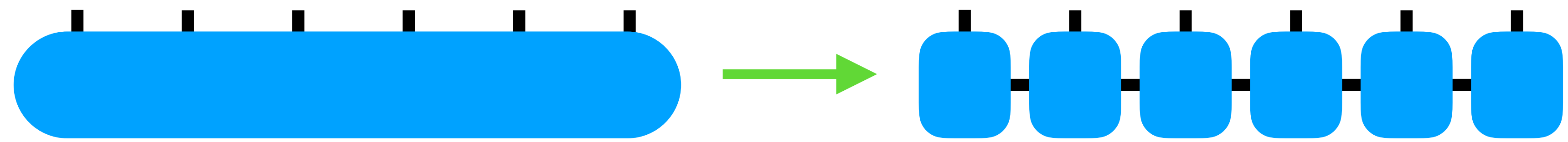
Choose a random CPS: $|i\rangle$ $\quad |i\rangle = |i_1\rangle|i_2\rangle\ldots|i_N\rangle$

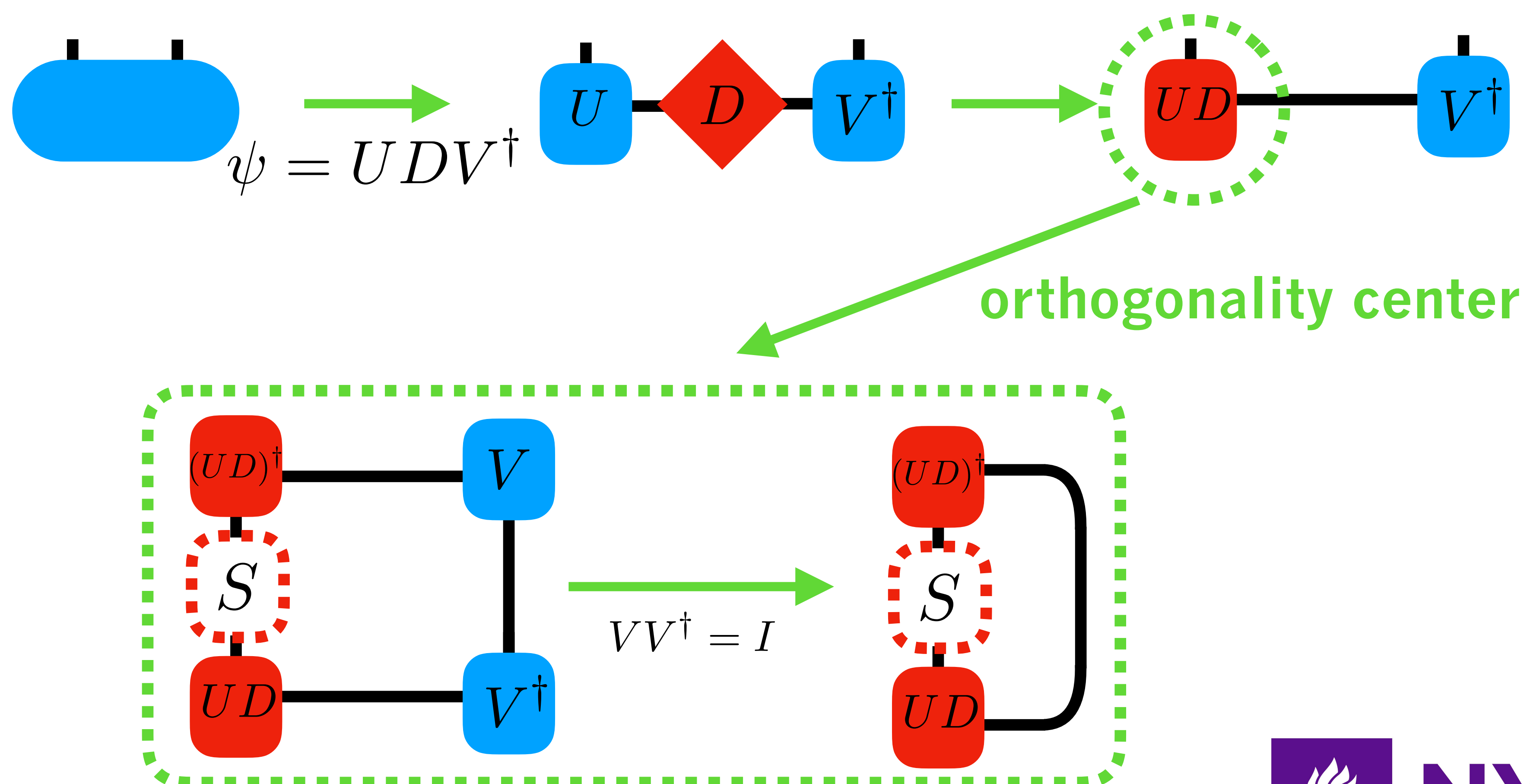
↓

1 Write $|i\rangle$ as a MPS

- Notion of matrix product state (MPS)



- Singular value decomposition and orthogonality centre.



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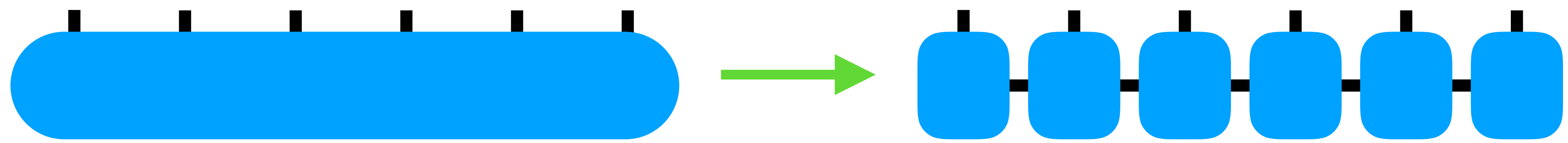

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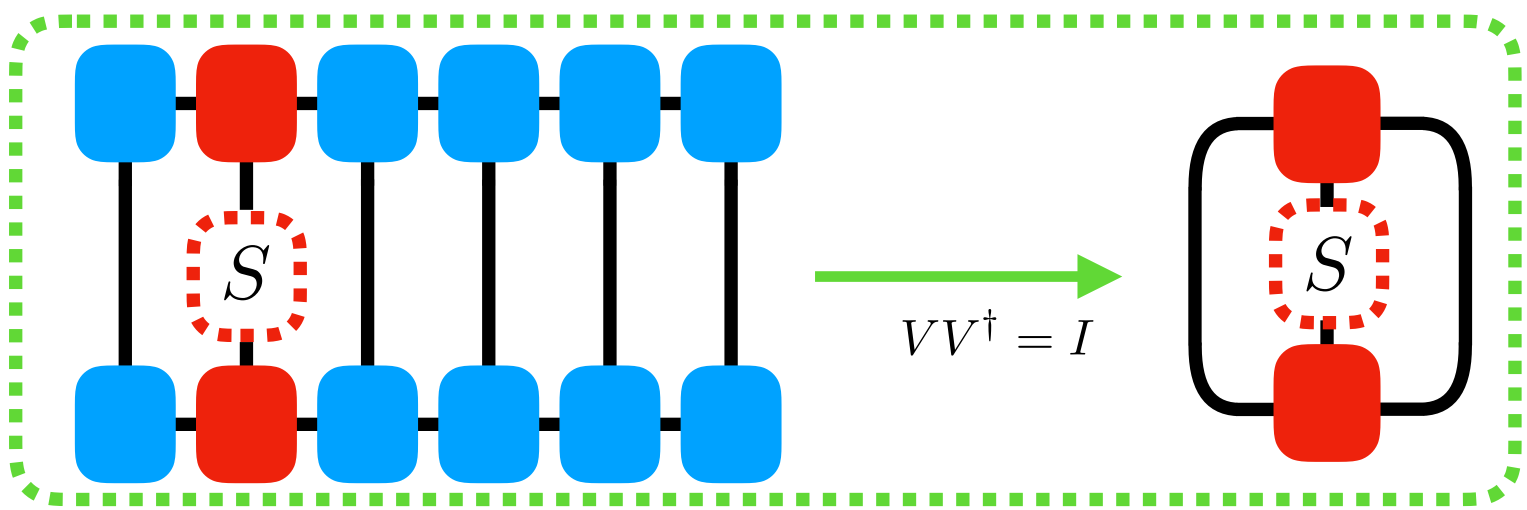
Polynomial time



Polynomial time!

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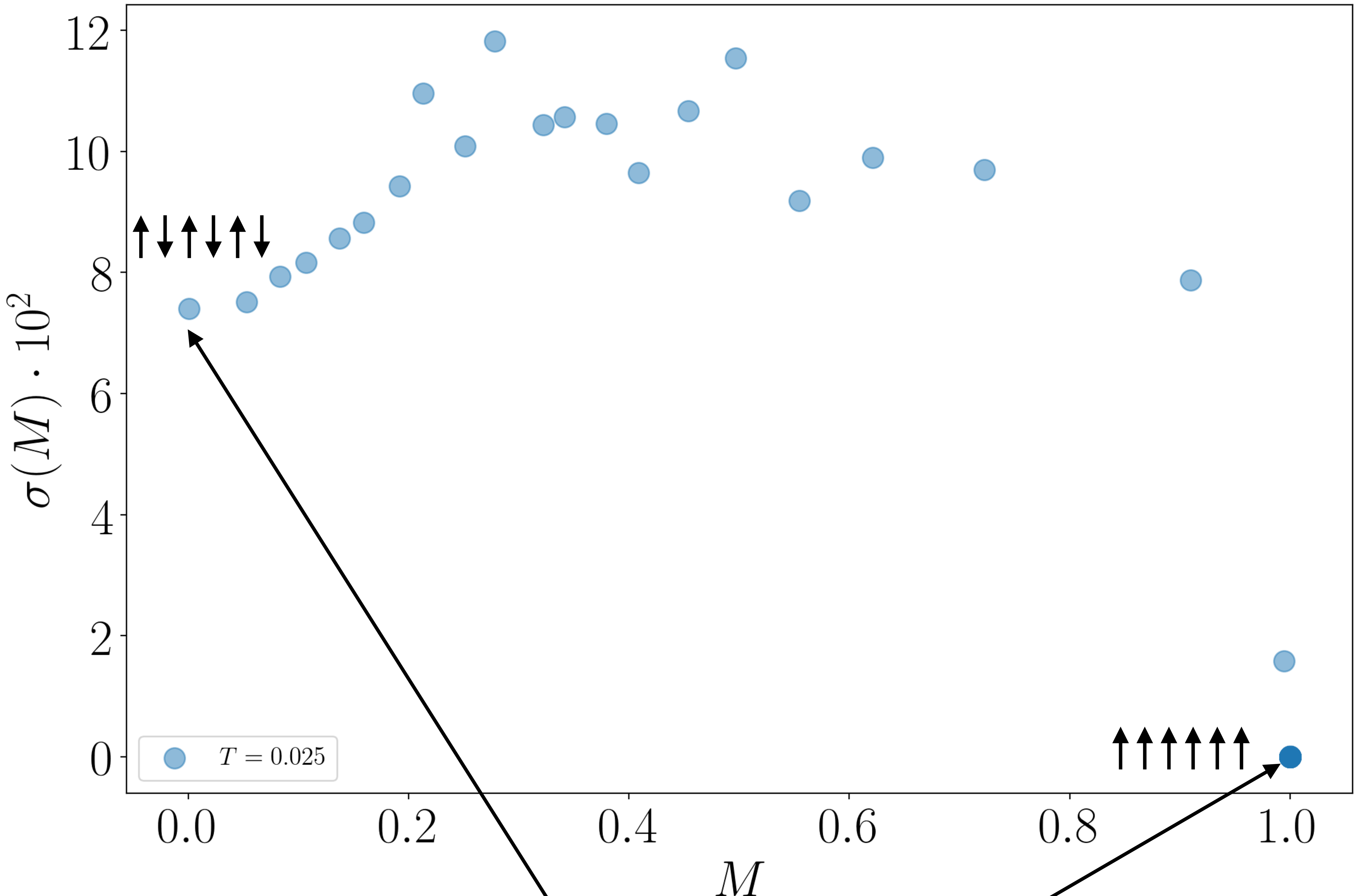
RESULTS: 1D NEAREST NEIGHBOUR



Ordering suppresses thermal fluctuations of the magnetisation.

COLLAPSING STEP ENSURES THE RIGHT SAMPLING DISTRIBUTION

- Randomly chose a CPS $|i\rangle$, the probability of collapsing into a CPS $|i'\rangle$ is:

$$\begin{aligned}
\sum_i \frac{P(i)}{Z} P(i \to i') &= \sum_i \frac{P(i)}{Z} |\langle i' | \psi(i) \rangle|^2 \\
&= \sum_i \frac{P(i)}{Z} \frac{|\langle i' | e^{-\beta H/2} | i \rangle|^2}{P(i)} \\
&= \langle i' | e^{-\beta H} | i' \rangle / Z \\
&= P(j)/Z
\end{aligned}$$

COMPUTATIONAL COST OF METTS

- Cost of producing the METTS: $O(N_x N_y^2 \beta m^3)$
- Cost of measuring magnetisation: $O(N_x N_y m^3 d^2)$
- Cost of collapsing to a new CPS: $O(m^3 d^2)$