Algebraic Methods for Efficient Hamiltonian Simulation via Quantum Computers

Efekan Kökcü

Lawrence Berkeley National Laboratory

ekokcu@lbl.gov

Outline

- Quantum computing
  - Qubits and quantum gates
- Quantum simulation of spin1/2 systems via quantum computers
  - Simulation overall: state prep, time evolution, measurement
  - Time evolution: Trotter-Suzuki approach
- Beyond spin 1/2 systems:
  - Fermions
  - Bosons
- Algebraic Compression of Free Fermionic Evolution

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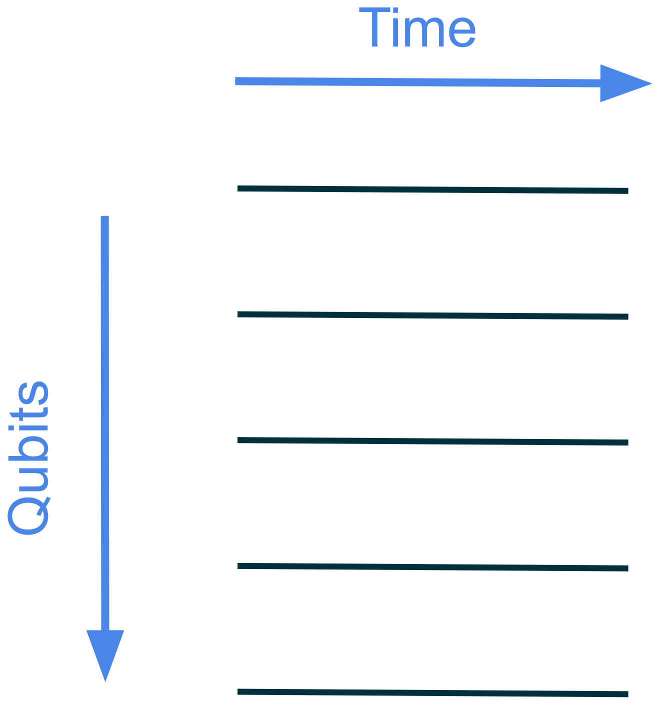
Quantum Computing: Qubits



- Qubits are two level systems which are labeled as 0 and 1

- n qubits can store 2^n complex numbers at once! Thus, quantum computers are powerful candidates for quantum simulation

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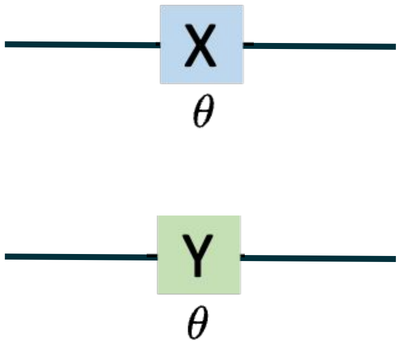
Quantum Computing: Quantum gates

- Commonly, 1-qubit gates are defined as exponentials of Pauli matrices



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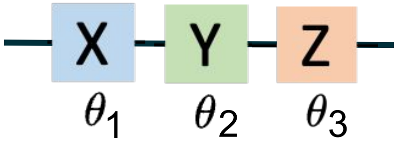
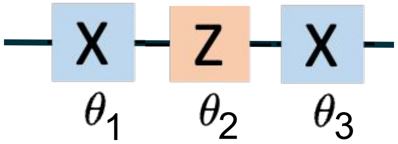
Quantum Computing: Quantum gates

- Commonly, 1-qubit gates are defined as exponentials of Pauli matrices

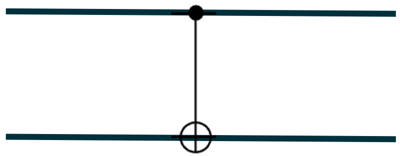
- Any 1-qubit unitary can be written as follows:





Quantum Computing: Quantum gates

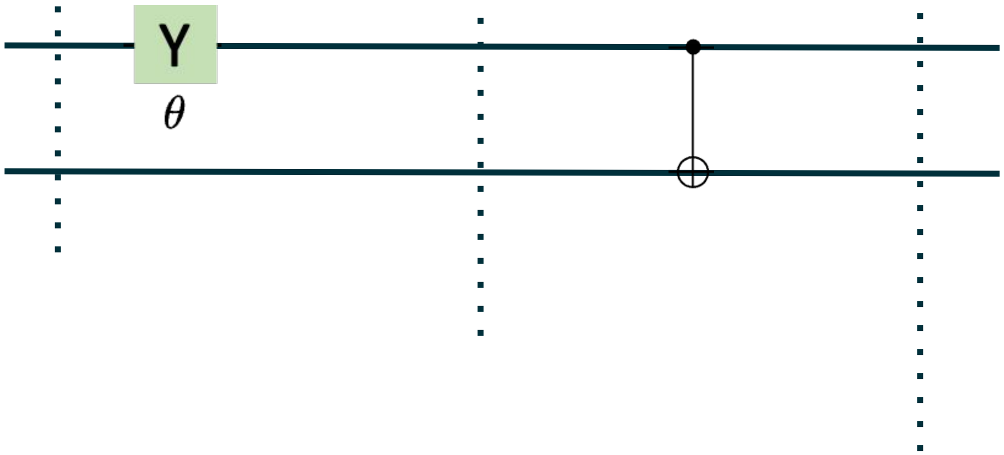
- Controlled not gate is defined as follows:



- It flips the target qubit if the control qubit is in 1 state
- Currently, these are more expensive and more noisy. In the fault tolerant era, the 1-q gates are going to be more expensive.

Quantum Computing: Quantum gates

- Example: the following generates Bell state for



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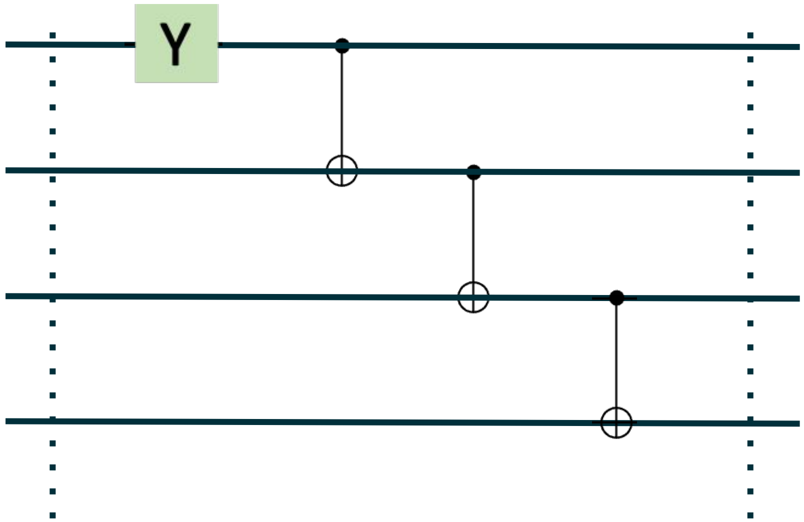
Quantum Computing: Quantum gates

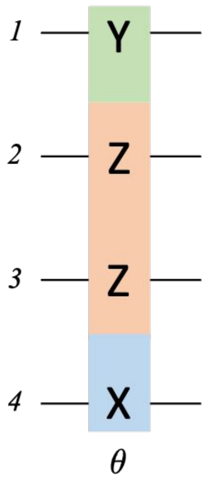
- Similarly, the GHZ state can be generated as follows:



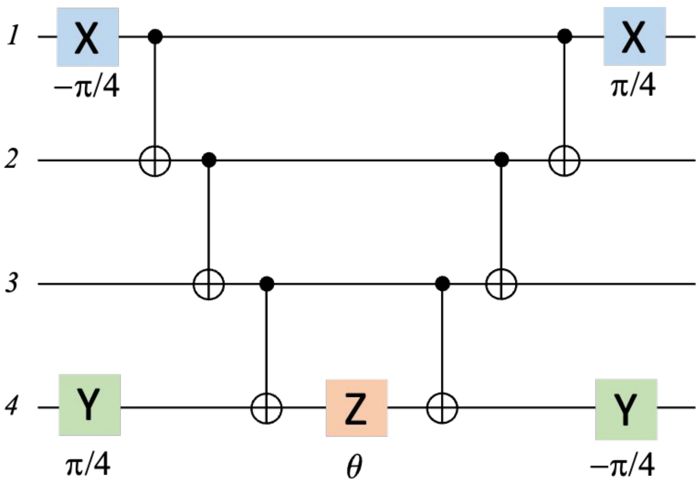
Quantum Computing: Quantum gates

- Using these gates, we can implement rotations of any tensor product of Pauli matrices

$$e^{i\theta Y_1 Z_2 Z_3 X_4} =$$



$$=$$



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Quantum simulation of spin 1/2 systems

- To simulate physical models, one need to map physical degrees of freedom to the d.o.f. of the quantum computer

- For spin 1/2 systems, we can map as follows:

$$|0\rangle \equiv |\uparrow\rangle \qquad |1\rangle \equiv |\downarrow\rangle$$

- Then, each spin operator correspond to the same 1-q quantum gate (to a factor of 2)!

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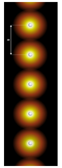
Quantum simulation via quantum computing



Ground state
Excited state
Thermal (Gibbs) state

Time evolution

Measurement

Time evolution: Trotter-Suzuki decomposition

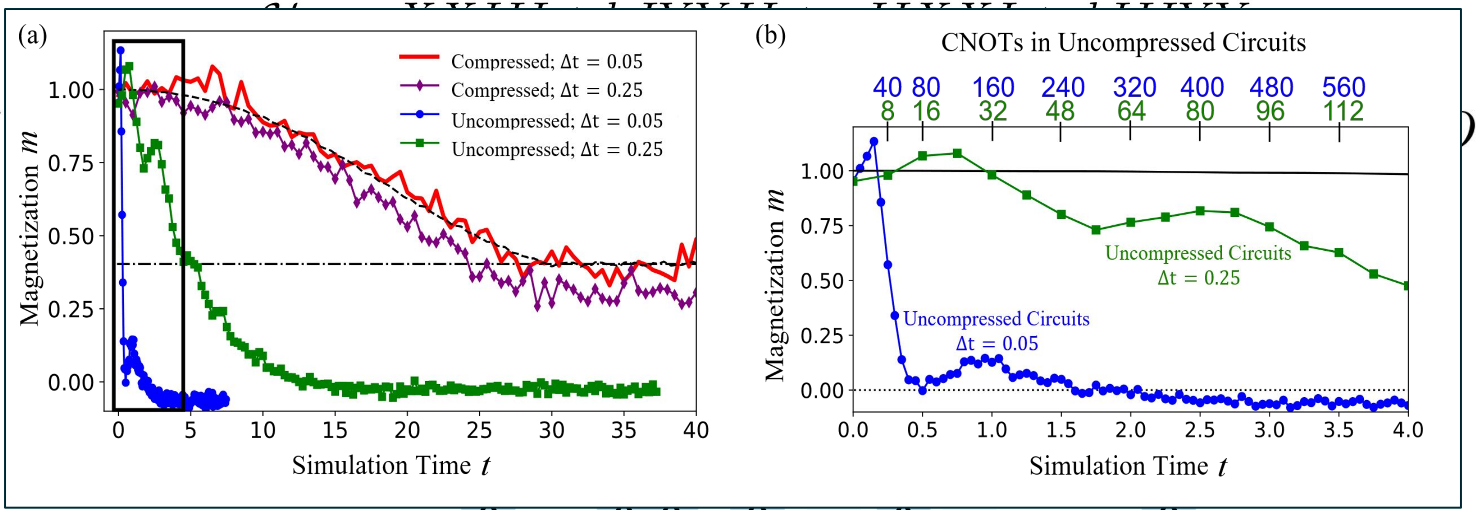
- Consider Kitaev spin chain on 5 spins:

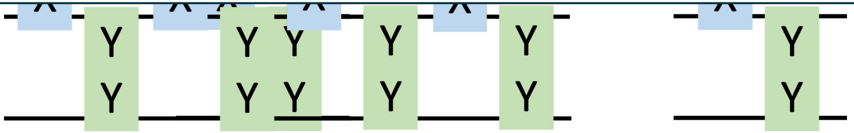
$$\mathcal{H} = a\,XXIII + b\,IYYII + c\,IIXXI + d\,IIIYY$$

$$U(t) = e^{-it\mathcal{H}} \neq e^{-ita\,XXIII}e^{-itb\,IYYII}e^{-itc\,IIXXI}e^{-itd\,IIIYY}$$

Time evolution: Trotter-Suzuki decomposition

- Consider Kitaev spin chain on 5 spins:





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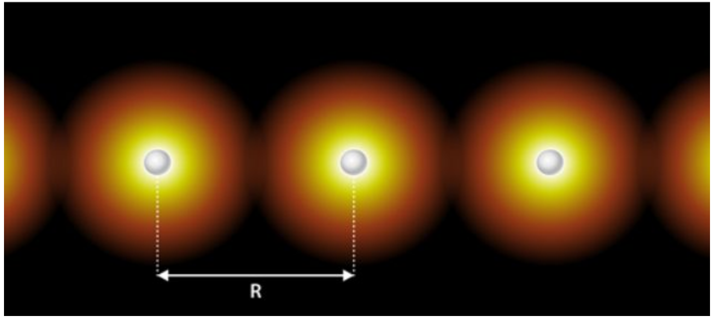
Beyond spin 1/2 systems: Fermions

- Fermionic systems in condensed matter consist of the following states



$|\text{vac}\rangle$ $|\text{vac}\rangle$ $|\text{vac}\rangle$

$c^\dagger|\text{vac}\rangle$ $c^\dagger|\text{vac}\rangle$ $c^\dagger|\text{vac}\rangle$

- These states can directly be mapped to qubits:

$$|0\rangle \equiv |\text{vac}\rangle$$

$$|1\rangle \equiv c^\dagger|\text{vac}\rangle$$

- One needs to make sure that the fermions generate a minus sign under exchange.

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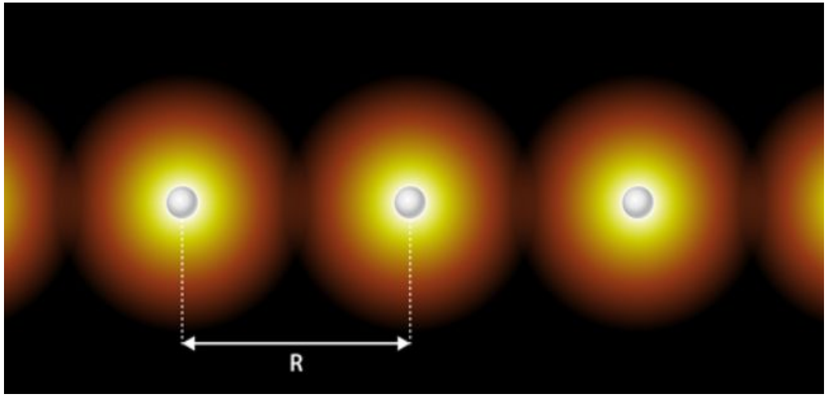
Beyond spin 1/2 systems: Fermions

- One example of these mappings is the Jordan-Wigner mapping:

- There are other mappings such as Bravyi-Kitaev, and generic ternary tree mappings [1,2]

[1] A. Miller et al (2023), PRX Quantum
[2] Y. Liu et al (2025), IEEE Int. Symp. HPCA

Beyond spin 1/2 systems: Bosons



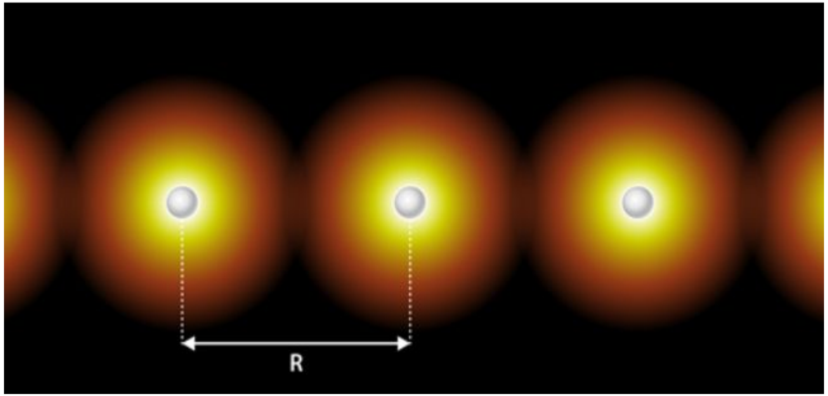
$|\mathrm{vac}\rangle \quad |\mathrm{vac}\rangle \quad |\mathrm{vac}\rangle$

$\vdots \quad \vdots \quad \vdots$

- Boson modes can be seen as quantum harmonic oscillators.
- If truncated in N states, each boson mode can be mapped to N qubits (unary mapping) or $\log_2 N$ qubits (binary mapping)
- Because the qubit operators commute, bosonic statistics is readily satisfied!

[1] R. Somma et al. Inter. Jour. Quant. Inf. 1.02 (2003): 189-206
[2] A. Miessen et al, PRR 3.4 (2021): 043212
[3] N. Sawaya et al, npjQI 6.1 (2020): 49
[4] B. Peng et al, Quant. Sci. Tech. 10.2 (2025):023002

Beyond spin 1/2 systems: Bosons



- Boson modes can be seen as quantum harmonic oscillators.
- Jordan-Lee-Preskill mapping maps each state to an n-qubit state, digitizing the field space.

[1] N. Klyco et al, PRA 99.5 (2019): 052335
[2] R. Ferrel et al, PRD 109.11 (2024): 114510
[3] S. P. Jordan, K. S. M. Lee, and J. Preskill (2011), [Quant. Inf. Comput.14,1014(2014)], 1112.4833

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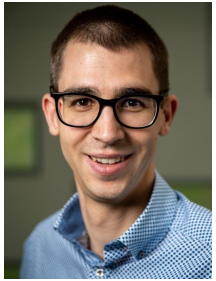
Acknowledgements

Daan Camps
NERSC



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LBNL

Alexander Kemper
NCSU

E. Kökcü et al (2022), PRA 105(3), 032420

D. Camps et al (2022), SIAM, 43(3), 1084-1108.

E. Kökcü et al (2023), arXiv:2303.09538

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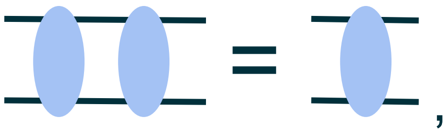
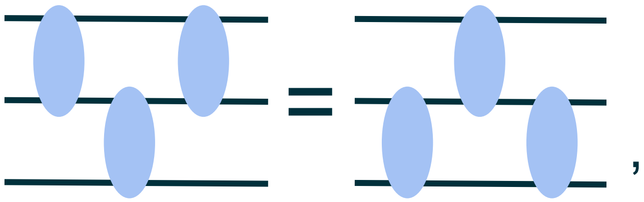
Algebraic Compression

Consider quantum gates that satisfy the following relations:

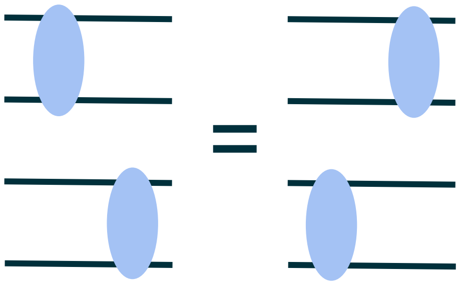
Fusion



Turnover



Commutation

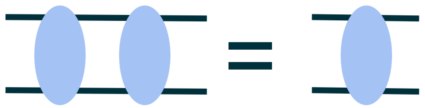


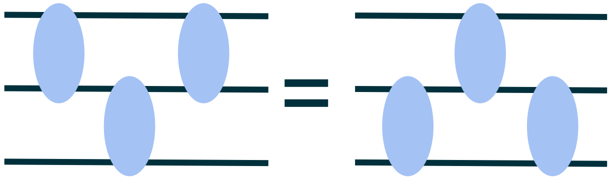
We call them **blocks**. Sequences of blocks can be simplified via algebraic compression [1-2]

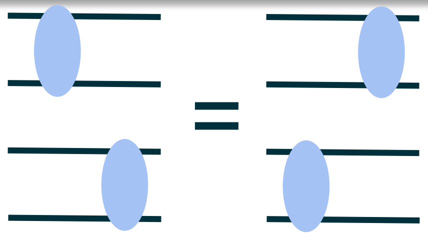
[1] E. Kökcü et al (2022), PRA 105(3), 032420

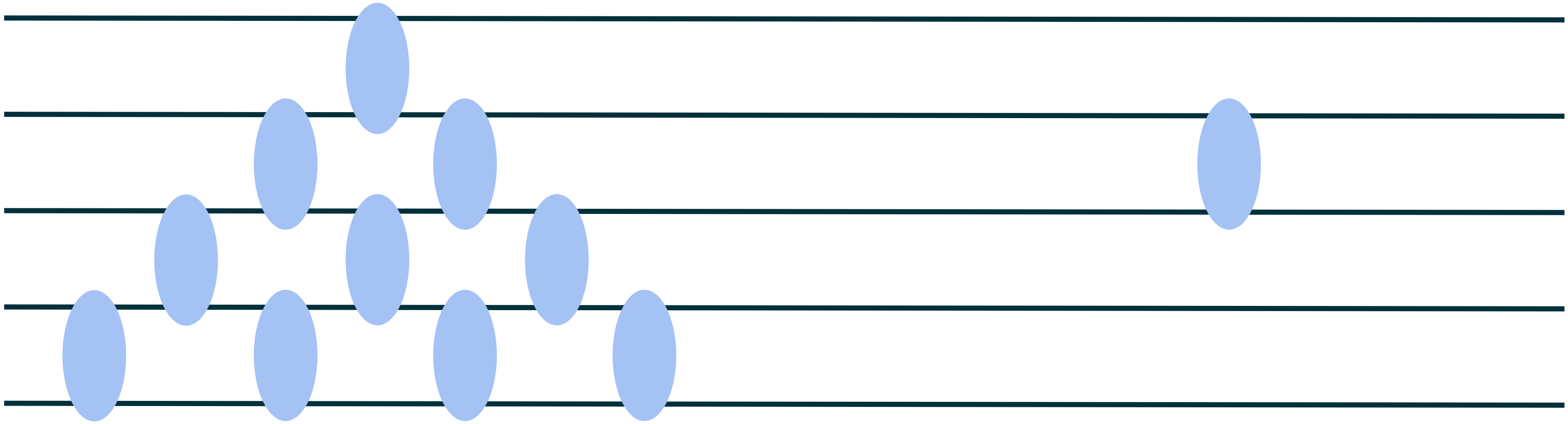
[2] D. Camps et al (2022), SIAM, 43(3), 1084-1108.

Simplification of blocks









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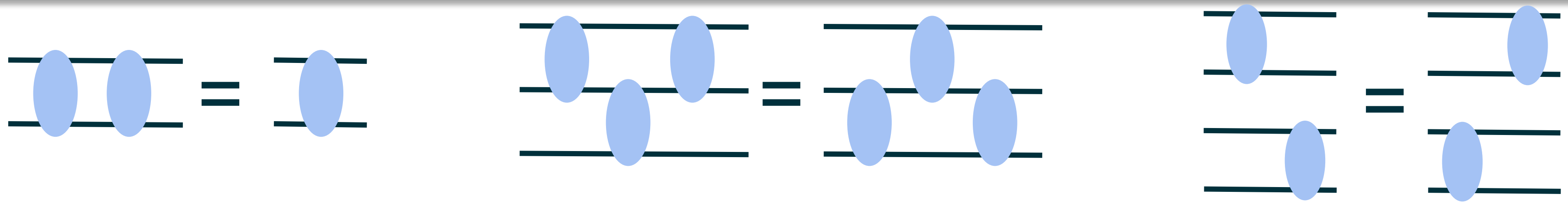

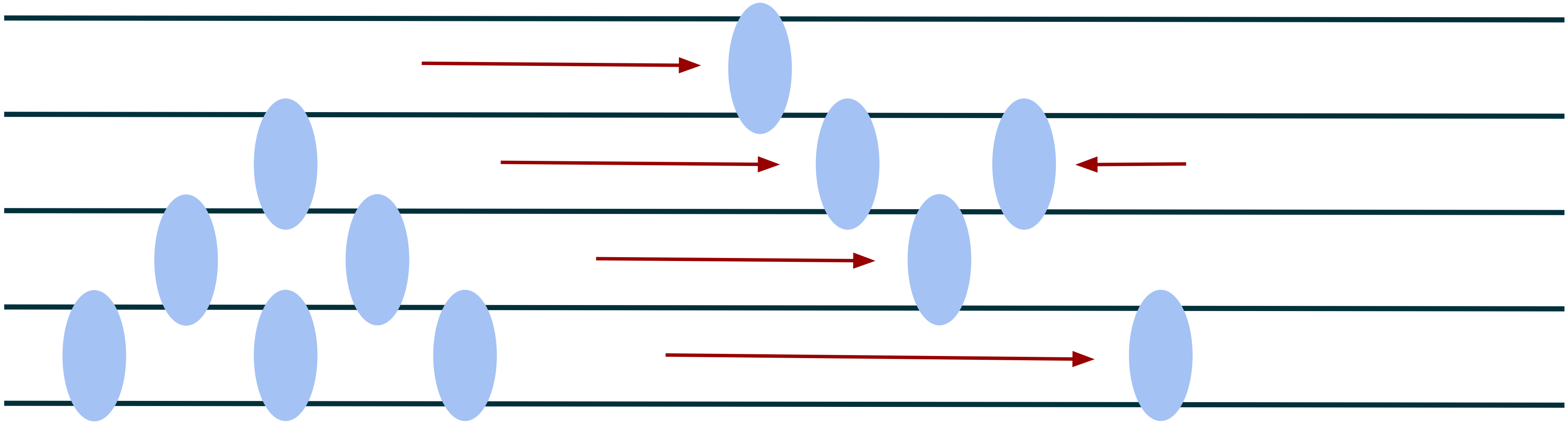

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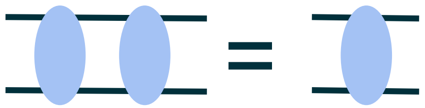

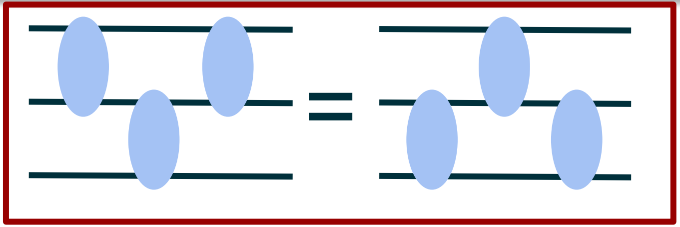

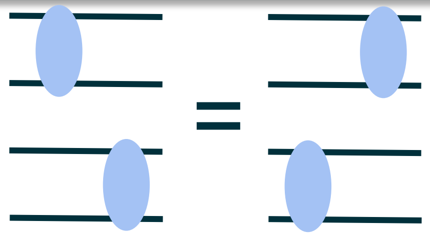

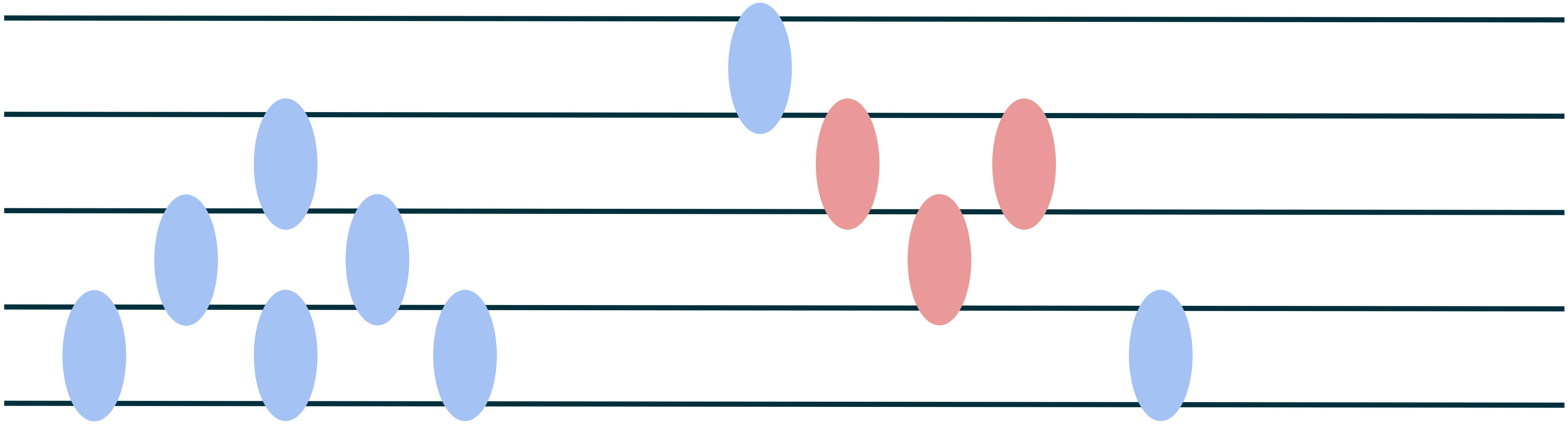

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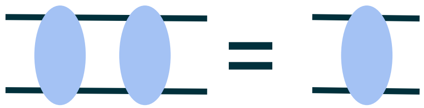

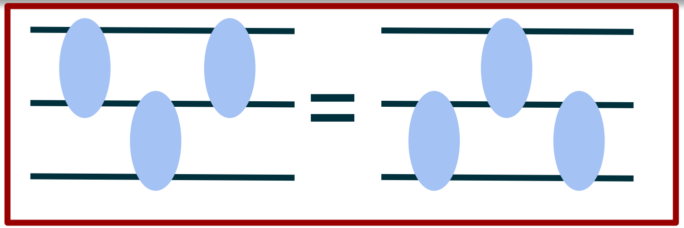

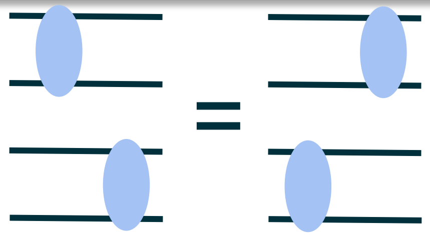

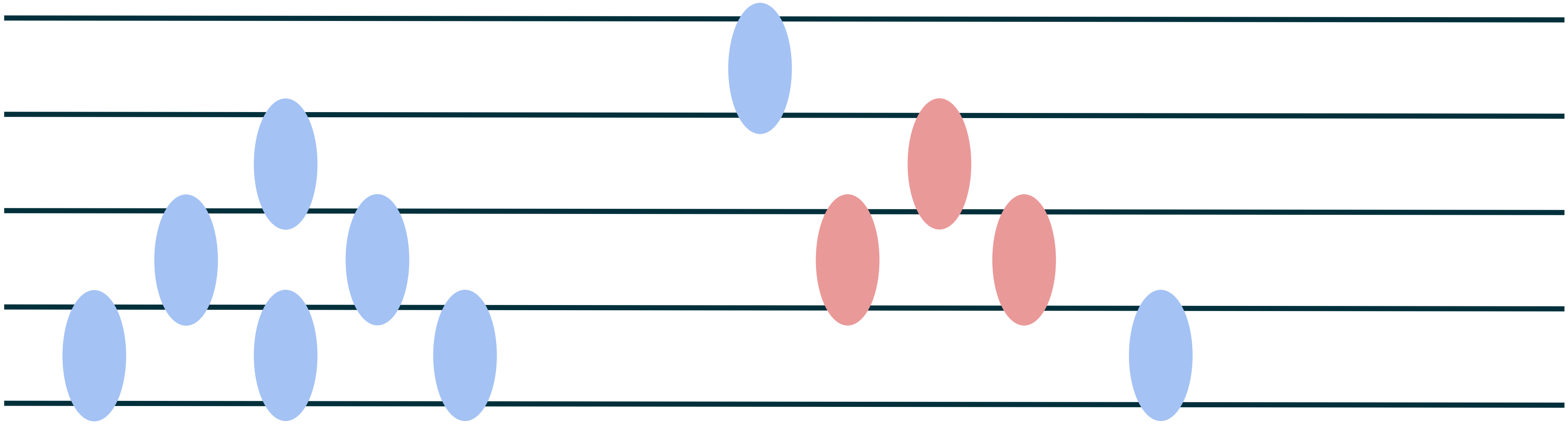

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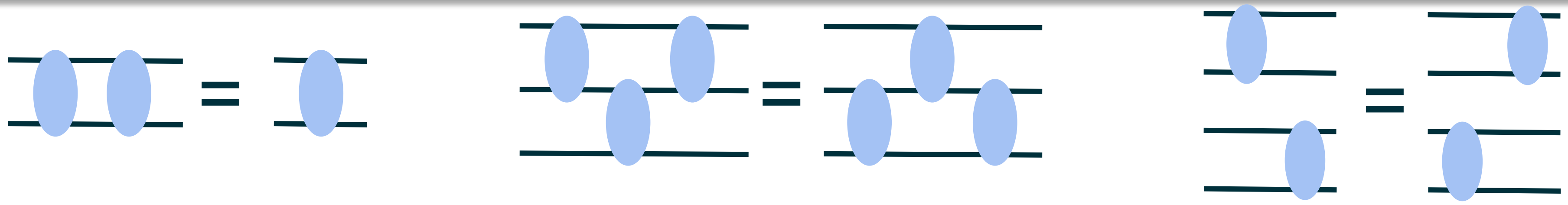

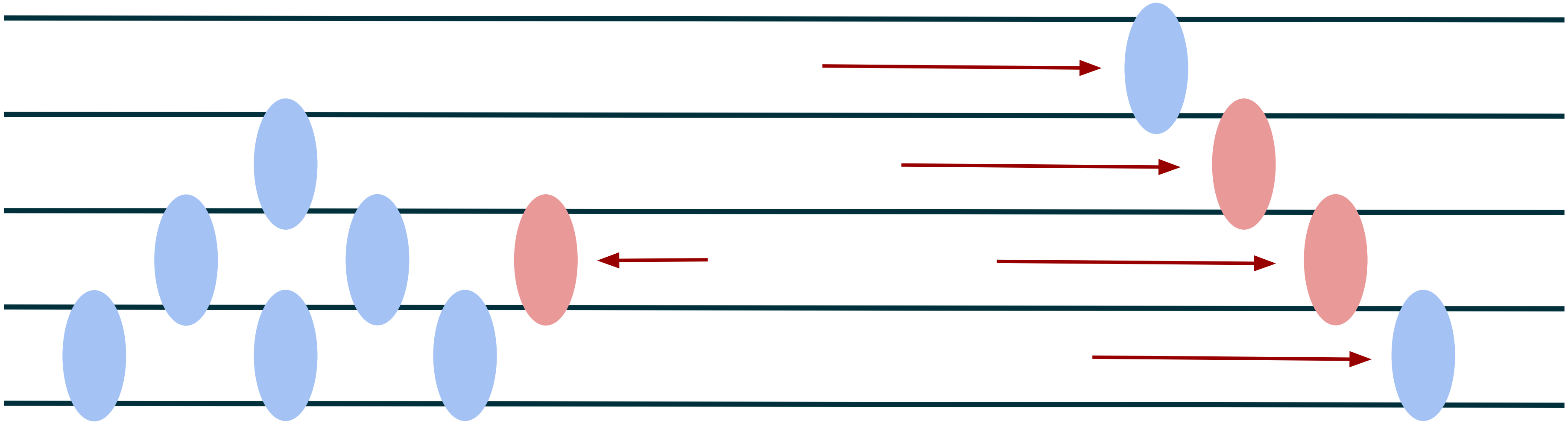

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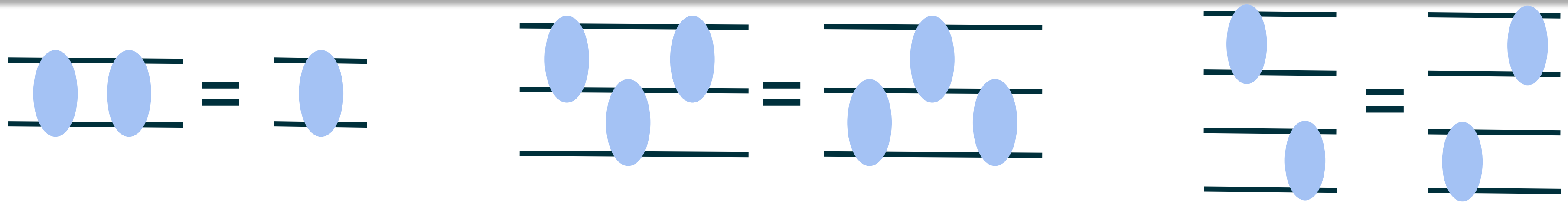

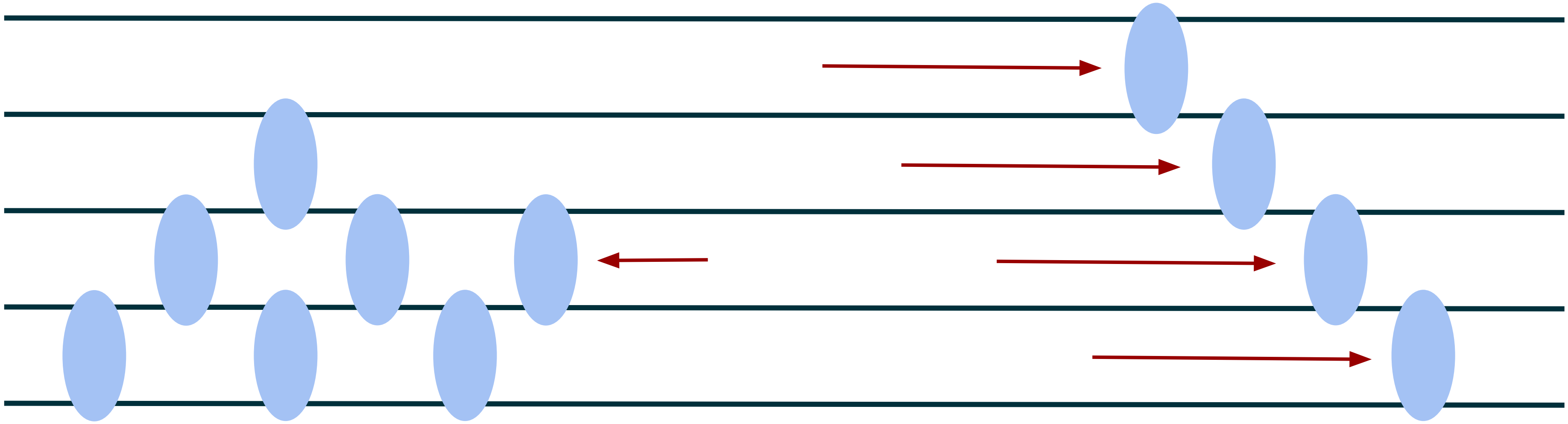

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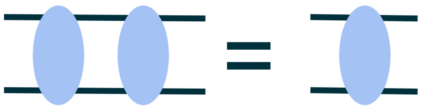

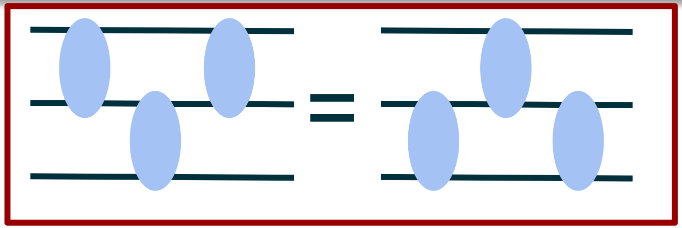

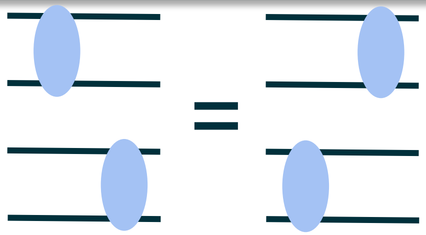

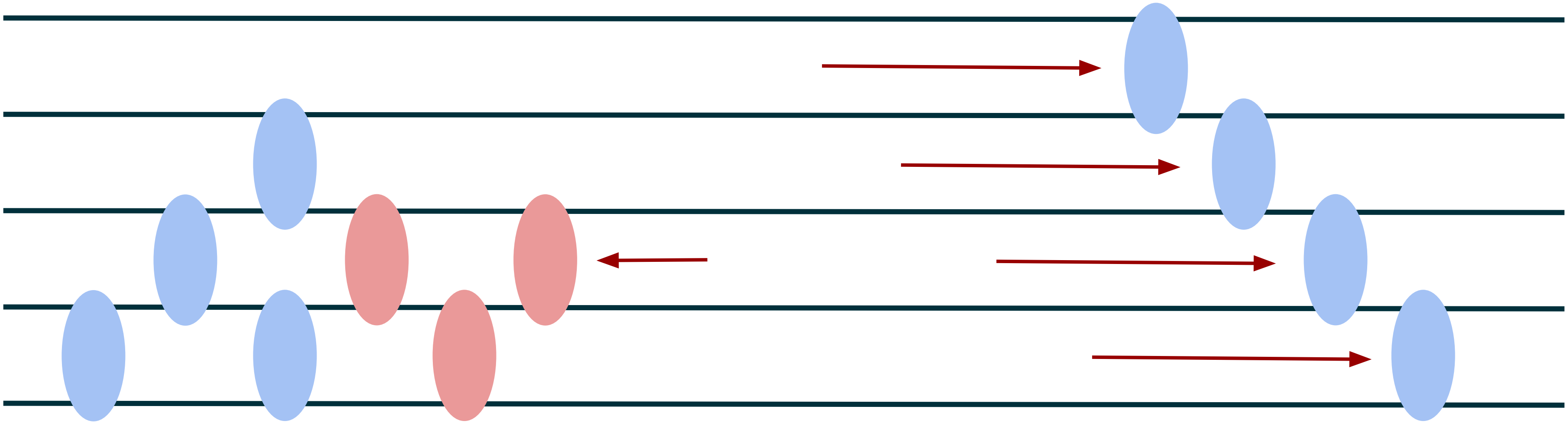

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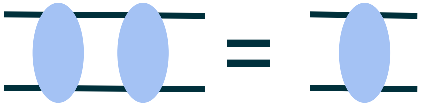

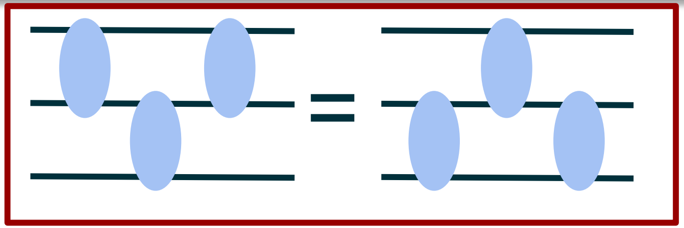

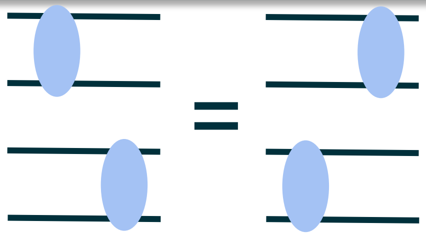

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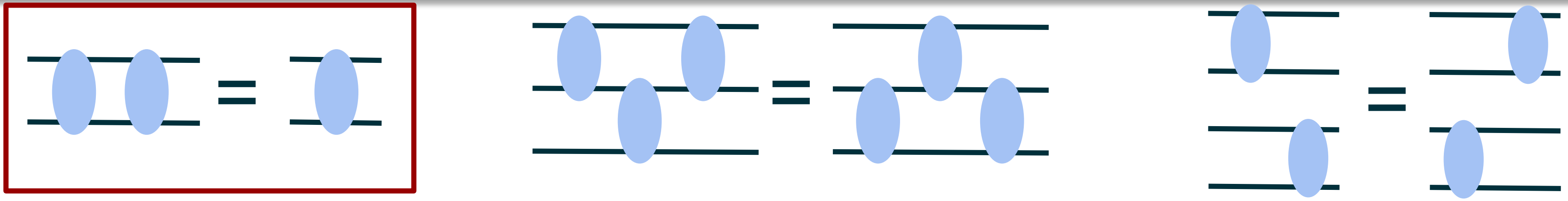

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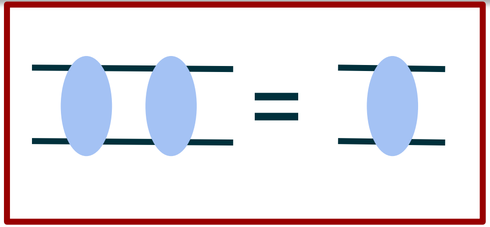

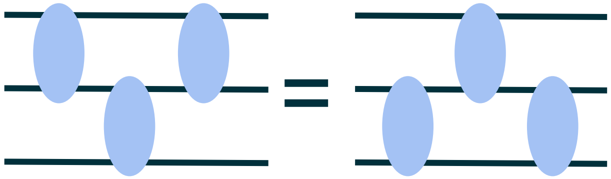

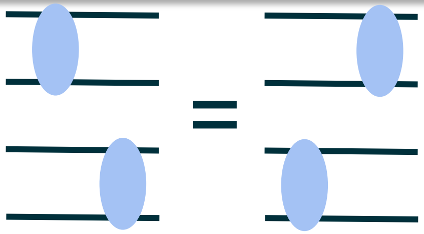

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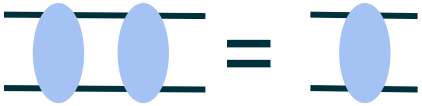

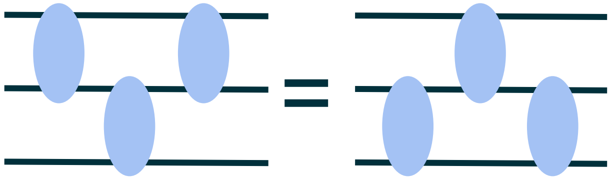

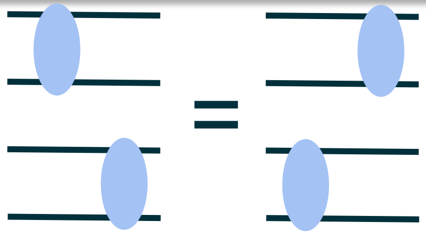

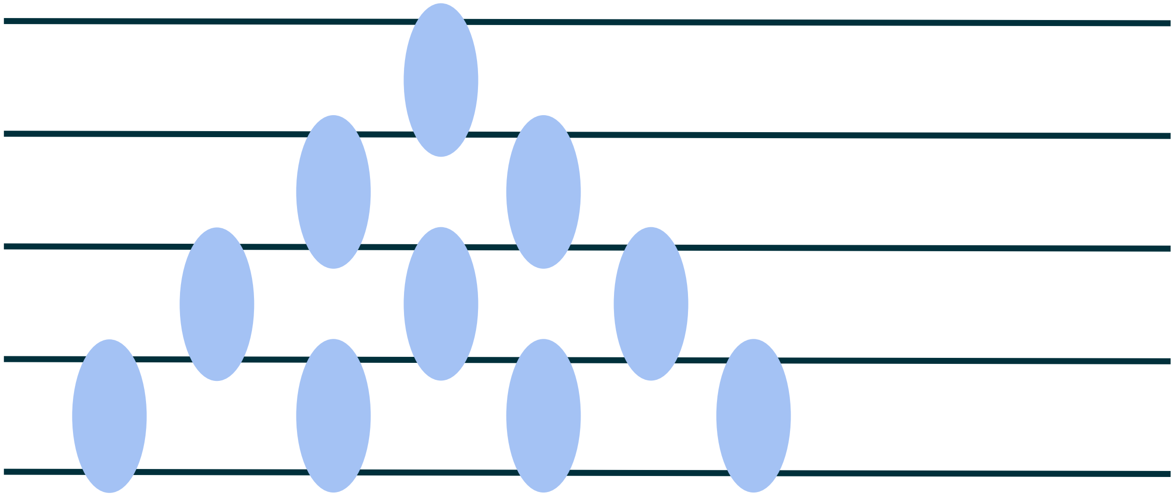

- Triangle can eat any other block!
- This allows us to reduce the number of gates significantly for certain models

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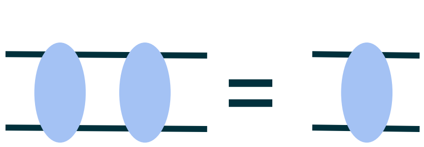
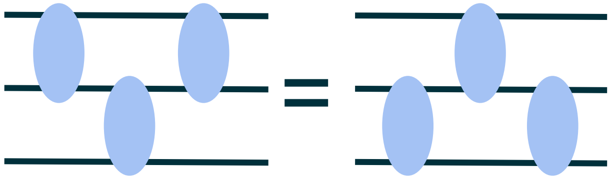
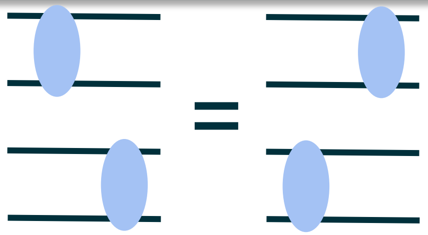
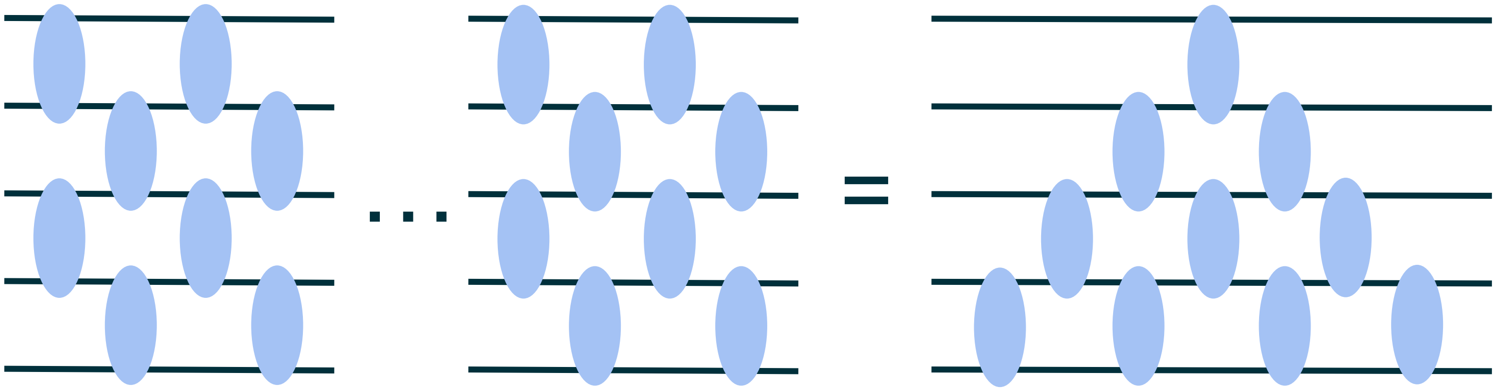
Simplification of blocks

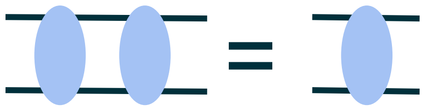


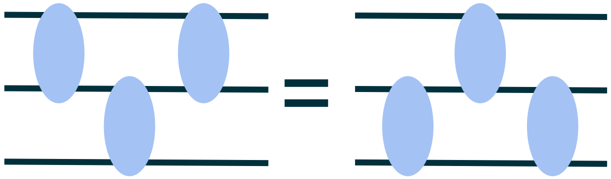


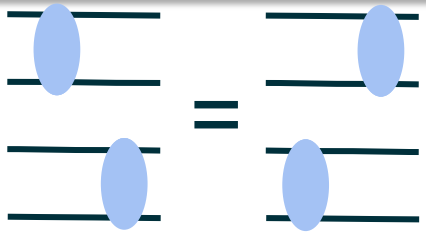




Free fermion models consist of blocks!





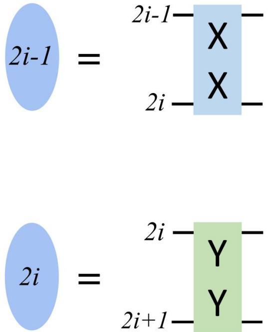


In [1-2], we show that the following models can be represented and compressed via the following blocks

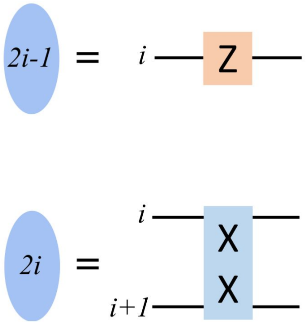
[1] E. Kökcü et al (2022), PRA 105(3), 032420

[2] D. Camps et al (2022), SIAM, 43(3), 1084-1108.

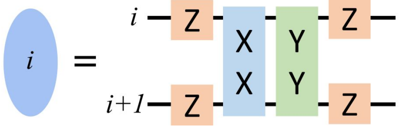
Kitaev Chain / XY model



Transverse Field Ising Model



Transverse Field XY Model



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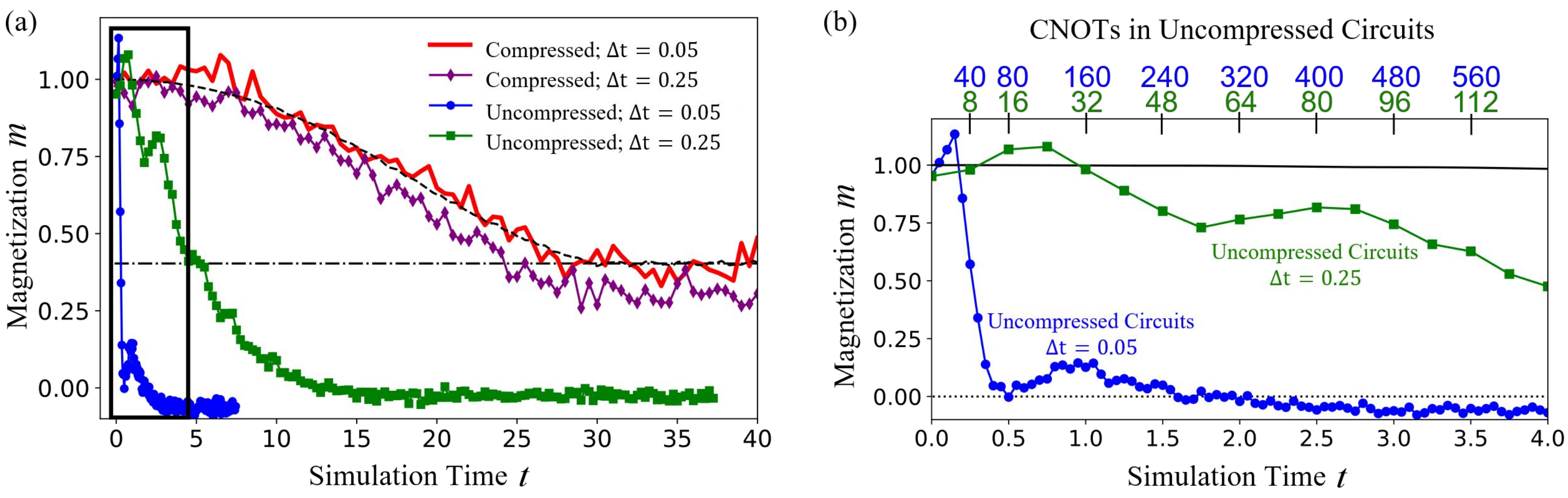
5-site Transverse Field Ising

$$\mathcal{H}_{ASP}(t) = J(t)\sum_{i=1}^{n-1} X_i X_{i+1} + h_z \sum_{i=1}^{n} Z_i \qquad \langle m(t)\rangle \equiv \frac{1}{n}\sum_i \sigma_i^z(t)$$

ibmq_brooklyn results:



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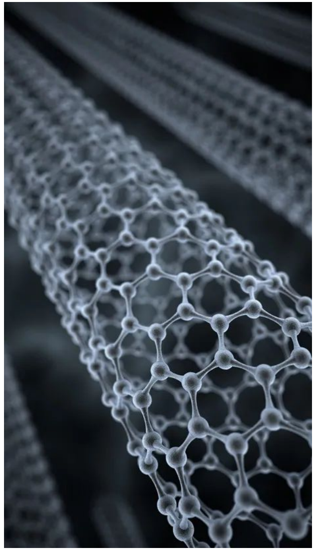
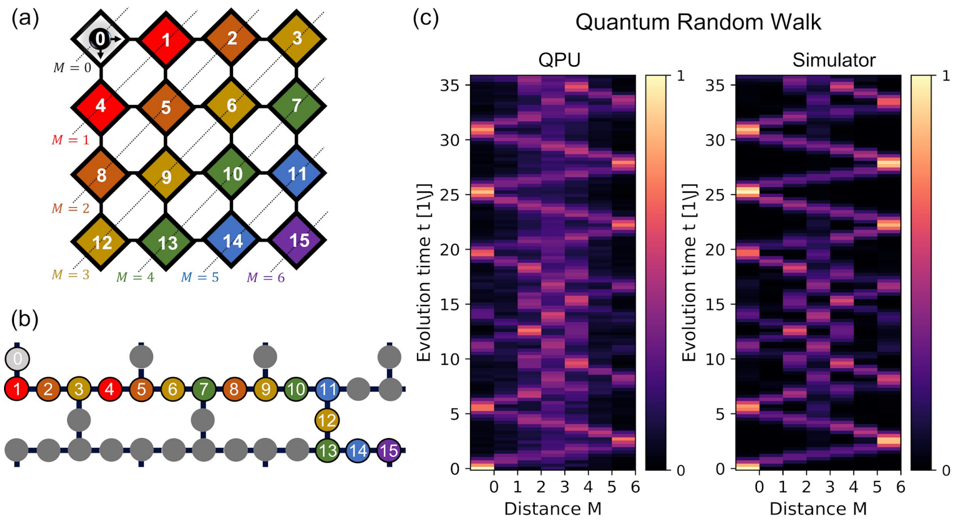
4x4 free tight binding model

We extend algebraic compression to free fermions with long range interactions as well, and simulate a 2-D 4x4 tight binding model on *ibmq_washington:*

E. Kökcü et al (2023), arXiv:2303.09538



https://www.newscientist.com/article/2093356



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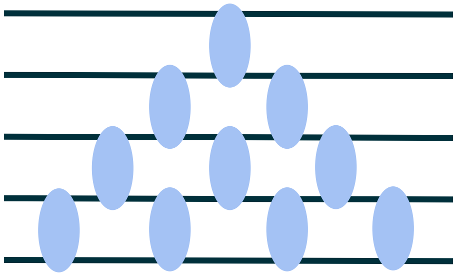
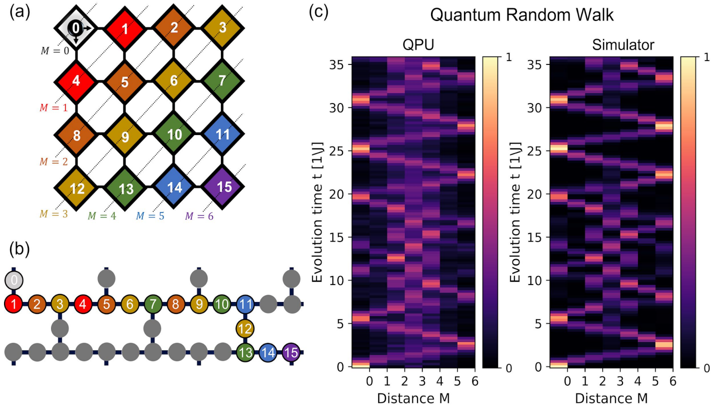
Conclusions and outlook

- We introduced a method to compress time evolution of free fermionic models on any graph



- We are applying the same method to impurity models (in progress)



- We introduced a method to compress time evolution of free fermionic models on any graph

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