Why statistical physics is the best course you take: Introduction to quantum information with entanglement renormalization

Thomas E. Baker
Canada Research Chair in Quantum Computing for Modelling of Molecules and Materials

Department of Physics & Astronomy
Department of Chemistry
Centre for Advanced Materials and Related Technology
University of Victoria

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Outline

Thermodynamics

- What is…?
  - Entropy
  - Density matrices
  - Renormalization group

Phase transitions and Information theory

- Renormalization
- Entropy
- Entanglement

Quantum information

- Entanglement renormalization
  - Entanglement renormalisation

DMRjulia

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Introduction paper

NRC Research Press

TUTORIAL

Méthodes de calcul avec réseaux de tenseurs en physique

Thomas E. Baker, Samuel Desrosiers, Maxime Tremblay et Martin P. Thompson

Résumé : Cet article se veut un survol des réseaux de tenseurs et s'adresse aux débutants en la matière. Nous y mettons l'accent sur les outils nécessaires à l'implémentation concrète d'algorithmes. Quatre opérations de base (remodelage, permutation d'indices, contraction et décomposition) qui sont couramment utilisées dans les algorithmes de réseaux de tenseurs y sont décrites. Y seront aussi couverts la notation diagrammatique, intrication, les états en produit de matrices (MPS), les opérateurs en produit de matrices (MPO), état projeté de paires intriquées (PEPS), l'approche par renormalisation d'enchevêtrement multi-échelle (MERA), la décimation par bloc d'évolution temporelle (TEBD) et le groupe de renormalisation de tenseurs (TRG).

Mots-clés : réseaux de tenseurs, décomposition en valeurs singulières, intrication.

Abstract : This article is an overview of tensor networks and is intended for beginners in this field. We focus on the tools required for the concrete implementation of algorithms. Four basic operations (remodelling, permutation of indices, contraction, and decomposition) commonly used in tensor network algorithms are described. This study also covers diagrammatic notation, entanglement, matrix product states (MPS), matrix product operators (MPO), projected entangled pair state (PEPS), multi-scale entanglement renormalization ansatz (MERA), time evolving block decimation (TEBD), and tensor renormalization group (TRG).

Keywords : tensor networks, singular value decomposition, entanglement.

1. Introduction

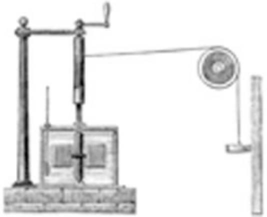
Les méthodes exactes de résolution de systèmes quantiques

Dans cette revue des réseaux de tenseurs, nous nous concentrons sur les opérations de base nécessaires à la manipulation des tenseurs. À la section 2, nous commençons par une discussion de

Thermodynamics

Energy equivalence

- Is energy different depending on how it is used?



APSNews December **18**, 11 (2009)

- Energy is energy (First Law of Thermodynamics):

$$\Delta U = Q + W$$

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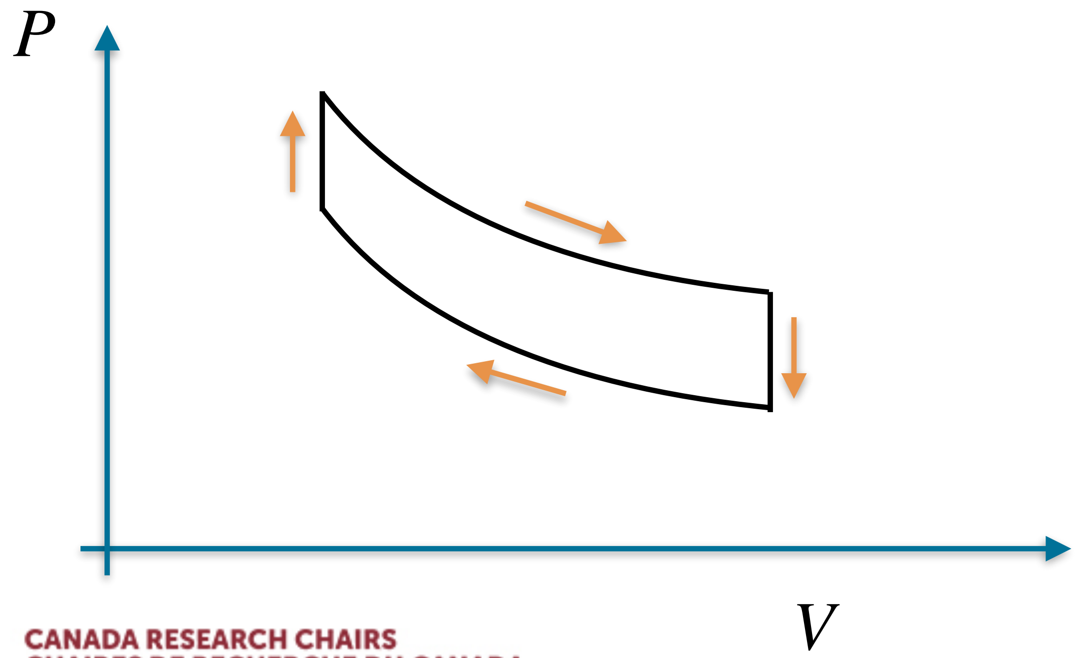
Thermodynamics

Ideal engine efficiency:



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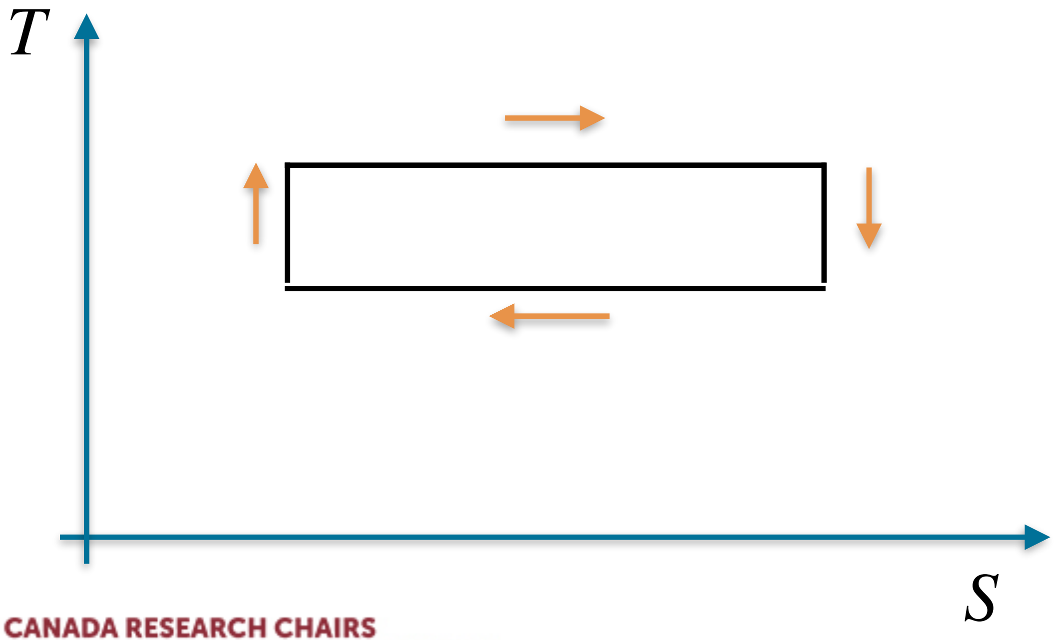
Thermodynamics

Legendre transformation (Maxwell relations): $dU = TdS - pdV$



Thermodynamics

What is *S*?

- “En” like energy
- *Verwandlungsinhalt* - German for transformation-content
  - en + “transform” = entropy

$$dS = \left(\frac{dQ}{T}\right)_V$$

- But what is it? Admittedly… $\Delta S \geq 0$

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Thermodynamics

Other form

- Boltzmann entropy

$$S = k_B \ln \Omega$$

- Density matrices

$$\langle O \rangle = \mathrm{Tr}(\rho O)$$

$$S = -k_b \sum_i \rho_i \ln \rho_i$$

  - Reduces when all probabilities are equal

https://en.wikipedia.org/wiki/Ludwig_Boltzmann

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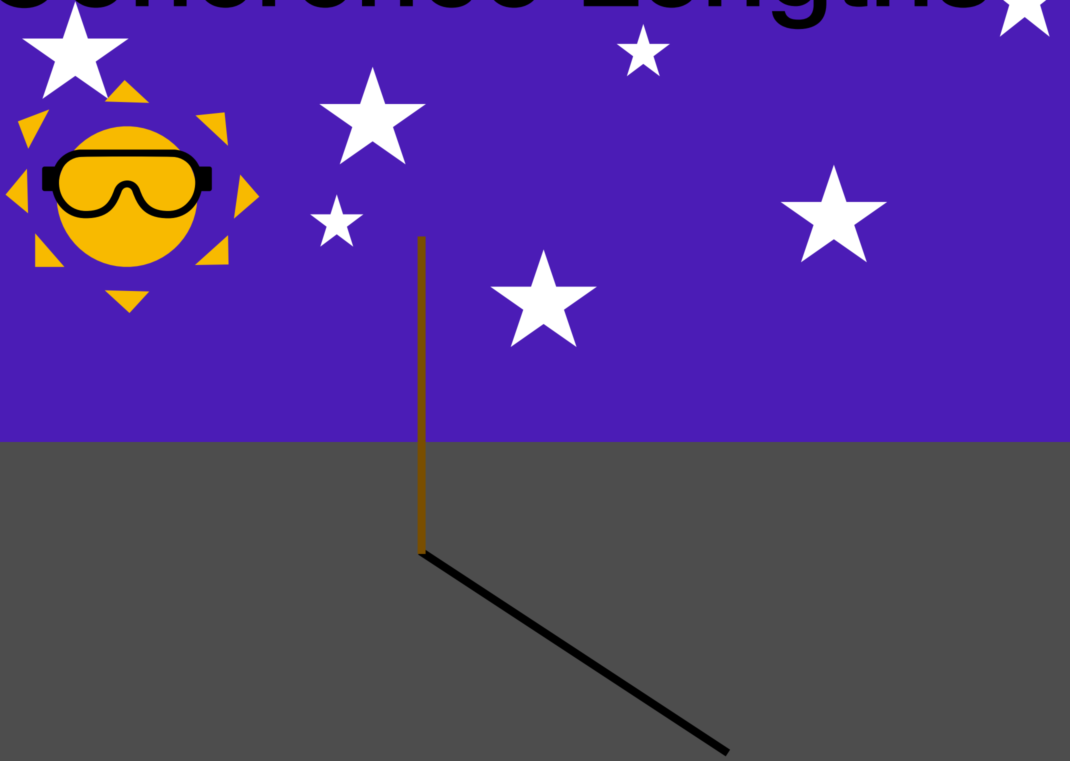
Part 2a. Phase transitions

Coherence Lengths



Coherence lengths

Mandelbrot noted:

- Measure the coastline
  - Satellite vs. Ant
- Different answers but both valid
- Depends on what measurement was used

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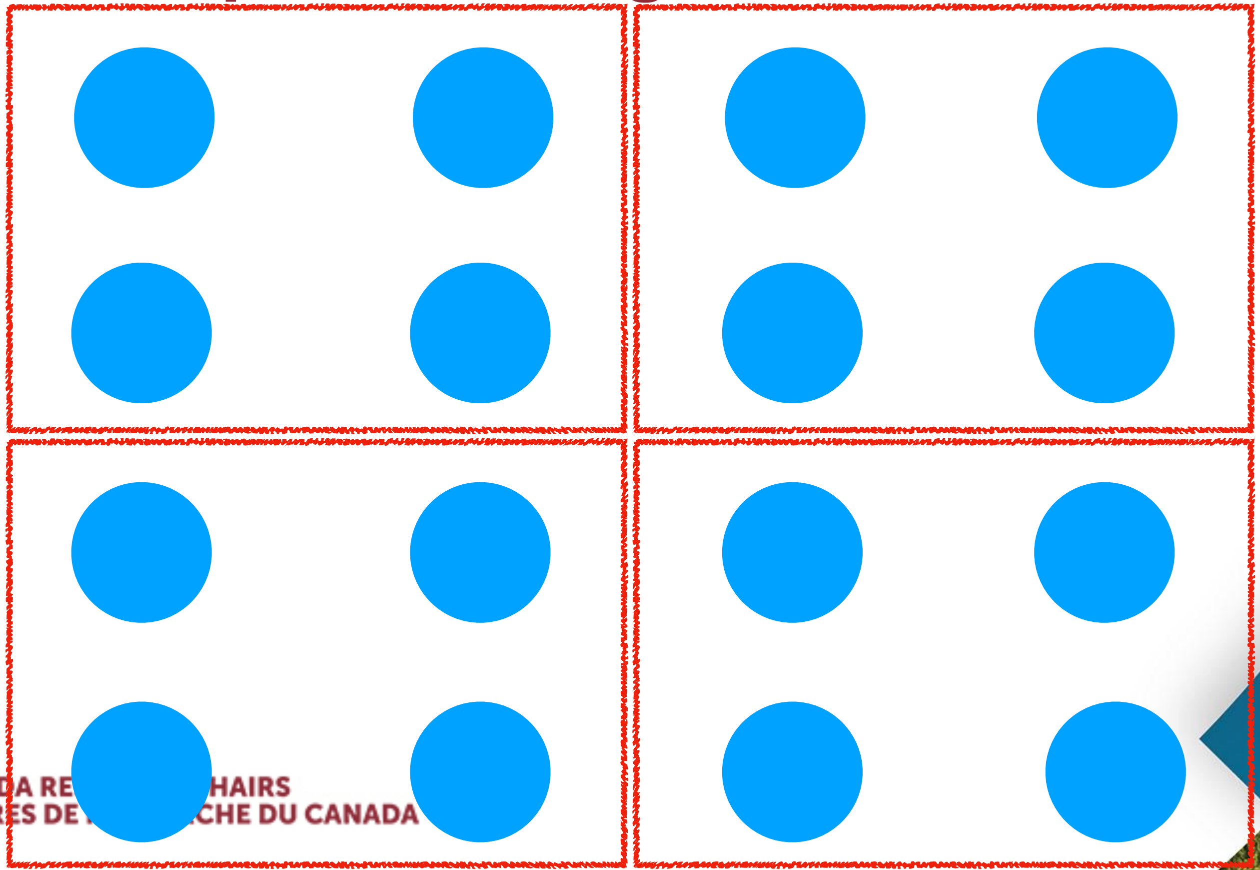
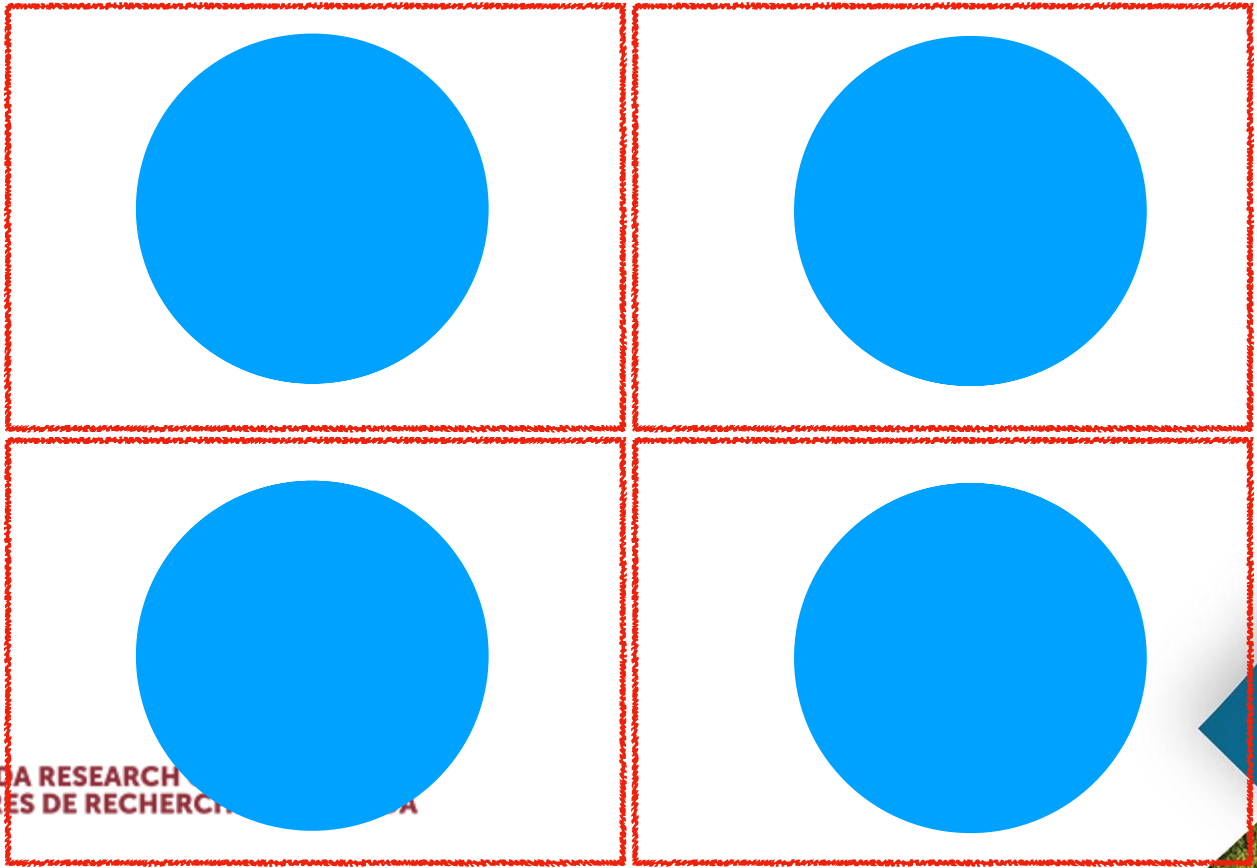
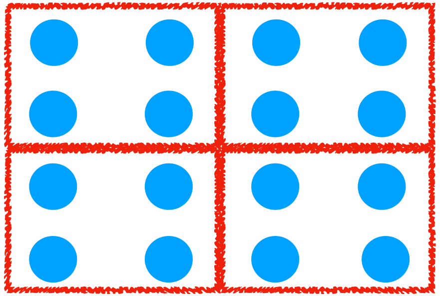
Kadanoff: Spin Blocking

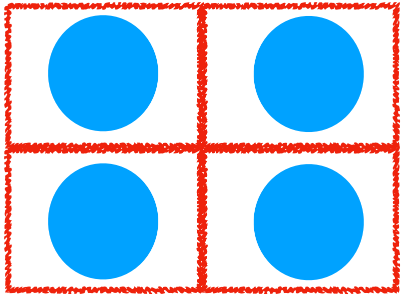


Kadanoff: Spin Blocking



Kadanoff: Spin Blocking

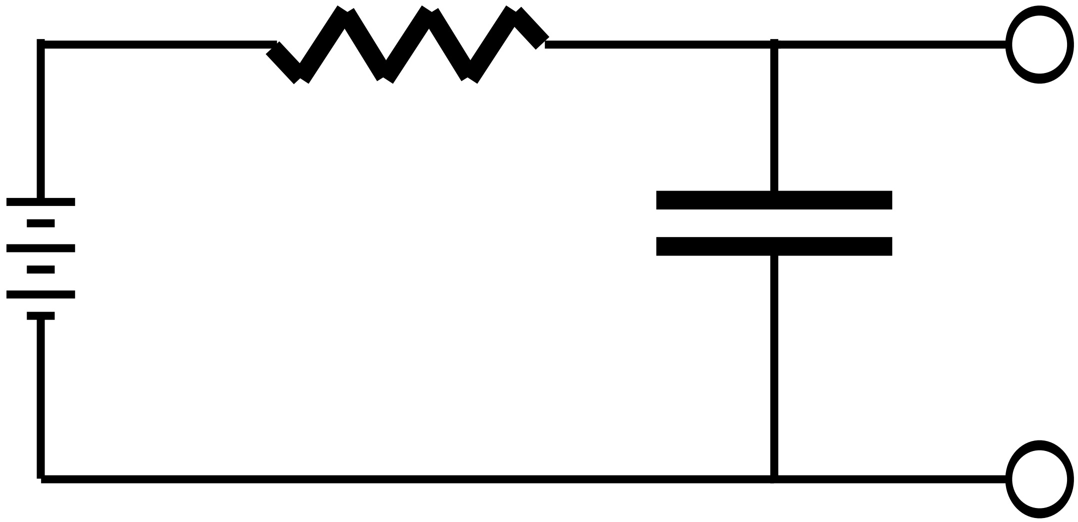




- Less terms
- Better near a critical point
- Same energy
  - Different *J*

$$H = -J \sum_{i,j} S_i^z \cdot S_j^z$$

Keep the most relevant degrees of freedom



Low pass filter

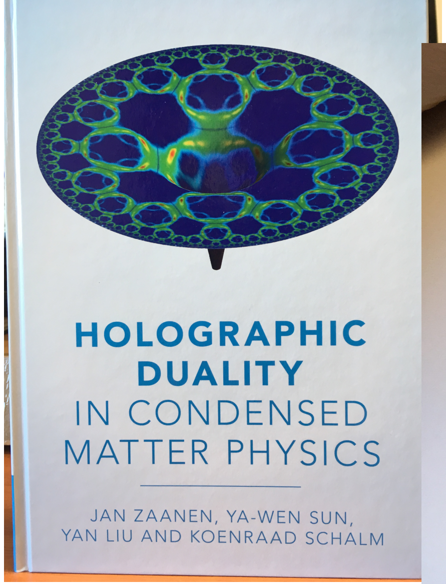
Wilson: renormalization group

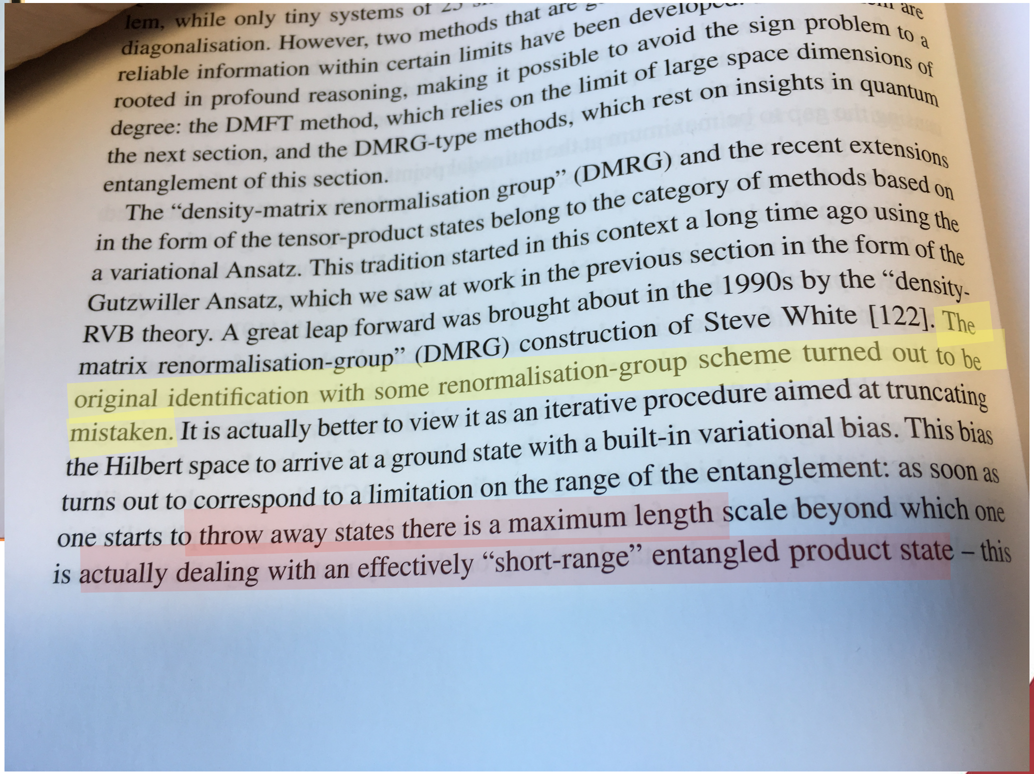
- Quantum field theory
- Condensed matter too:

$$\frac{V}{2\pi^2 c_s^3}\int_0^{\omega_D} \omega^2 d\omega = N$$

  - Debye frequency
  - Cutoff to regularize integrals
  - In condensed matter: lattice cutoff

- Also made the numerical renormalization group (NRG)





lem, while only tiny systems of … diagonalisation. However, two methods that are … have been developed … are reliable information within certain limits … rooted in profound reasoning, making it possible to avoid the sign problem to a degree: the DMFT method, which relies on the limit of large space dimensions of the next section, and the DMRG-type methods, which rest on insights in quantum entanglement of this section.

The "density-matrix renormalisation group" (DMRG) and the recent extensions in the form of the tensor-product states belong to the category of methods based on a variational Ansatz. This tradition started in this context a long time ago using the Gutzwiller Ansatz, which we saw at work in the previous section in the form of the RVB theory. A great leap forward was brought about in the 1990s by the "density-matrix renormalisation-group" (DMRG) construction of Steve White [122]. The original identification with some renormalisation-group scheme turned out to be mistaken. It is actually better to view it as an iterative procedure aimed at truncating the Hilbert space to arrive at a ground state with a built-in variational bias. This bias turns out to correspond to a limitation on the range of the entanglement: as soon as one starts to throw away states there is a maximum length scale beyond which one is actually dealing with an effectively "short-range" entangled product state – this

Part 3. Classical algorithms for quantum problems

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Algorithms to solve problems: Exact Diagonalization

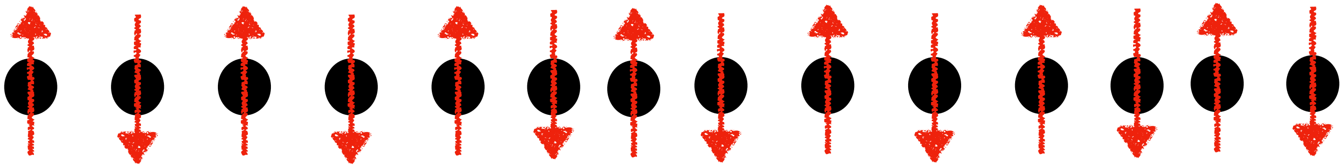
- Large Hamiltonian operators
  - Scales as d^N
    - d local Fock space size
    - N sites
- Realistically 5-20
  - Record as of 2018: 50 sites

    A. Wietek and A.M. Laüchli. *Phys. Rev. E*, 98, 033309 (2018)
- Too expensive for large systems!
  - Especially fermions

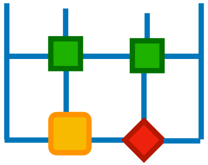
$$\sigma_i^z = I \otimes I \otimes \sigma^z \otimes I \otimes \ldots \otimes I$$

Renormalize what?

- Decompose wavefunction?



- But how?



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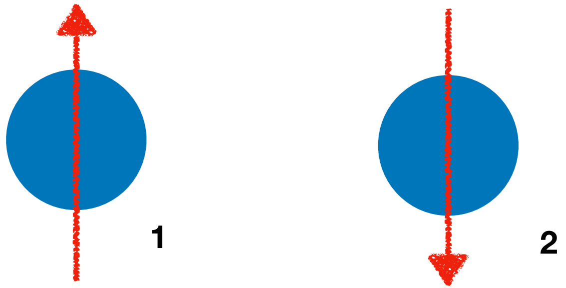
2-site Spin-1/2 State

$$\psi(\uparrow,\downarrow) =$$



$$= |\uparrow_1\downarrow_2\rangle = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$

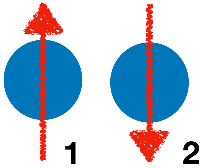
$$= |\uparrow\rangle_1 \otimes |\downarrow\rangle_2 = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}$$

How to split left and right?

- Right way: grouping basis functions on the left and on the right

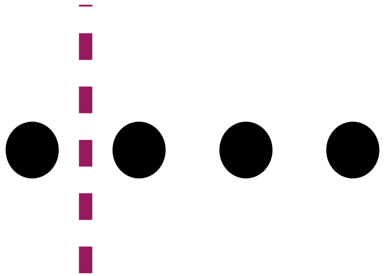
Left states

Right states



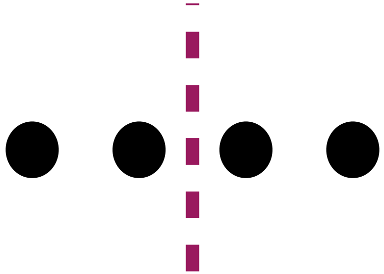
$$= \begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix} = \begin{pmatrix} 0_1 \\ 1_2 \\ 0_3 \\ 0_4 \end{pmatrix} \overset{\text{reshape}}{=} \begin{array}{cc} & \begin{array}{cc} \uparrow_2 & \downarrow_2 \end{array} \\ \begin{array}{c} \uparrow_1 \\ \downarrow_1 \end{array} & \begin{pmatrix} 0_1 & 1_2 \\ 0_3 & 0_4 \end{pmatrix} \end{array}$$

Reshaping: 4-sites



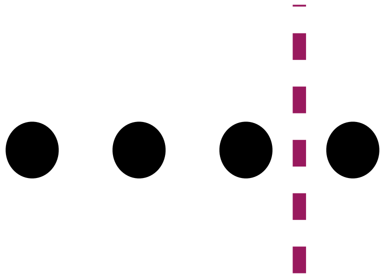
$$2\times(\text{rest of lattice})$$

Reshaping: 4-sites



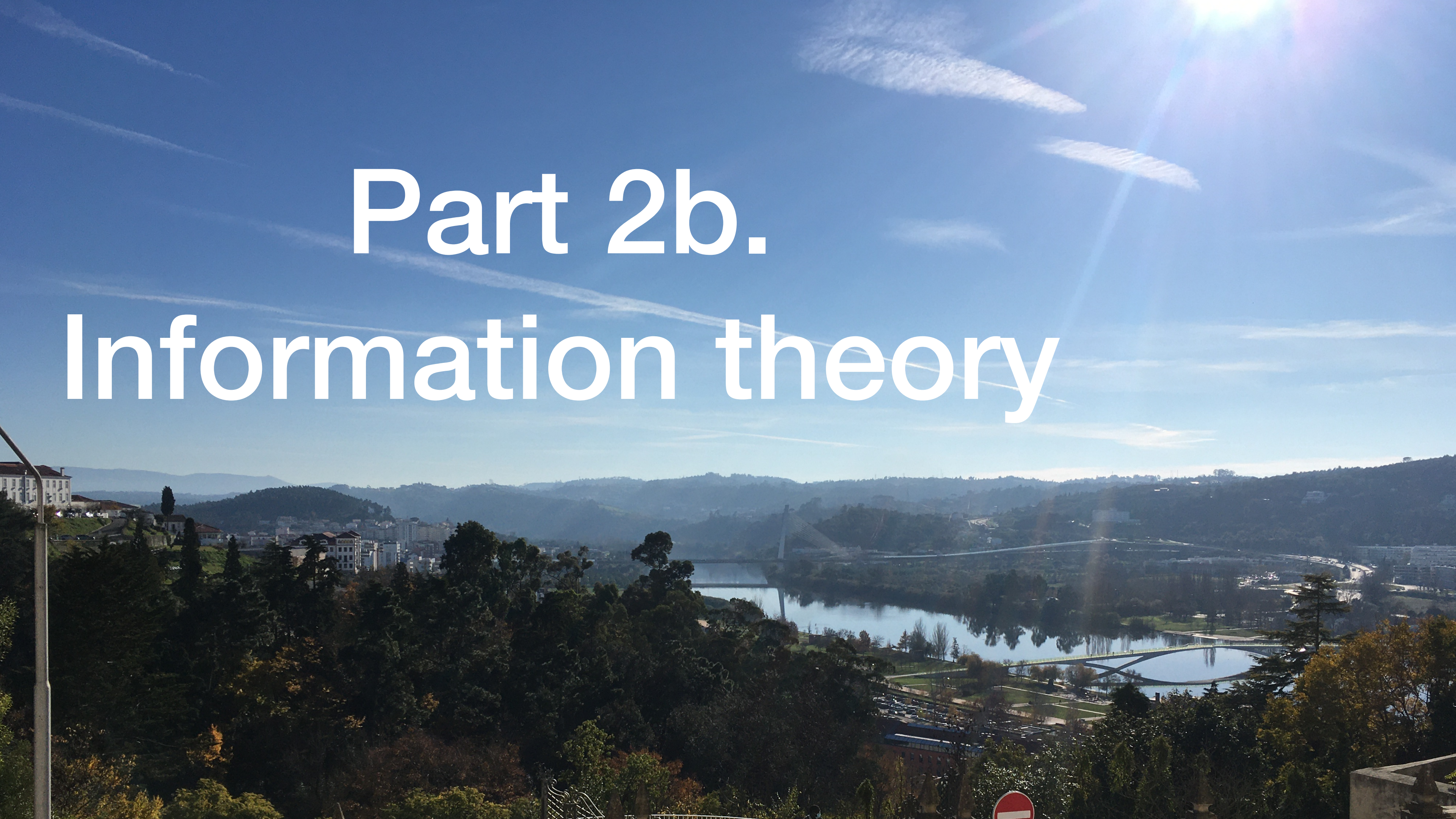
$$4 \times 4$$

Reshaping: 4-sites

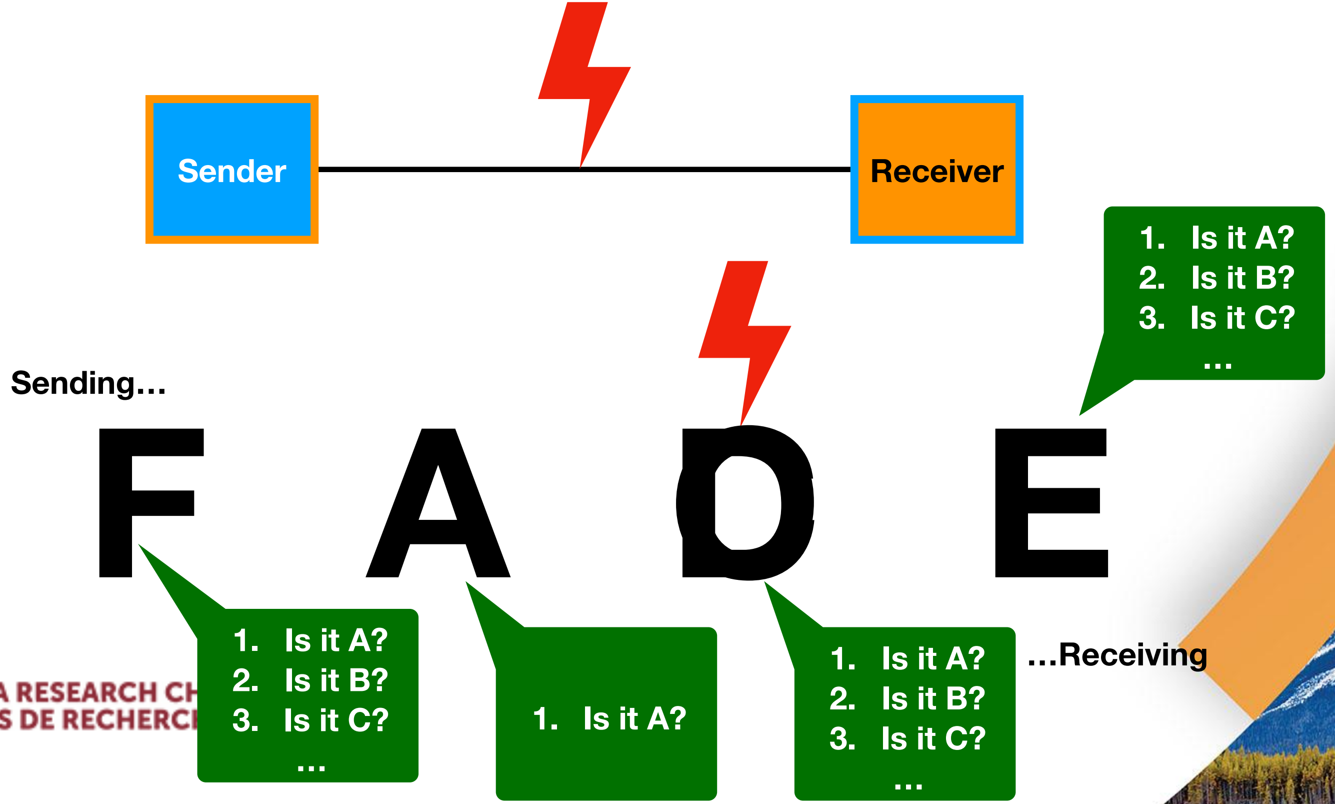


$$(\text{rest of lattice}) \times 2$$

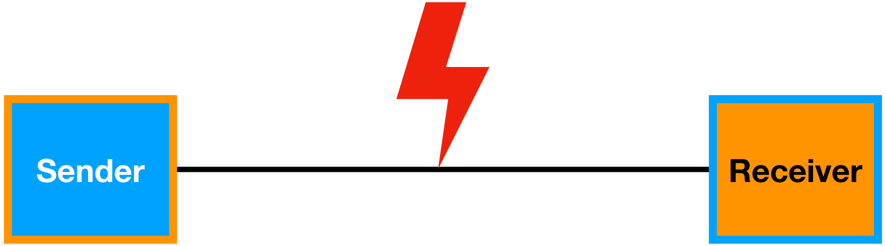
Part 2b. Information theory



Information Theory



How many questions do I have to ask?



- Monotonically increasing function
- Adds like a logarithm
- Grouping Axiom
- Continuous

Density matrix elements!

$$S = -\sum_i \rho_i \ln \rho_i$$

Shannon entropy
(After quantization: von Neumann entropy or entanglement entropy)

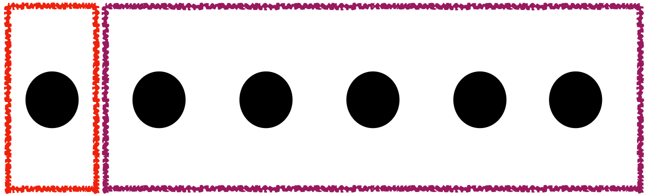
The Density Matrix

- Density matrix of a subsystem

$$\hat{\rho} = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$$

$$\hat{\rho} = \psi\psi^\dagger \quad \textbf{or} \quad \psi^\dagger\psi$$

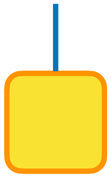
$$\boxed{\hat{\rho}_{\text{left}}} = UD^2U^\dagger \qquad\qquad \boxed{\hat{\rho}_{\text{right}}} = V^\dagger D^2 V$$



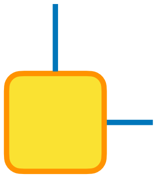
- Need U and V in one expression

$$\psi = UDV^\dagger$$

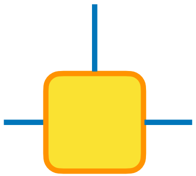
Easy to Read Diagrams



A^{μ}

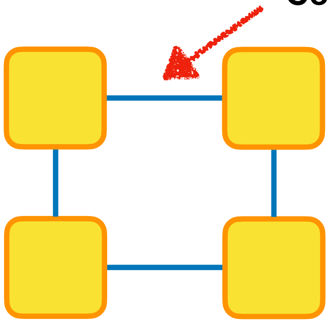


$A^{\mu\nu}$



$A^{\mu\nu\gamma}$

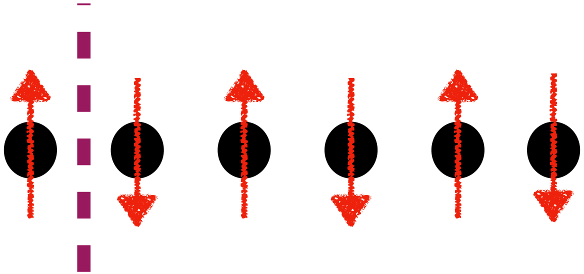
Contraction



$\mathrm{Tr}(A^{\alpha\beta}A^{\beta\gamma}A^{\gamma\delta}A^{\delta\zeta})$

Matrix Product State: 6-sites

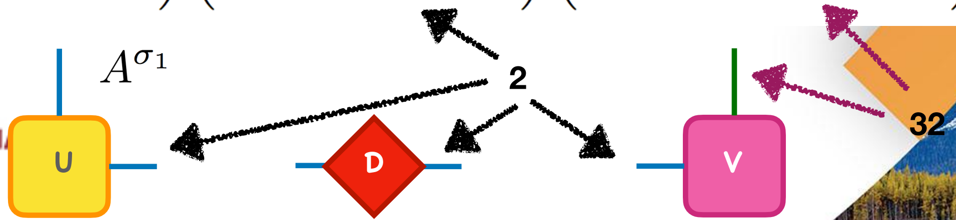
- Reshape (2 x 32)



$$\psi = \frac{1}{8}\begin{pmatrix} 1 & 0 & 1 & \dots \\ 1 & 0 & 0 & \dots \end{pmatrix}$$

- Singular Value Decomposition

$$\psi = UDV = \begin{pmatrix} -0.92388 & -0.382683 \\ -0.382683 & 0.92388 \end{pmatrix}\begin{pmatrix} 0.23097 & 0 \\ 0 & 0.0956709 \end{pmatrix}\begin{pmatrix} -0.707107 & 0 & -0.5 & \dots \\ 0.707107 & 0 & -0.5 & \dots \end{pmatrix}$$



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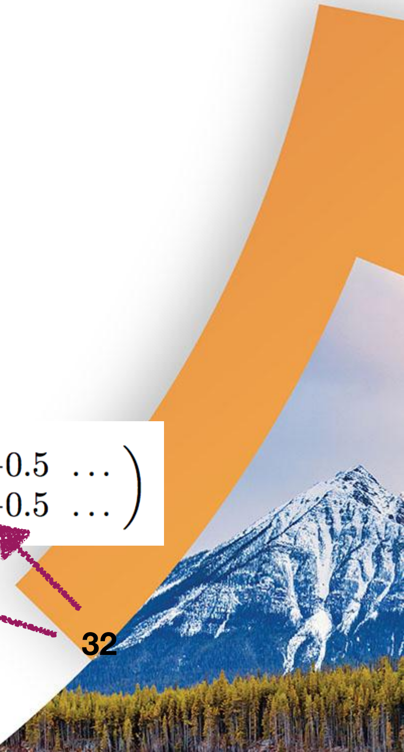
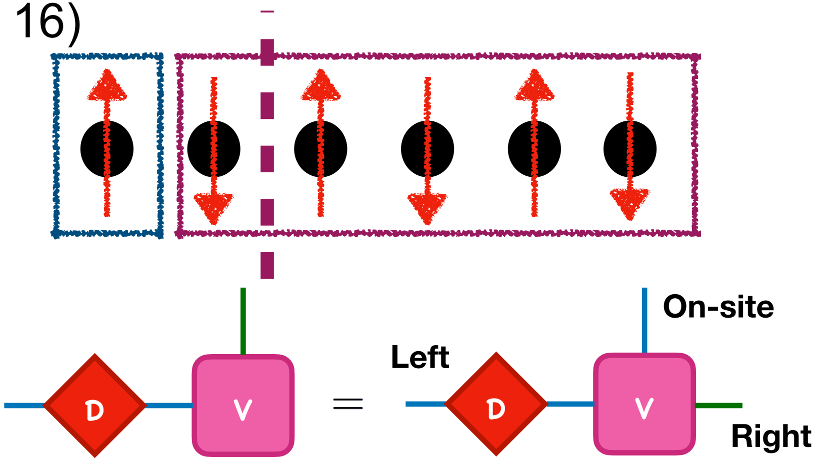
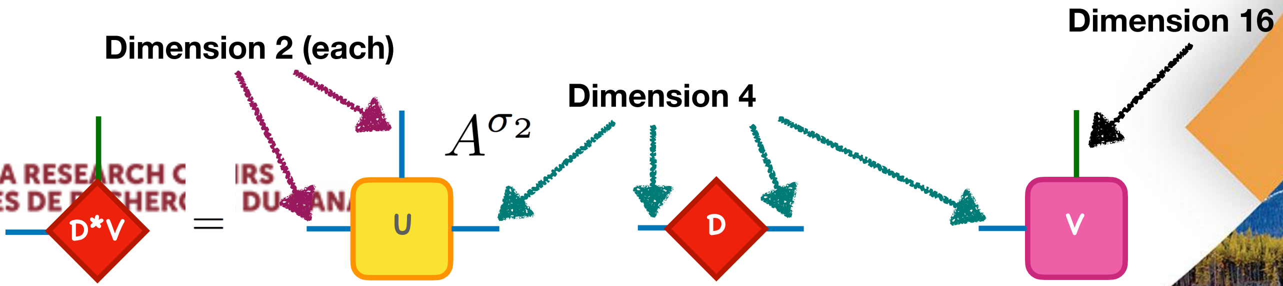


Matrix Product State: 6-sites

- Reshape (2 x 2 x 16)

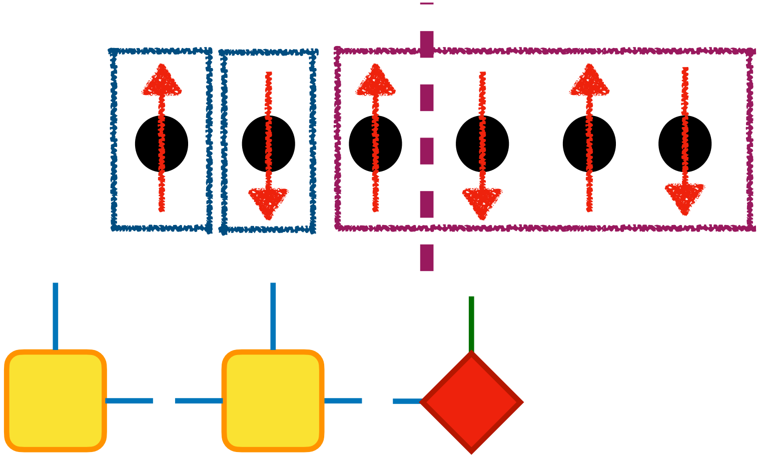


- Singular Value Decomposition



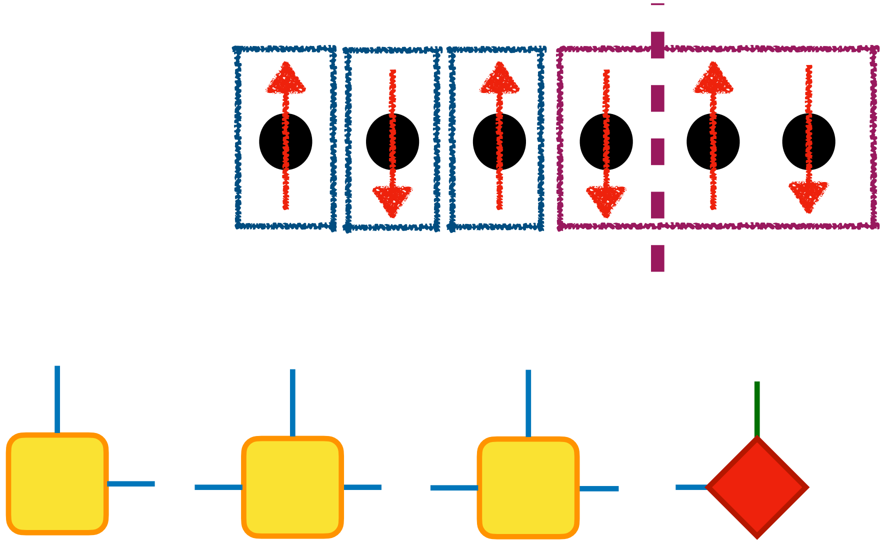
Matrix Product State:
6-sites

- Reshape



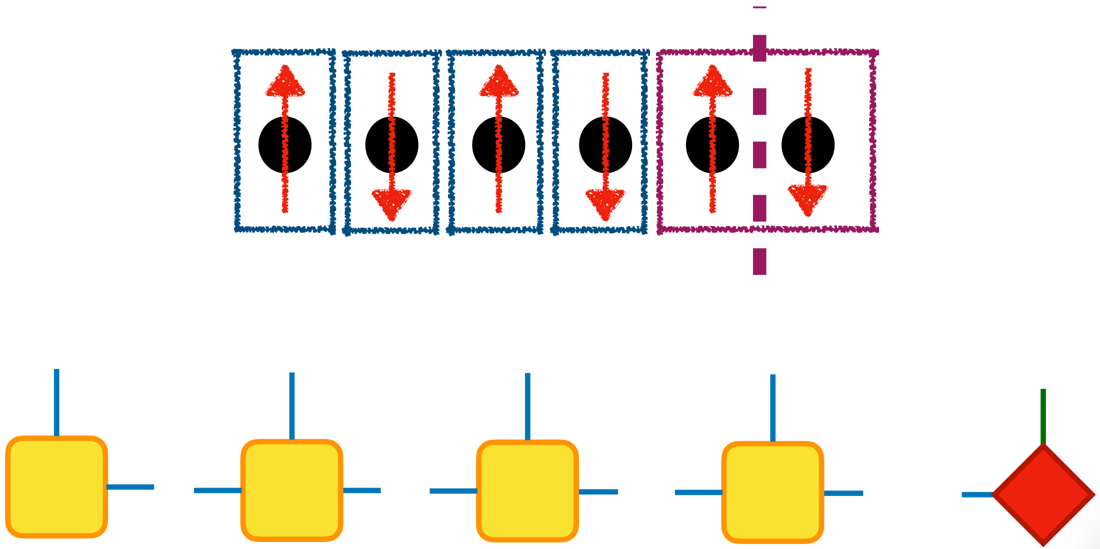
Matrix Product State:
6-sites

- Reshape



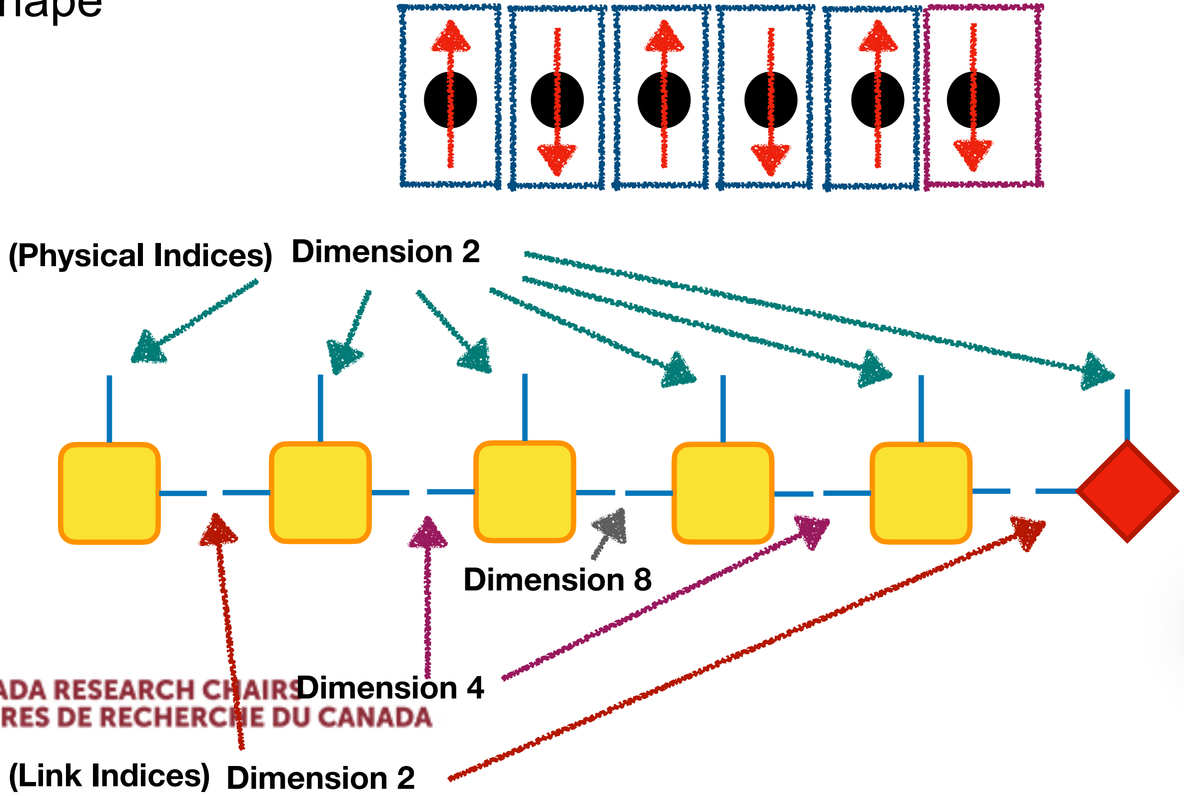
Matrix Product State: 6-sites

- Reshape



Matrix Product State:
6-sites

- Reshape



Truncation

- Density matrix of a subsyste
  - Truncation of small weights

$$\hat{\rho} = \psi\psi^\dagger = \begin{pmatrix} 0.98 & 0 & 0 & 0 & 0 \\ 0 & 0.01 & 0 & 0 & 0 \\ 0 & 0 & \cancel{0.0005} & 0 & 0 \\ 0 & 0 & 0 & \cancel{0.0003} & 0 \\ 0 & 0 & 0 & 0 & \cancel{0.0002} \end{pmatrix}$$

$$E = \mathrm{Tr}(\rho\mathcal{H})$$

  - Quantum Chemistry: weights of the natural orbitals from the 1-particle reduced density matrix
  - Control size of wavefunctions
  - Truncation error

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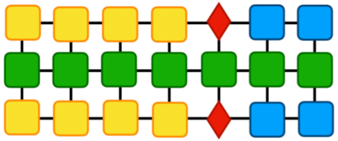
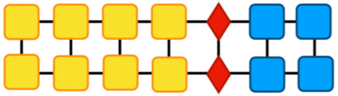
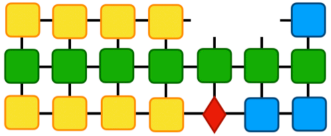
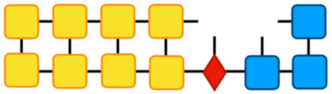
Density matrix renormalization group

 $-E$  $= 0$

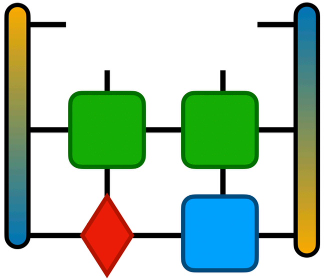
$$\frac{\partial^2}{\partial A^{*\sigma_i}_{a_{i-1}a_i}\partial A^{*\sigma_{i+1}}_{a_i a_{i+1}}}\Big(\langle\Psi|\mathcal{H}|\Psi\rangle - E\langle\Psi|\Psi\rangle\Big) = 0$$

 $-E$  $= 0$

T.E. Baker and M.P. Thompson, arxiv: 2019.03120

Density matrix renormalization group

1.

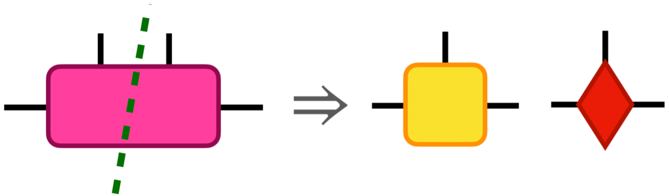


2.

$$|\psi_{n+1}\rangle = \mathcal{H}|\psi_n\rangle - \alpha_n|\psi_n\rangle - \beta_n|\psi_{n-1}\rangle$$

$$\alpha_n = \langle\psi_n|\mathcal{H}|\psi_n\rangle \quad \text{and} \quad \beta_n^2 = \langle\psi_{n-1}|\psi_{n-1}\rangle$$

3.



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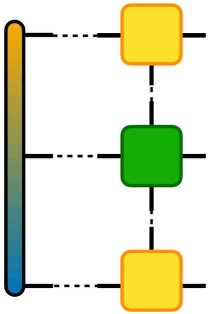

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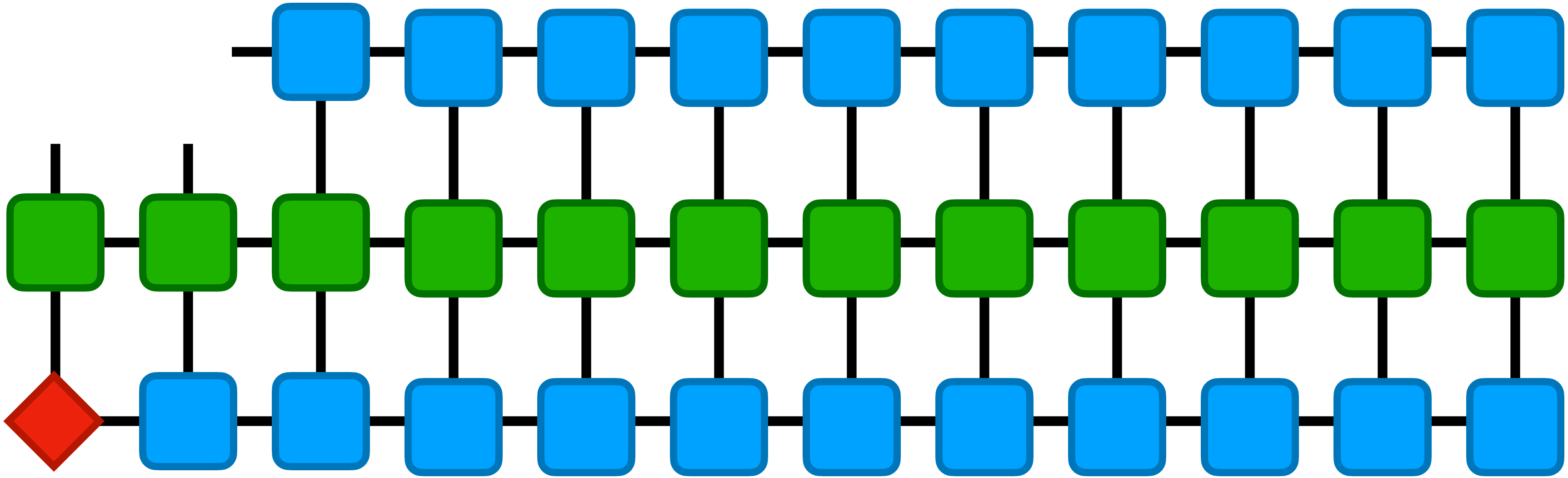
Density matrix renormalization group



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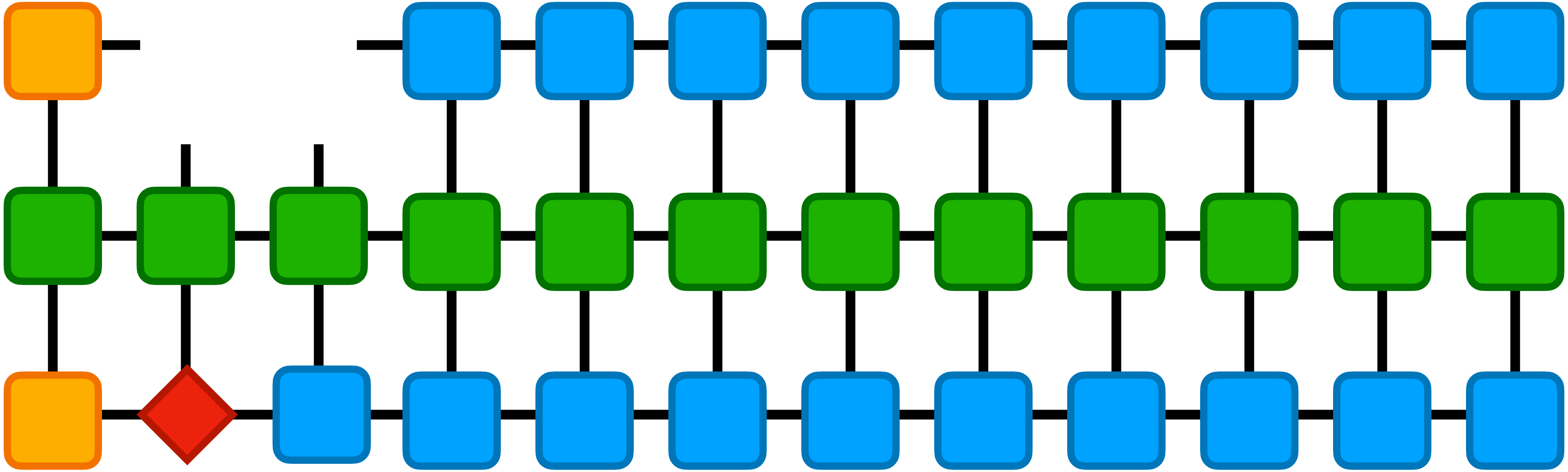
Density matrix renormalization group



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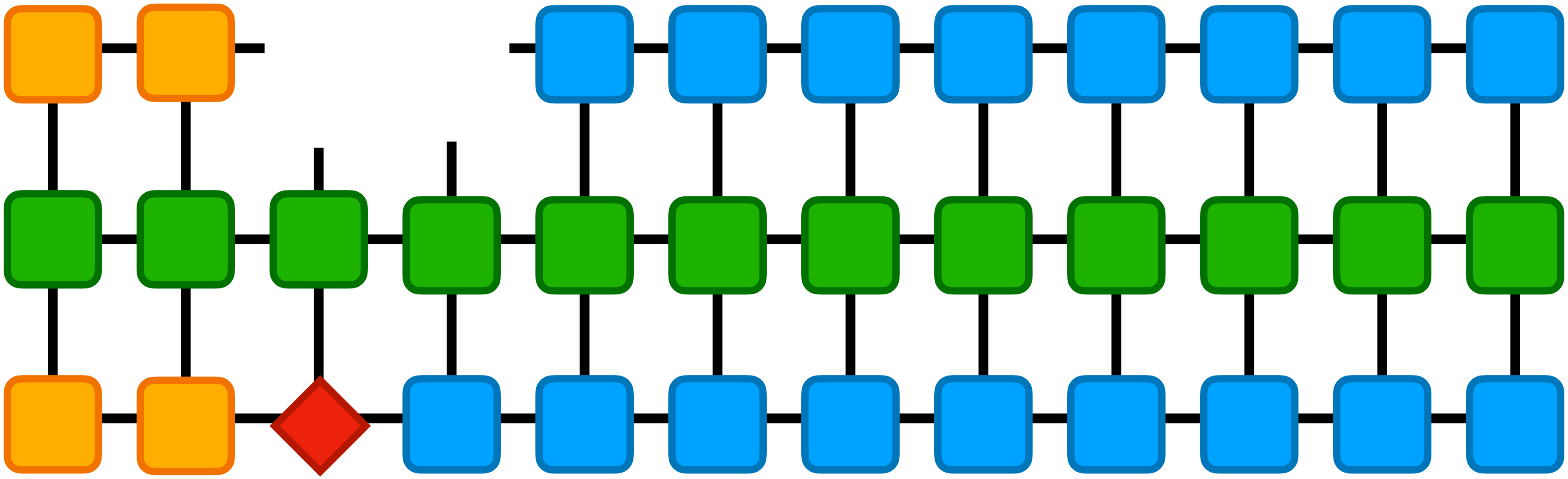
Density matrix renormalization group



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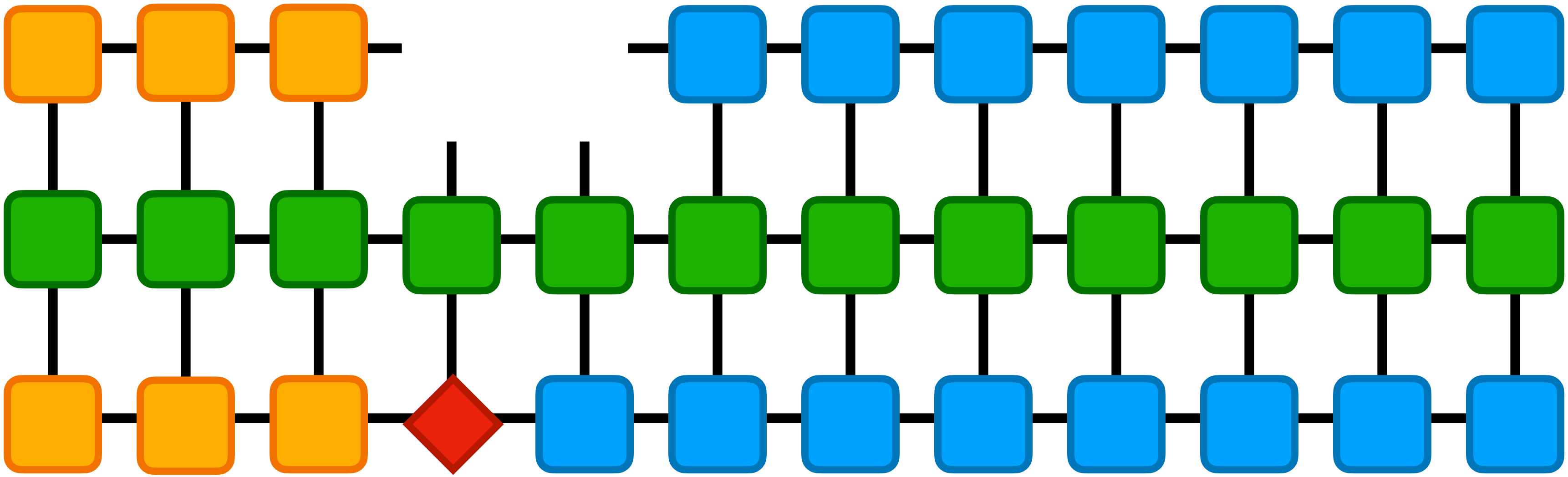
Density matrix renormalization group



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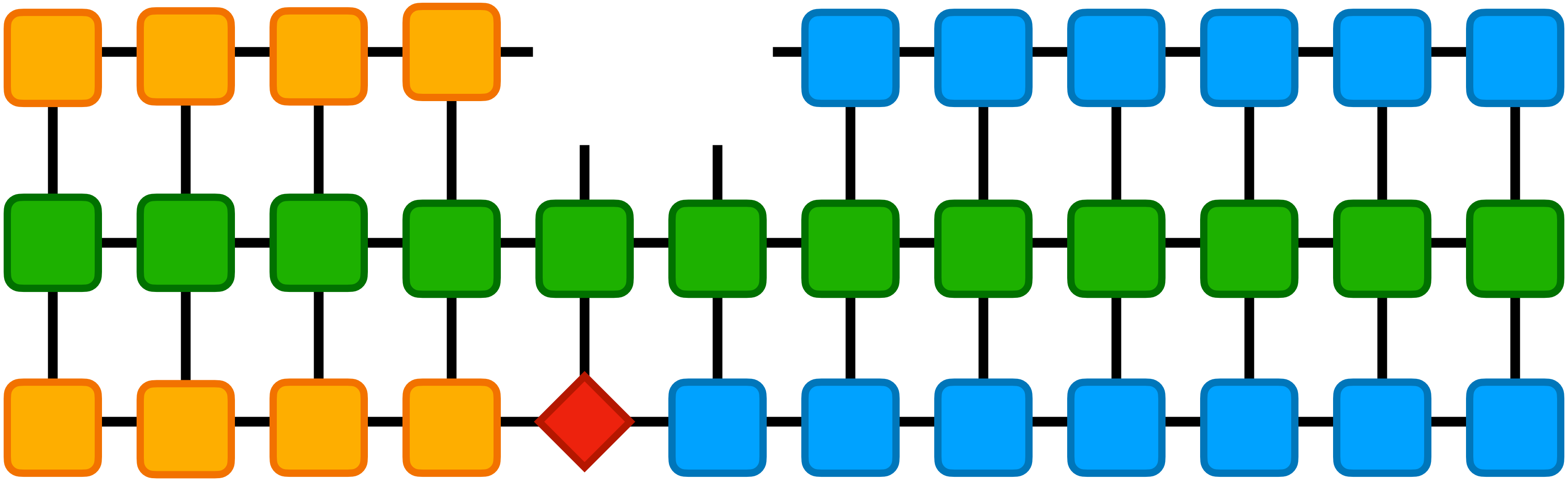

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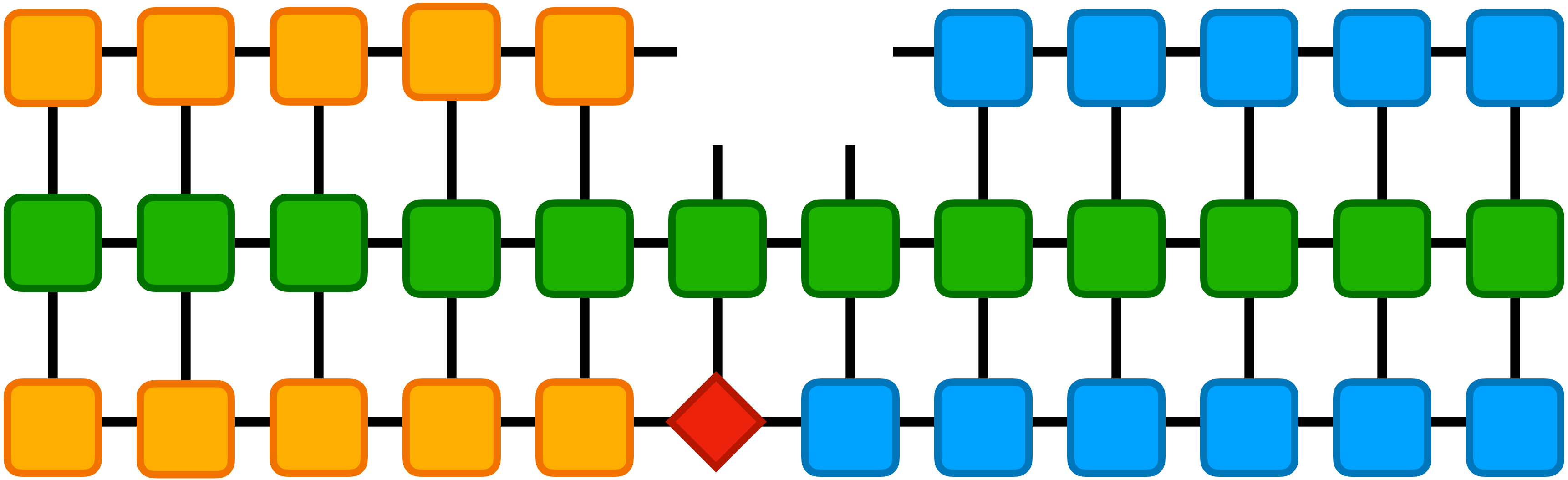

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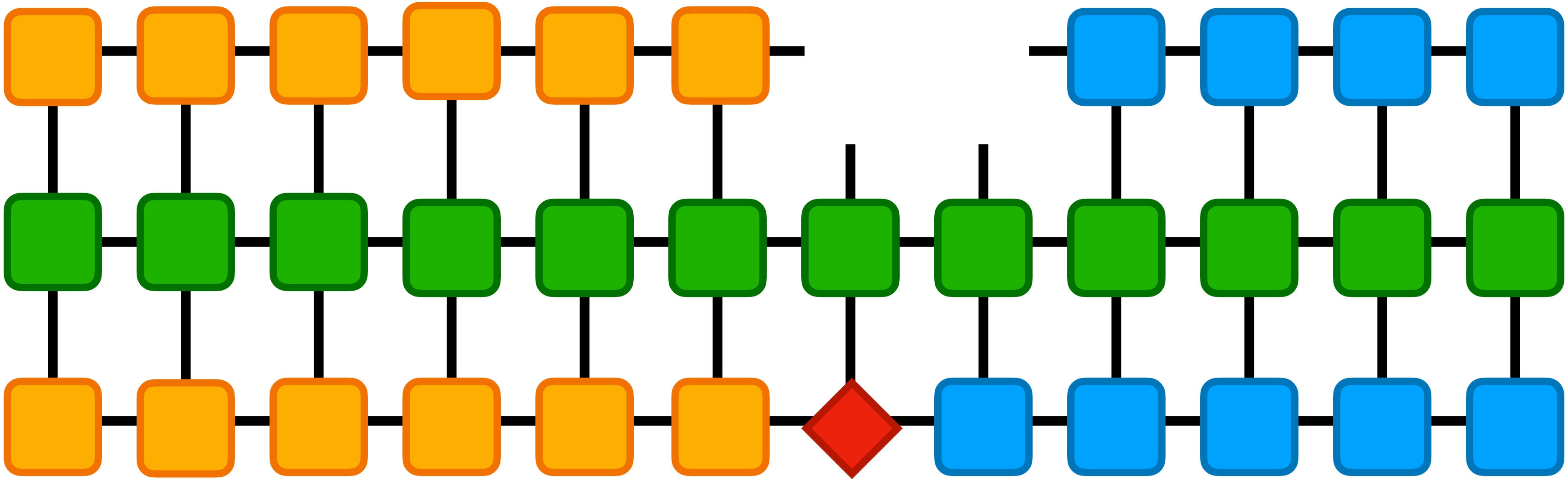

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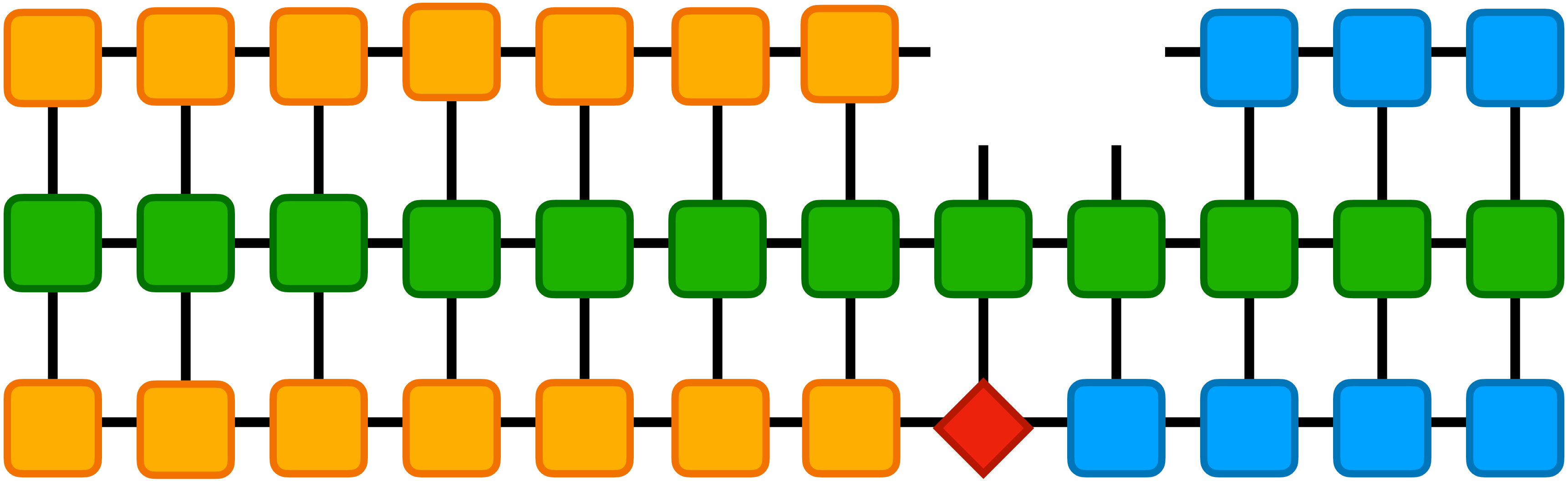

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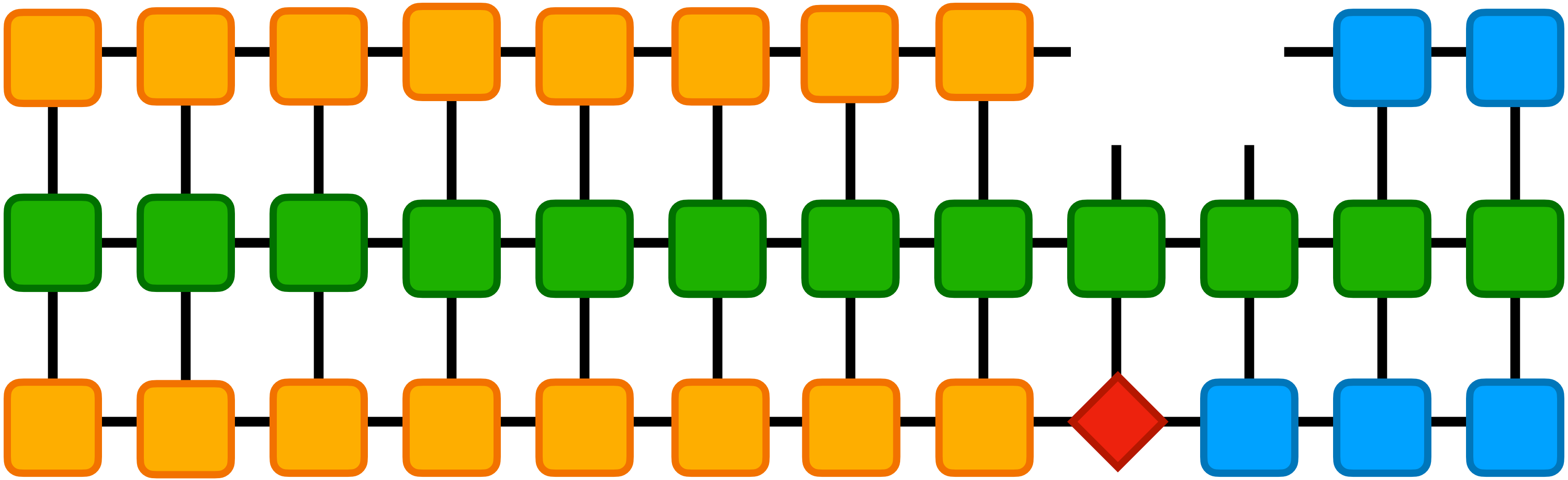

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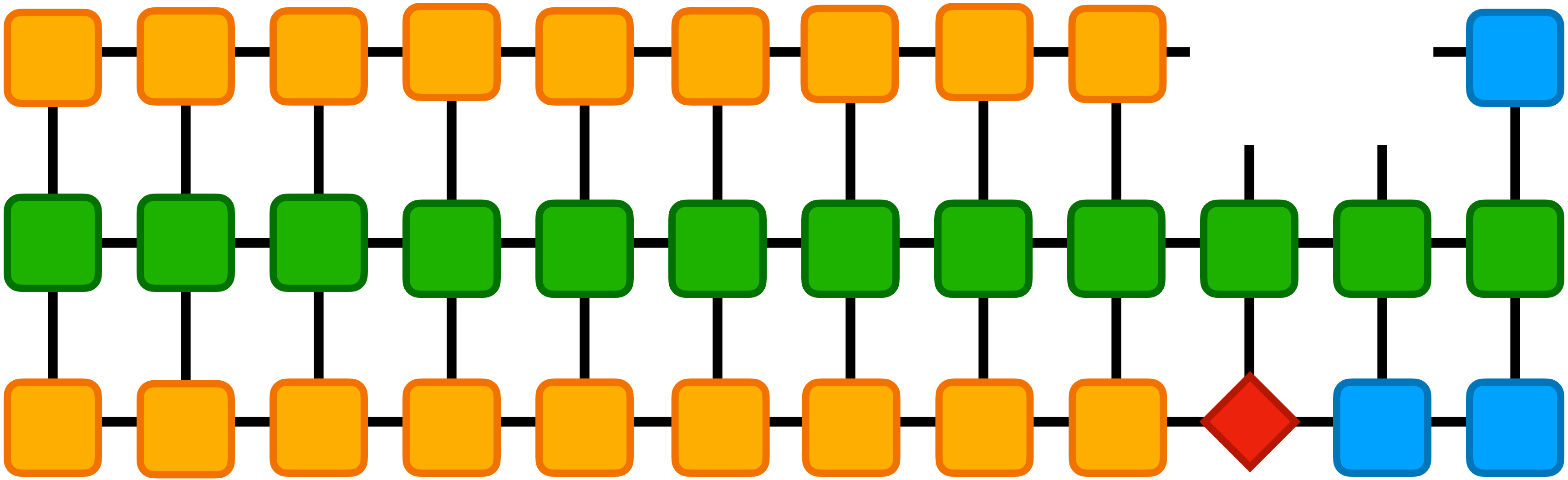

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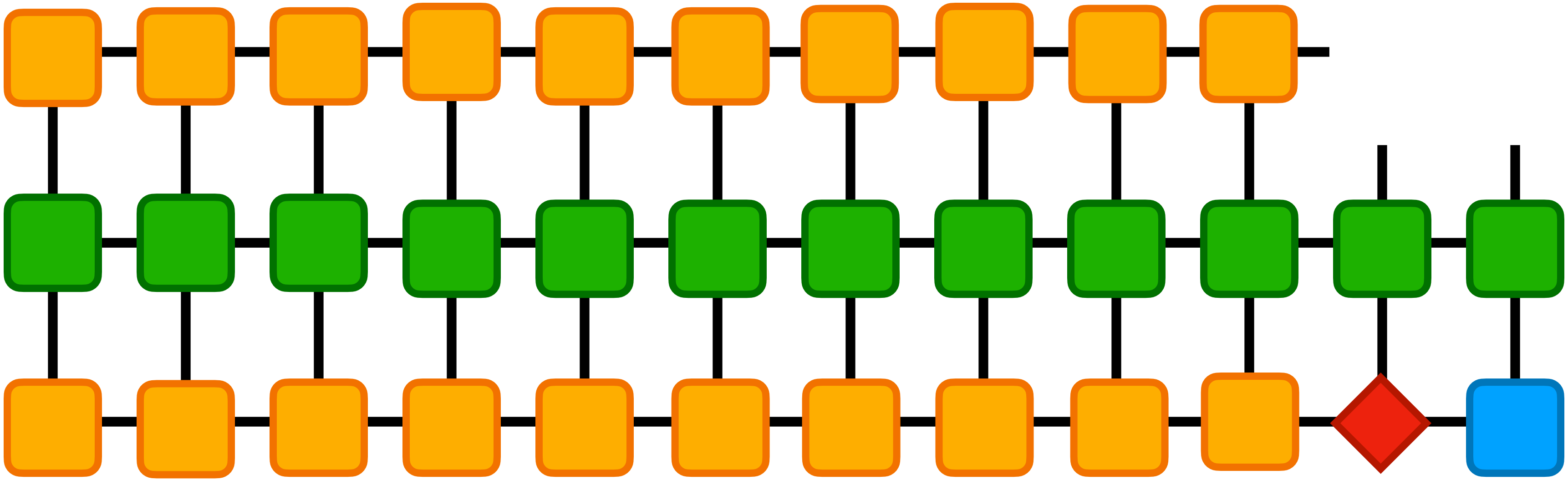

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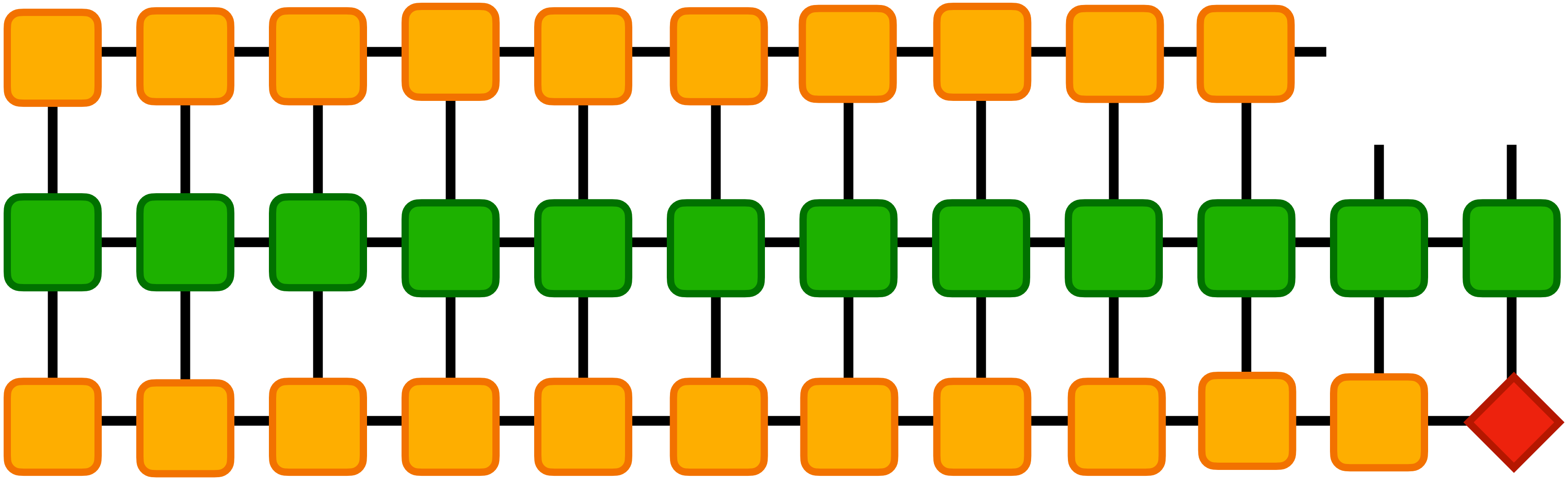

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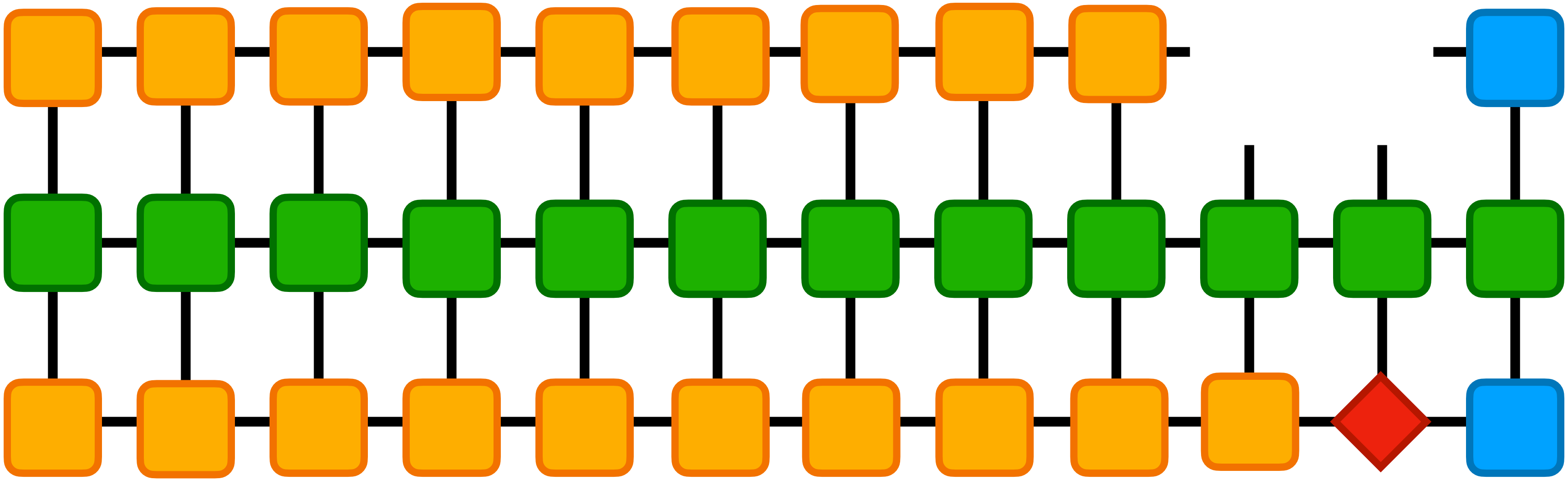

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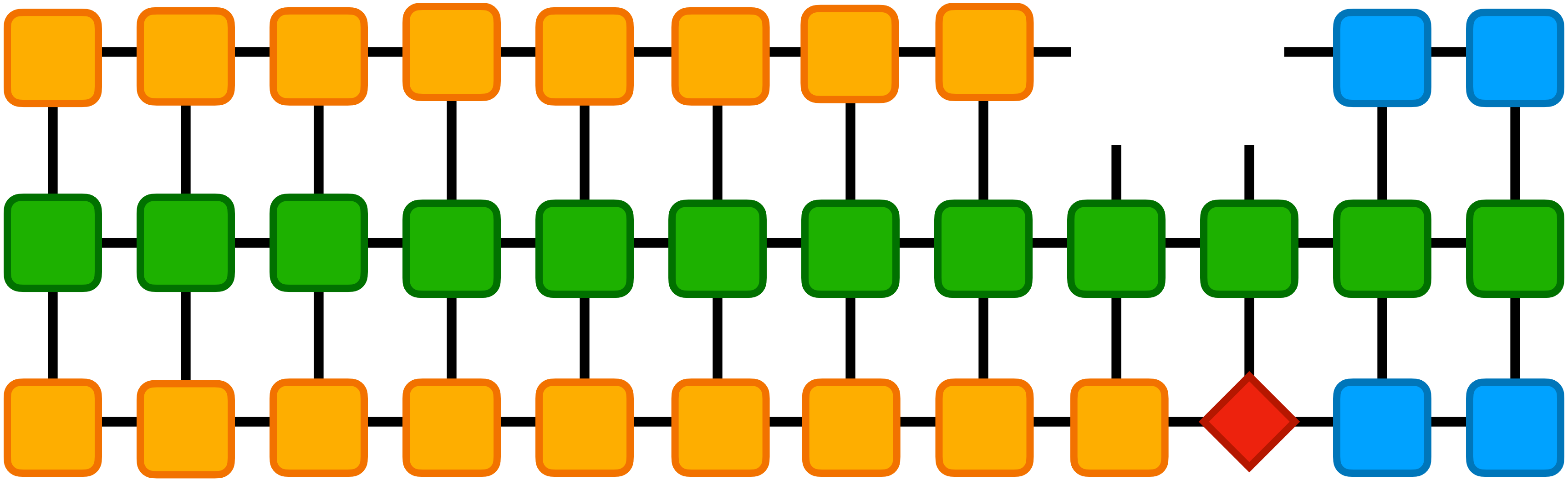

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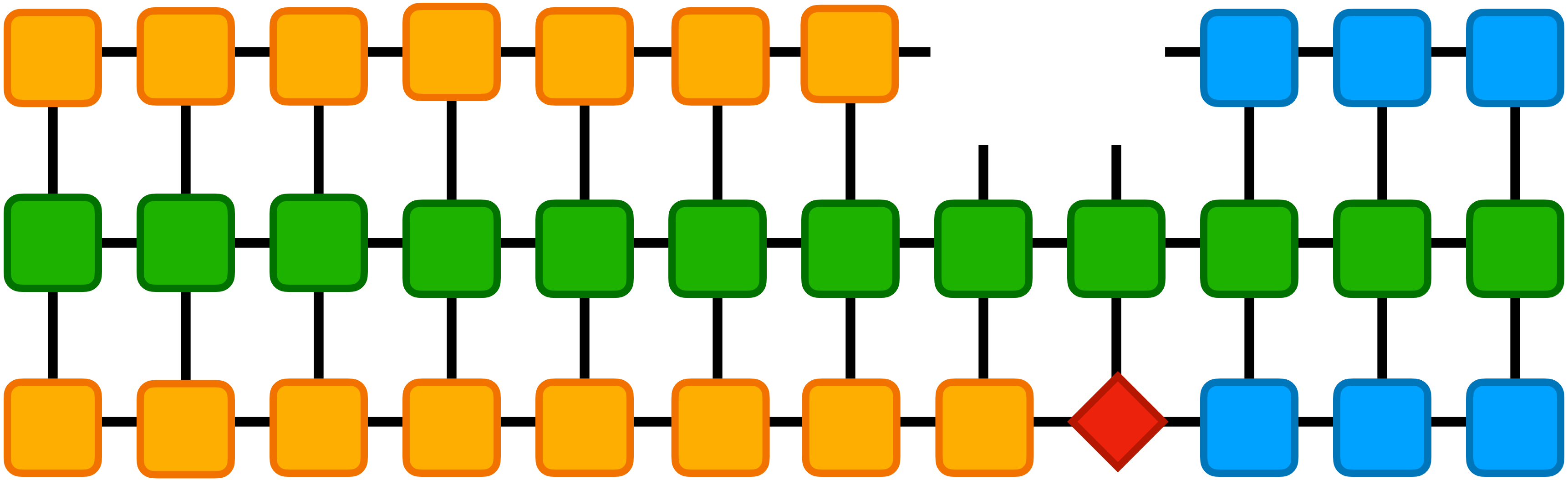

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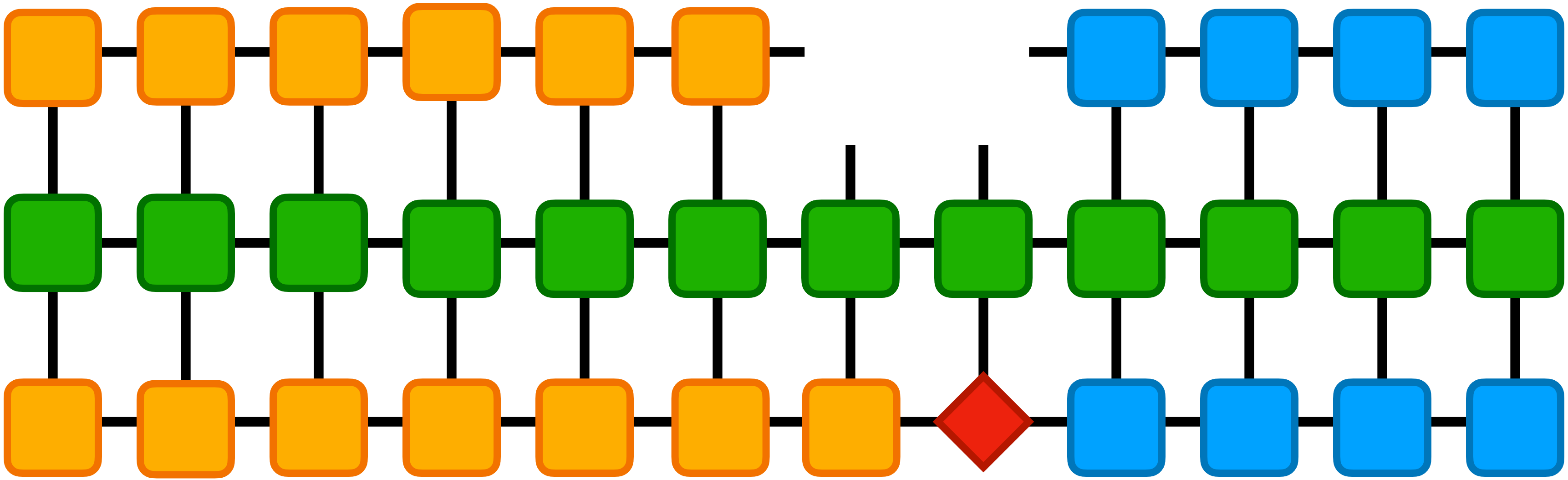

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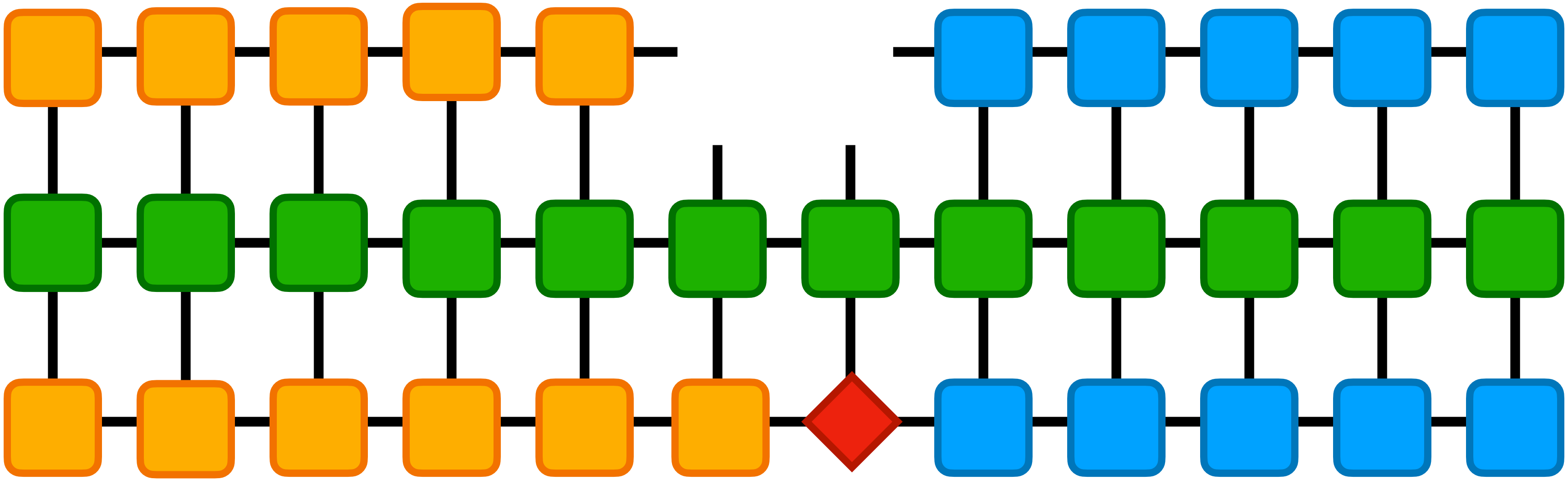

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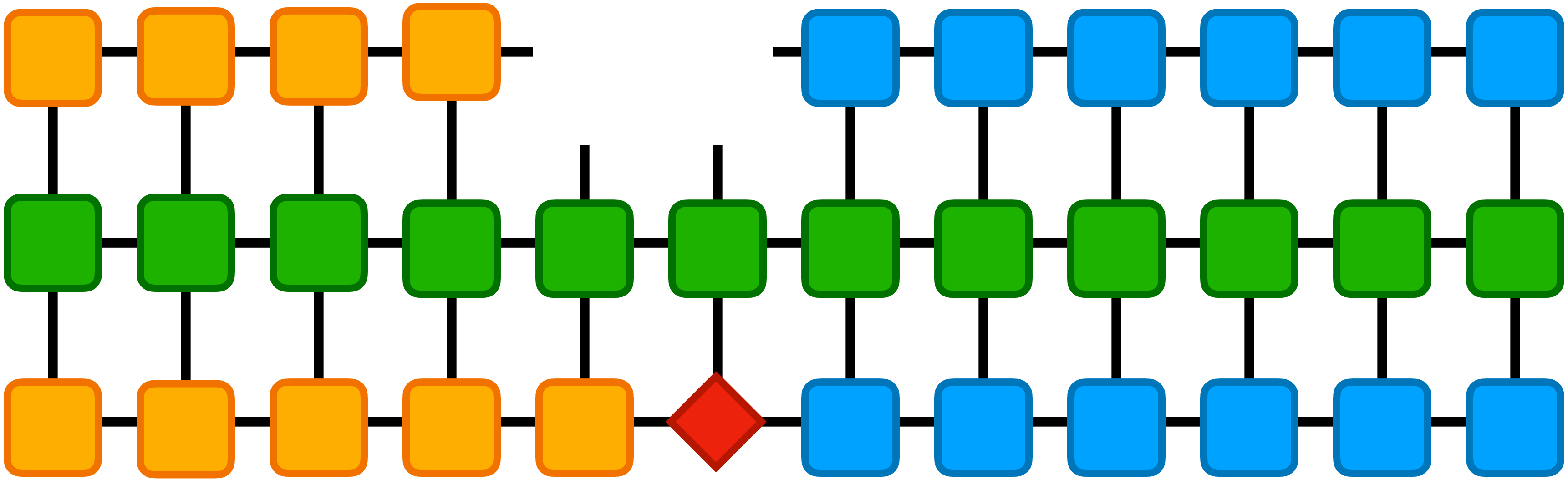

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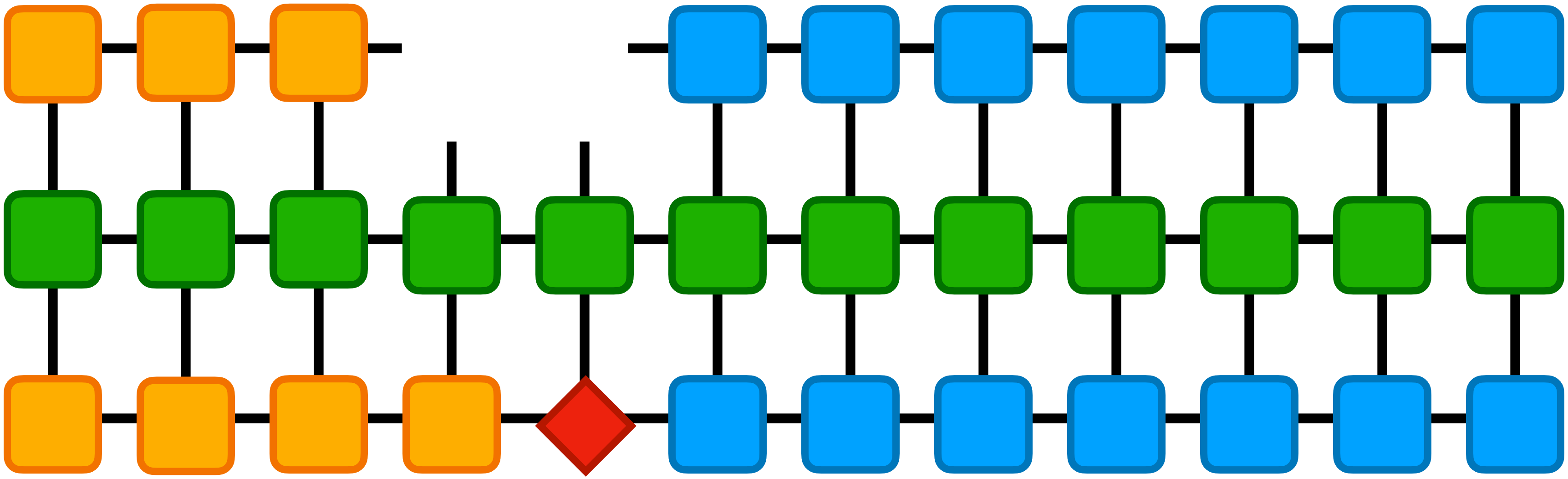

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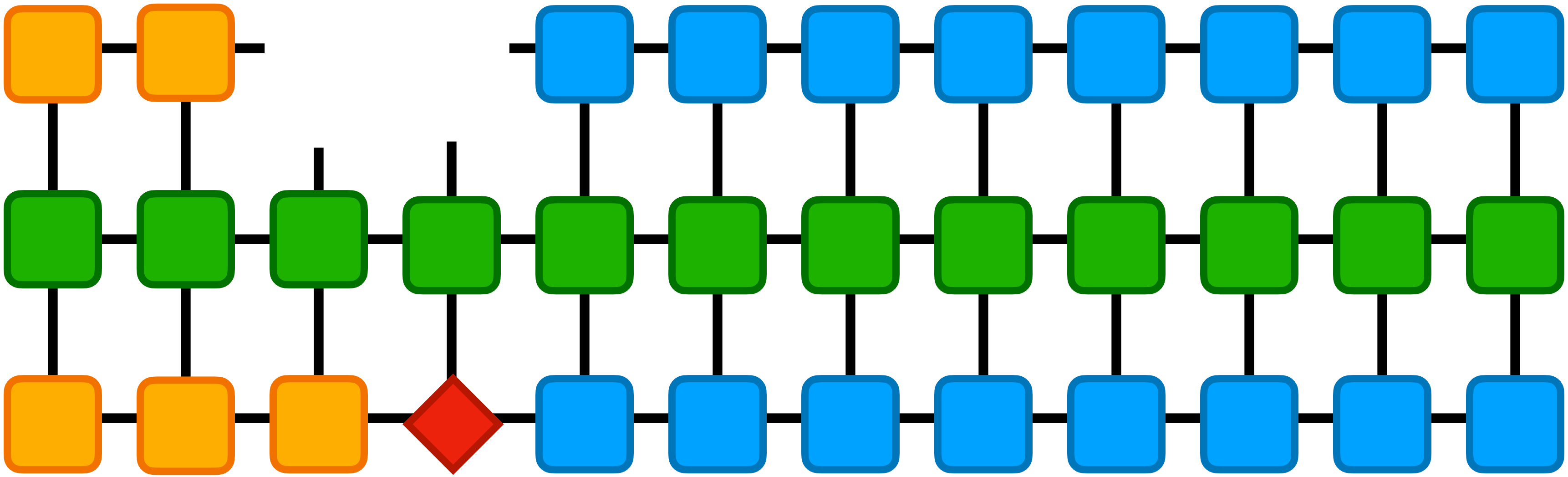

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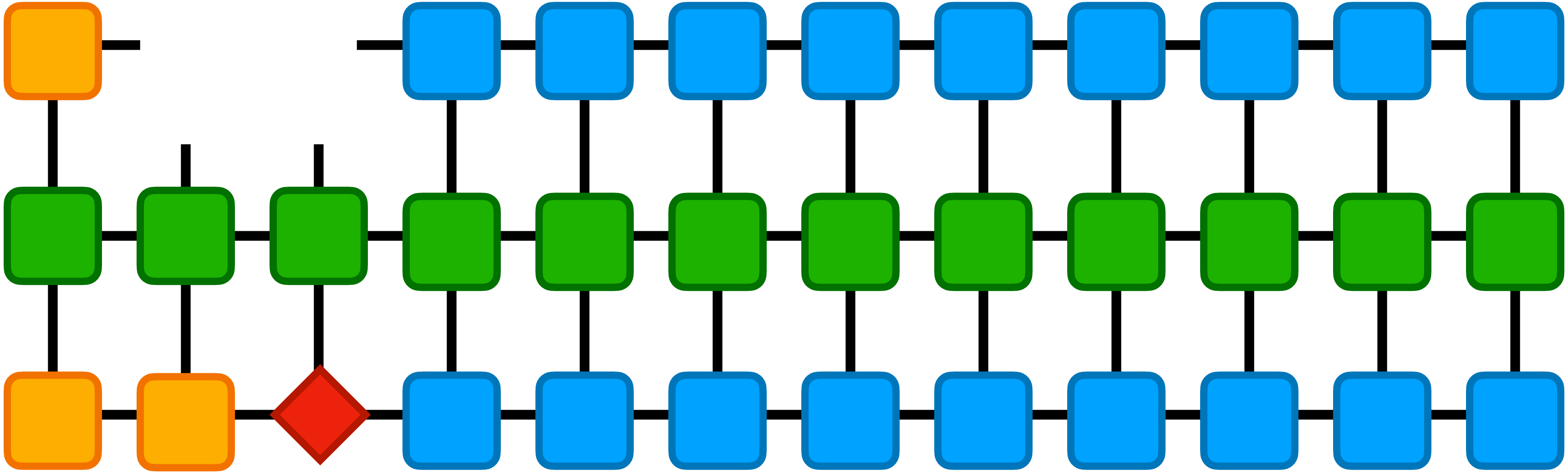

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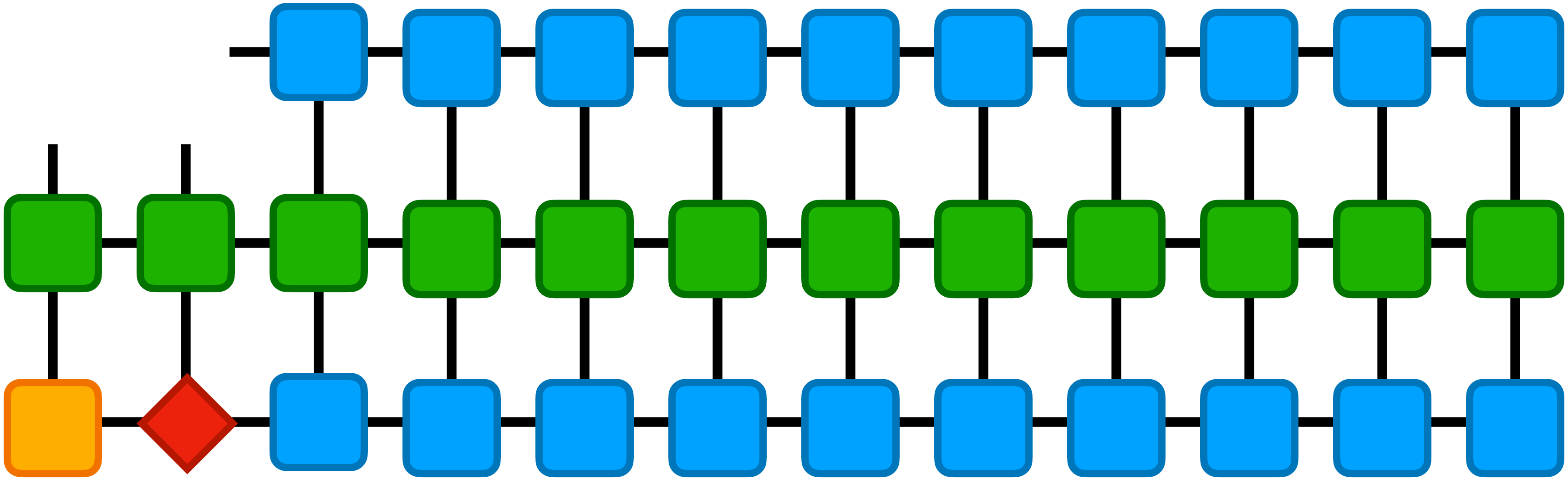
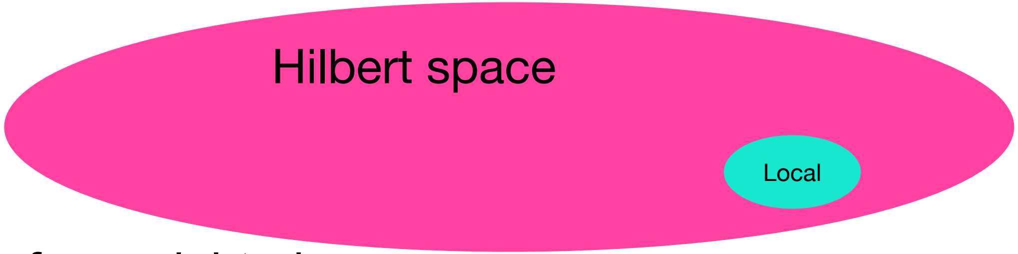
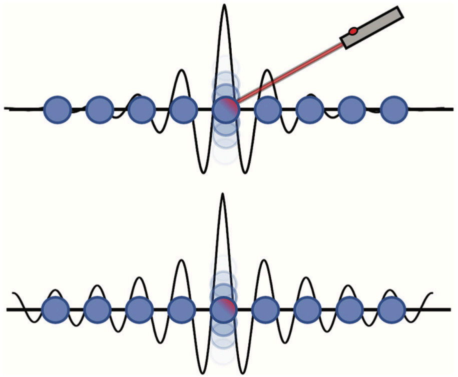


T.E. Baker and M.P. Thompson, arxiv: 2019.03120

When does DMRG work well?



- Area law
- Kohn's principle of nearsightedness



$$\begin{cases} \exp(-x/\xi) & \text{gapped} \\ 1/x^{\gamma} & \text{gapless} \end{cases}$$

T.E. Baker, et. al., *Can. J. Phys.* **99**, 4 (2021)

ibid, arxiv: 1911.11566

Conclusion

- Entanglement renormalization
    - Use of entanglement
- Custom library
    - Well documented
    - Near the v1.0 release
    - New algorithms
    - Highly efficient

DMRjulia

Build your own tensor network library:
DMRjulia I. Basic library for the density matrix renormalization group

Thomas E. Baker[1,2] and Martin P. Thompson[2]

[1]*Department of Physics, University of York, Heslington, York YO10 5DD, United Kingdom*
[2]*Institut quantique & Département de physique, Université de Sherbrooke, Sherbrooke, Québec J1K 2R1 Canada*
(Dated: September 8, 2021)

An introduction to the density matrix renormalization group is contained here, including coding examples. The focus of this code is on basic operations involved in tensor network computations, and this forms the foundation of the DMRjulia library. Algorithmic complexity, measurements from the matrix product state, convergence to the ground state, and other relevant features are also discussed. The present document covers the implementation of operations for dense tensors into the Julia language. The code can be used as an educational tool to understand how tensor network computations are done in the context of entanglement renormalization or as a template for other codes in low level languages. A comprehensive Supplemental Material is meant to be a "Numerical Recipes" style introduction to the core functions and a simple implementation of them. The code is fast enough to be used in research and can be used to make new algorithms.

CONTENTS

NRC Research Press

TUTORIA

Méthodes de calcul avec réseaux de tenseurs en physique

Thomas E. Baker, Samuel Desrosiers, Maxime Tremblay et Martin P. Thompson

Résumé : Cet article se veut un survol des réseaux de tenseurs et s'adresse aux débutants en la matière. Nous y metton cent sur les outils nécessaires à l'implémentation concrète d'algorithmes. Quatre opérations de base (remodelage, pern tion d'indices, contraction et décomposition) qui sont couramment utilisées dans les algorithmes de réseaux de tense sont décrites. Y seront aussi couverts la notation diagrammatique, intrication, les états en produit de matrices (les opérateurs en produit de matrices (MPO), état projeté de paires intriquées (PEPS), l'approche par renormalis d'enchevêtrement multi-échelle (MERA), la décimation par bloc d'évolution temporelle (TEBD) et le groupe de renor sation de tenseurs (TRG).

Mots-clés : réseaux de tenseurs, décomposition en valeurs singulières, intrication.

Abstract : This article is an overview of tensor networks and is intended for beginners in this field. We focus on the required for the concrete implementation of algorithms. Four basic operations (remodelling, permutation of indices traction, and decomposition) commonly used in tensor network algorithms are described. This study also covers dia matic notation, entanglement, matrix product states (MPS), matrix product operators (MPO), projected entangled pair (PEPS), multi-scale entanglement renormalization ansatz (MERA), time evolving block decimation (TEBD), and t renormalization group (TRG).

Keywords : tensor networks, singular value decomposition, entanglement.

1. Introduction

Les méthodes exactes de résolution de systèmes quantiques sont difficiles à appliquer aux problèmes de grande taille. Il est alors nécessaire d'utiliser des méthodes approximatives et les réseaux de tenseurs figurent parmi les méthodes les plus utilisées à cet effet. Les méthodes des réseaux de tenseurs se basent

Dans cette revue des réseaux de tenseurs, nous nous co trons sur les opérations de base nécessaires à la manipulatio tenseurs. À la section 2, nous commençons par une discussi ce que sont les tenseurs. À la section 3, nous introduisons notation schématique qui permet de simplifier le traitemen lytique des réseaux de tenseurs. À la section 4, nous présen quatre opérations de base s'appliquant aux tenseurs. Da