



UNIVERSITÀ  
DEGLI STUDI  
DI PADOVA



Dipartimento  
di Fisica  
e Astronomia  
Galileo Galilei



QUANTUM  
Information and Matter



# Lattice QED photonic wavepackets on ladder geometries

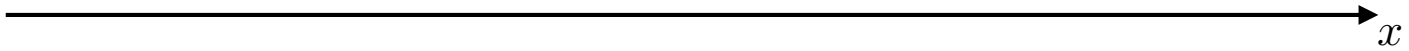
**Mattia Morgavi**, M. Rigobello, L. Maffi, P. Silvi and S. Montangelo

September 3, 2024, QuantHEP Conference, LMU, München

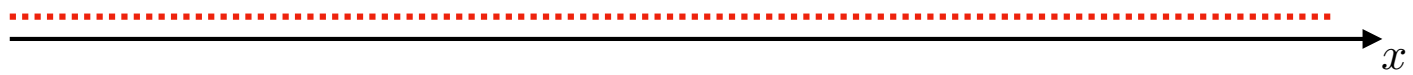


# Introduction

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$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$$

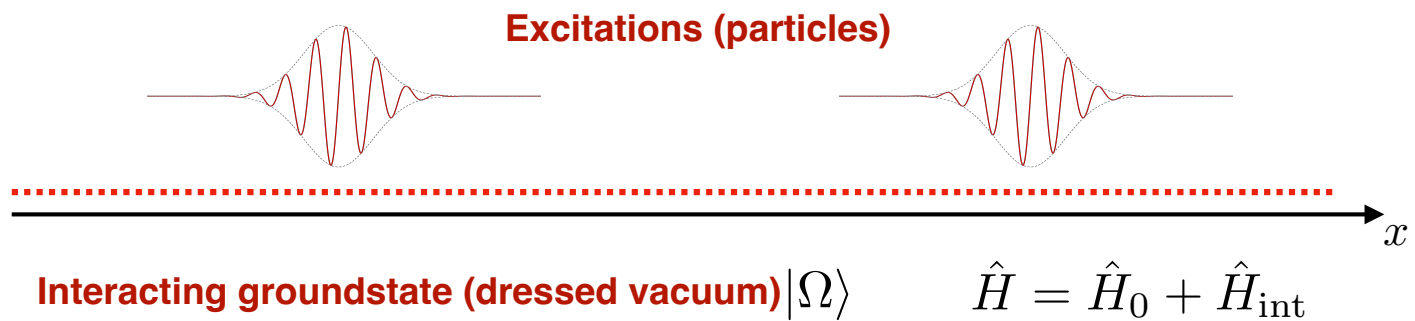
# Introduction



Interacting groundstate (dressed vacuum)  $|\Omega\rangle$        $\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$

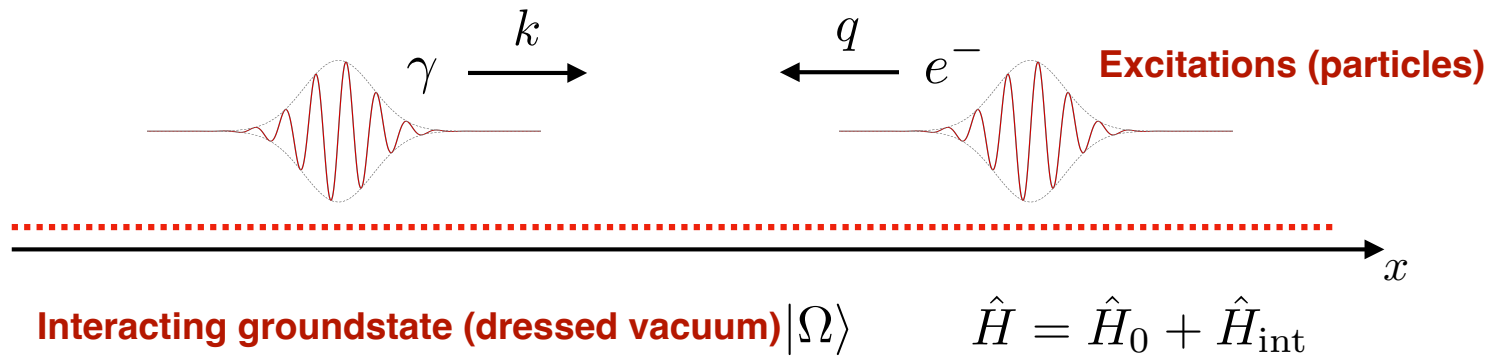


# Introduction

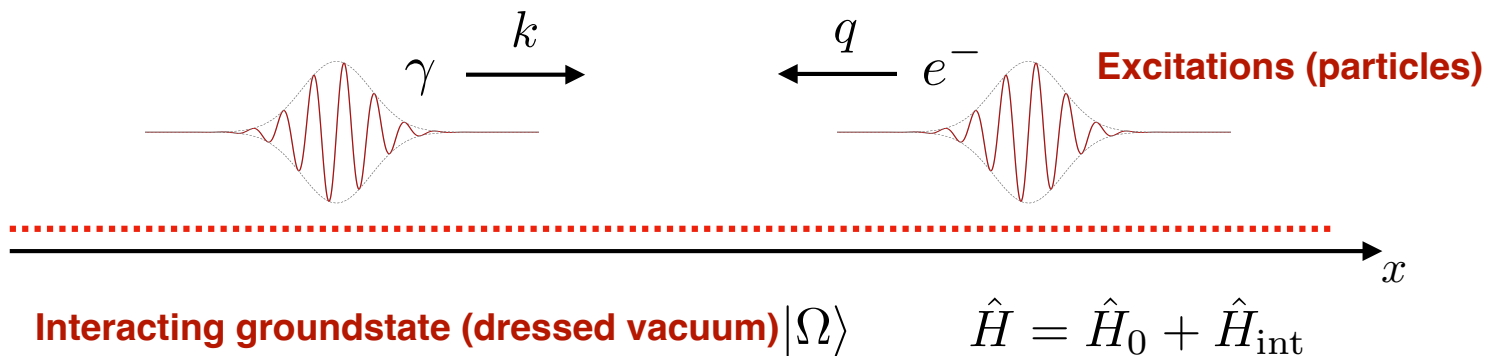


# Introduction

**Scattering!**



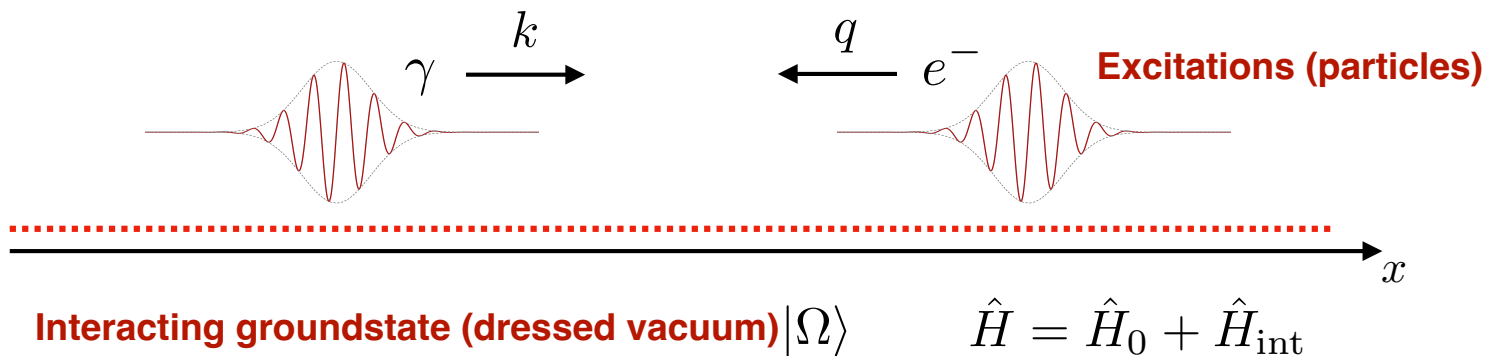
# Introduction



continuous...

Model: 1D  
|  
first step

# Introduction

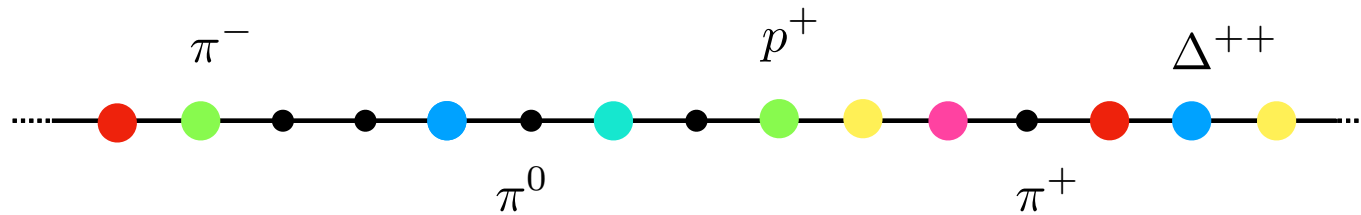
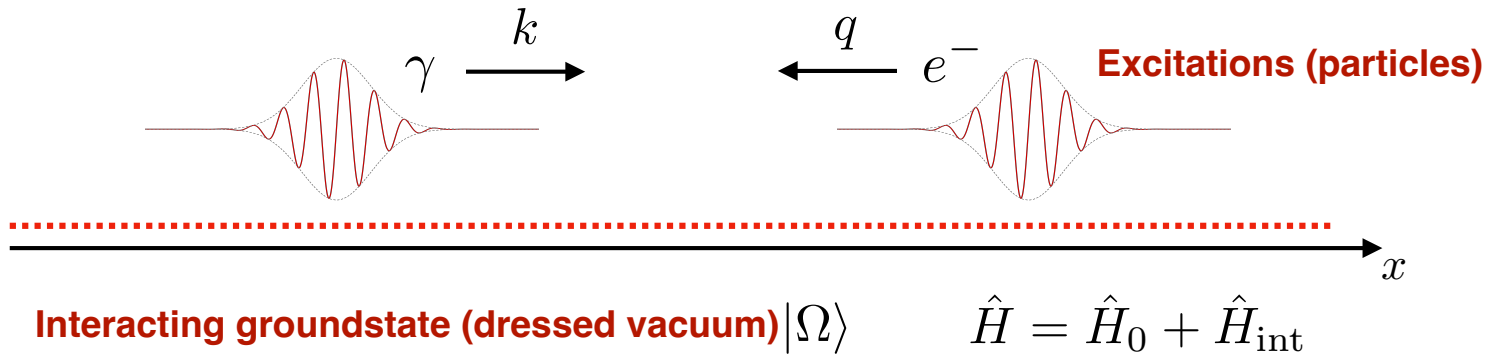


Toy Model:

1D Lattice

first step computable

# Introduction

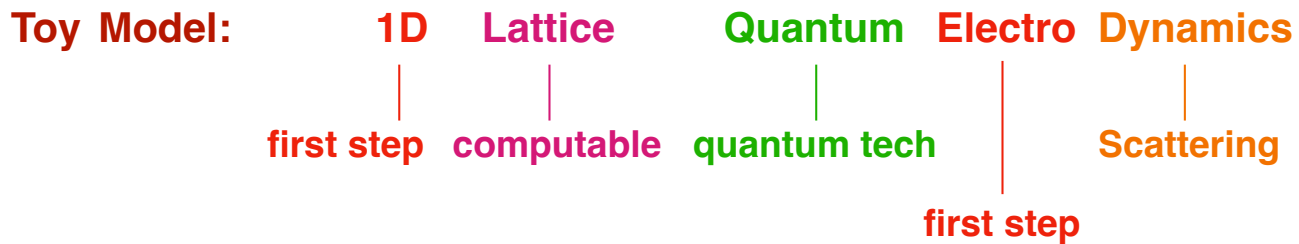
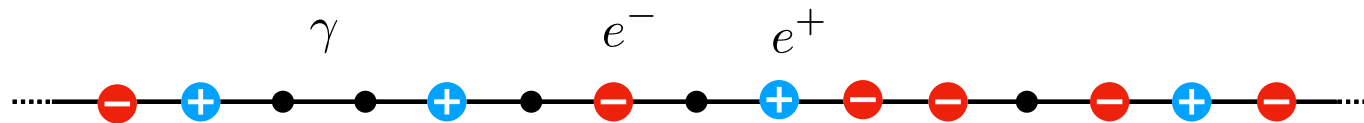
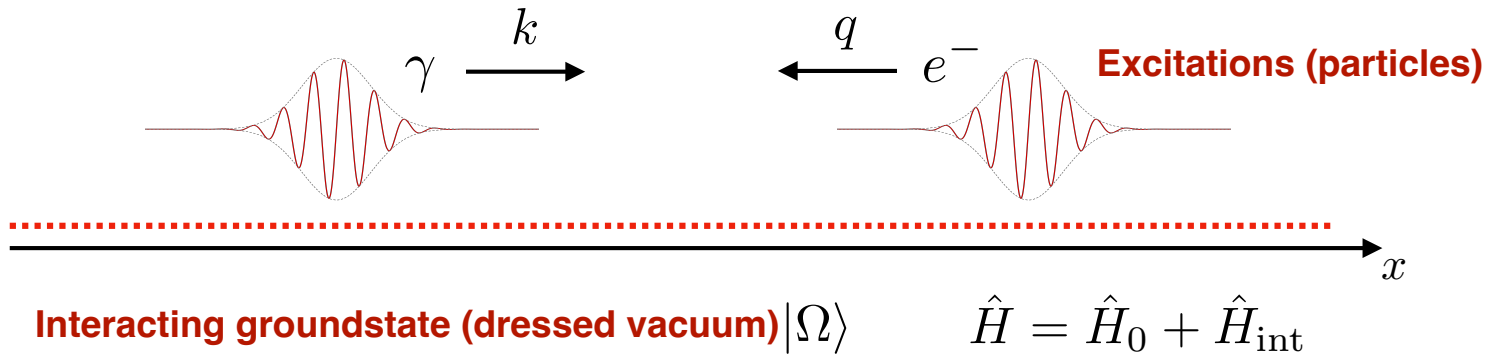


Challenging (maybe next year...)

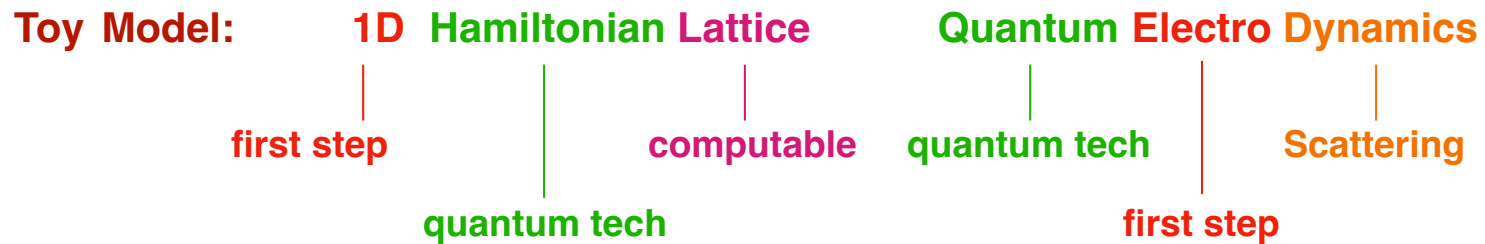
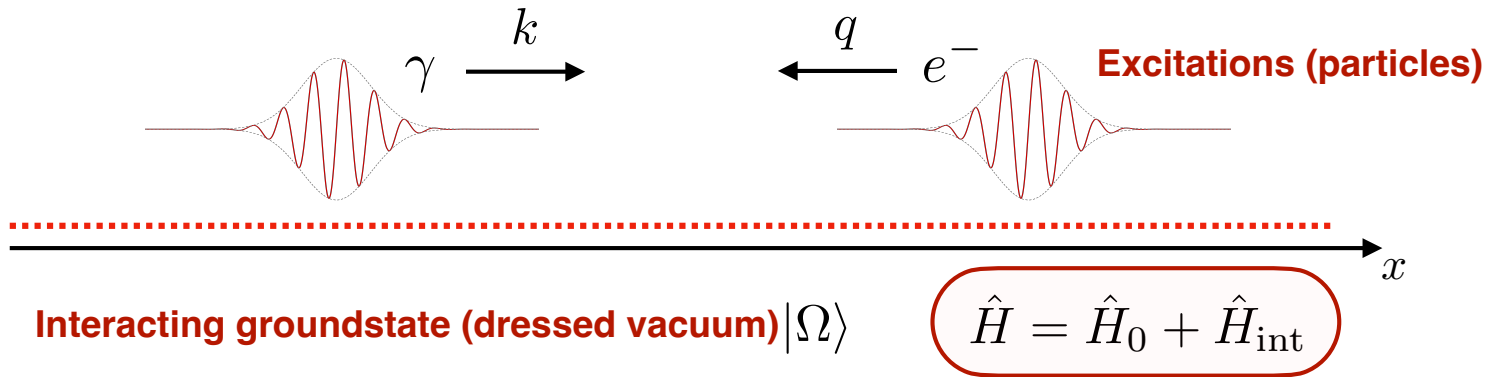
Toy Model: 1D Lattice Quantum Chromo Dynamics

first step computable quantum tech Scattering

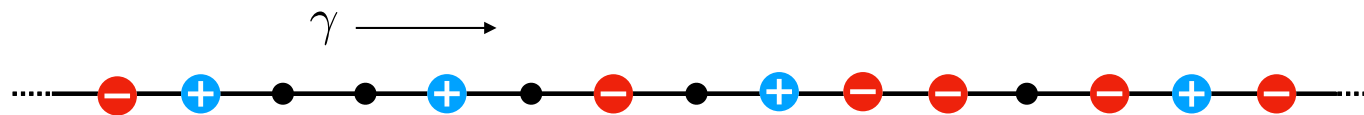
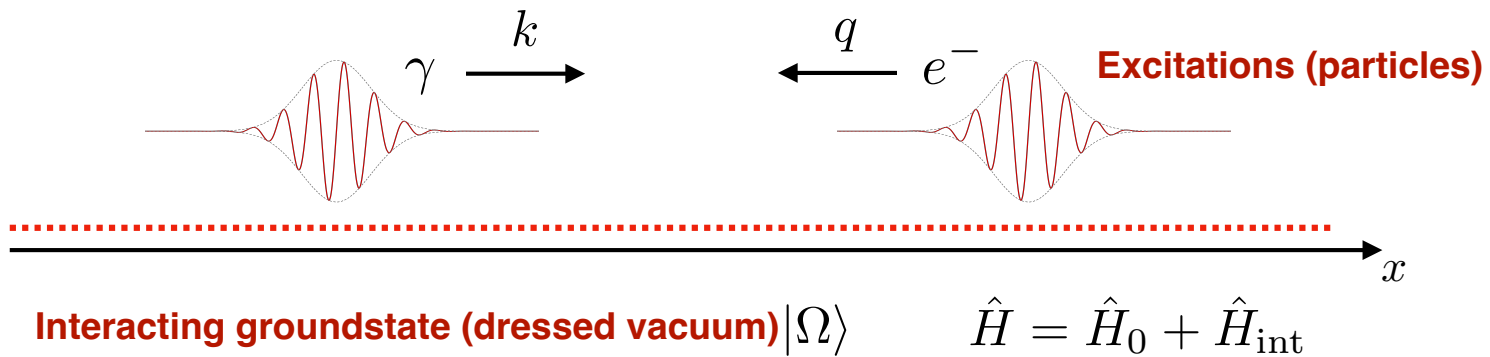
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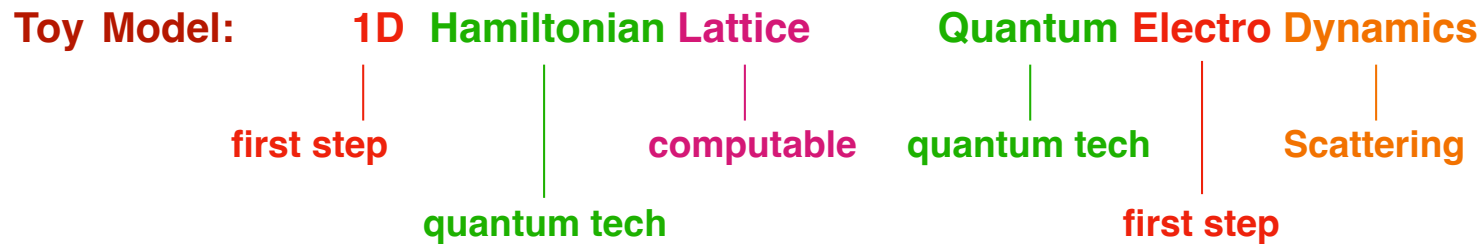
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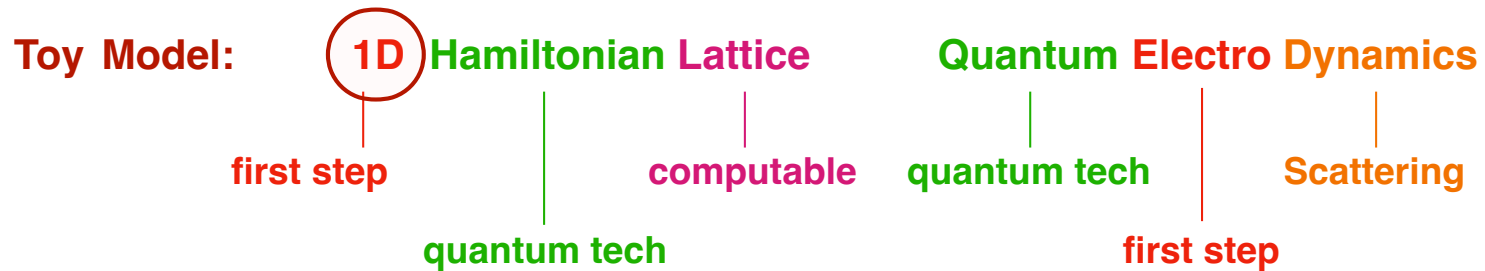
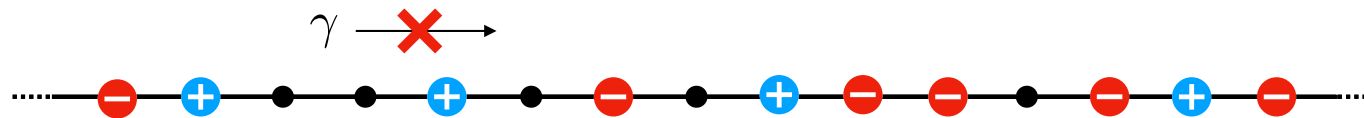
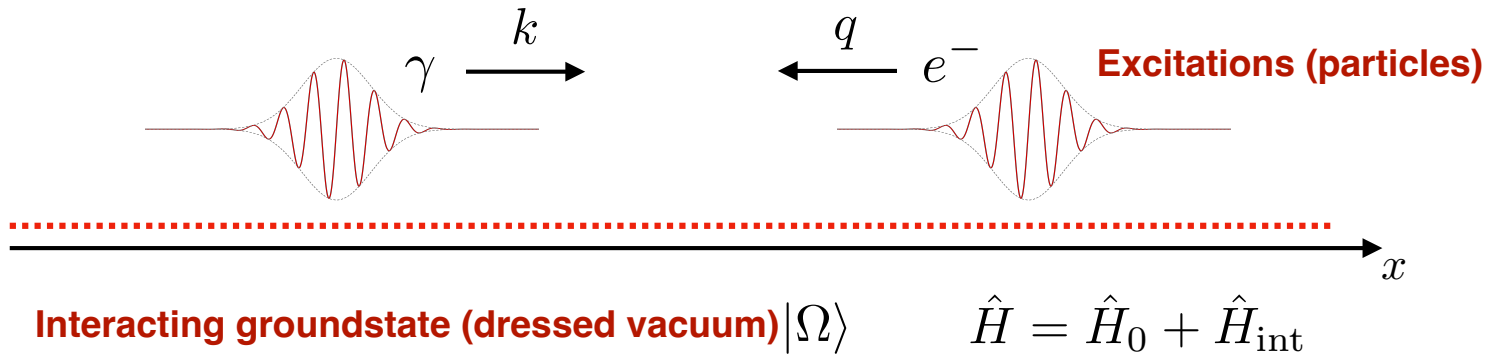


Goal: Compton scattering  
...we need a photon...



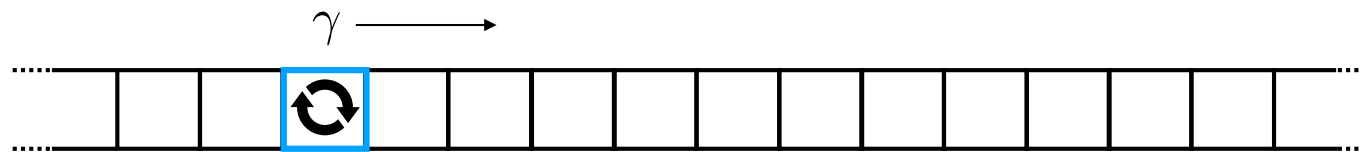
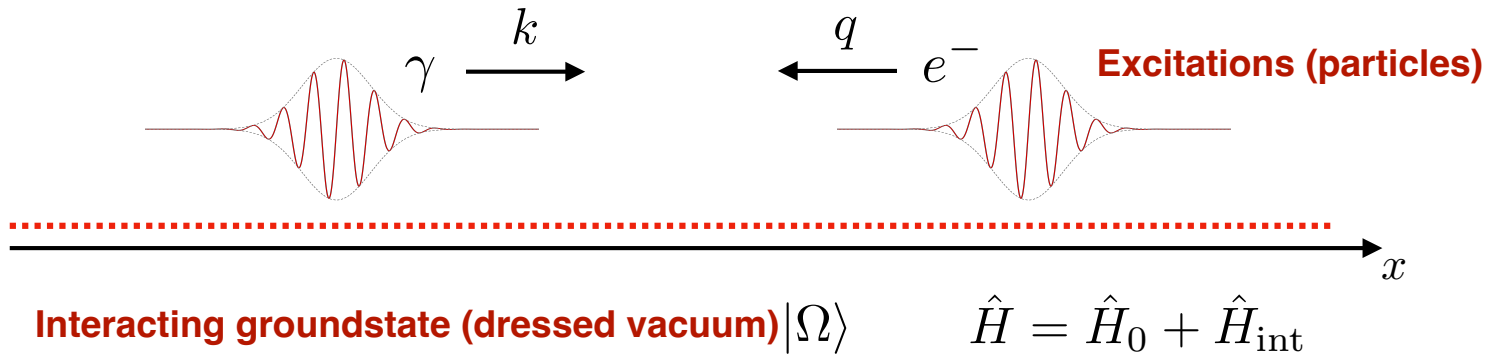


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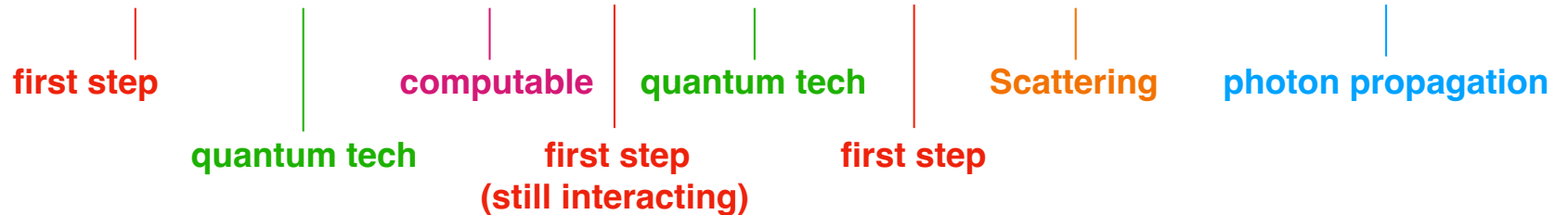




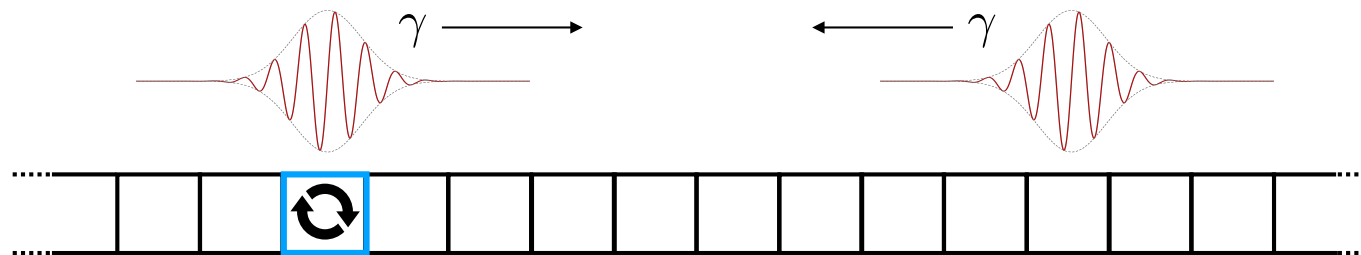
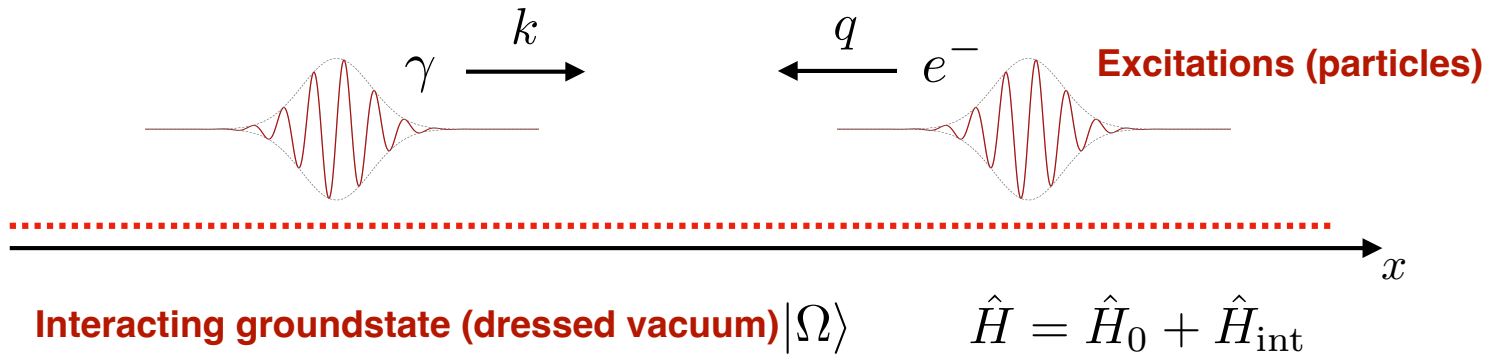
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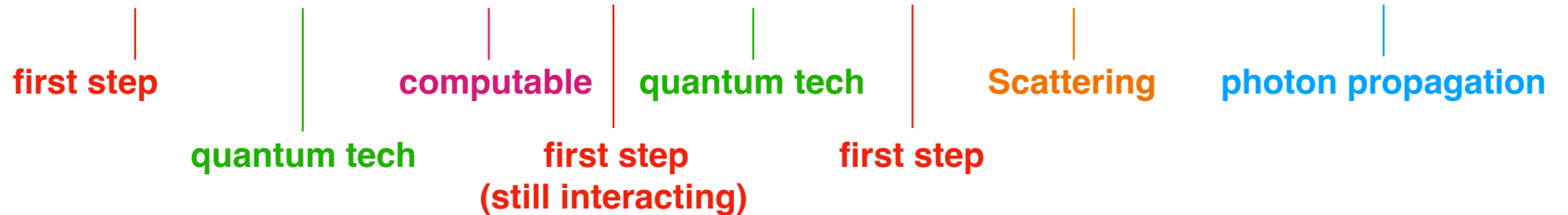
Toy Model: (quasi)-1D Hamiltonian Lattice Pure Quantum Electro Dynamics on Ladder Geometries



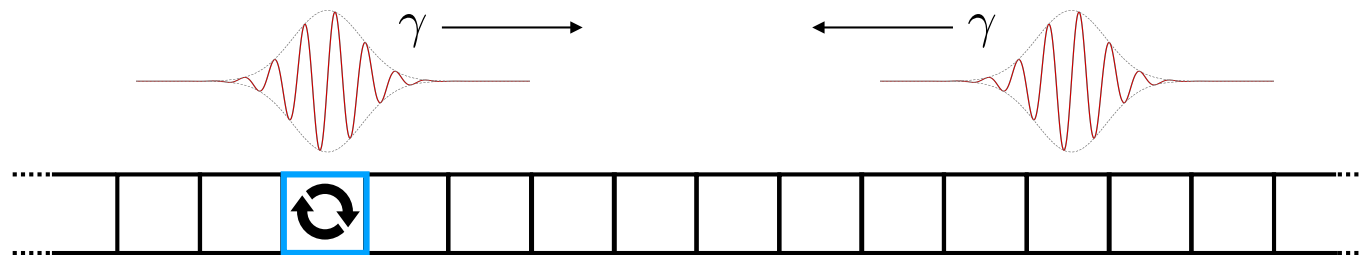
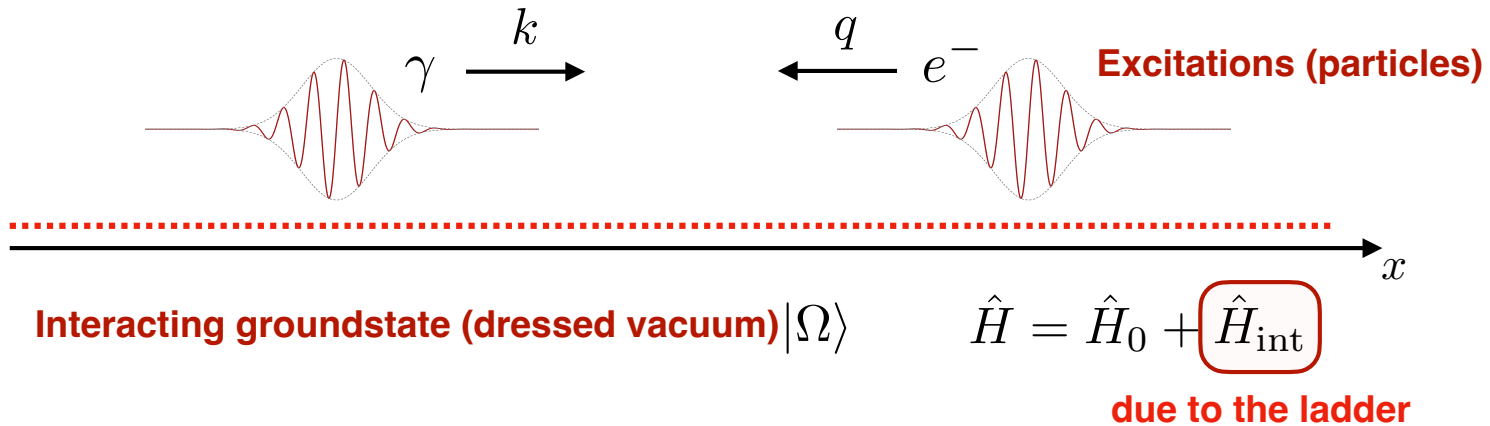
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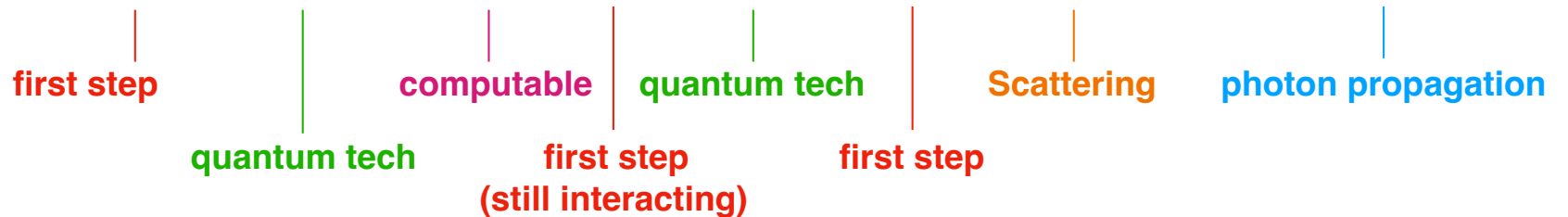
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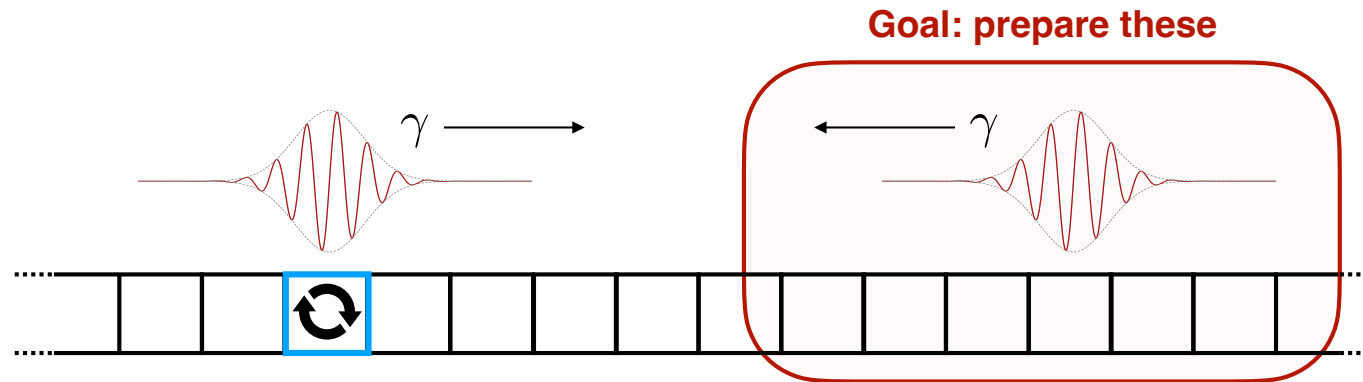
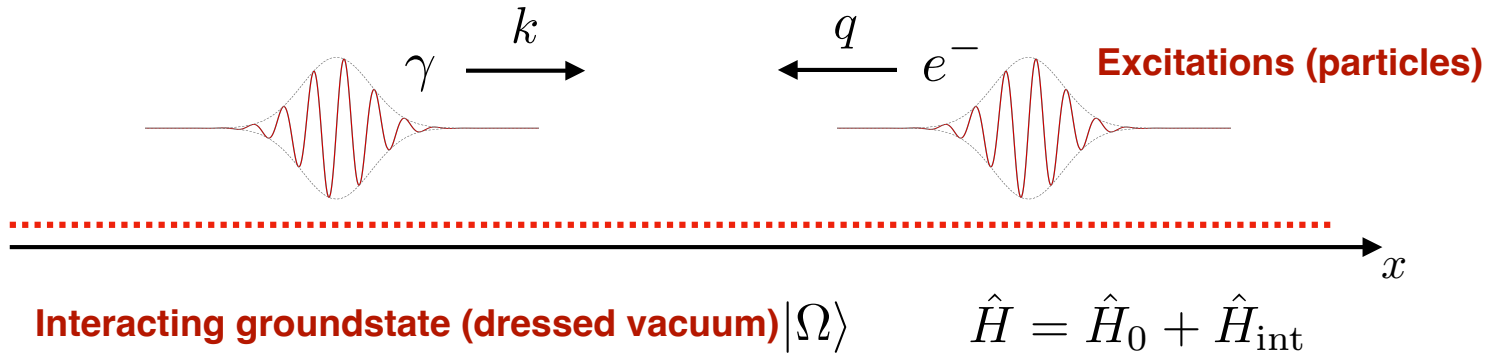
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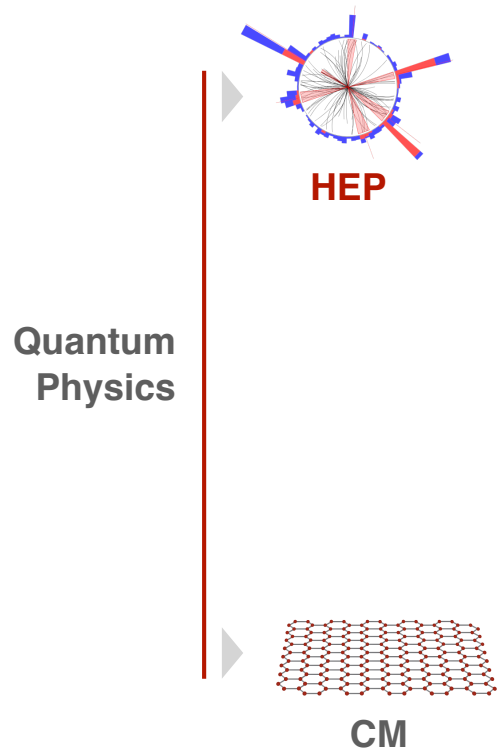
# Motivation: problems and solutions

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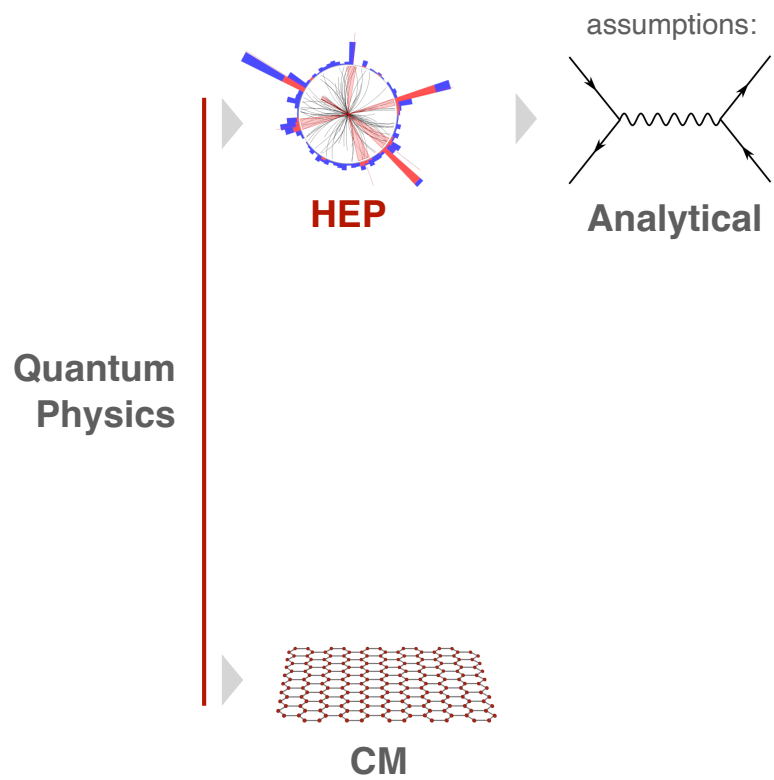
Quantum  
Physics



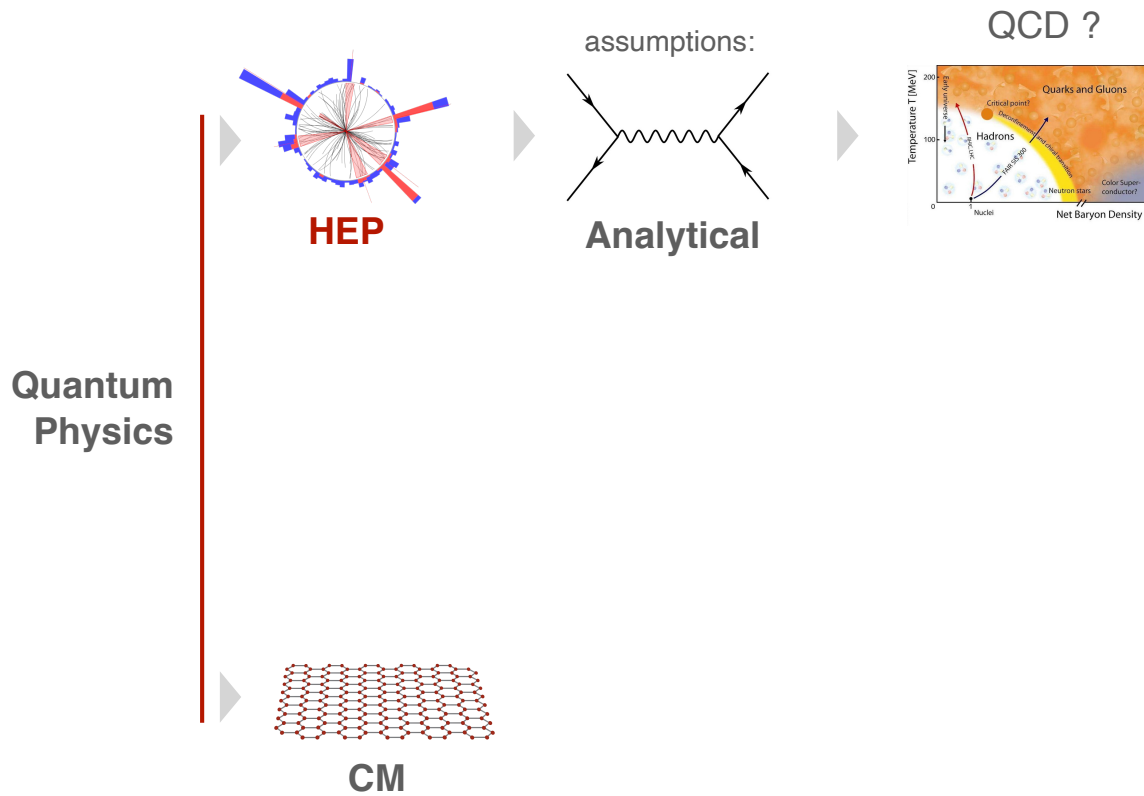
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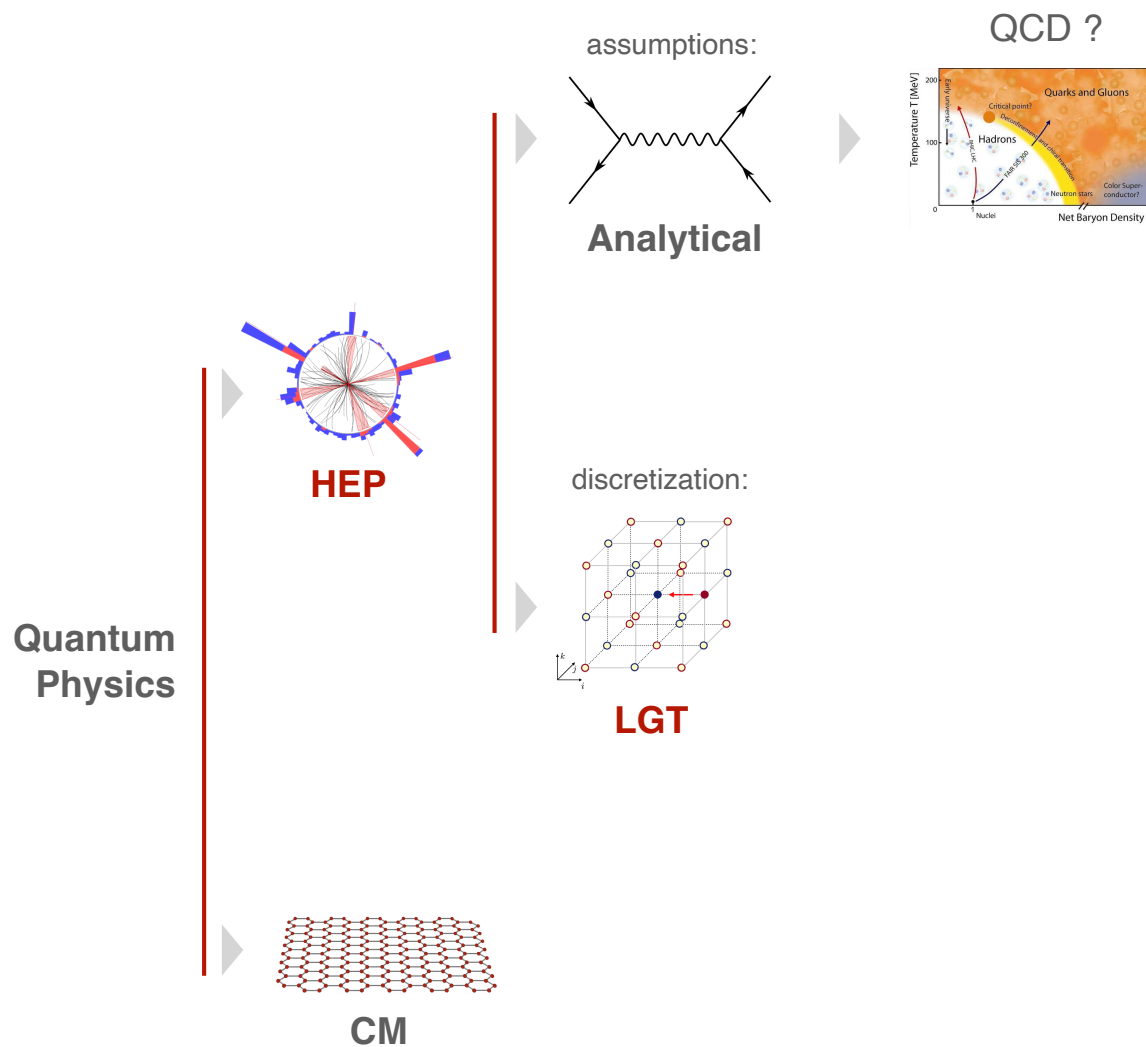


# Motivation: problems and solutions



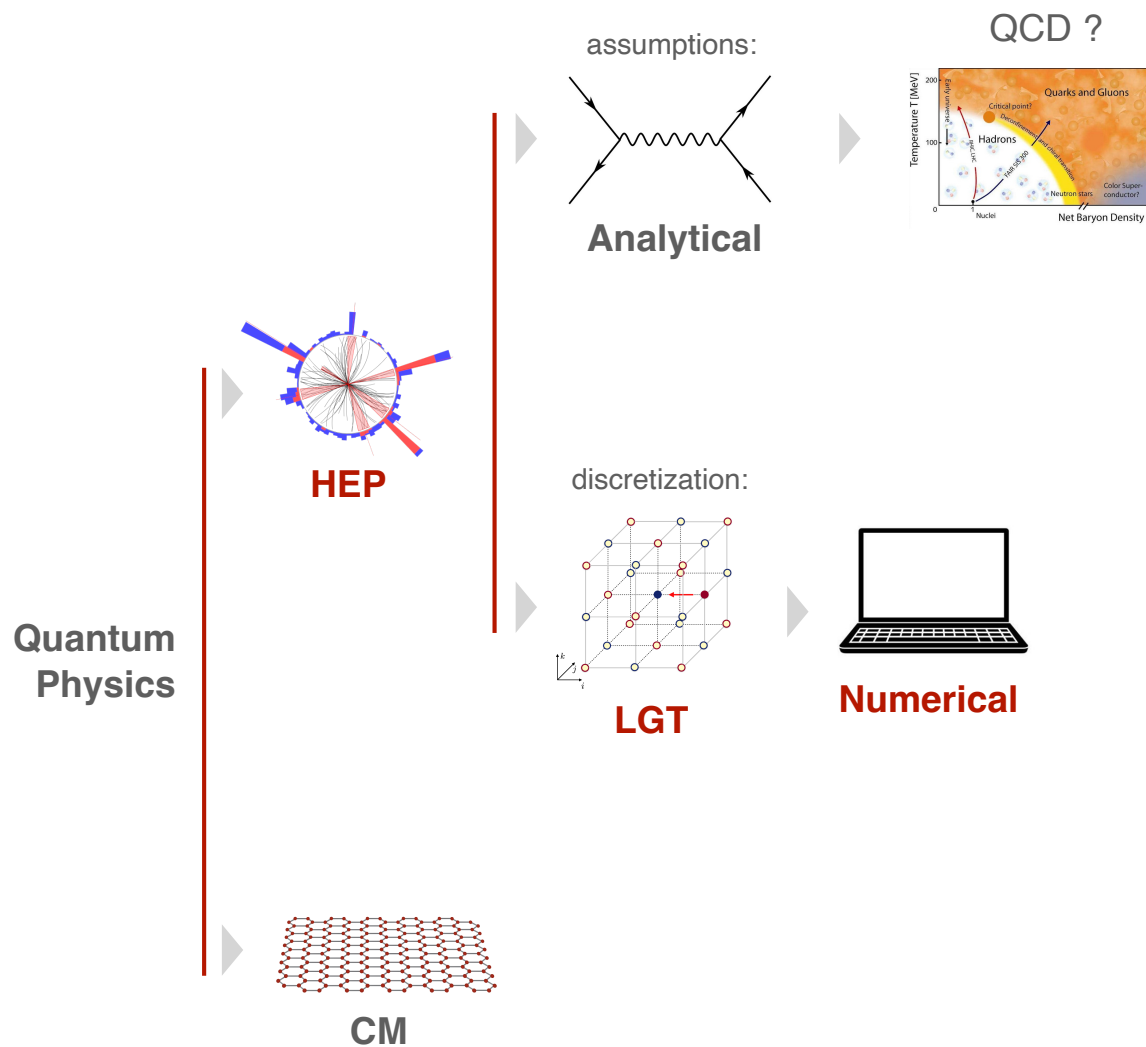
Some problems remain intractable...

# Motivation: problems and solutions



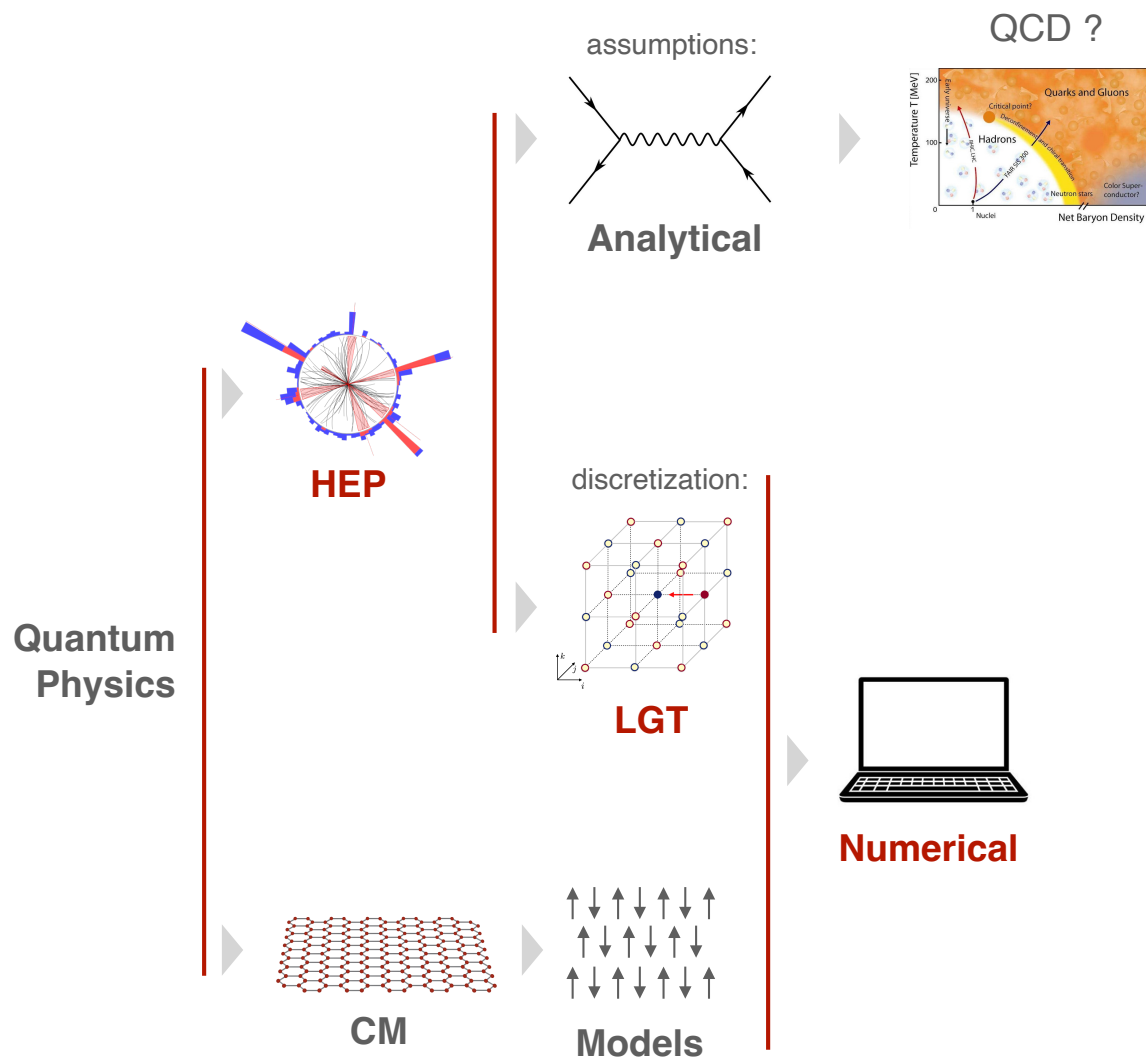
Some problems remain intractable...

# Motivation: problems and solutions



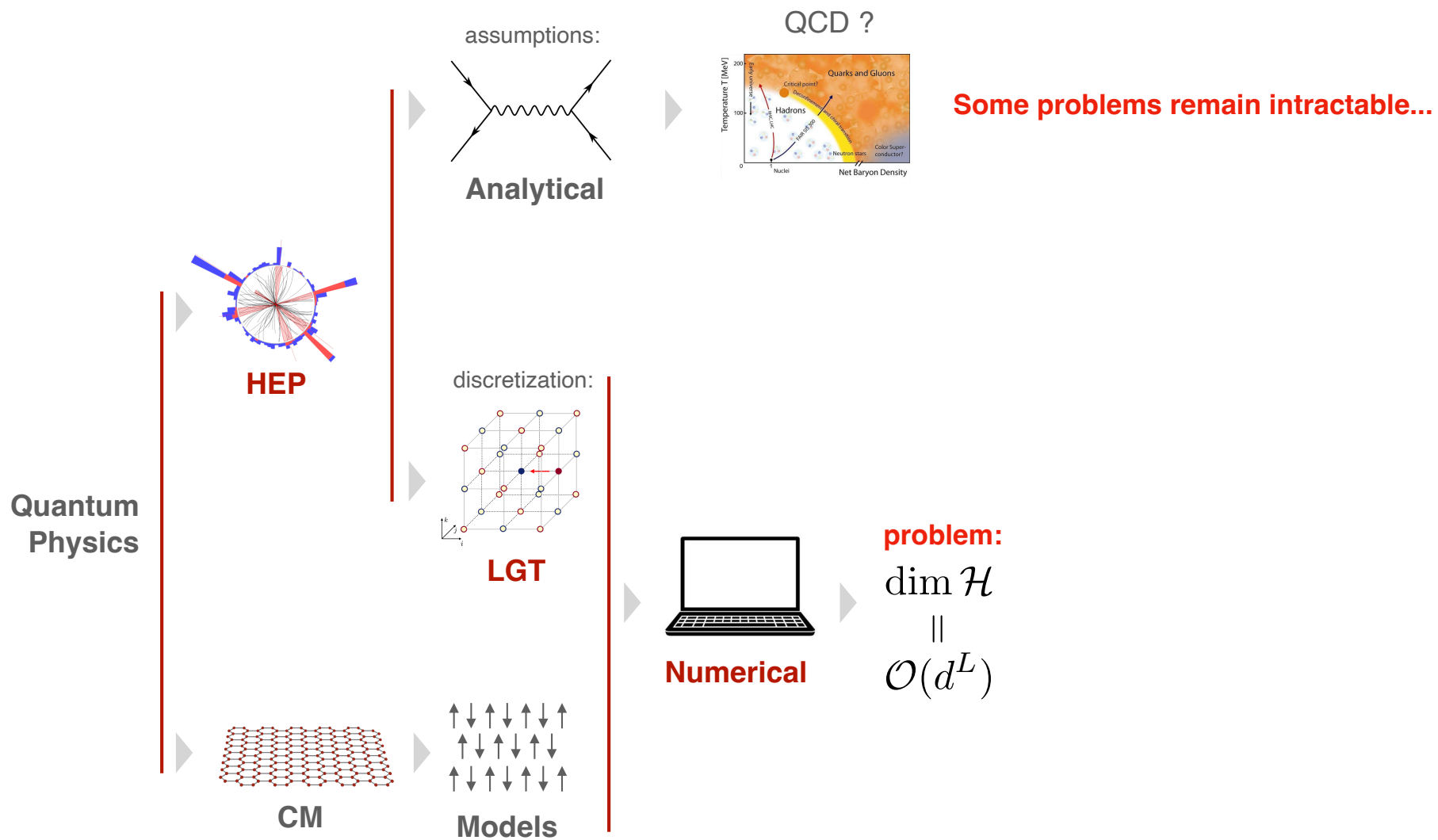
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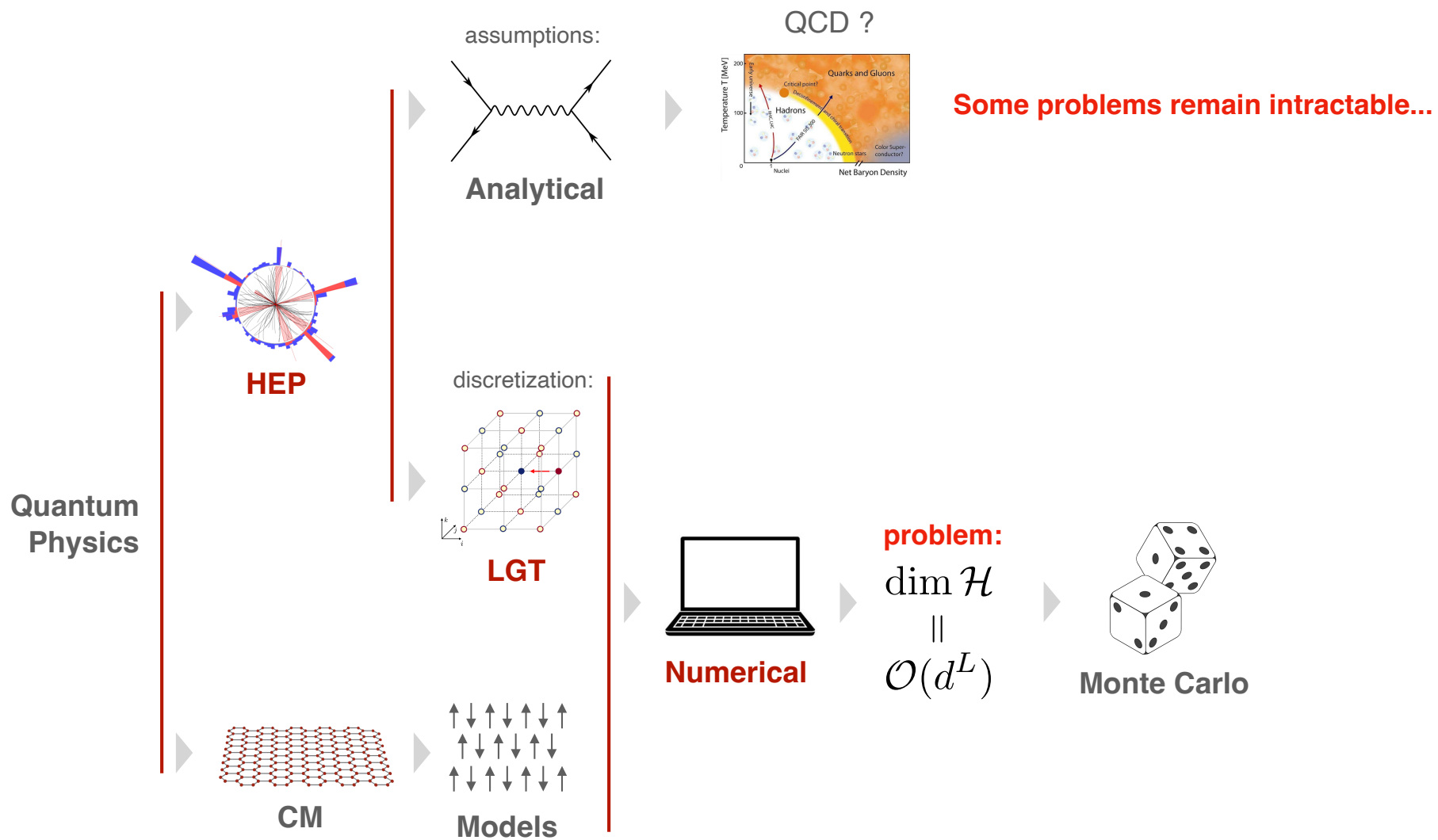


Some problems remain intractable...

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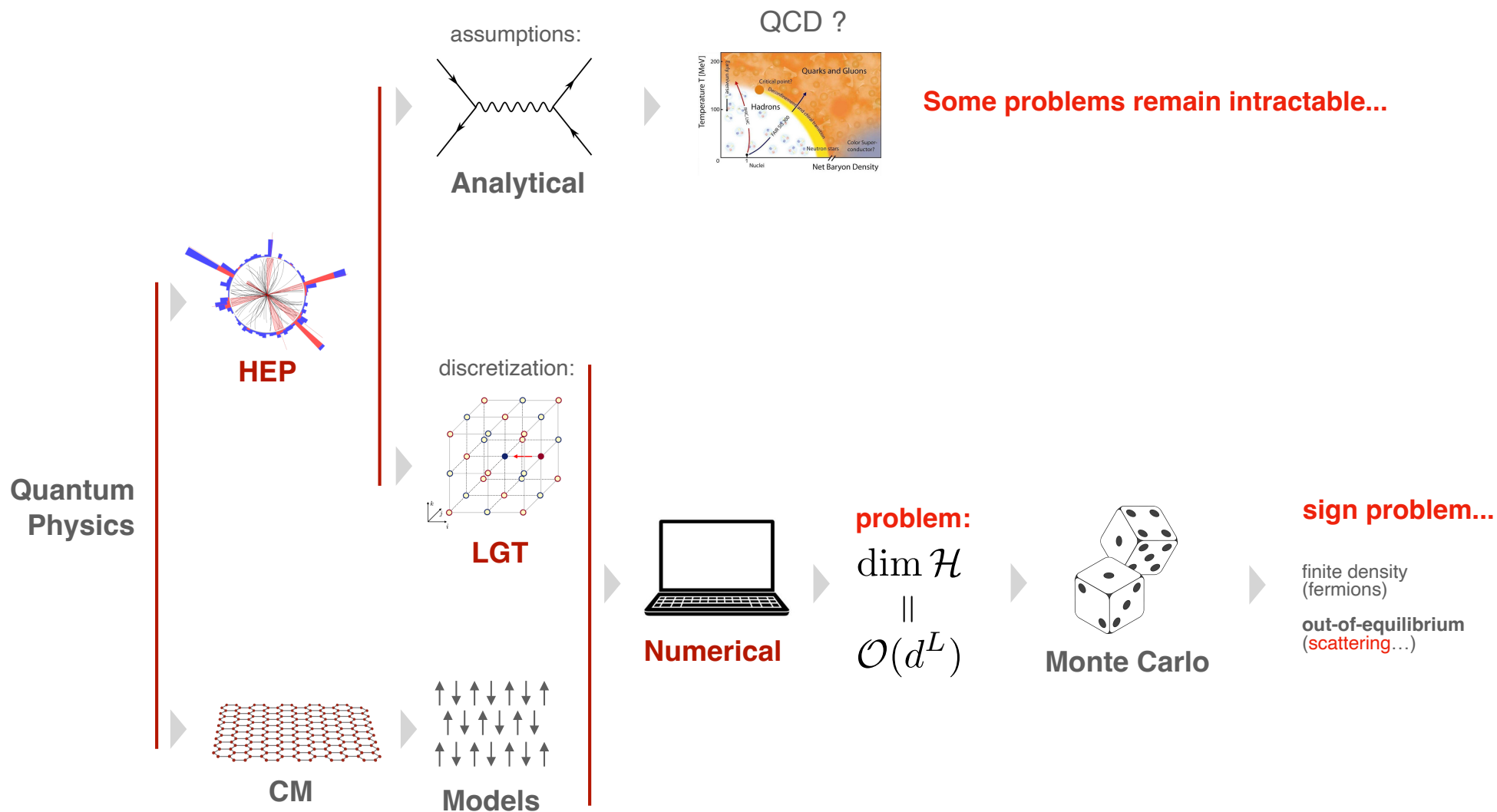


# Motivation: problems and solutions

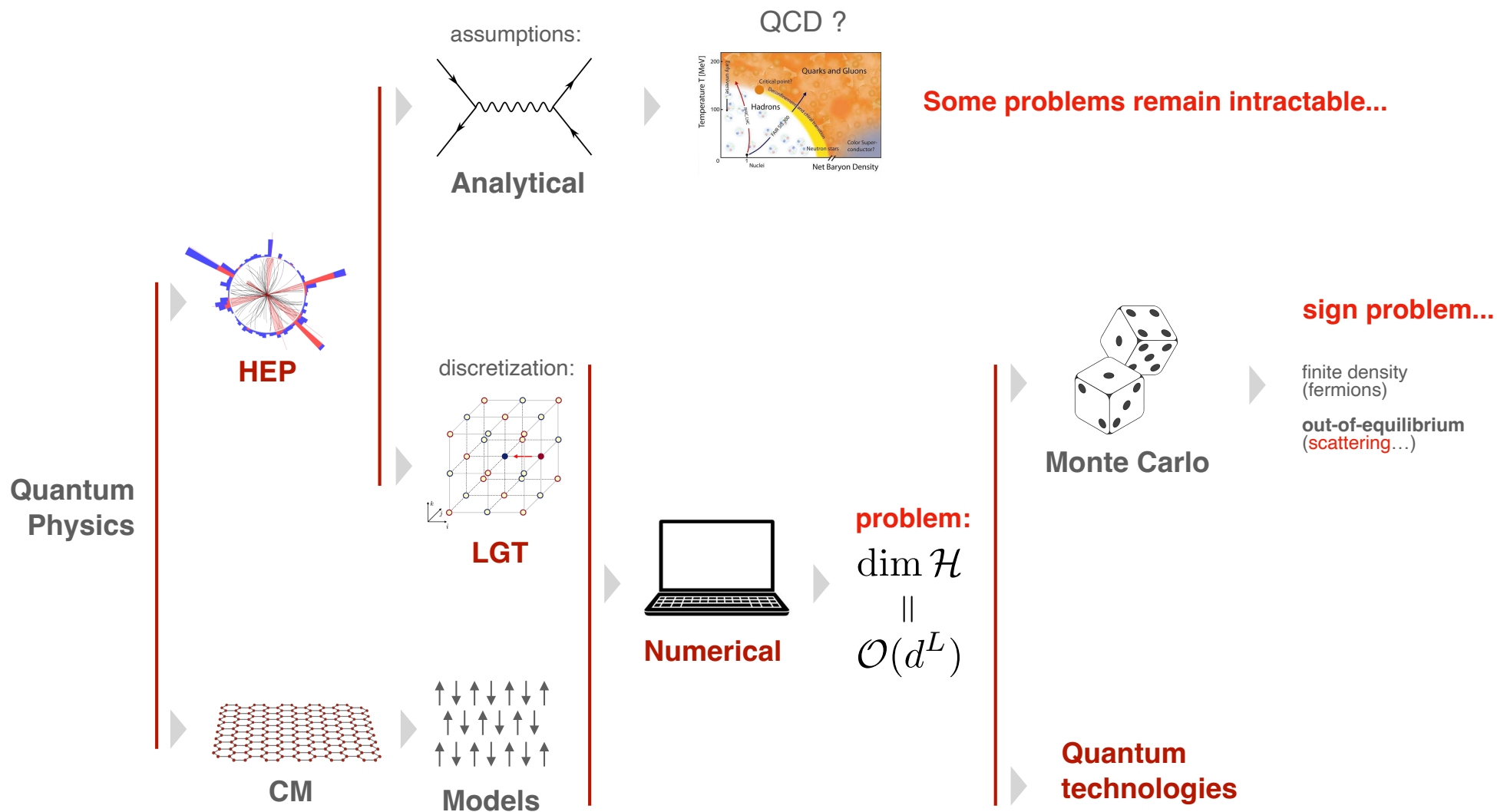




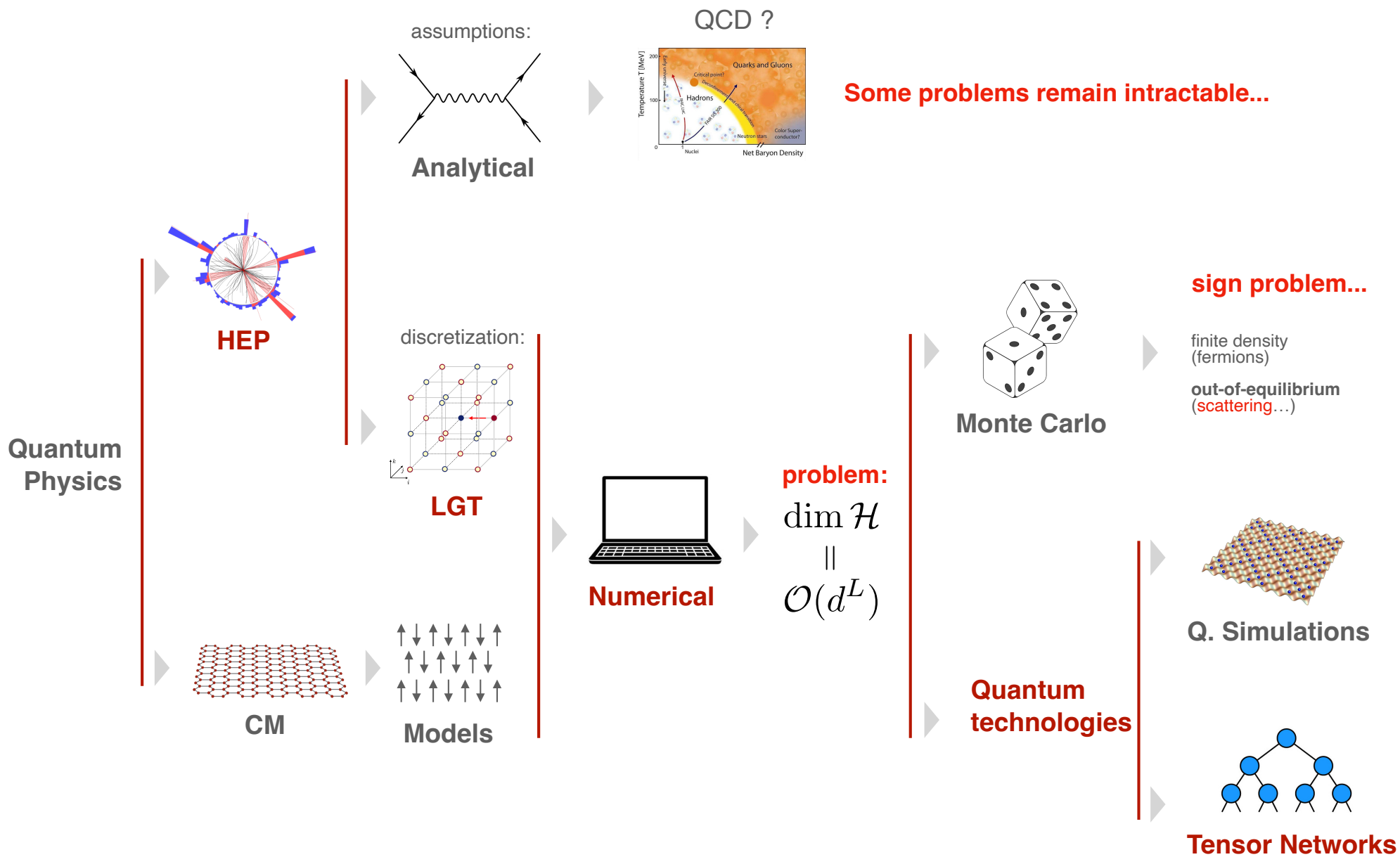
# Motivation: problems and solutions



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# Motivation: problems and solutions



# 1. Theoretical background

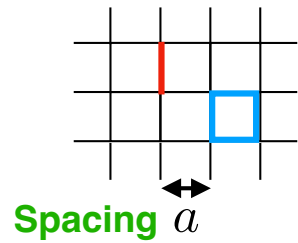
# 1. Theoretical background

● (2+1)D pure EM Hamiltonian  $H = \frac{1}{2} \int d^2x (E^2 + B^2)$

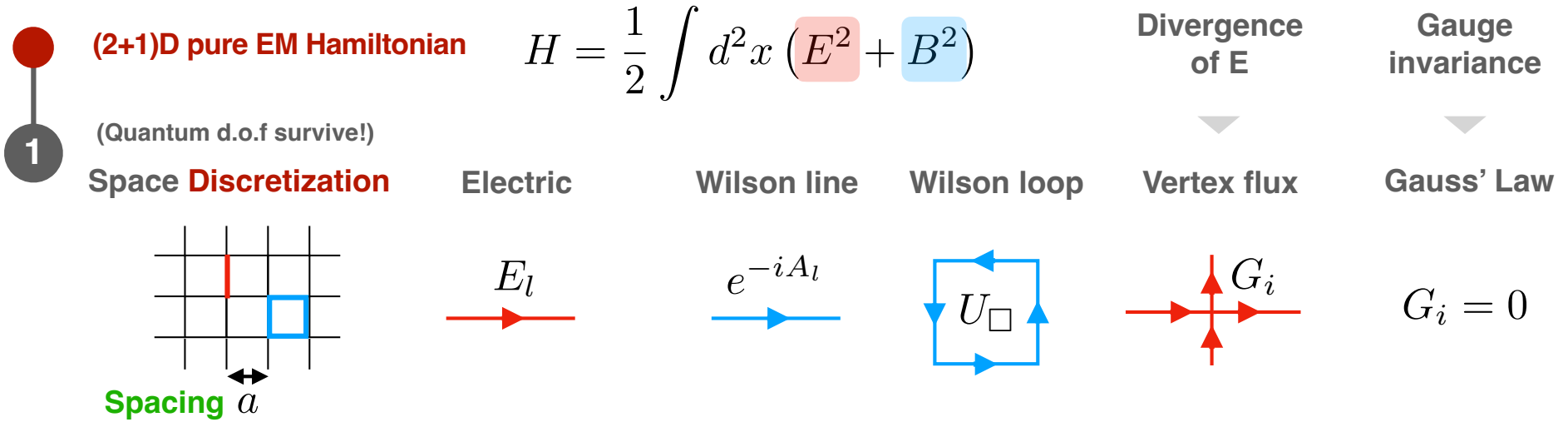
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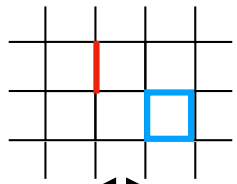

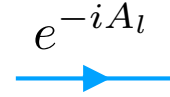
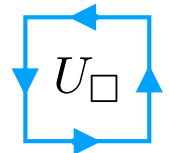

1 (Quantum d.o.f survive!)  
Space **Discretization**



# 1. Theoretical background

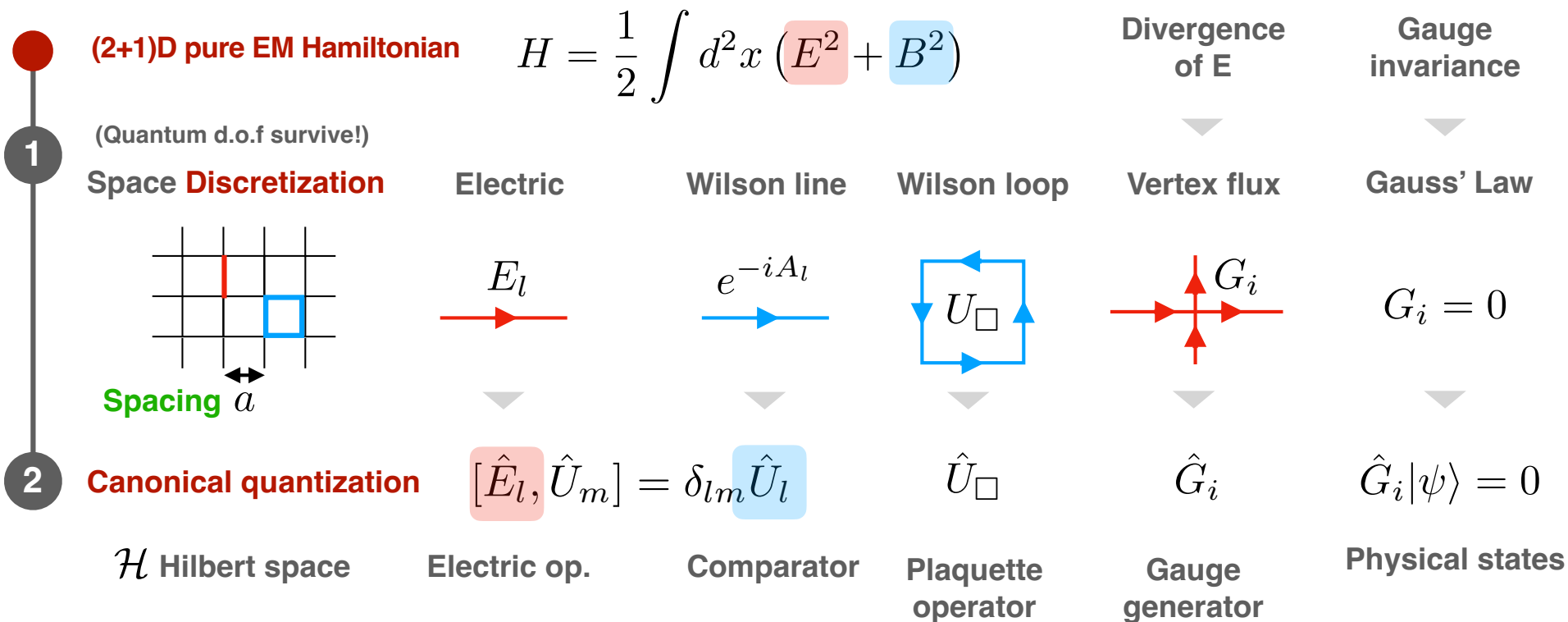


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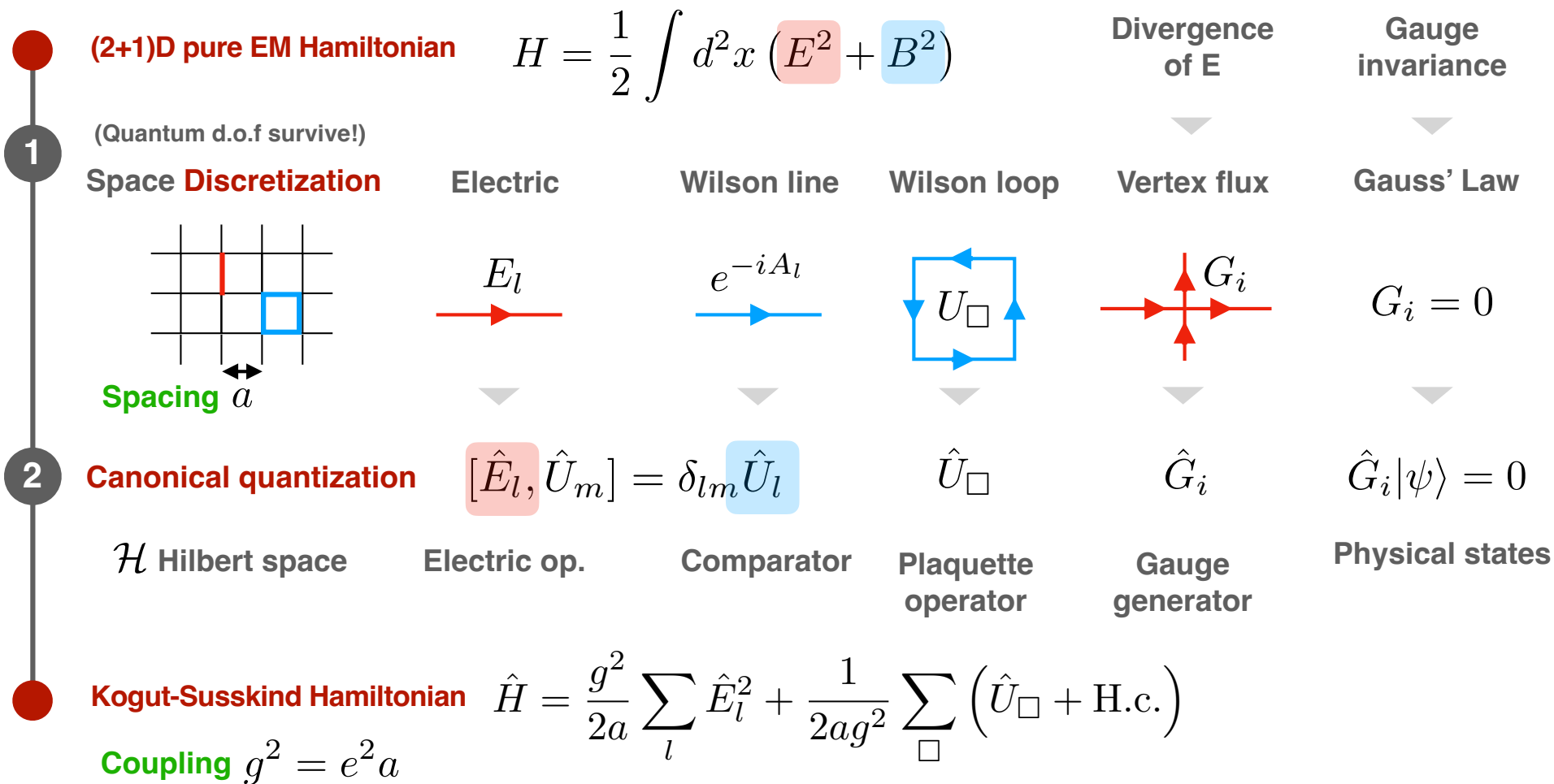
<p>●</p> <p>1</p> <p>2</p>	<p><b>(2+1)D pure EM Hamiltonian</b></p> <p>(Quantum d.o.f survive!)</p> <p><b>Space Discretization</b></p>  <p>Spacing <math>a</math></p>	$H = \frac{1}{2} \int d^2x (E^2 + B^2)$	<p><b>Electric</b></p>  <p><math>E_l</math></p>	<p><b>Wilson line</b></p>  <p><math>e^{-iA_l}</math></p>	<p><b>Wilson loop</b></p>  <p><math>U_{\square}</math></p>	<p><b>Divergence of E</b></p> <p>▼</p> <p><b>Vertex flux</b></p>  <p><math>G_i</math></p>	<p><b>Gauge invariance</b></p> <p>▼</p> <p><b>Gauss' Law</b></p> <p><math>G_i = 0</math></p>
	<p><b>Canonical quantization</b></p> <p><math>\mathcal{H}</math> Hilbert space</p>	$[\hat{E}_l, \hat{U}_m] = \delta_{lm} \hat{U}_l$					



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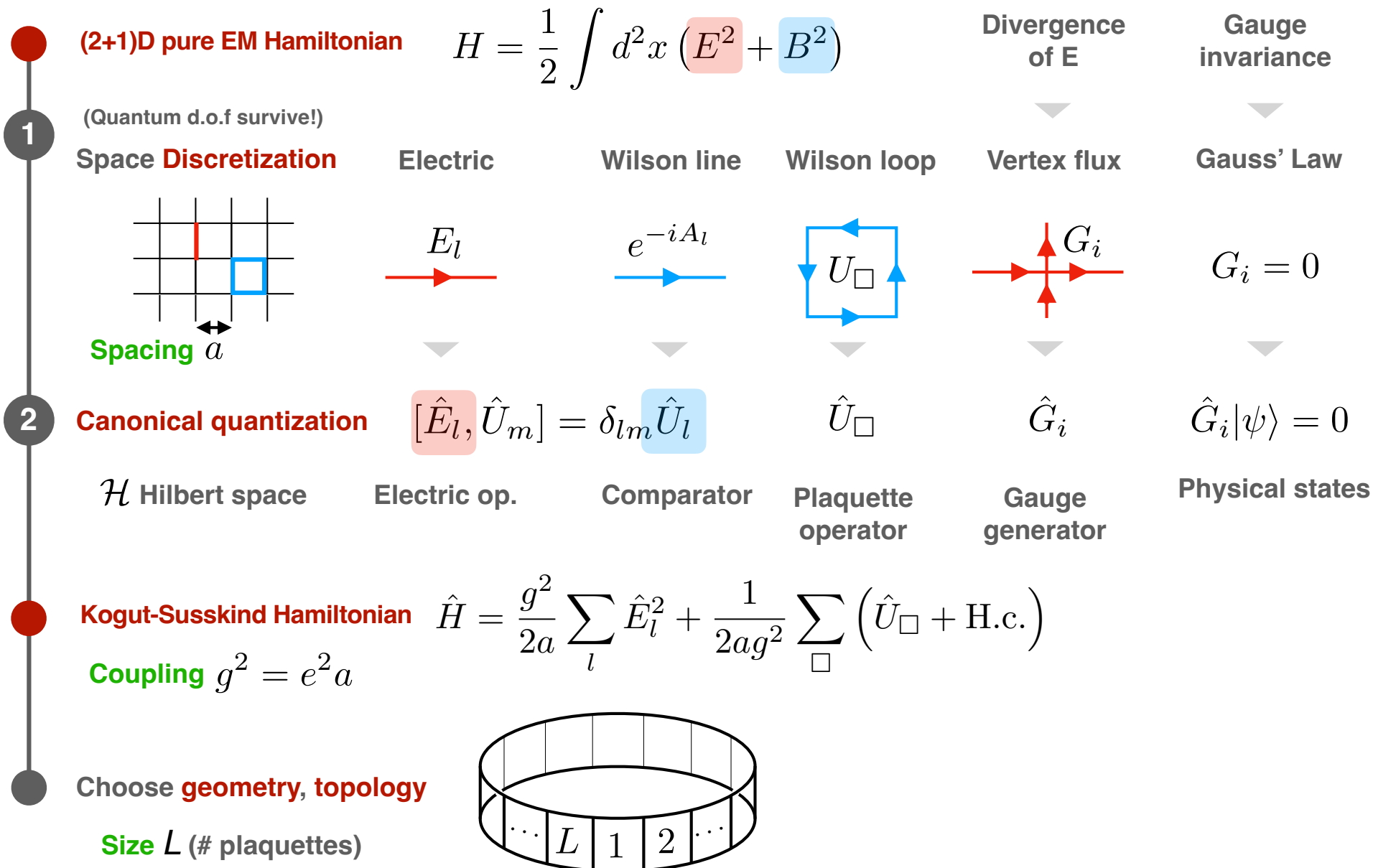


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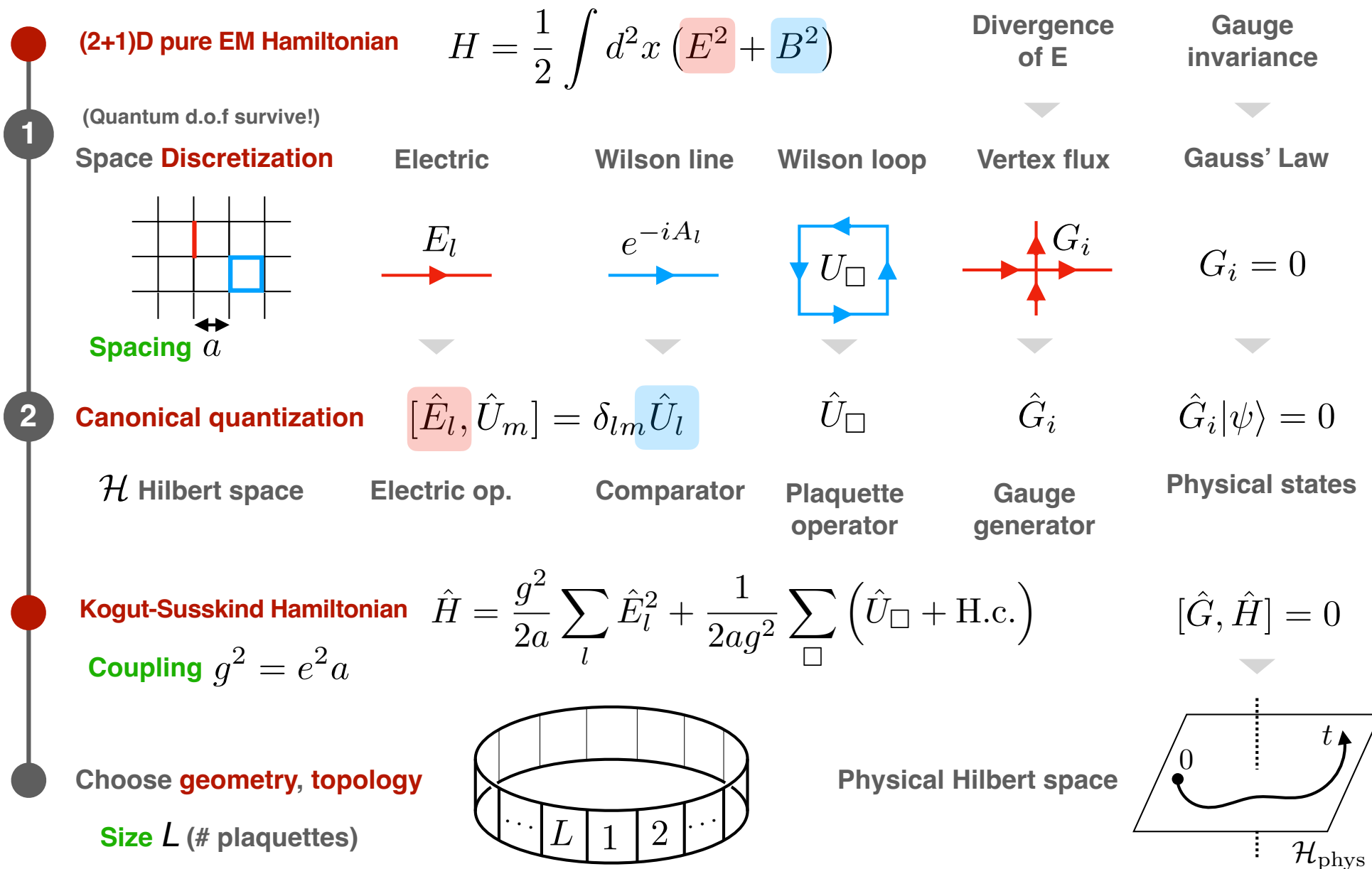


J. Kogut, L. Susskind, Phys. Rev. D (1975) 395-408

# 1. Theoretical background



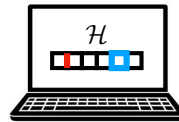
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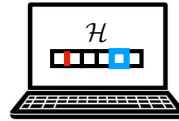
To simulate  $\mathcal{H}$  



We want  $\mathcal{H}$  **finite**-dimensional!

# 1. Theoretical background

To simulate  $\mathcal{H}$  



We want  $\mathcal{H}$  **finite**-dimensional!

**U(1) Lattice QED**

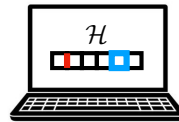


**U(1) Quantum Link Model (QLM)**

U. J. Wiese, Nuc. Phys. B 492 (1997) 455-471

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**U(1) Quantum Link Model (QLM)**

$\forall$  link Hilbert space  $\mathcal{H}_{\text{link}}$

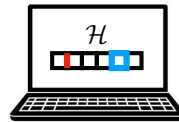


SU(2) irreducible representations  $\mathfrak{s} \in \mathbb{N}/2$



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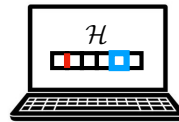


SU(2) irreducible representations  $\mathfrak{s} \in \mathbb{N}/2$

Operators		$\hat{E}$	▶	$\hat{S}^z$
		$\hat{U}$	▶	$\hat{S}^+$
		$\hat{U}^\dagger$	▶	$\hat{S}^-$

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**Operators**  $\left| \begin{array}{l} \hat{E} \\ \hat{U} \\ \hat{U}^\dagger \end{array} \right.$



$\hat{S}^z$



$\hat{S}^+$



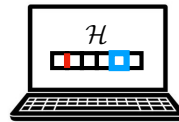
$\hat{S}^-$

Arrow notation

$\longrightarrow$   $s_z = 1/2$   
 $\longrightarrow\longrightarrow$   $s_z = 1$   
 $\longrightarrow\longrightarrow\longrightarrow$   $s_z = 3/2$   
 $\vdots$

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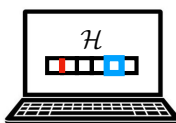
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SU(2) irreducible representations  $s \in \mathbb{N}/2$

<b>Operators</b>	$\hat{E}$	$\hat{S}^z$	$\longrightarrow$	$s_z = 1/2$
	$\hat{U}$	$\hat{S}^+$	Arrow notation $\longrightarrow$	$s_z = 1$
	$\hat{U}^\dagger$	$\hat{S}^-$	$\longrightarrow$	$s_z = 3/2$
			$\vdots$	
	$\sigma(\hat{E})$	$\sigma(\hat{S}^z) = \{-s, \dots, s\}$		<b>finite!</b> ✓

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$\hat{S}^z$   
 $\hat{S}^+$   
 $\hat{S}^-$

Arrow notation  $\begin{array}{l} \longrightarrow s_z = 1/2 \\ \longrightarrow\longrightarrow s_z = 1 \\ \longrightarrow\longrightarrow\longrightarrow s_z = 3/2 \\ \vdots \end{array}$

$\sigma(\hat{E})$

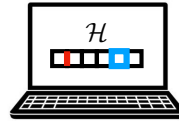
$\sigma(\hat{S}^z) = \{-s, \dots, s\}$  **finite!** ✓

**CCR**  $[\hat{E}, \hat{U}] = \hat{U}$

$[\hat{S}^z, \hat{S}^+] = \hat{S}^+$  ✓

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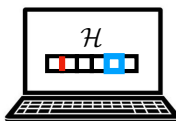
$[\hat{S}^z, \hat{S}^+] = \hat{S}^+$  ✓

**Unitarity**  $\hat{U}\hat{U}^\dagger = \mathbb{I}$

$\hat{S}^+\hat{S}^- \neq \mathbb{I}$  ✗

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Operators  $\left| \begin{array}{l} \hat{E} \\ \hat{U} \\ \hat{U}^\dagger \end{array} \right.$

$\hat{S}^z$

$\hat{S}^+ / s$

$\hat{S}^- / s$

Arrow notation

$\longrightarrow$   $s_z = 1/2$

$\longrightarrow\longrightarrow$   $s_z = 1$

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$\vdots$

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$\sigma(\hat{S}^z) = \{-s, \dots, s\}$  **finite!** ✓

**CCR**  $[\hat{E}, \hat{U}] = \hat{U}$

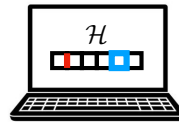
$[\hat{S}^z, \hat{S}^+] = \hat{S}^+$  ✓

**Unitarity**  $\hat{U}\hat{U}^\dagger = \mathbb{I}$

$\hat{S}^+\hat{S}^- / s^2$

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$\hat{S}^z$

$\hat{S}^+ / s$

$\hat{S}^- / s$

Arrow notation

$\longrightarrow$   $s_z = 1/2$

$\longrightarrow\longrightarrow$   $s_z = 1$

$\longrightarrow\longrightarrow\longrightarrow$   $s_z = 3/2$

$\vdots$

$\sigma(\hat{E})$

$\sigma(\hat{S}^z) = \{-s, \dots, s\}$  **finite!** ✓

**CCR**  $[\hat{E}, \hat{U}] = \hat{U}$

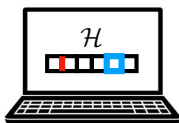
$[\hat{S}^z, \hat{S}^+] = \hat{S}^+$  ✓

**Unitarity**  $\hat{U}\hat{U}^\dagger = \mathbb{I}$

$\hat{S}^+ \hat{S}^- / s^2 \rightarrow \mathbb{I}$  ✓ **Kogut - Susskind limit**  $s \rightarrow \infty$

# 1. Theoretical background

To simulate  $\mathcal{H}$  



We want  $\mathcal{H}$  **finite**-dimensional!

**U(1) Lattice QED**

**U(1) Quantum Link Model (QLM)**

$\forall$  link Hilbert space  $\mathcal{H}_{\text{link}}$

SU(2) irreducible representations  $s \in \mathbb{N}/2$

Operators  $\left\{ \begin{array}{l} \hat{E} \\ \hat{U} \\ \hat{U}^\dagger \end{array} \right.$

$\hat{S}^z$

$\hat{S}^+ / s$

$\hat{S}^- / s$

Arrow notation

$\longrightarrow$   $s_z = 1/2$

$\longrightarrow\longrightarrow$   $s_z = 1$

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$\sigma(\hat{E})$

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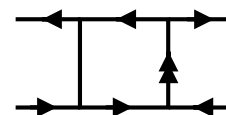
Unitarity  $\hat{U}\hat{U}^\dagger = \mathbb{I}$

$\hat{S}^+ \hat{S}^- / s^2 \rightarrow \mathbb{I}$  ✓

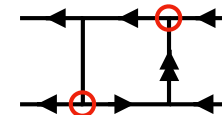
**Kogut - Susskind limit**  $s \rightarrow \infty$

Gauge generator  $\hat{G}$

$\hat{S}_i^z + \hat{S}_k^z - \hat{S}_j^z$



Allowed ✓



Not allowed ✗



## d | 2. The pure Lattice QED on ladder geometry

## 2. The pure Lattice QED on ladder geometry

### Spin representation

Translation and reflection inv.



**Lowest** spin irrep assignments  
which admits gauge inv. configs:

$$\boxed{\frac{1}{2}}_1$$

## 2. The pure Lattice QED on ladder geometry

### Spin representation

Translation and reflection inv.

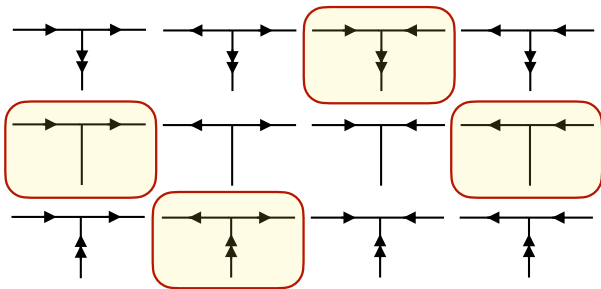


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### Gauss' Law on vertices



## 2. The pure Lattice QED on ladder geometry

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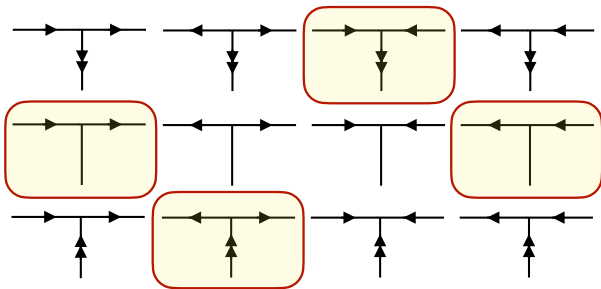
Translation and reflection inv.



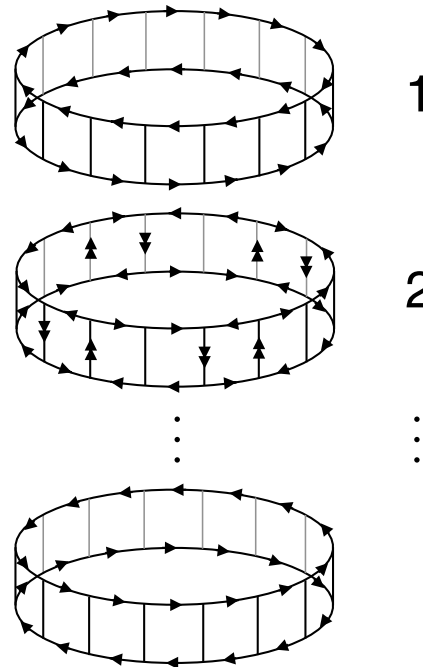
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### $L$ plaquettes ladder in PBC



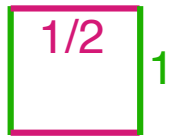
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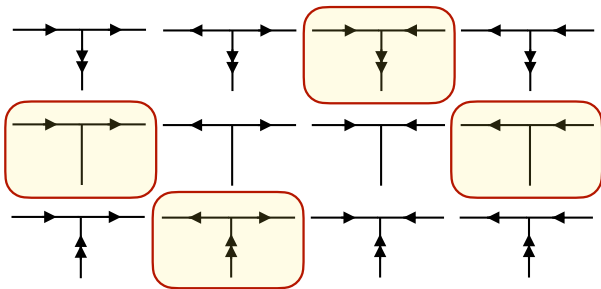
Translation and reflection inv.



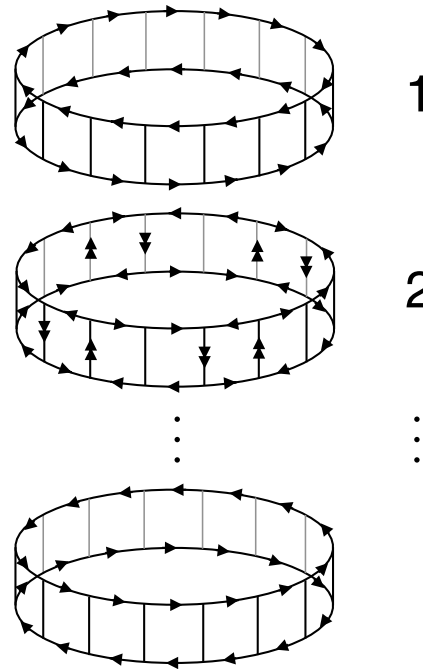
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### Gauss' Law on vertices



### $L$ plaquettes ladder in PBC



$$\dim \mathcal{H} = 2^L + 2$$

↑  
Exp scaling

## 2. The pure Lattice QED on ladder geometry

### Spin representation

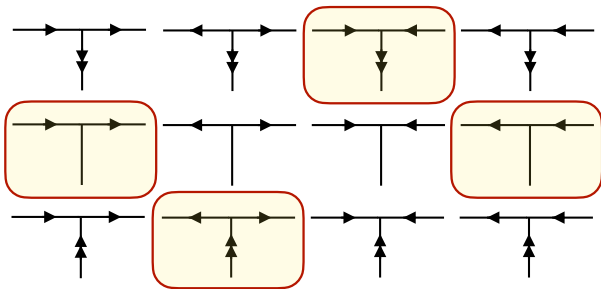
Translation and reflection inv.



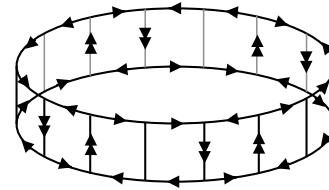
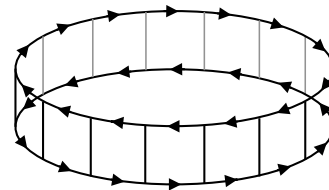
Lowest spin irrep assignments which admits gauge inv. configs:



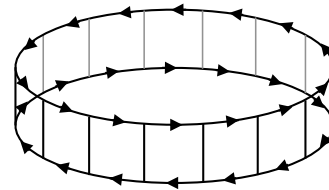
### Gauss' Law on vertices



### $L$ plaquettes ladder in PBC



⋮



1

2

⋮

Computational basis

$$\dim \mathcal{H} = 2^L + 2$$

↑  
Exp scaling

## 2. The pure Lattice QED on ladder geometry

### Spin representation

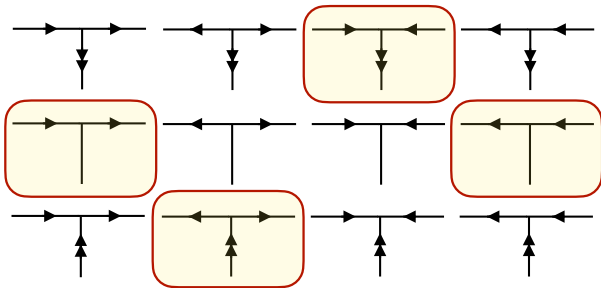
Translation and reflection inv.



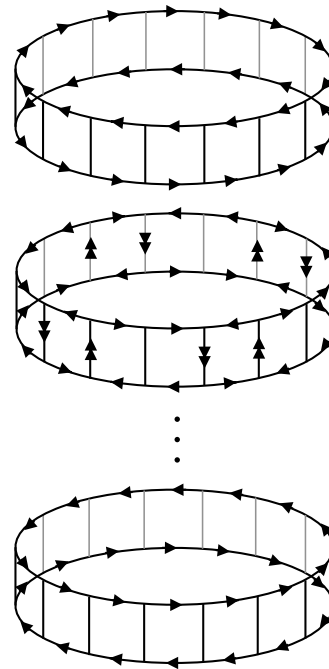
Lowest spin irrep assignments which admits gauge inv. configs:



### Gauss' Law on vertices



### $L$ plaquettes ladder in PBC



1

2

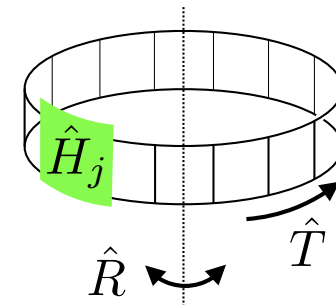
⋮

$$\dim \mathcal{H} = 2^L + 2$$

↑  
Exp scaling

### Construct operators

Computational basis



## 2. The pure Lattice QED on ladder geometry

### Spin representation

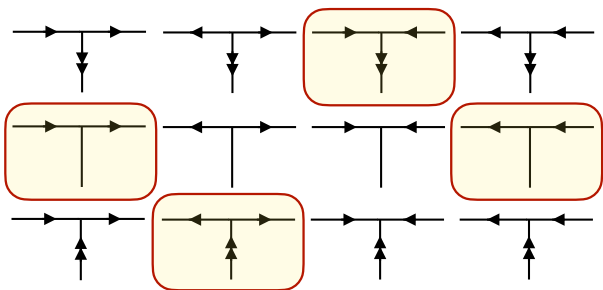
Translation and reflection inv.



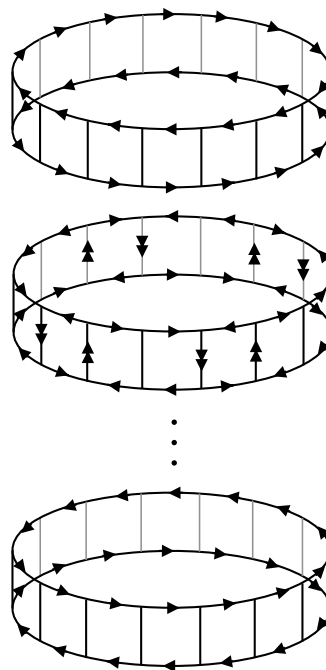
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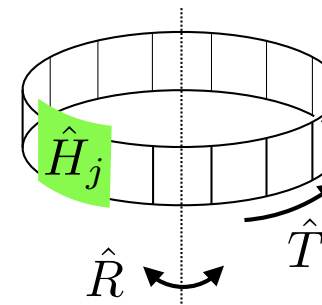


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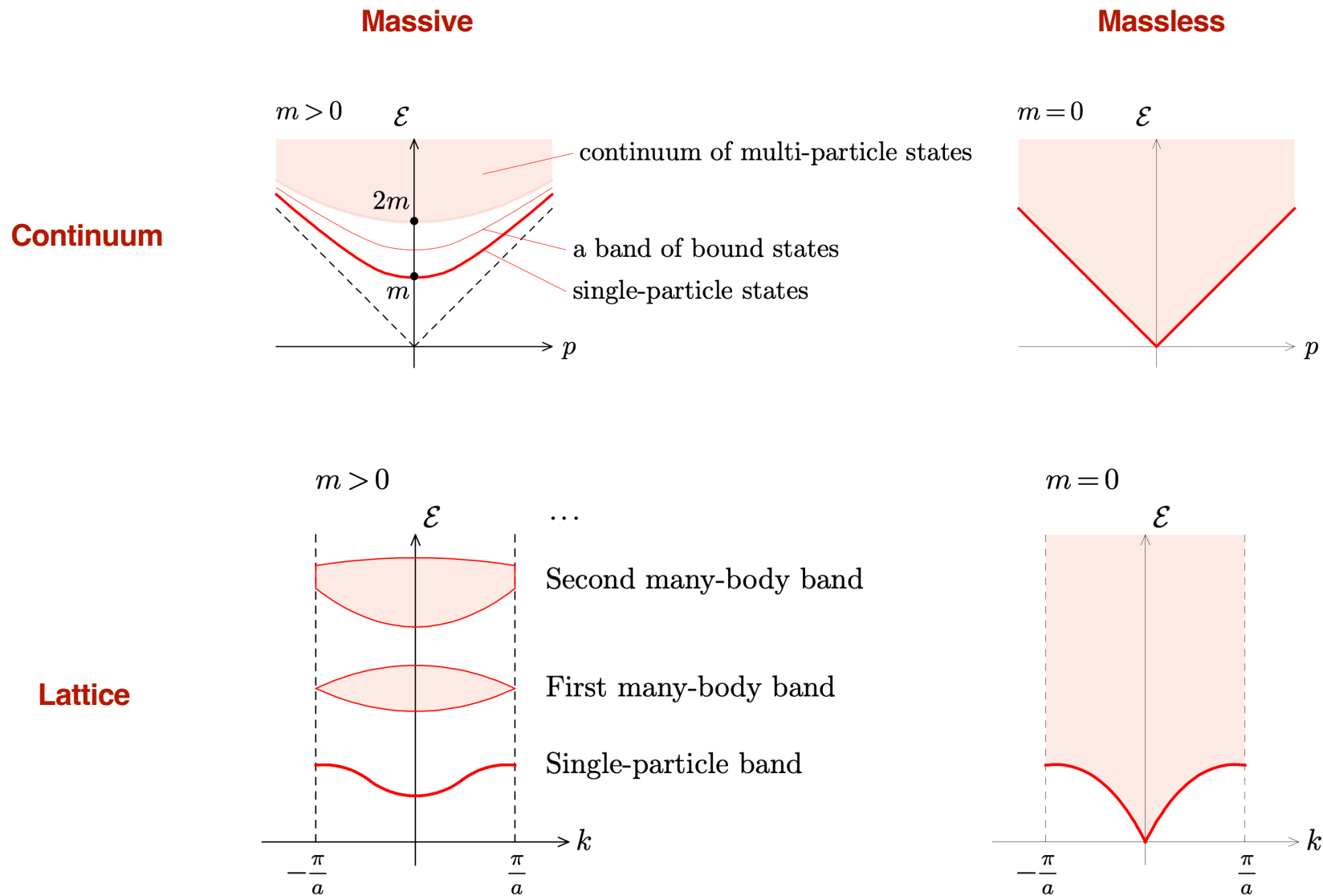


$$[\hat{H}, \hat{T}] = 0$$

**Dispersion relation!**

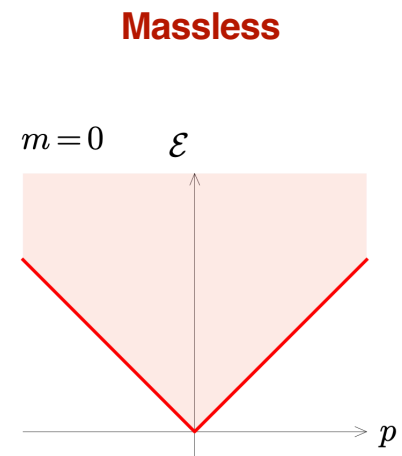
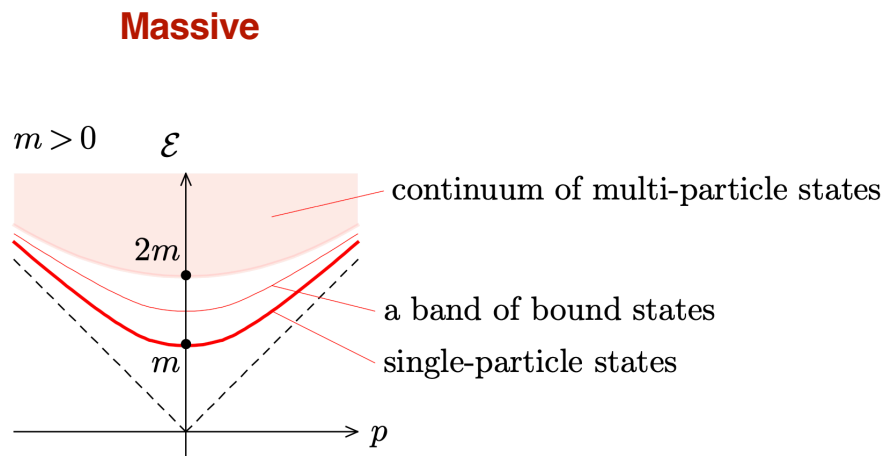


## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$

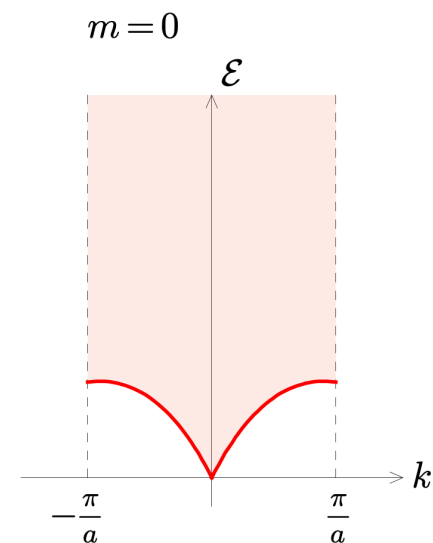
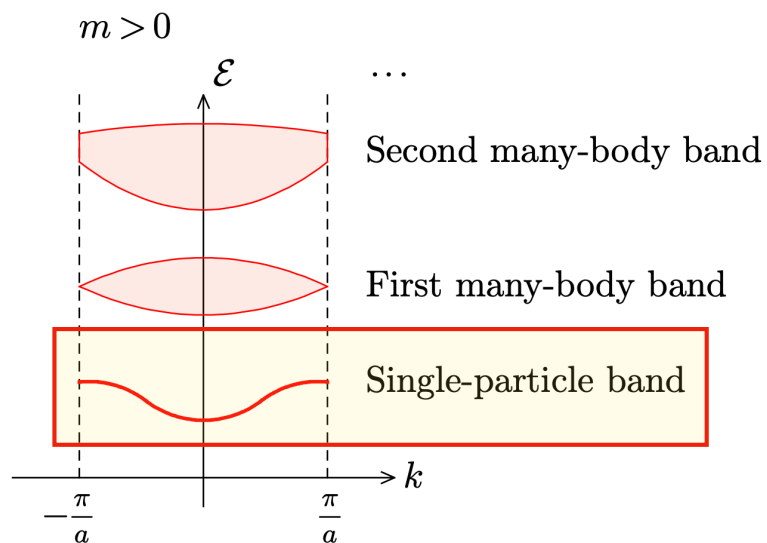


## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$

**Continuum**



**Lattice**



## 2. The pure Lattice QED on ladder geometry<sub>( $\frac{1}{2}, 1$ )</sub>

### Assuming

$[\hat{H}, \hat{T}] = 0$     Translational invar. (PBC)

$L = 13$     Intermediate system size

$\frac{1}{2}$   $\square$   $1$     Lowest spin rep.

$a = 1$     Unit lattice spacing

( varying the coupling  $g$  )

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$$1/2 \quad \square \quad 1 \quad \text{Lowest spin rep.}$$

$$a = 1 \quad \text{Unit lattice spacing}$$

( varying the coupling  $g$  )



**Simultaneous *exact* diagonalization  
(computationally difficult step)**

$$\dim \mathcal{H} = 8194$$

## 2. The pure Lattice QED on ladder geometry<sub>( $\frac{1}{2}, 1$ )</sub>

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**Simultaneous *exact* diagonalization**  
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**Dispersion relation**  
in our (interacting!) model:

## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$

**Assuming**

$[\hat{H}, \hat{T}] = 0$  Translational invar. (PBC)

$L = 13$  Intermediate system size

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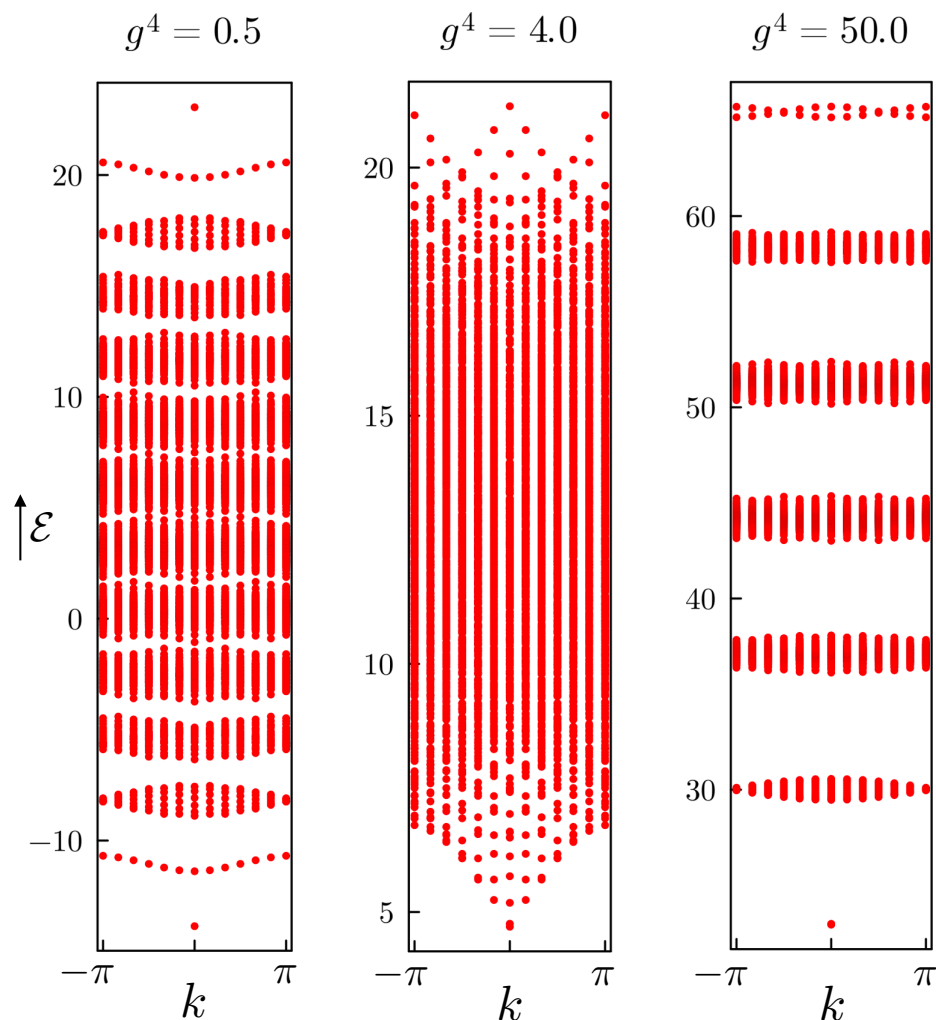
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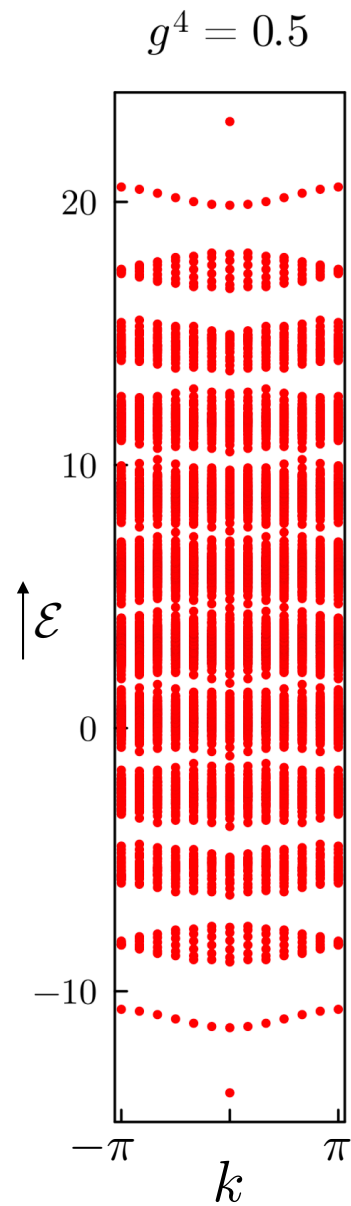


Gapped phase  
(massive photon)

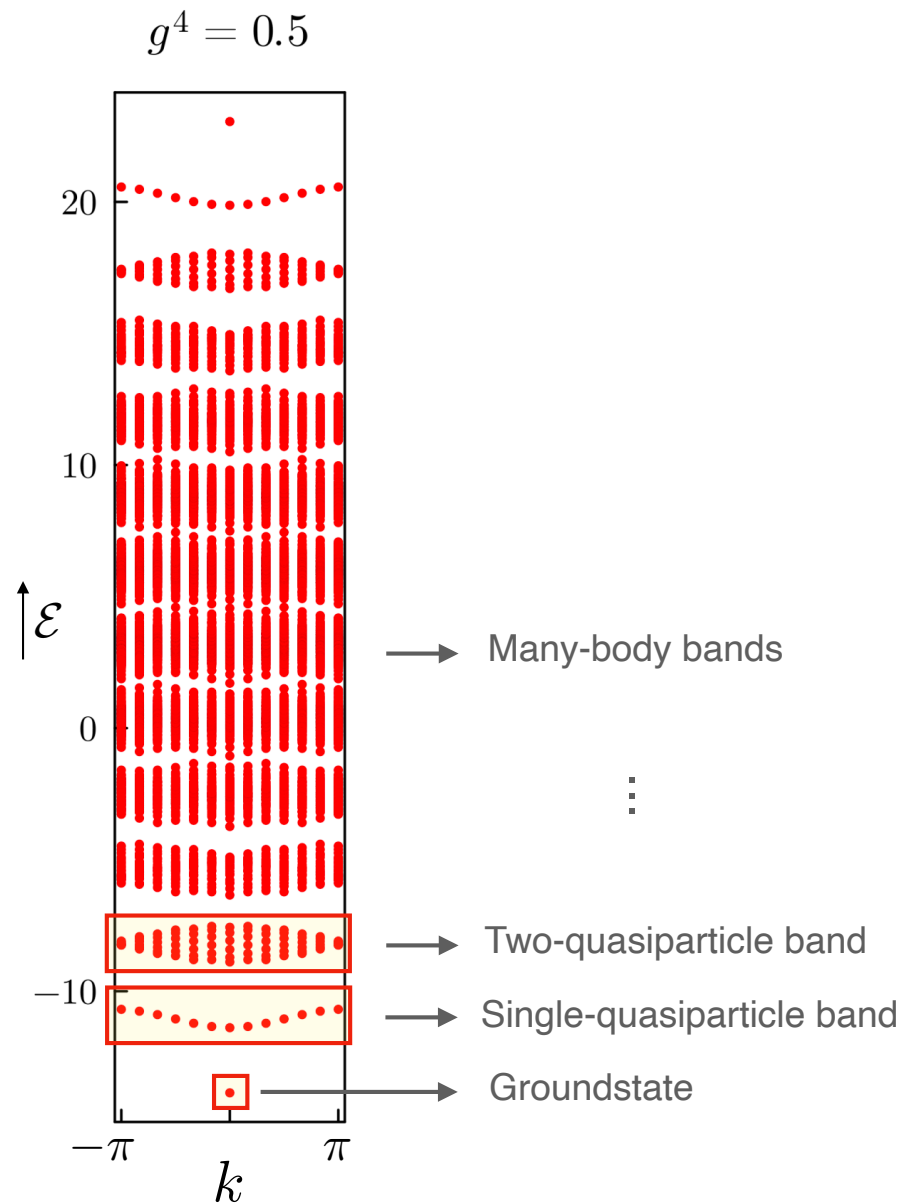
Critical point  
(massless photon)

Gapped SSB phase  
(degenerate g.s.)

## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$

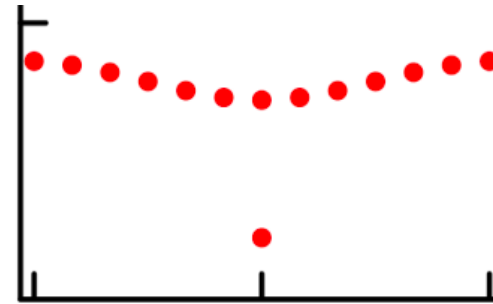
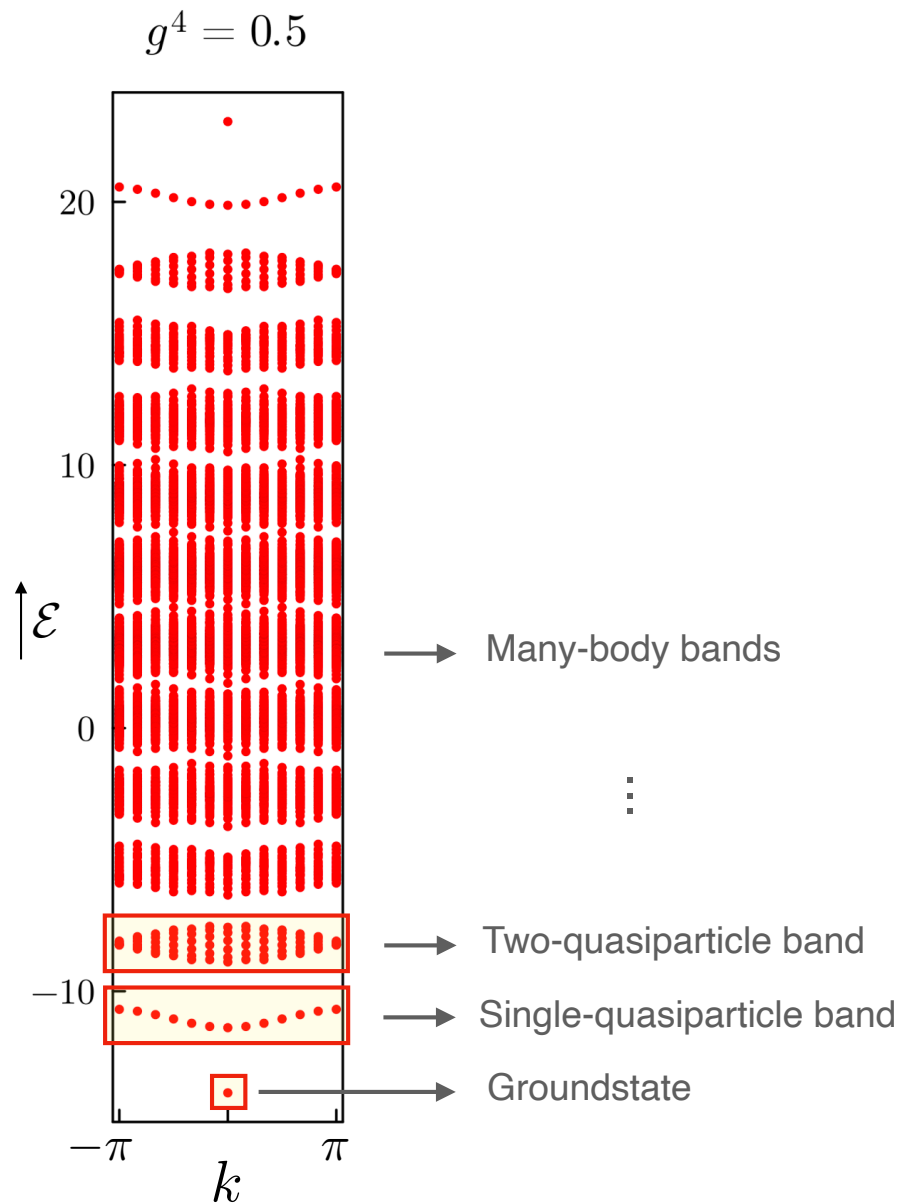


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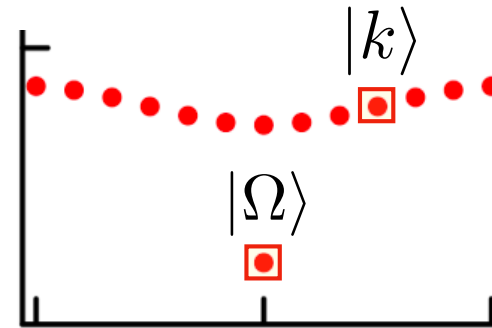
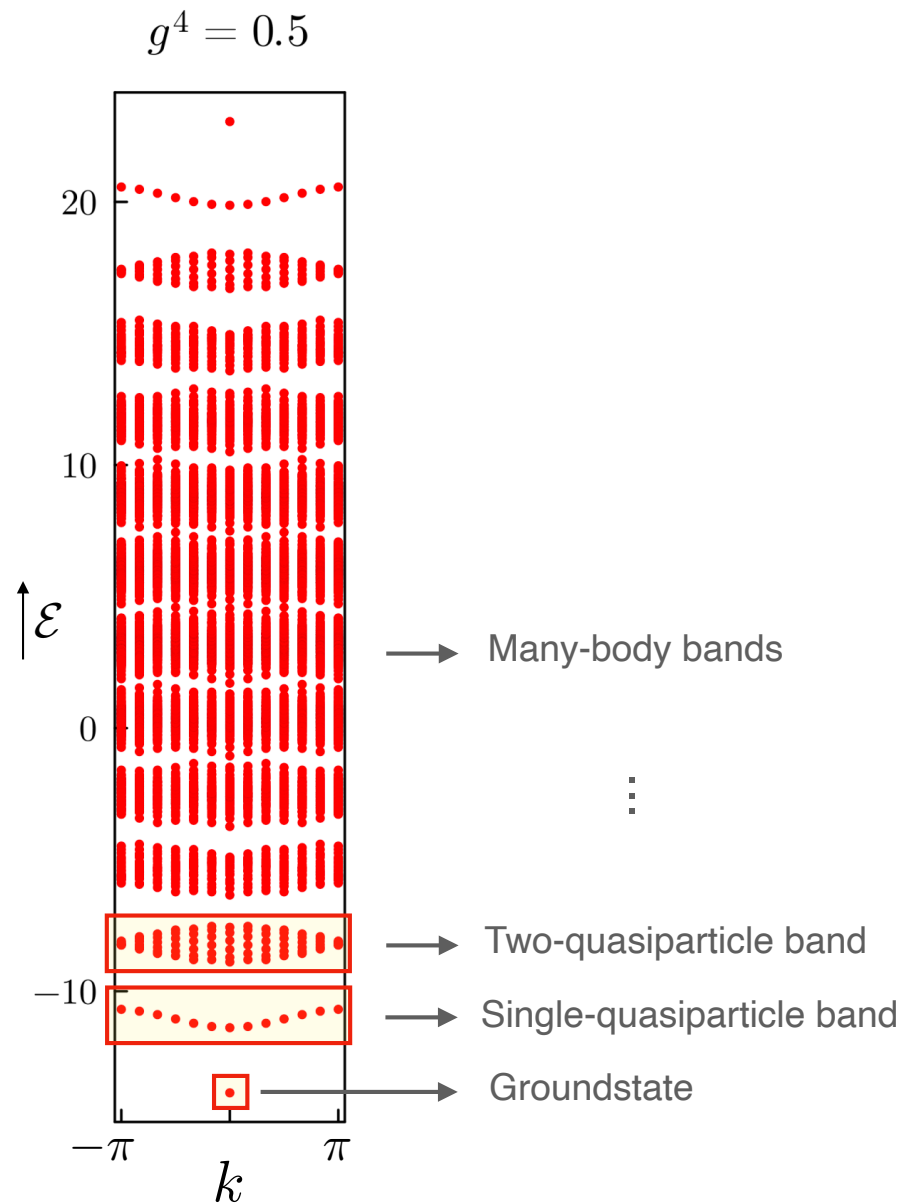




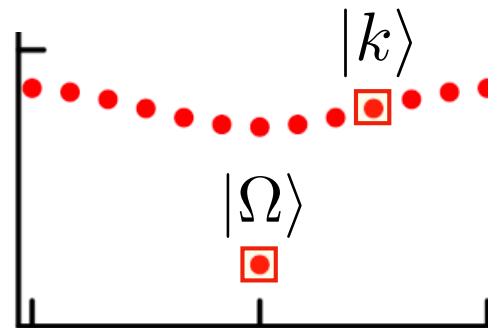
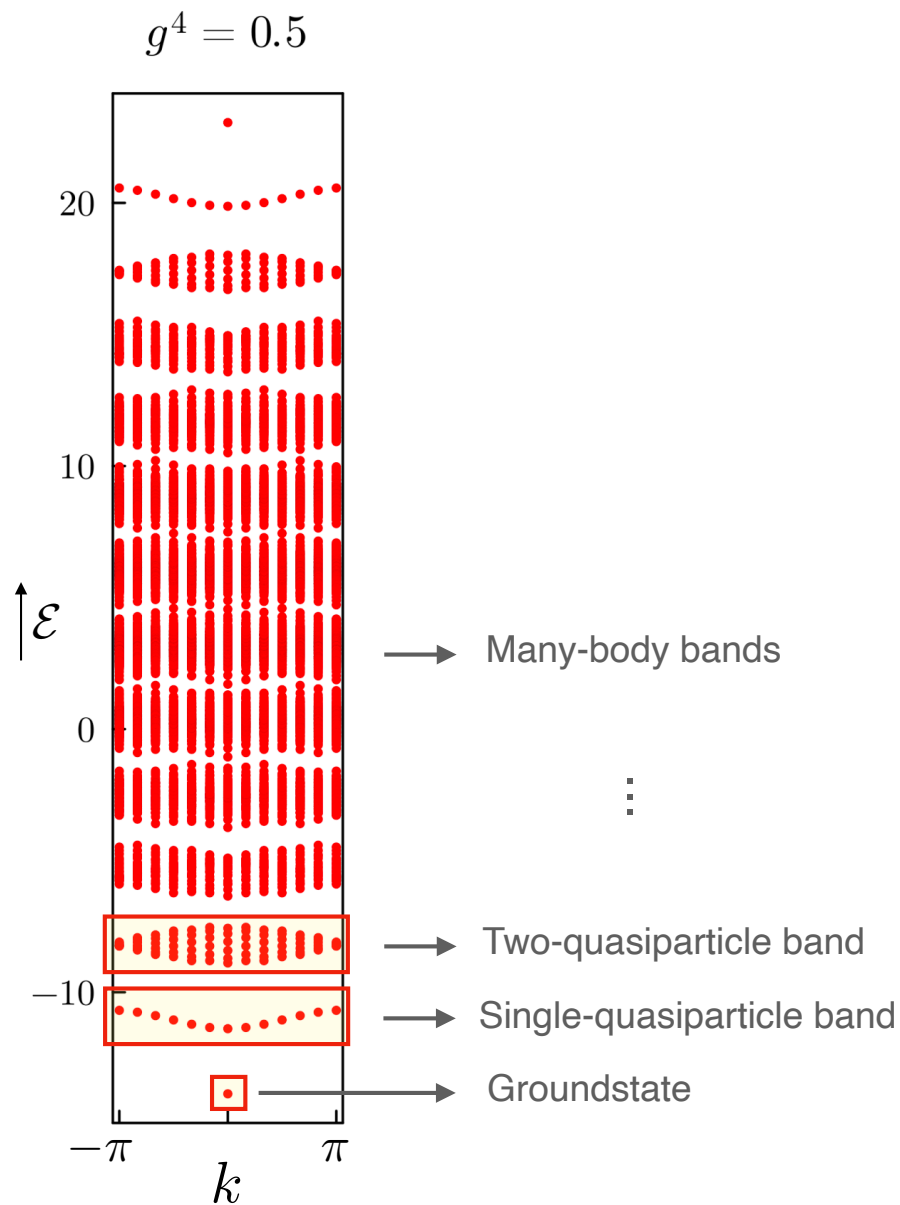
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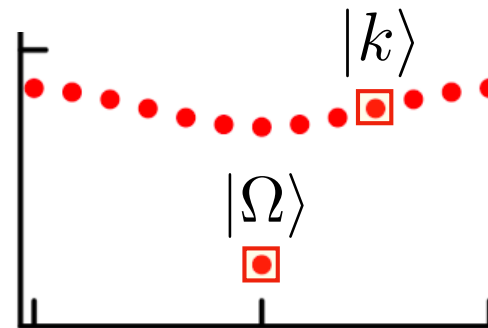
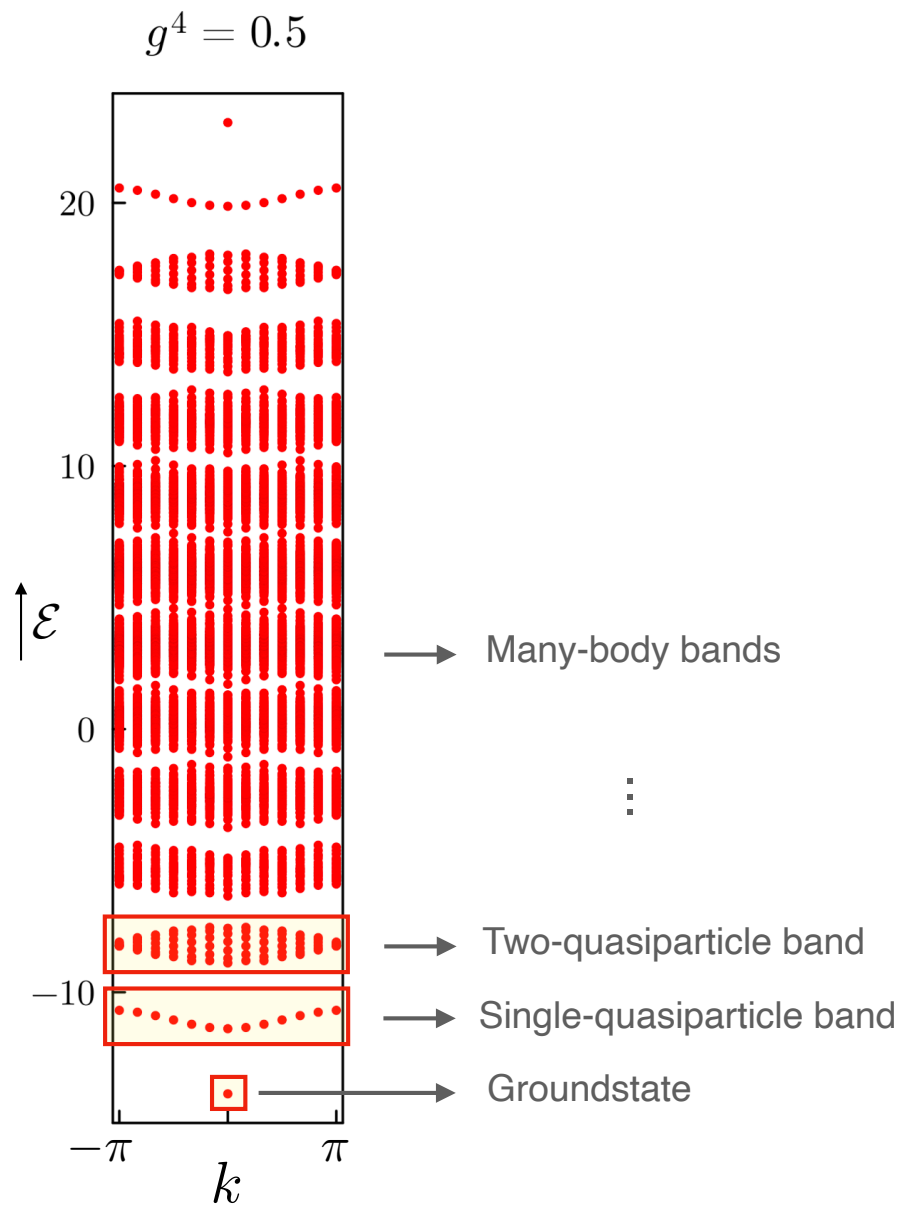
## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$



$$|\phi\rangle = \sum a_k |k\rangle$$

Single-particle state  
(Bloch basis)

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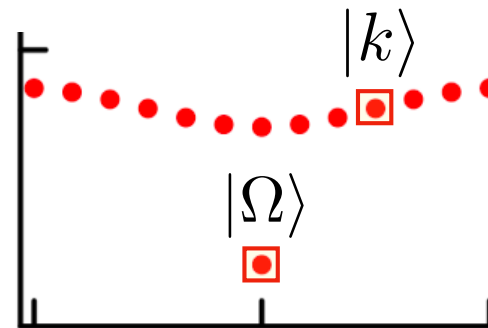
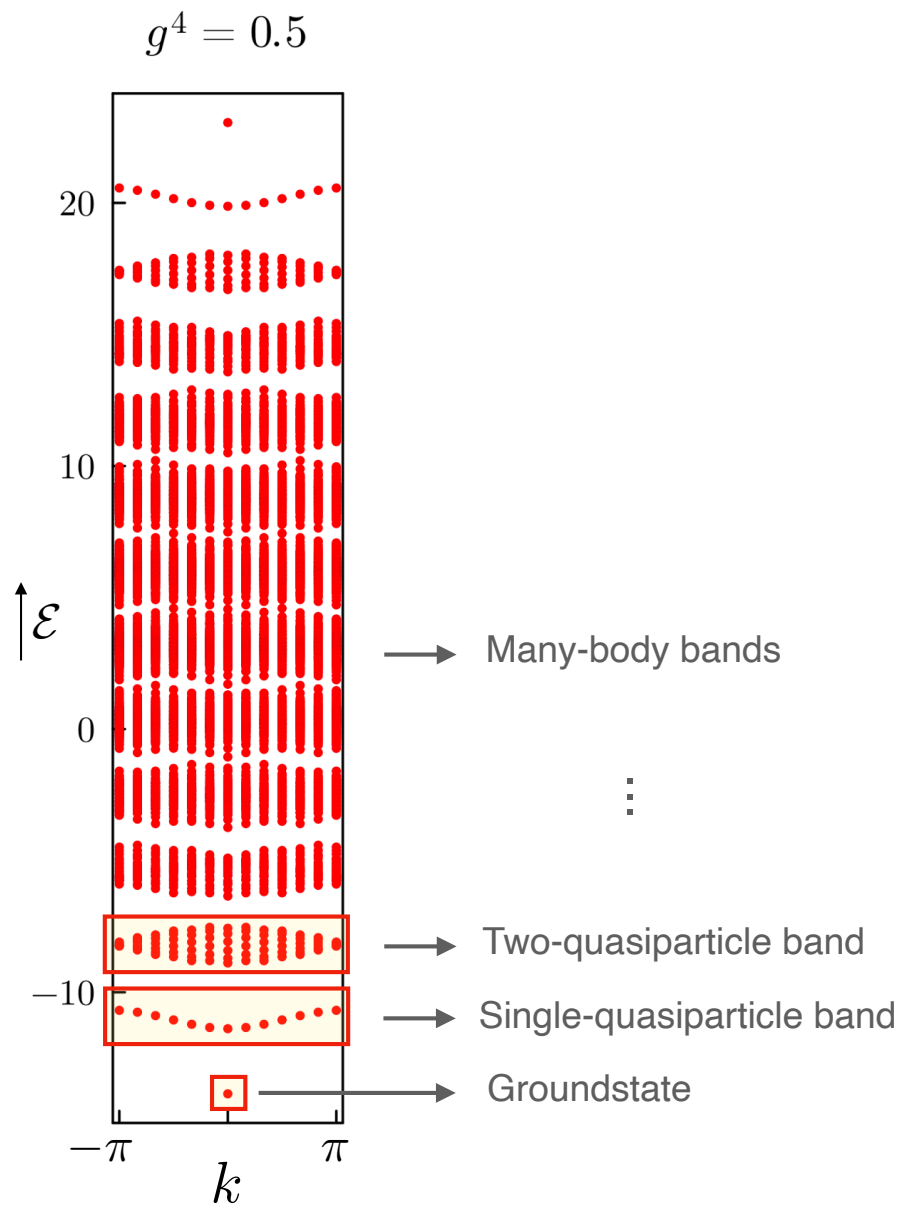


$$|\phi\rangle = \sum a_k |k\rangle$$

Single-particle state  
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Wannier Functions  
(real-space basis)

## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$



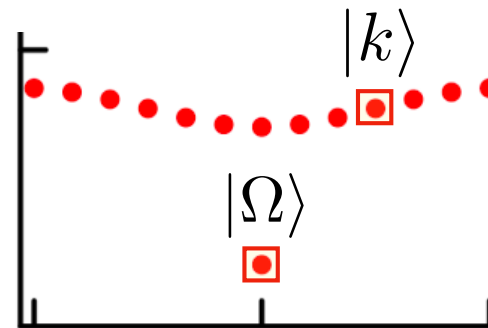
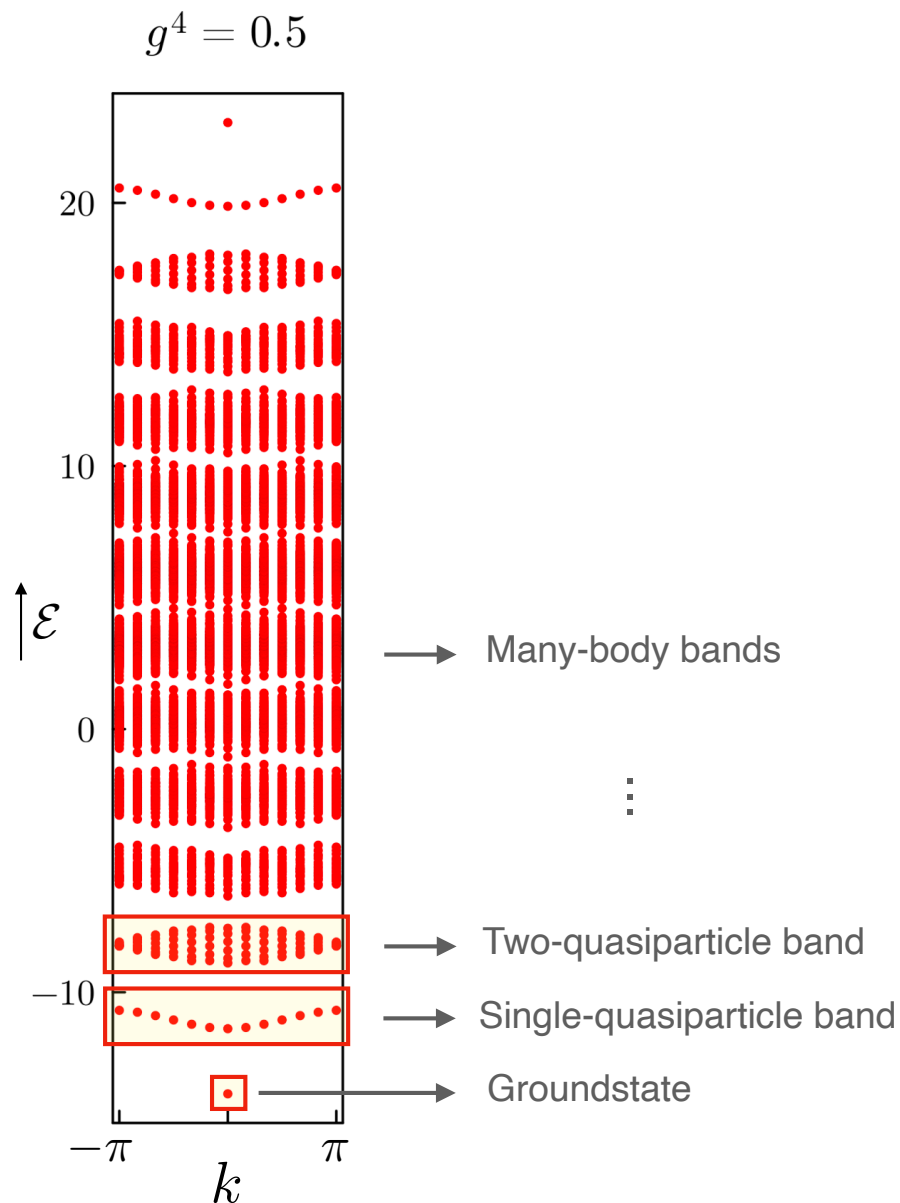
$$|\phi\rangle = \sum a_k |k\rangle$$

Single-particle state  
(Bloch basis)

Wannier Functions  
(real-space basis)

Wave-packet state

## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$



Program

$$|\phi\rangle = \sum a_k |k\rangle$$

Single-particle state  
(Bloch basis)

Wannier Functions  
(real-space basis)

Wave-packet state

### 3. Construction of the wavepackets

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**Wannier states**

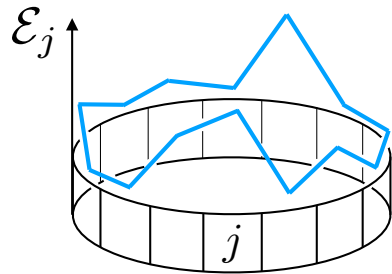
$$|W(\theta_k)\rangle = \frac{1}{\sqrt{L}} \sum_k e^{i\theta_k} |k\rangle$$



### 3. Construction of the wavepackets

#### Wannier states

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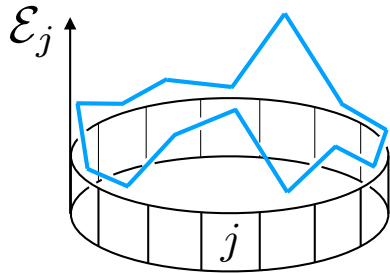
#### Energy density

$$\mathcal{E}_j[\phi] = \langle \phi | \hat{H}_j | \phi \rangle$$

### 3. Construction of the wavepackets

#### Wannier states

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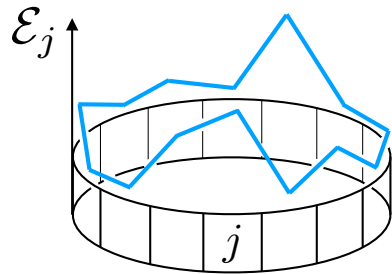
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$$\sigma^2[\phi] \equiv \frac{\sum_j j^2 \mathcal{E}_j[\phi]}{\sum_j \mathcal{E}_j[\phi]} - \left( \frac{\sum_j j \mathcal{E}_j[\phi]}{\sum_j \mathcal{E}_j[\phi]} \right)^2$$

### 3. Construction of the wavepackets

#### Wannier states

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$\theta \rightarrow \bar{\theta}$   
Minimize  $\sigma^2$

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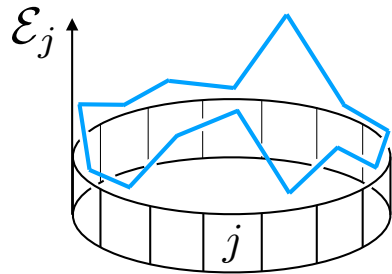
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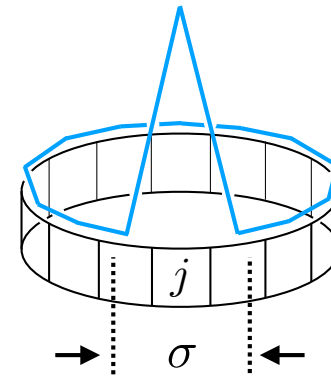
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Minimize  $\sigma^2$

#### Maximally localized Wannier states

$$|W_j\rangle \equiv |W_j(\bar{\theta})\rangle$$



#### Energy density

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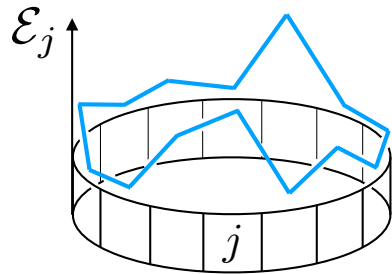
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# 3. Construction of the wavepackets

## Wannier states

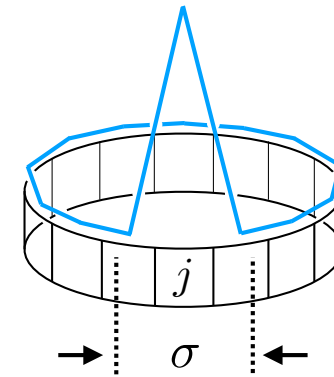
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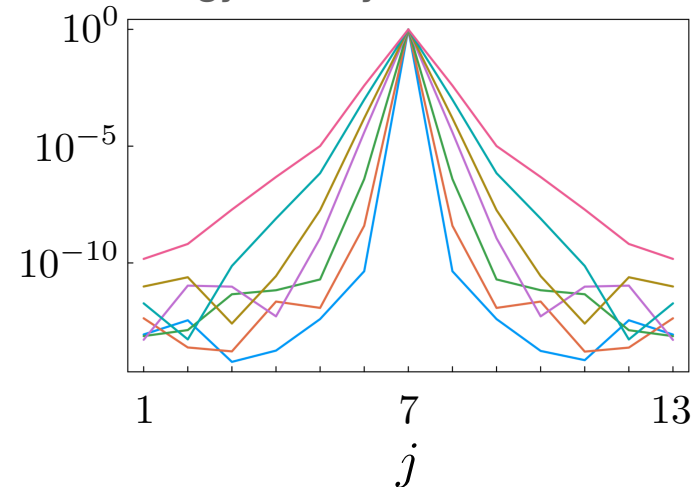
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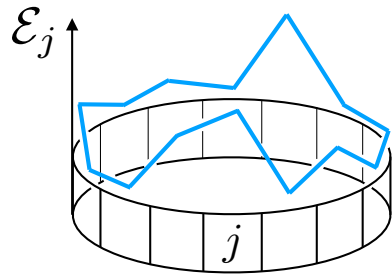
## Energy density after minimization



# 3. Construction of the wavepackets

## Wannier states

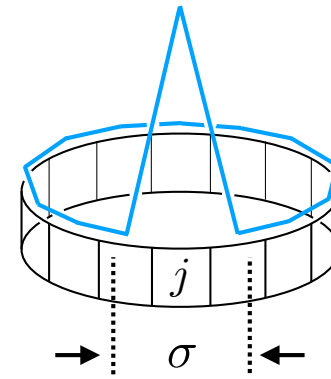
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Minimize  $\sigma^2$



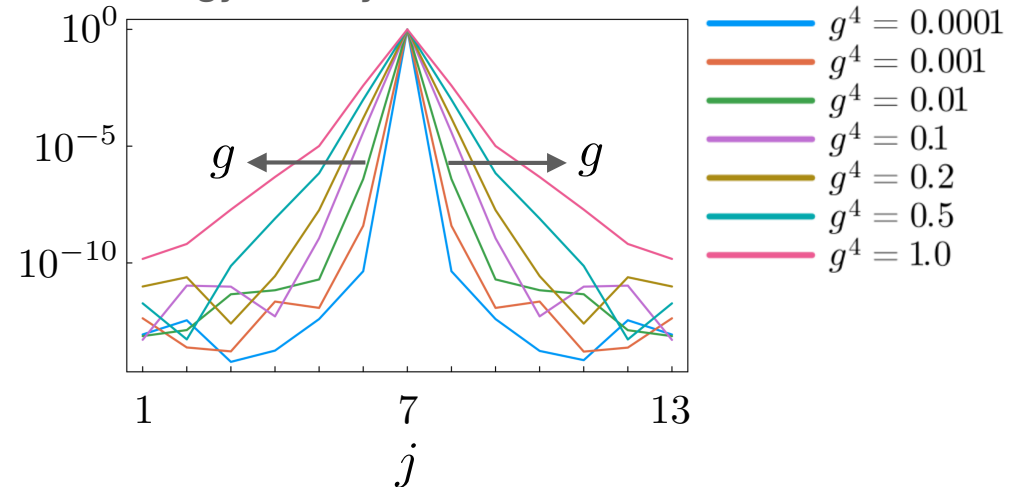
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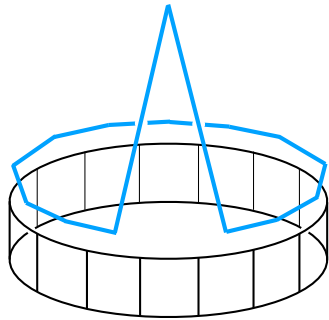
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## Energy density after minimization



### 3. Construction of the wavepackets

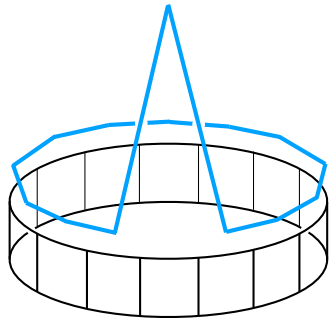
Wannier creation  
operator



$$\hat{W}|\Omega\rangle = |W\rangle$$

### 3. Construction of the wavepackets

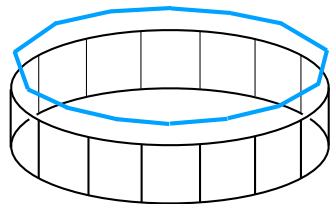
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||

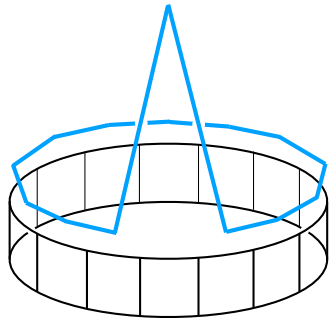
$|\Omega\rangle$  Interacting!





### 3. Construction of the wavepackets

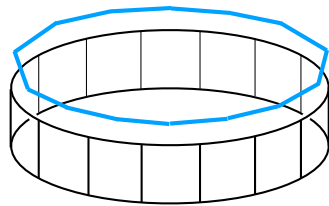
Wannier creation operator



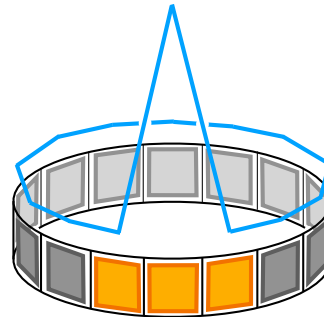
$$\hat{W}|\Omega\rangle = |W\rangle$$

||

$|\Omega\rangle$  **Interacting!**

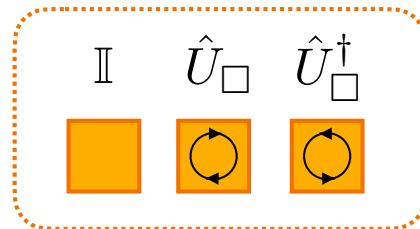


Wannier creation ansatz



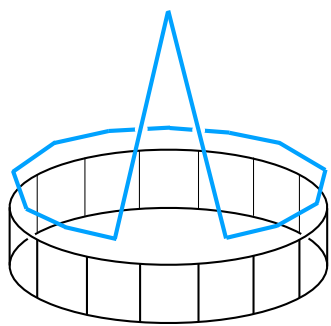
$\longleftrightarrow W \longrightarrow$

choose  $L_\alpha$



### 3. Construction of the wavepackets

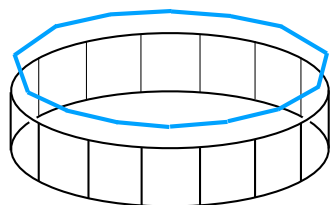
Wannier creation operator



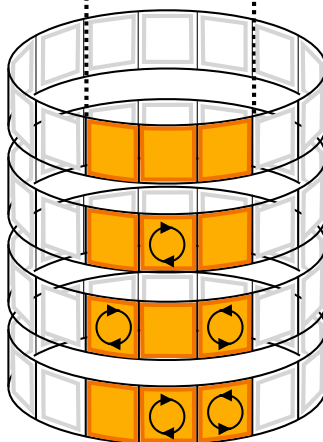
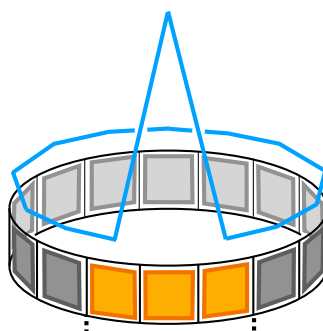
$$\hat{W}|\Omega\rangle = |W\rangle$$

||

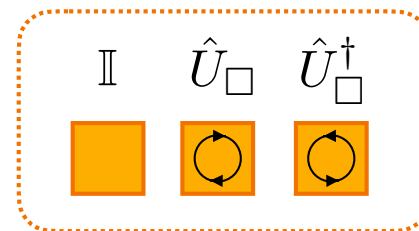
$|\Omega\rangle$  Interacting!



Wannier creation ansatz



choose  $L_\alpha$

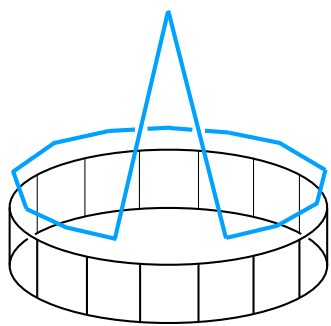


$$\begin{aligned}
 & c_1 \mathbb{I} \\
 & + c_2 \hat{U}_{\square,2}^\dagger \\
 & + c_3 \hat{U}_{\square,1}^\dagger \hat{U}_{\square,3} \\
 & + c_3 \hat{U}_{\square,2}^\dagger \hat{U}_{\square,3}
 \end{aligned}$$

$$= \sum_{\alpha_1 \dots \alpha_w} c_{\alpha_1 \dots \alpha_w} L_{\alpha_1} \dots L_{\alpha_w}$$

### 3. Construction of the wavepackets

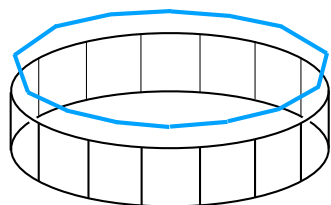
Wannier creation operator



$$\hat{W}|\Omega\rangle = |W\rangle$$

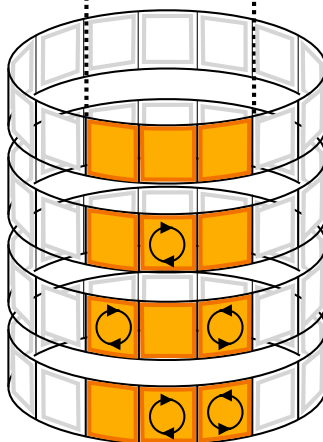
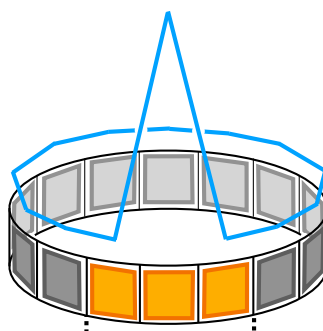
||

$|\Omega\rangle$  Interacting!



$$\hat{W} = \sum_{\alpha_1 \dots \alpha_w} c_{\alpha_1 \dots \alpha_w} L_{\alpha_1} \dots L_{\alpha_w}$$

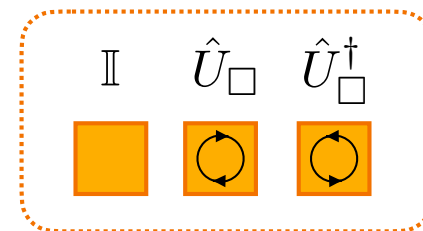
Wannier creation ansatz



$$\begin{aligned} & c_1 \mathbb{I} \\ & + c_2 \hat{U}_{\square,2}^\dagger \\ & + c_3 \hat{U}_{\square,1}^\dagger \hat{U}_{\square,3} \\ & + c_3 \hat{U}_{\square,2}^\dagger \hat{U}_{\square,3} \end{aligned}$$

Interpolation

choose  $L_\alpha$

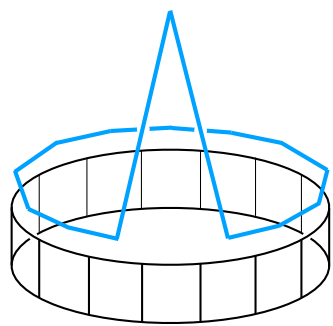


Minimize

$$\left| \hat{W}(\mathbf{c})|\Omega\rangle - |W\rangle \right|^2$$

### 3. Construction of the wavepackets

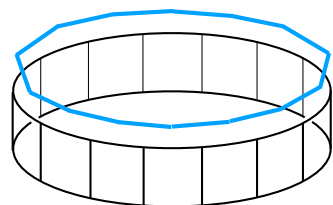
Wannier creation operator



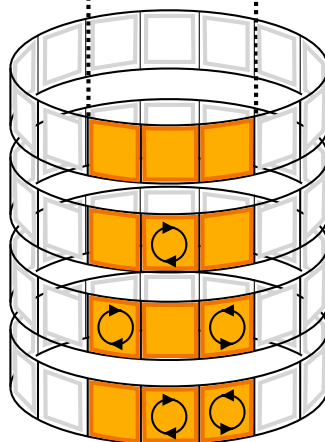
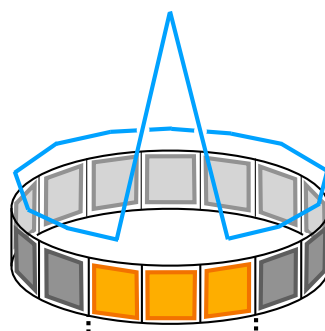
$$\hat{W}|\Omega\rangle = |W\rangle$$

||

$|\Omega\rangle$  Interacting!



Wannier creation ansatz

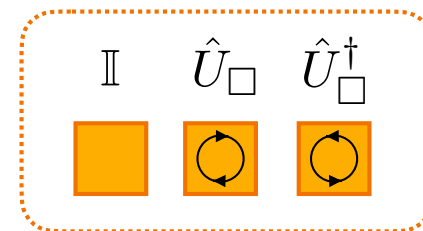


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$$\hat{W} = \sum_{\alpha_1 \dots \alpha_w} c_{\alpha_1 \dots \alpha_w} L_{\alpha_1} \dots L_{\alpha_w}$$

Interpolation

choose  $L_\alpha$



Minimize

$$\left| \hat{W}(c)|\Omega\rangle - |W\rangle \right|^2$$

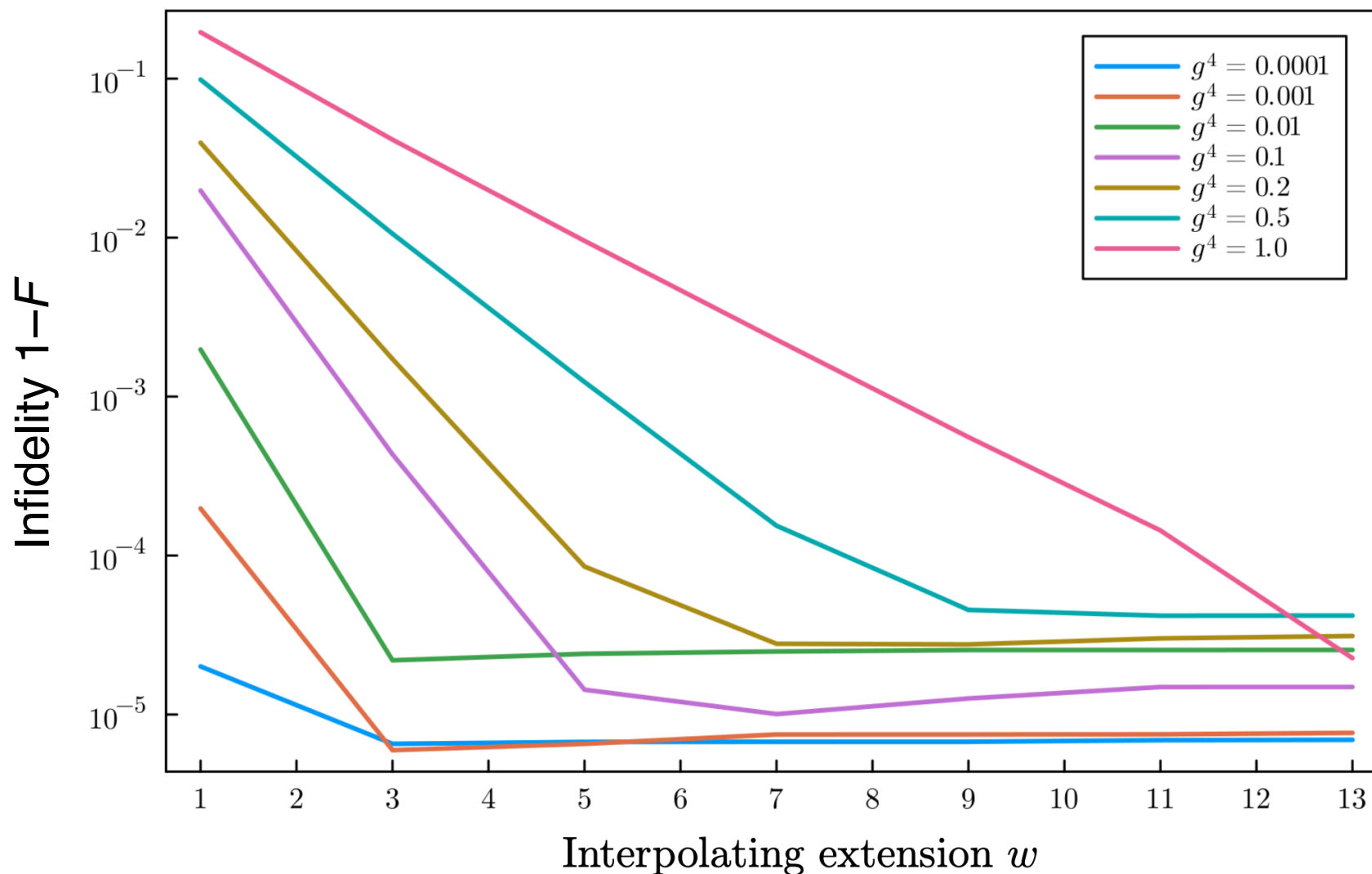


Linear system

$$Ac = b$$

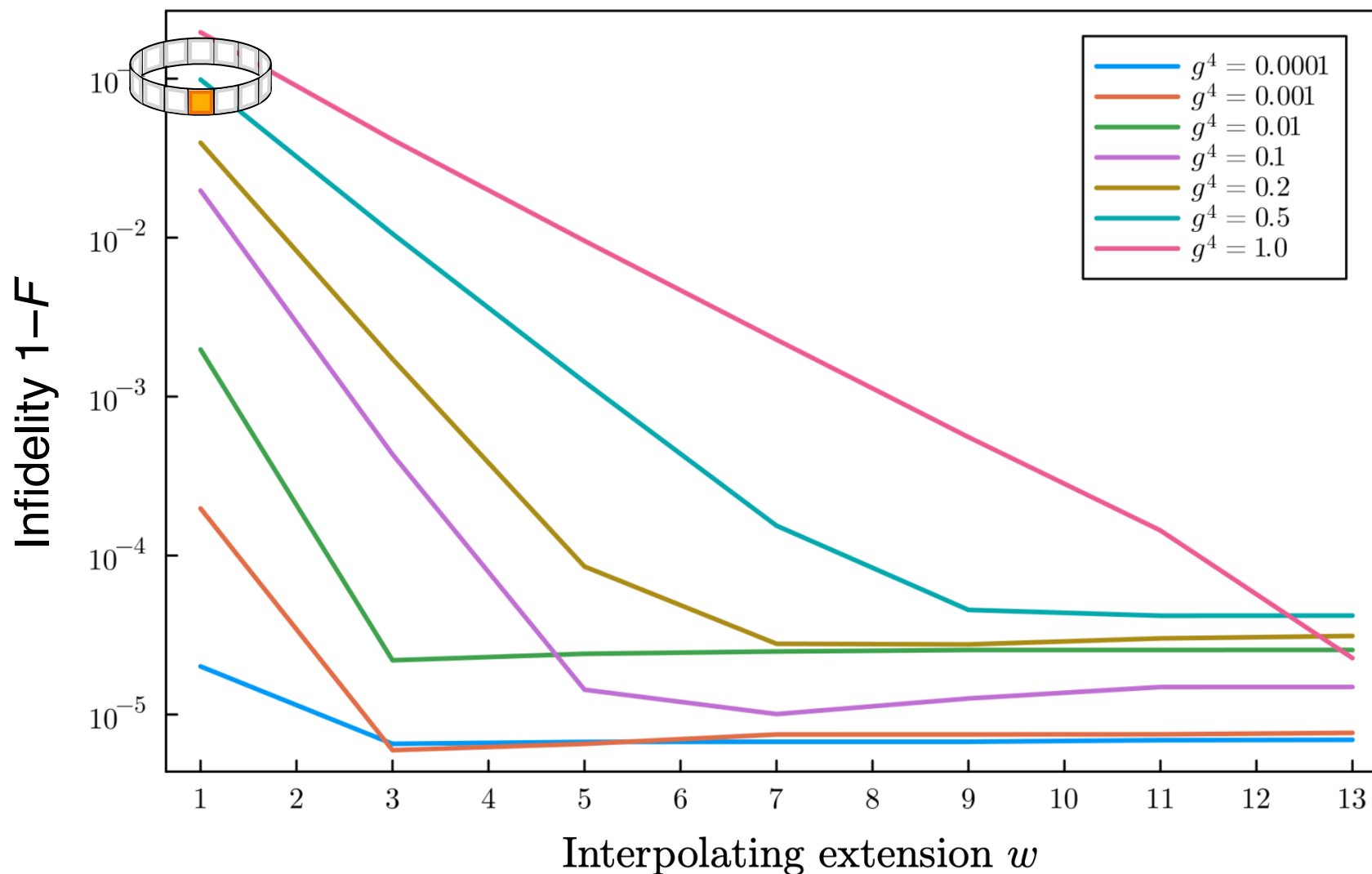
### 3. Construction of the wavepackets

Infidelity of the interpolation of the Wannier state  $|W_7\rangle$ ,  $L = 13$



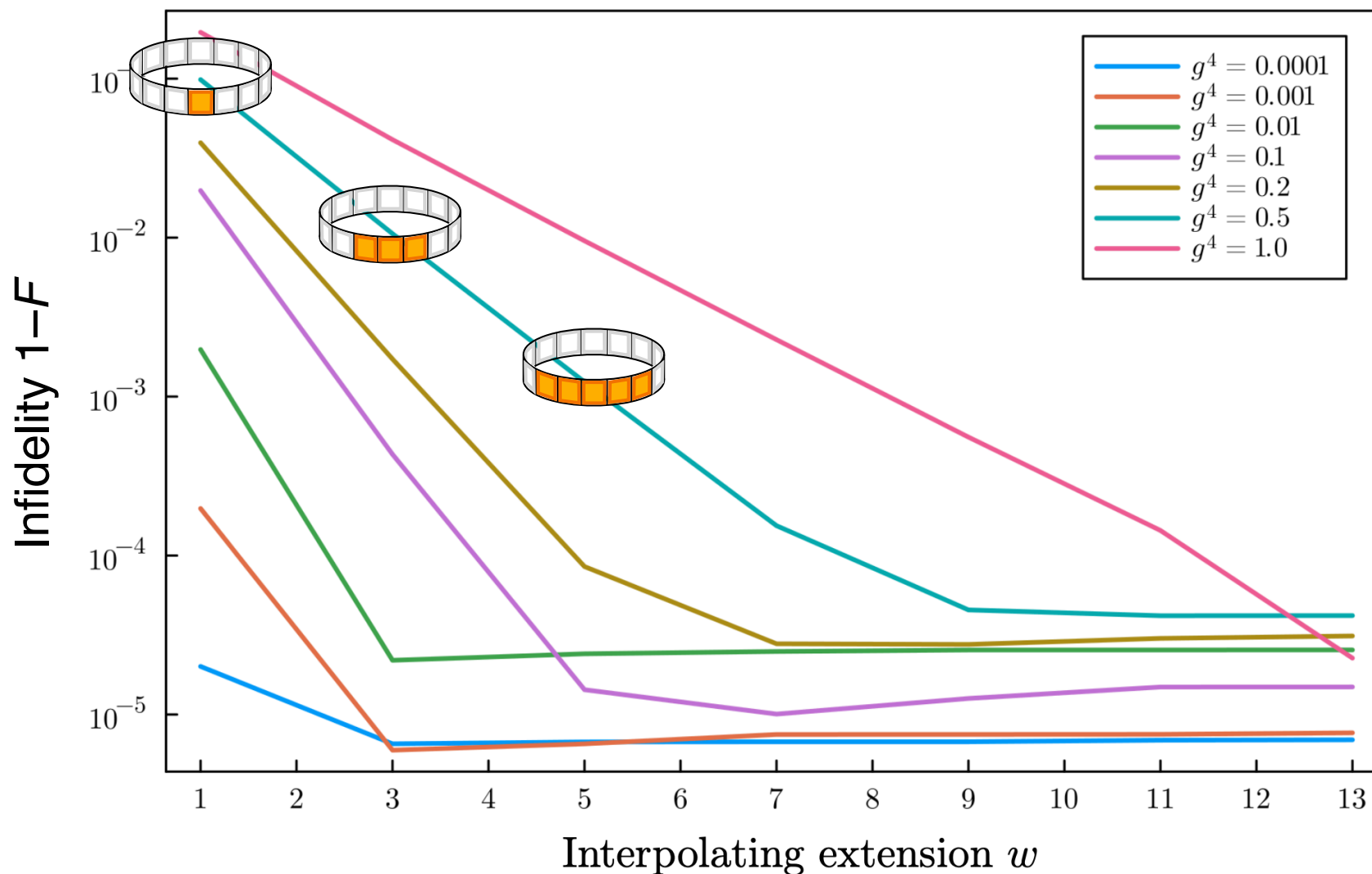
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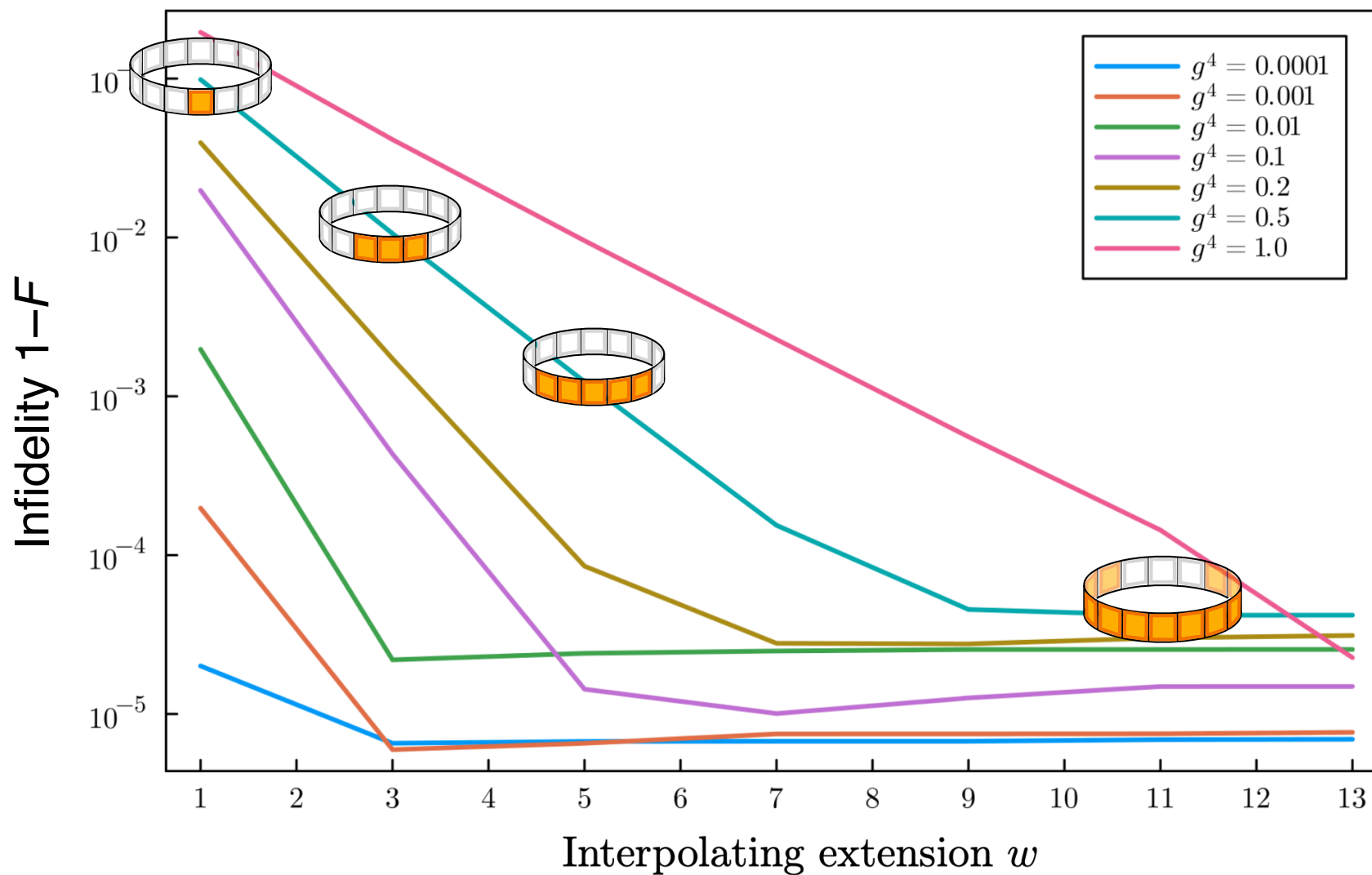
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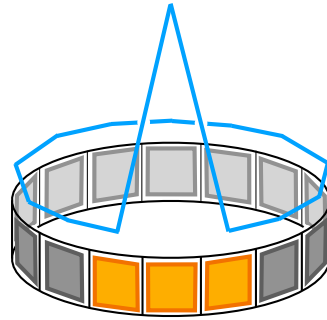
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Infidelity of the interpolation of the Wannier state  $|W_7\rangle$ ,  $L = 13$



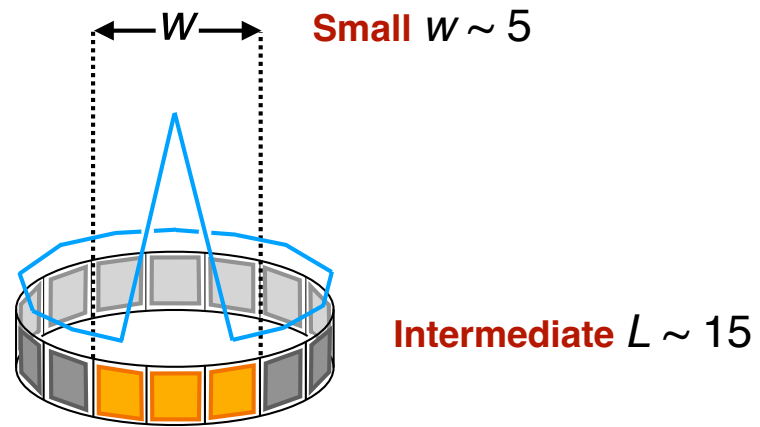


### 3. Construction of the wavepackets

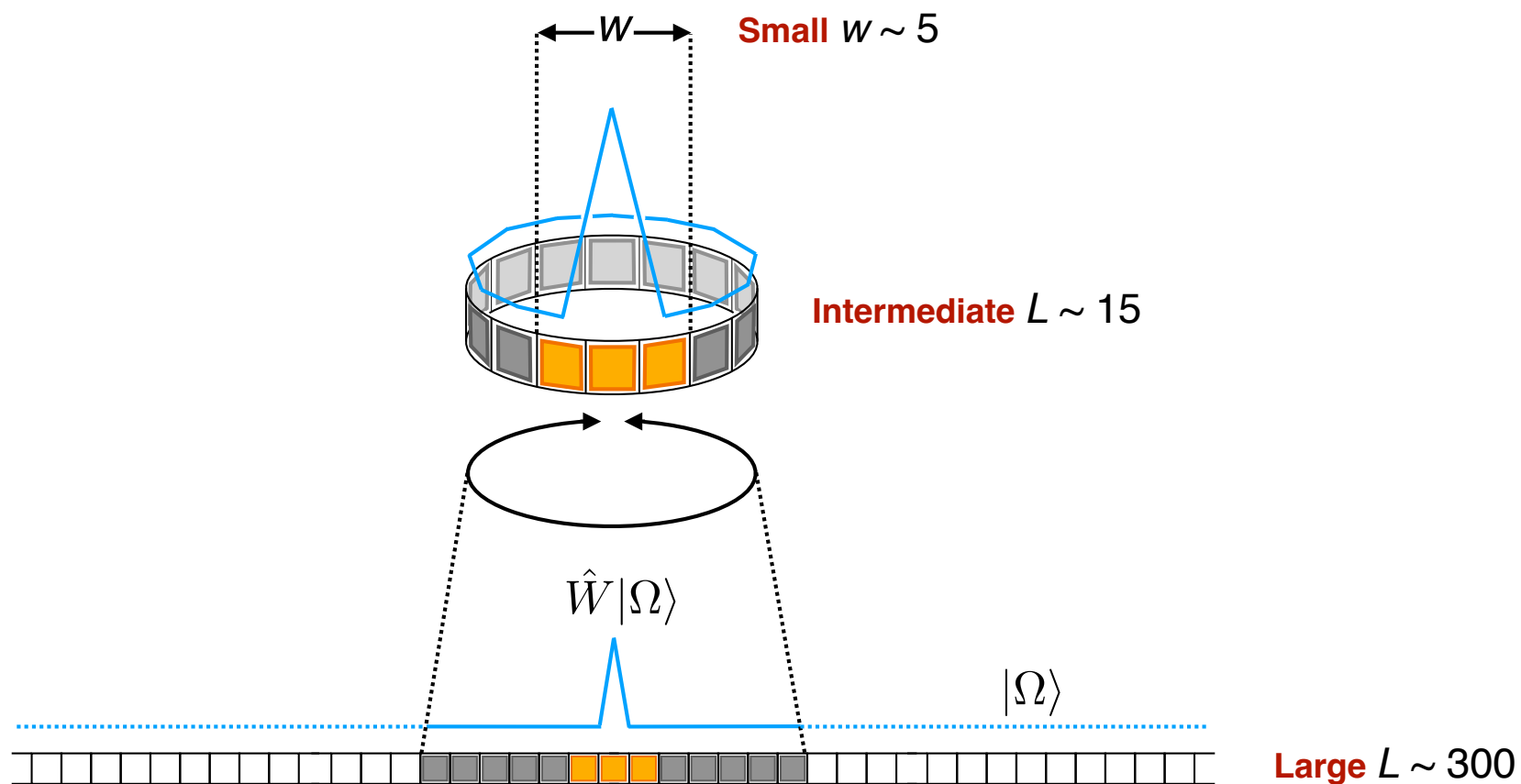


Intermediate  $L \sim 15$

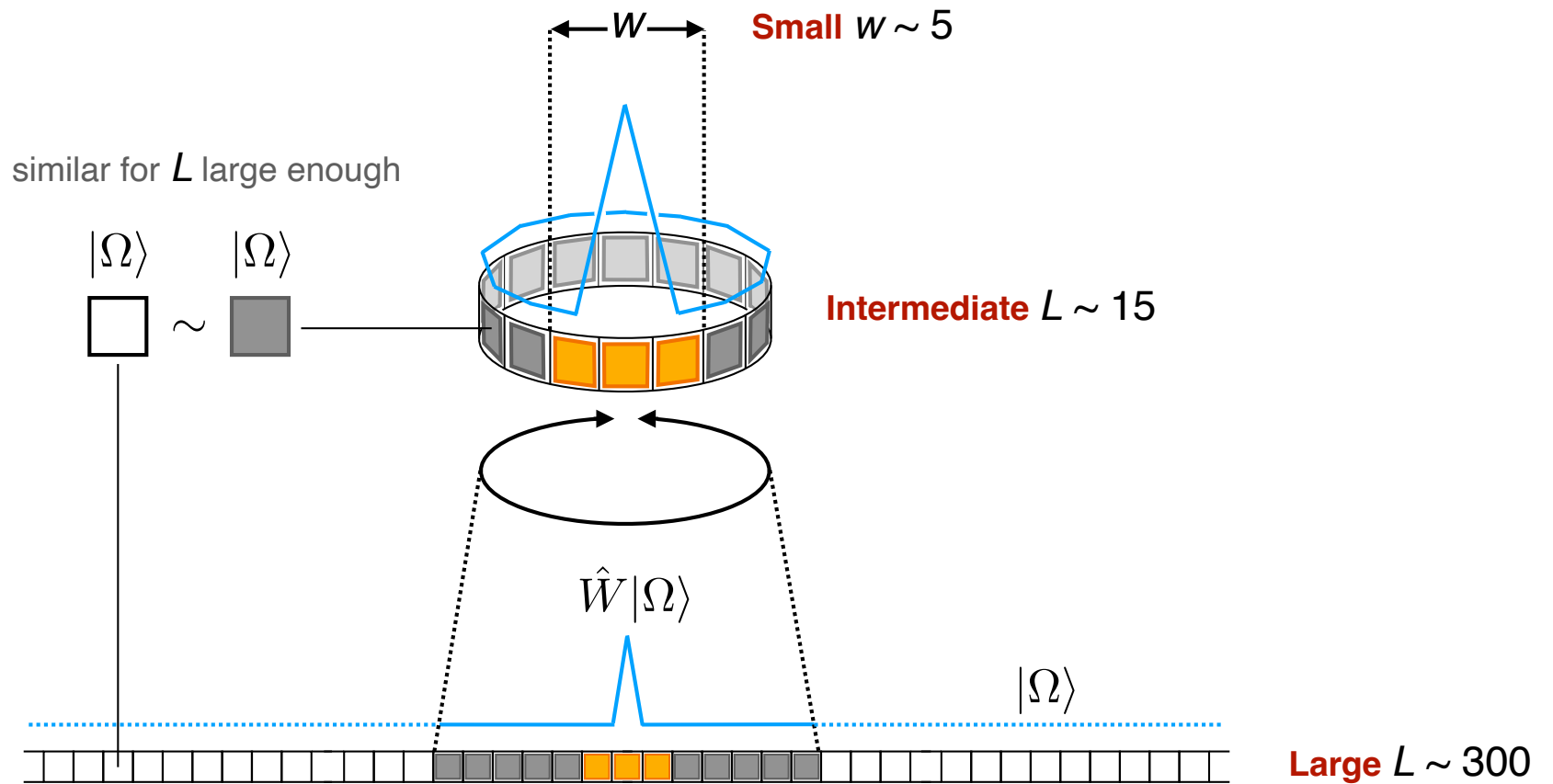
### 3. Construction of the wavepackets



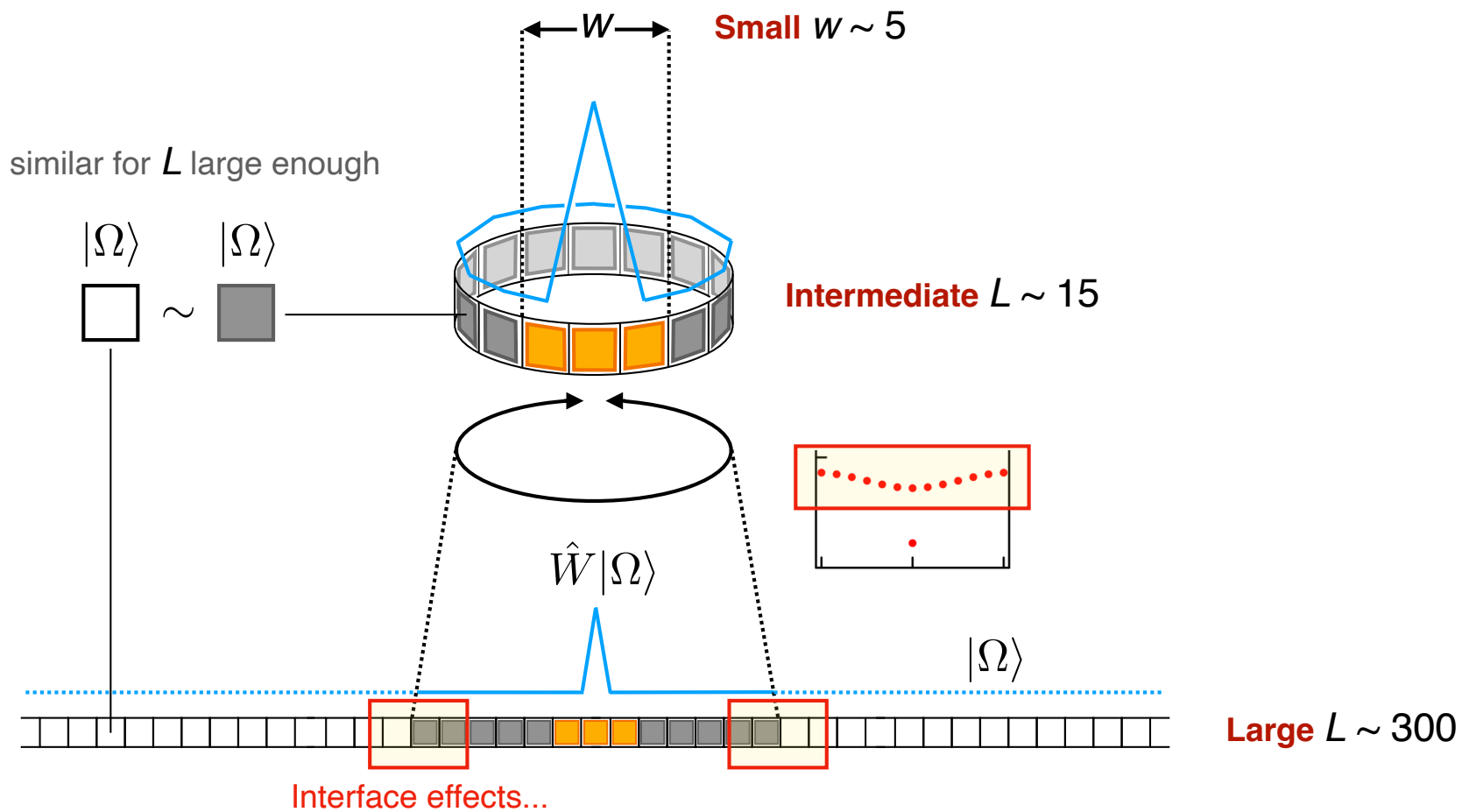
### 3. Construction of the wavepackets



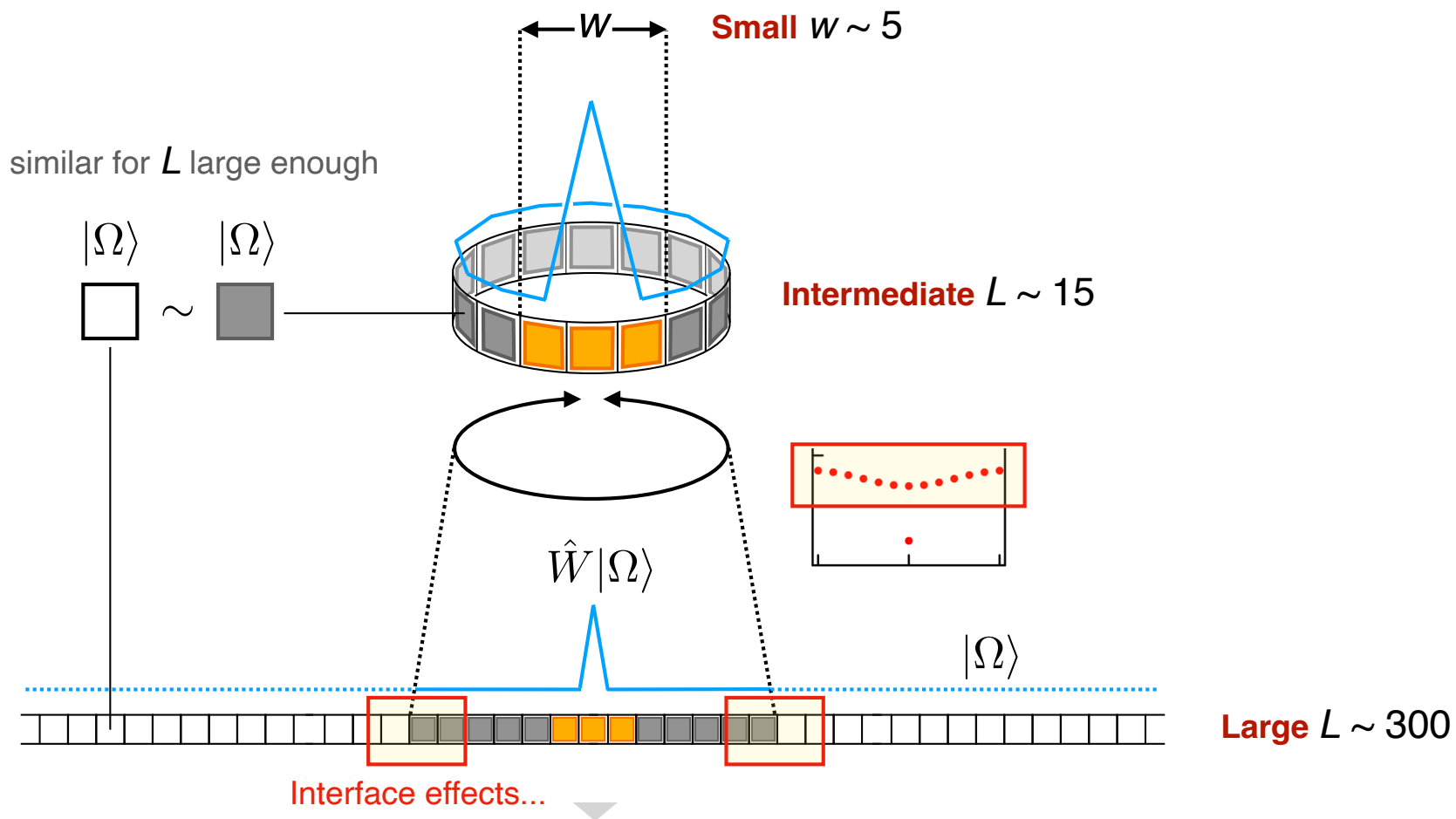
### 3. Construction of the wavepackets



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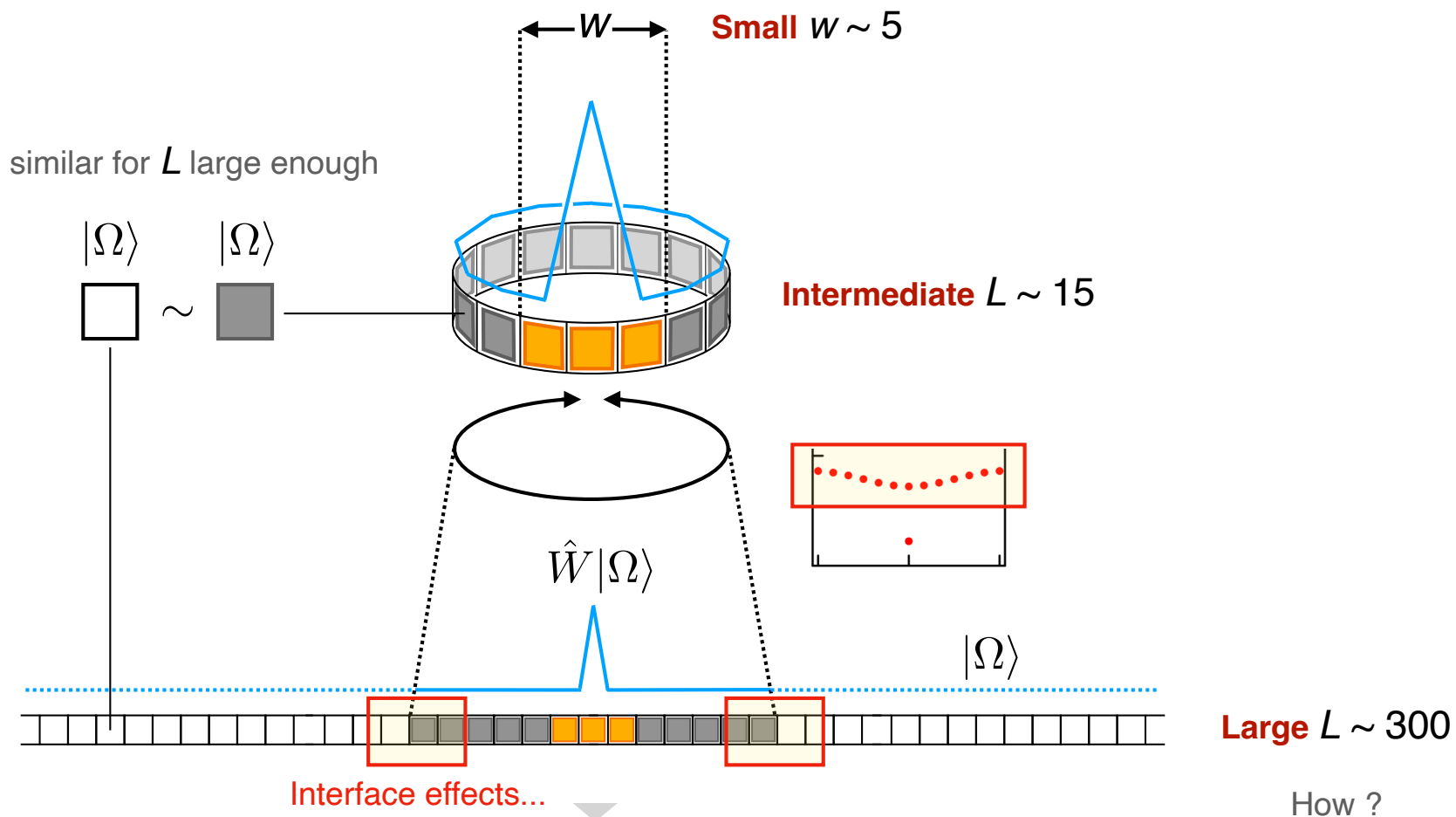


(On top of the interacting vacuum)

$$|W_j\rangle = T^j |W_0\rangle$$

Wannier function  $\rightarrow$  **building blocks** to construct any single-(quasi)particle state.

### 3. Construction of the wavepackets



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## 4. Tensor Network methods in a nutshell

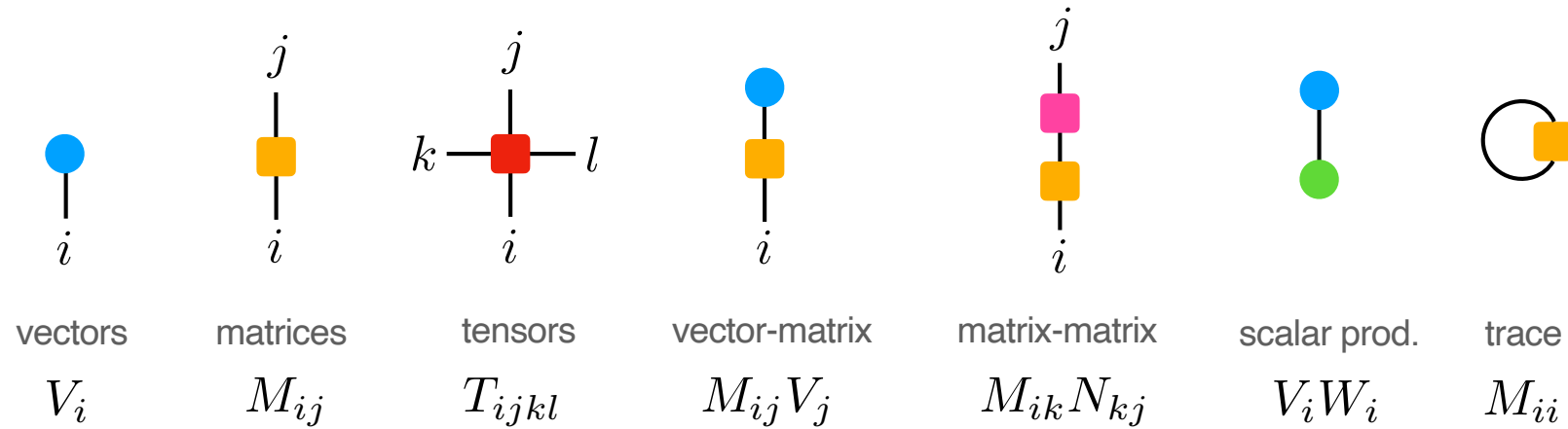


## 4. Tensor Network methods in a nutshell

**Tensor Networks notation:** each tensor  $T$  (node) has  $n$  indices  $i$  (links). Each index has a dimension  $d$  (size).

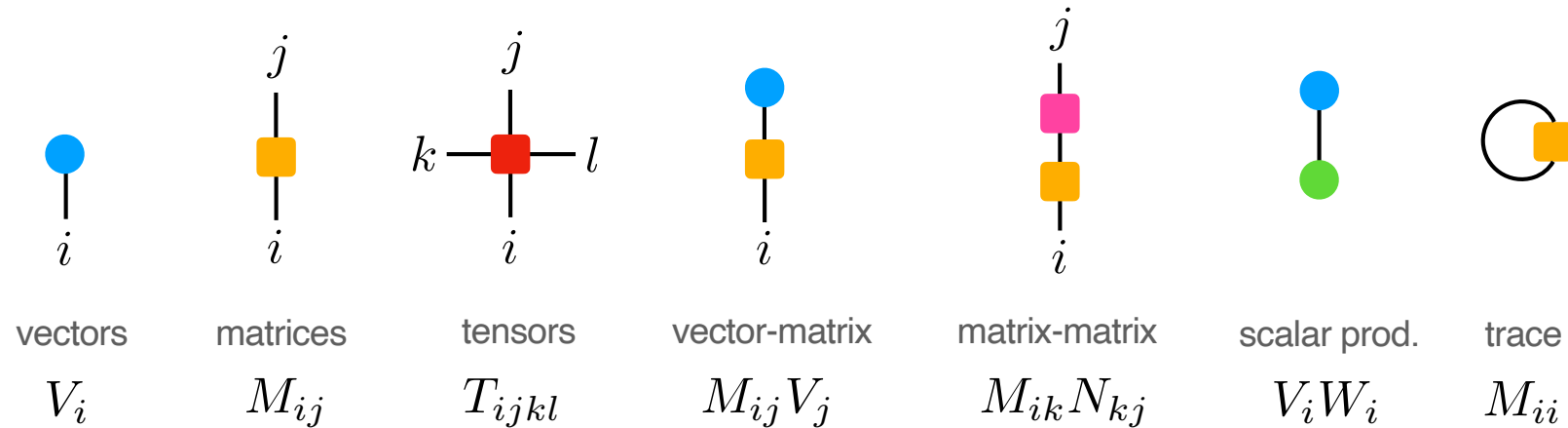
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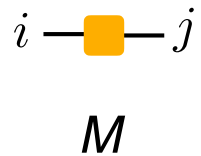


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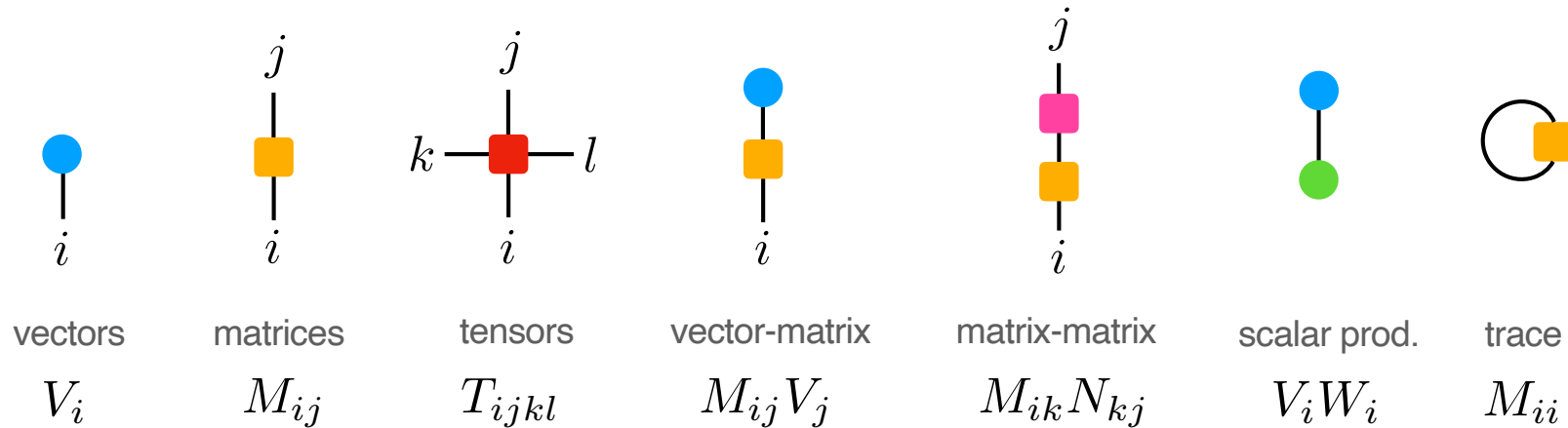


### Singular Value Decomposition (SVD)

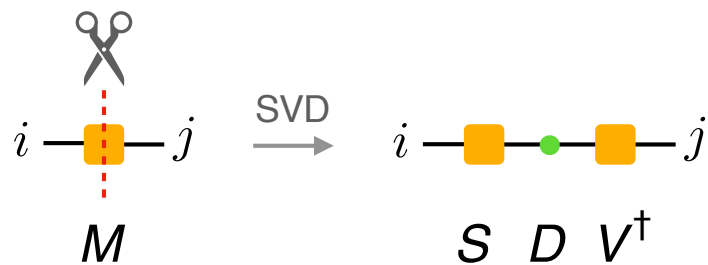


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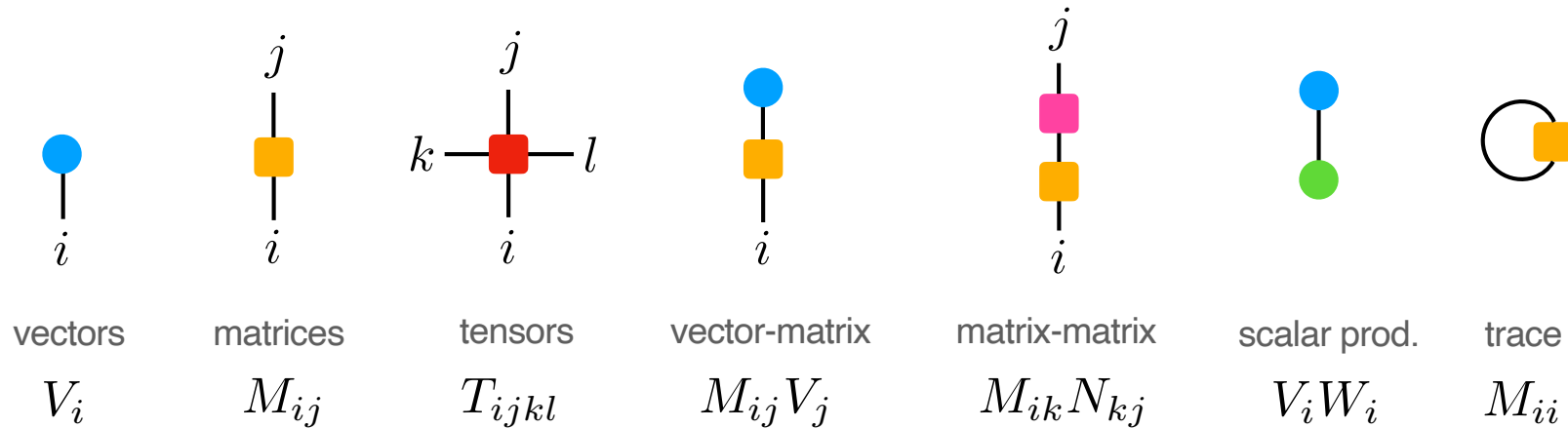


## Singular Value Decomposition (SVD)

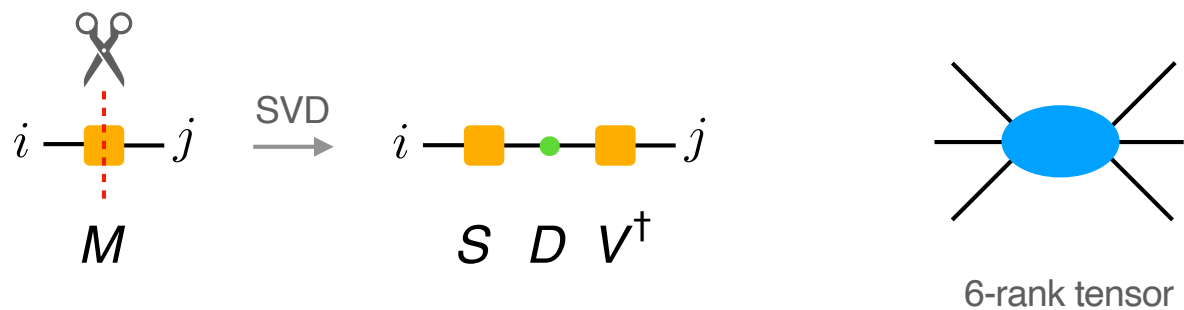


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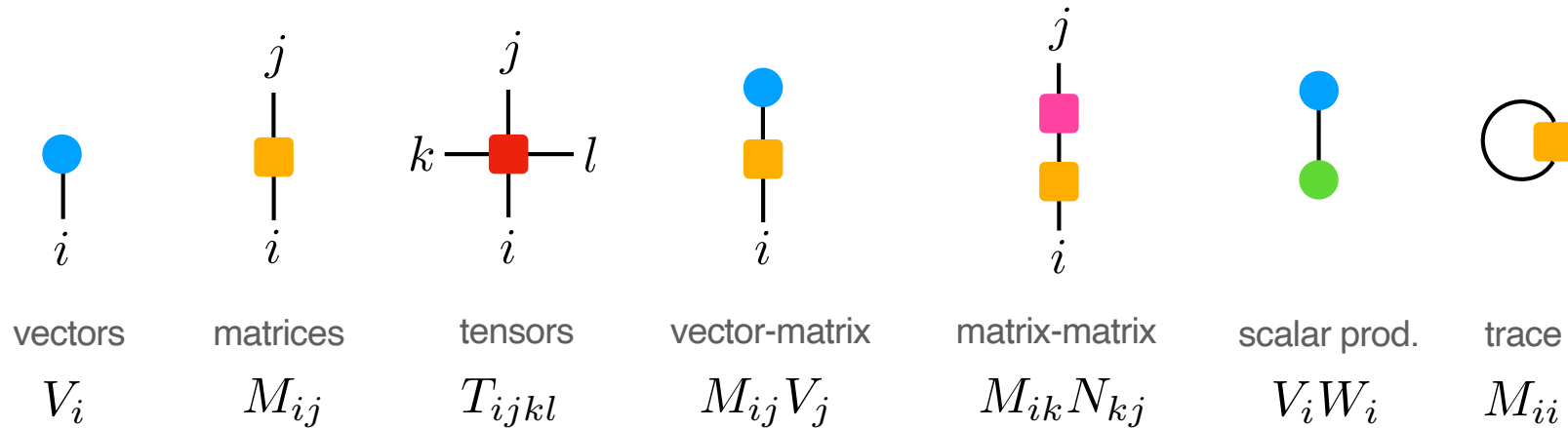


## Singular Value Decomposition (SVD)

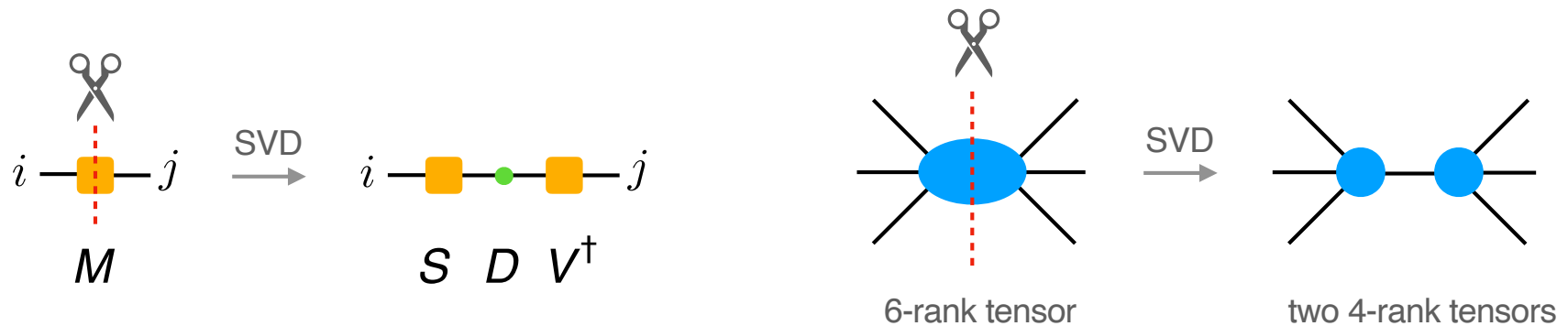


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## Singular Value Decomposition (SVD)

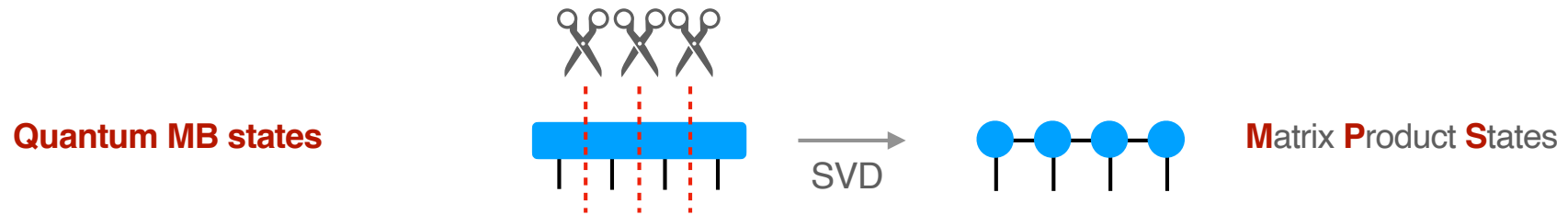


## 4. Tensor Network methods in a nutshell

Quantum MB states

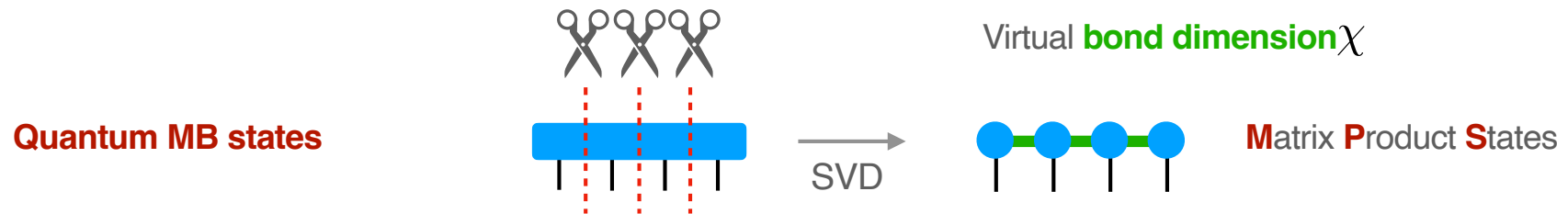


## 4. Tensor Network methods in a nutshell

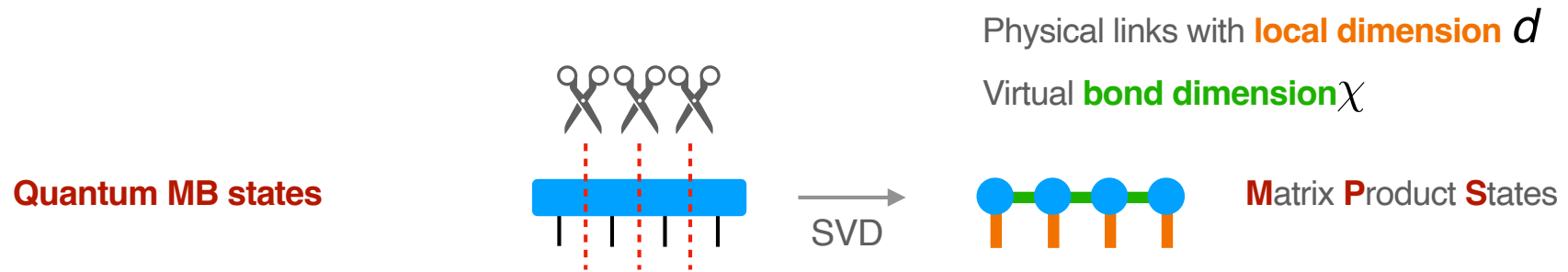




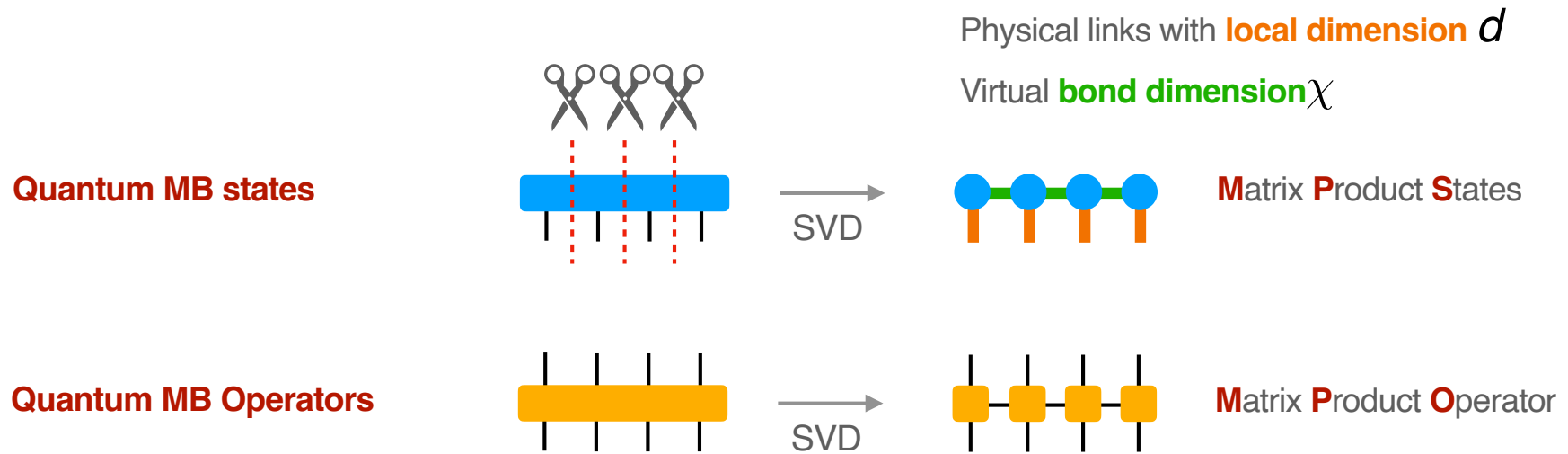
## 4. Tensor Network methods in a nutshell



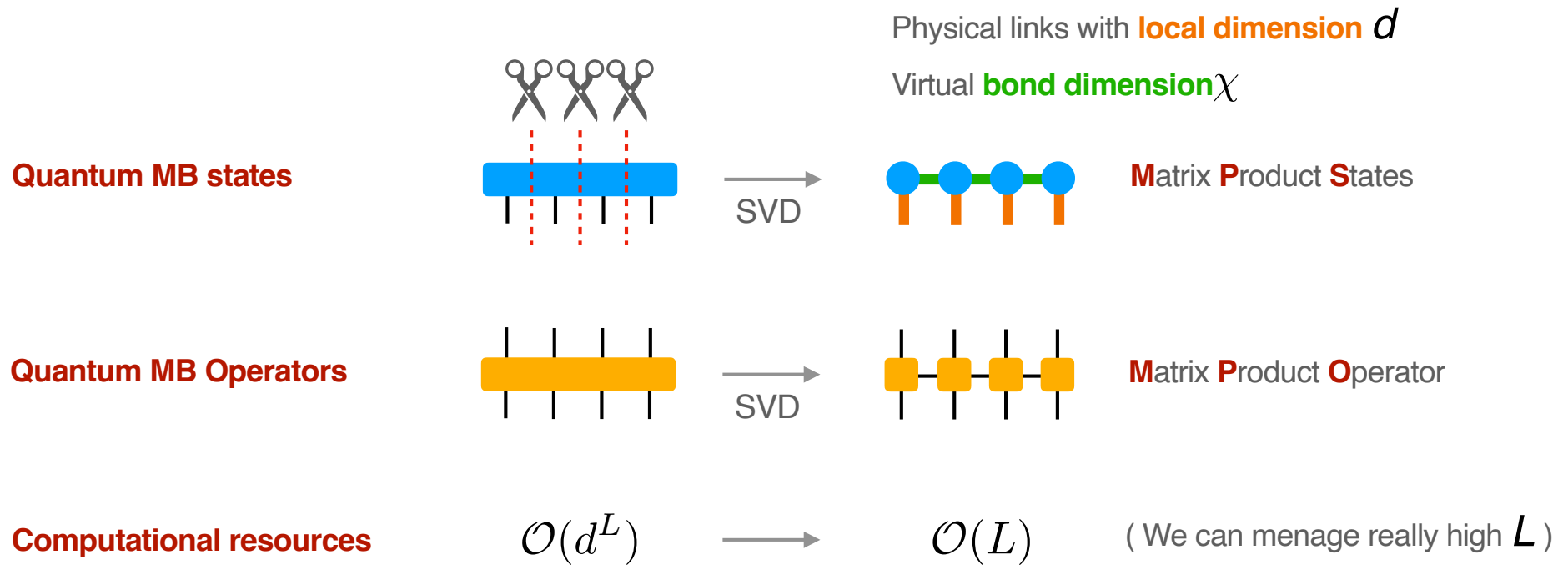
## 4. Tensor Network methods in a nutshell



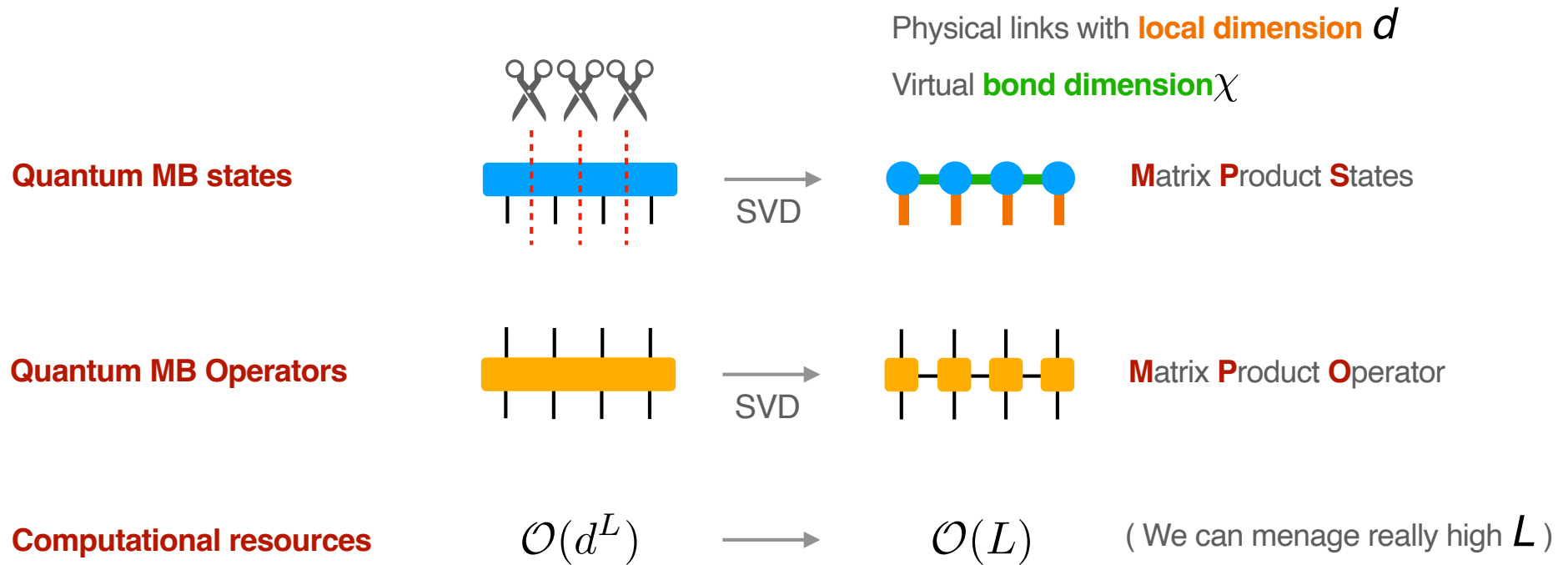
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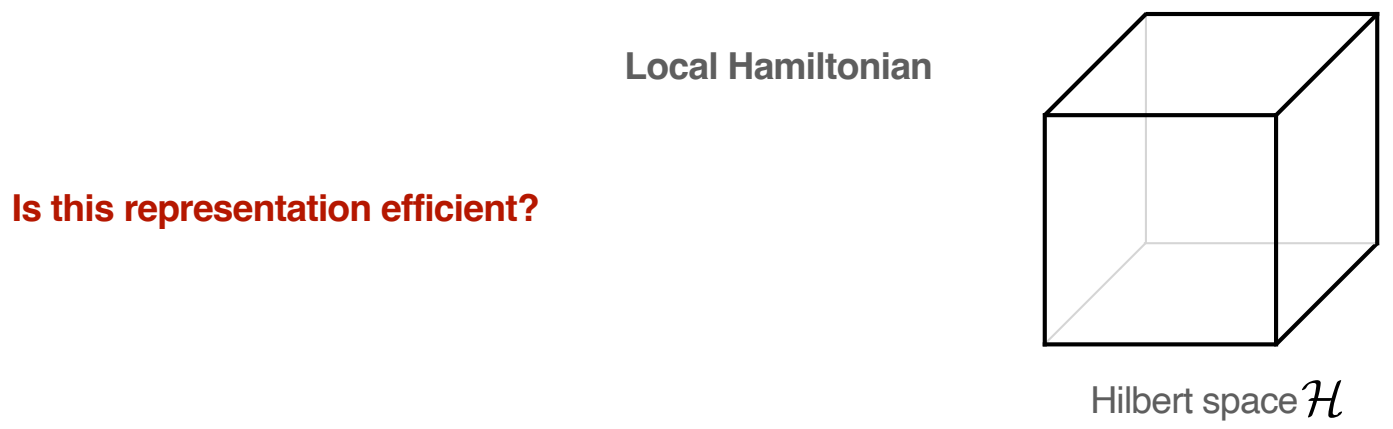
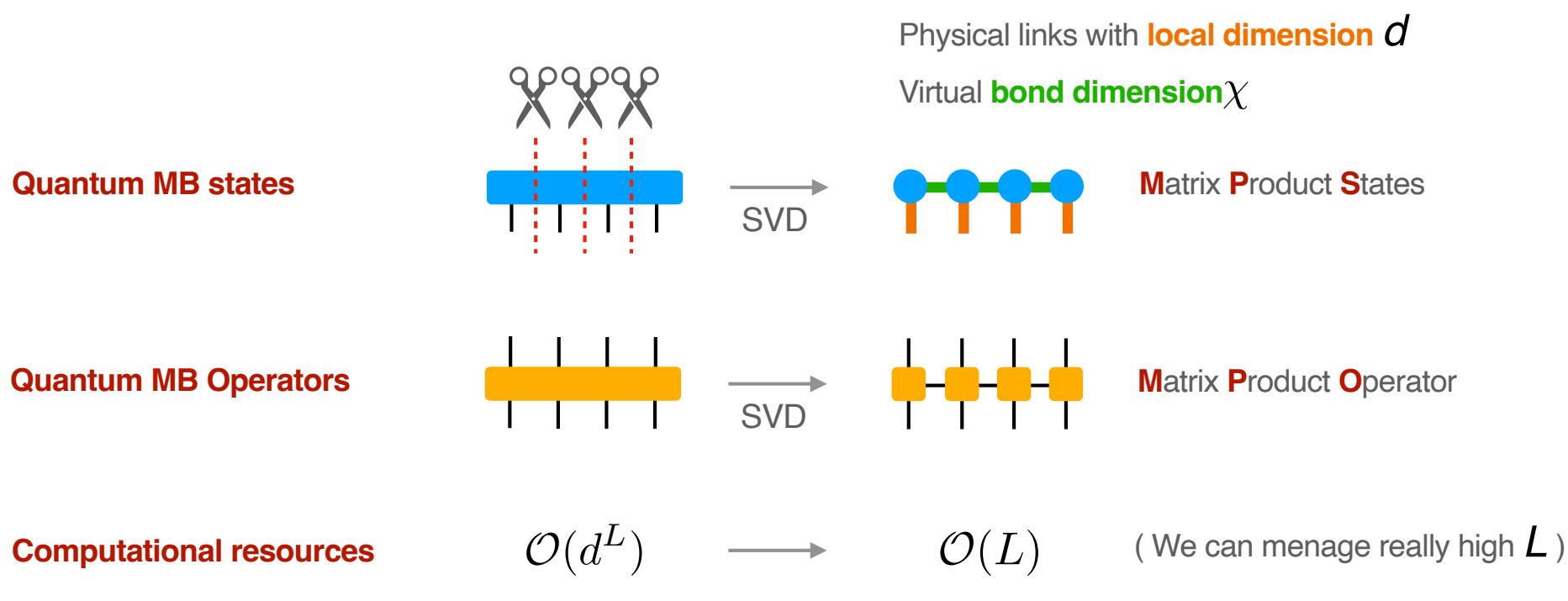


## 4. Tensor Network methods in a nutshell

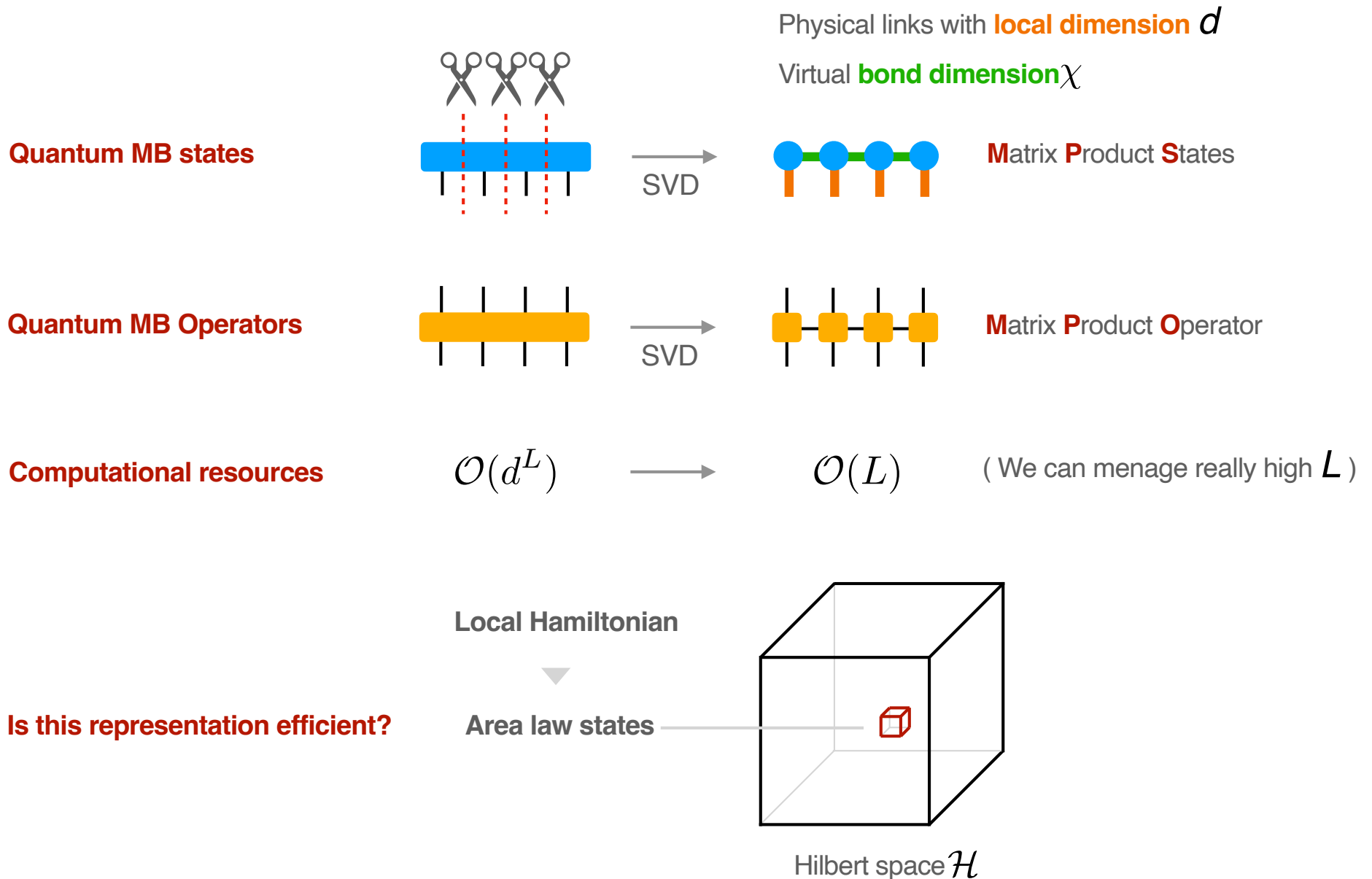


Is this representation efficient?

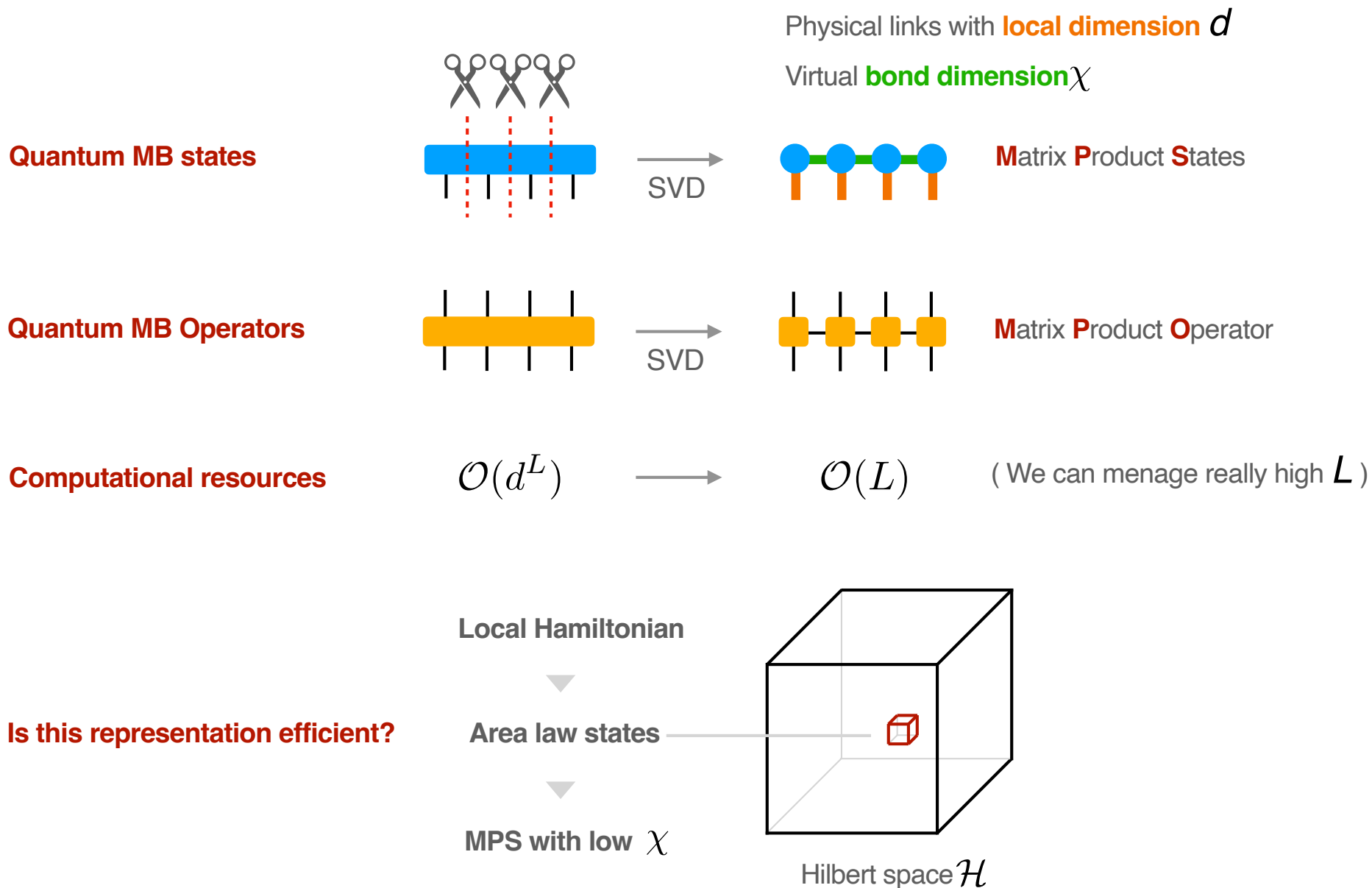
# 4. Tensor Network methods in a nutshell



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# 4. Tensor Network methods in a nutshell





## 4. Tensor Network methods in a nutshell

Useful MPS and MPO Algorithms

## 4. Tensor Network methods in a nutshell

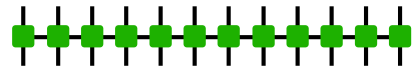
Useful MPS and MPO Algorithms

Ground-state search

# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

Ground-state search Density Matrix Renormalization Group

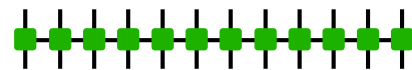


MPO Hamiltonian

# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

Ground-state search Density Matrix Renormalization Group



MPO Hamiltonian



DMRG

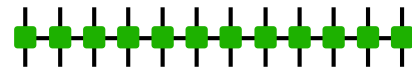


MPS ground-state  $|\Omega\rangle$

# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

Ground-state search Density Matrix Renormalization Group



MPO Hamiltonian



DMRG



MPS ground-state  $|\Omega\rangle$

Large systems  
(with just a laptop!)

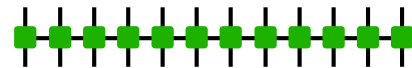
$$L \gtrsim 100$$



# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

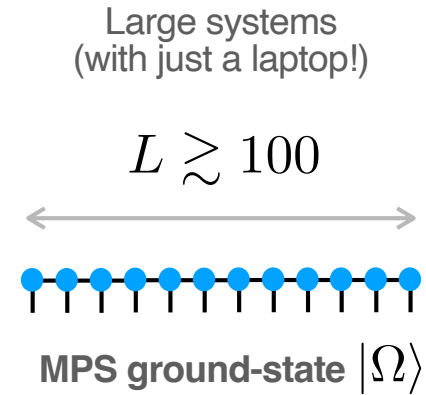
Ground-state search Density Matrix Renormalization Group



MPO Hamiltonian



DMRG

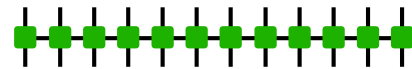


## Time evolution for MPS

# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

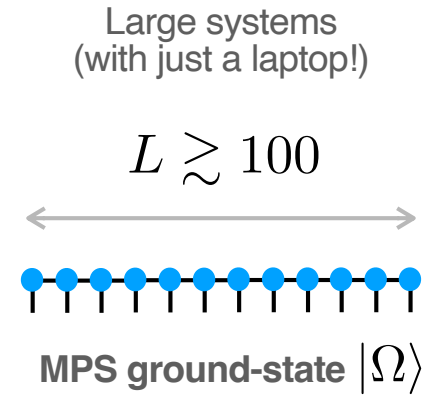
Ground-state search Density Matrix Renormalization Group



MPO Hamiltonian



DMRG



Time evolution for MPS Time Evolving Block Decimation (...but also TDVP)

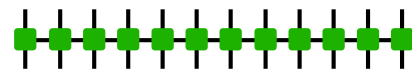


Time evolution operator

# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

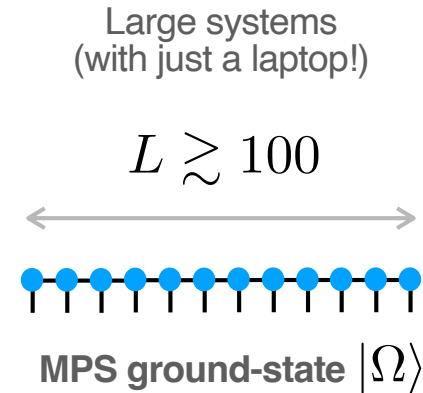
Ground-state search Density Matrix Renormalization Group



MPO Hamiltonian



DMRG



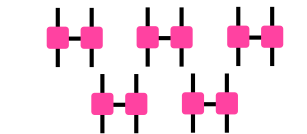
Time evolution for MPS Time Evolving Block Decimation (...but also TDVP)



Time evolution operator



Suzuki-Trotter  $\delta t$



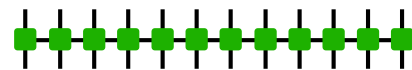
Iteration of gates



# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

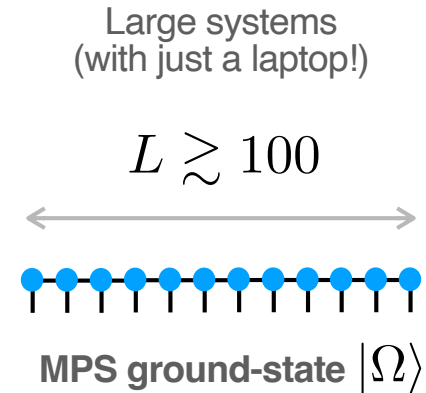
Ground-state search Density Matrix Renormalization Group



MPO Hamiltonian



DMRG



MPS ground-state  $|\Omega\rangle$

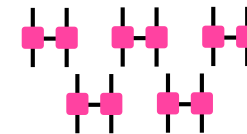
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Suzuki-Trotter  $\delta t$



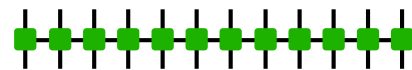
Iteration of gates

Operator to MPO conversion

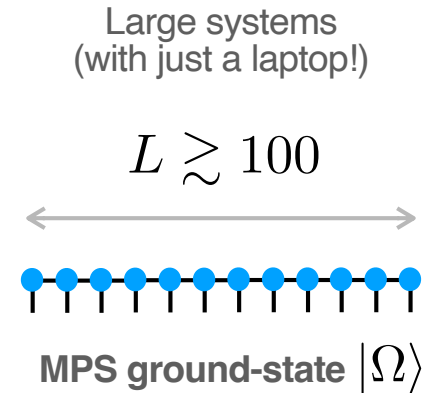
# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

Ground-state search Density Matrix Renormalization Group



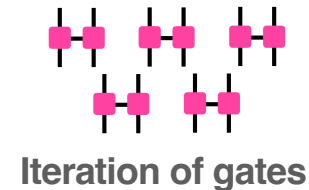
MPO Hamiltonian



Time evolution for MPS Time Evolving Block Decimation (...but also TDVP)



Time evolution operator



Operator to MPO conversion

$$\sum_{\alpha} \hat{L}_{\alpha} = \sum \text{[Diagram of yellow squares on a chain]}$$

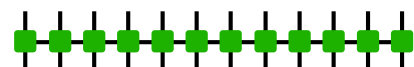
The diagram shows a horizontal chain of three yellow squares, each with a vertical line extending upwards and downwards from its center, representing the decomposition of a local operator into a sum of MPOs.

Sum of compositions of local operators

# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

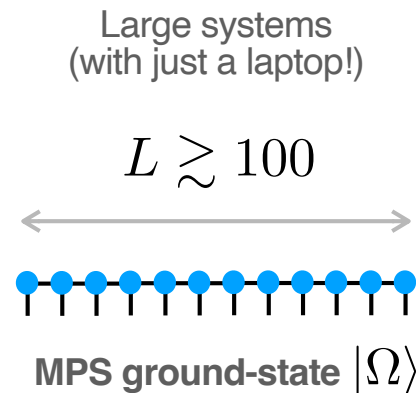
Ground-state search Density Matrix Renormalization Group



MPO Hamiltonian



DMRG



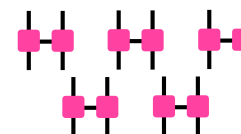
Time evolution for MPS Time Evolving Block Decimation (...but also TDVP)



Time evolution operator



Suzuki-Trotter  $\delta t$



Iteration of gates

Operator to MPO conversion

$$\sum_{\alpha} \hat{L}_{\alpha} = \sum \text{[Diagram of yellow squares on a chain]}$$

Sum of compositions of local operators



Automata procedure



Matrix Product Operator

## 4. Tensor Network methods in a nutshell

**Automata procedure** Fröwis et al. Phys. Rev. A 81 (2010) 062337

## 4. Tensor Network methods in a nutshell

### Automata procedure

1 Operator picture

$$\hat{O} = \sum_{\alpha} \hat{L}_{\alpha}$$

# 4. Tensor Network methods in a nutshell

## Automata procedure

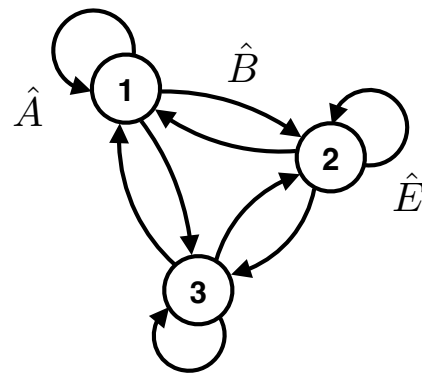
1

Operator picture

$$\hat{O} = \sum_{\alpha} \hat{L}_{\alpha}$$

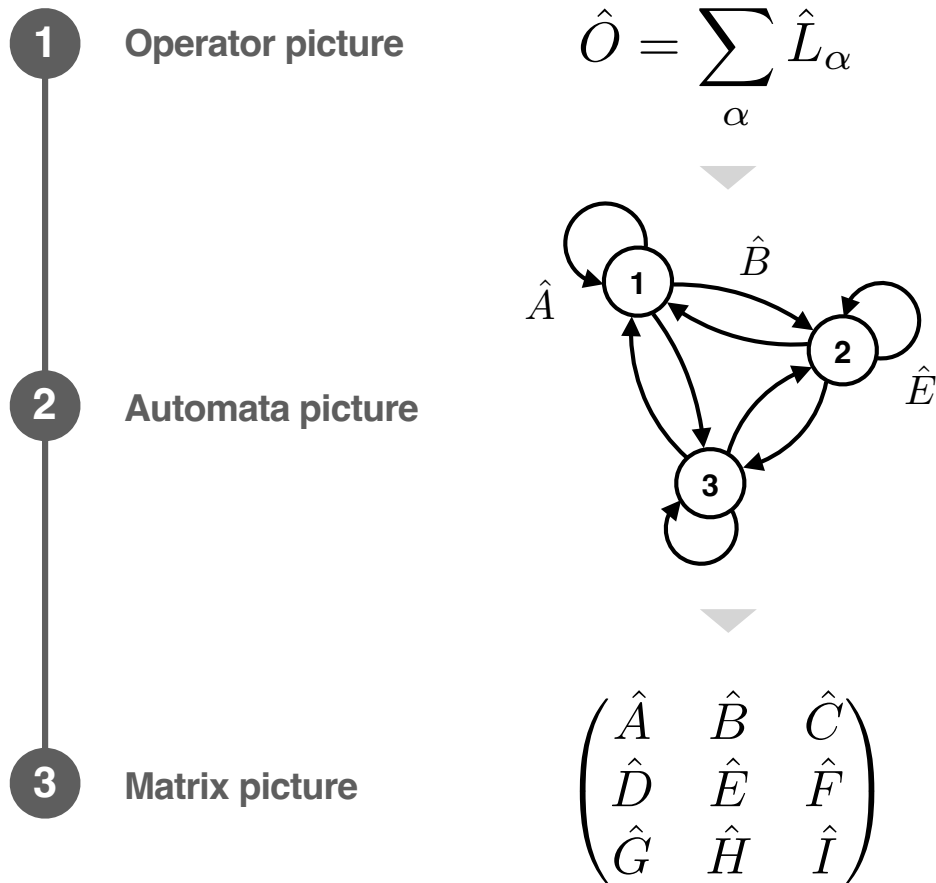
2

Automata picture



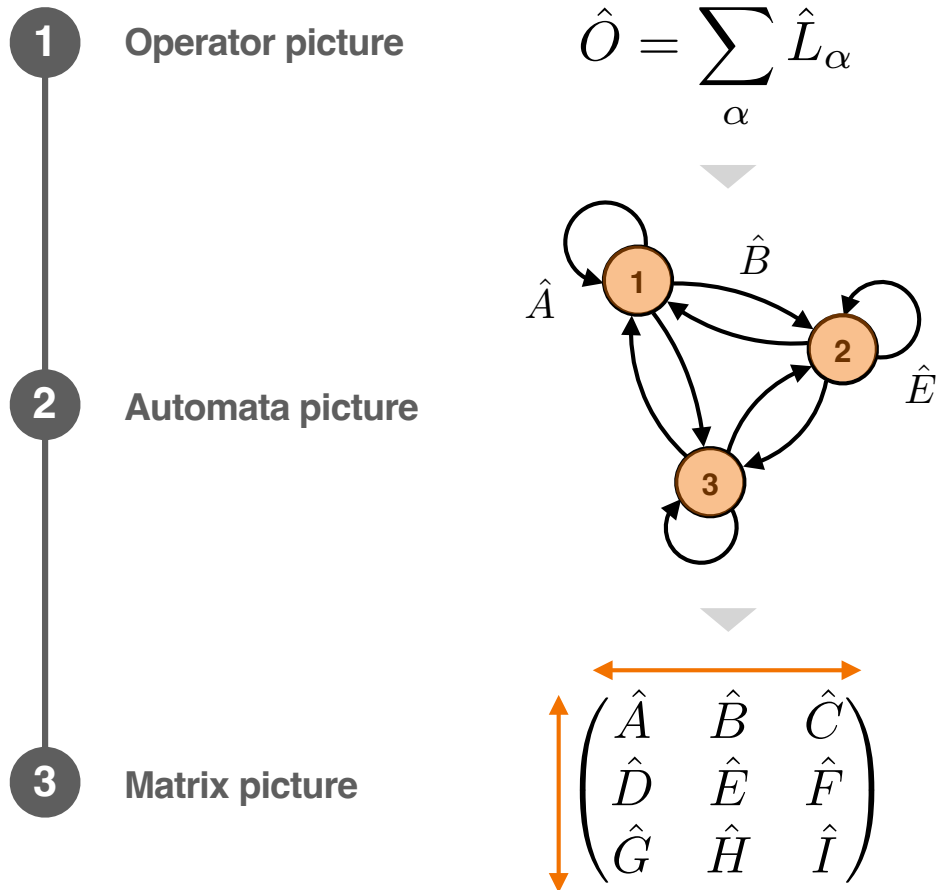
# 4. Tensor Network methods in a nutshell

## Automata procedure



# 4. Tensor Network methods in a nutshell

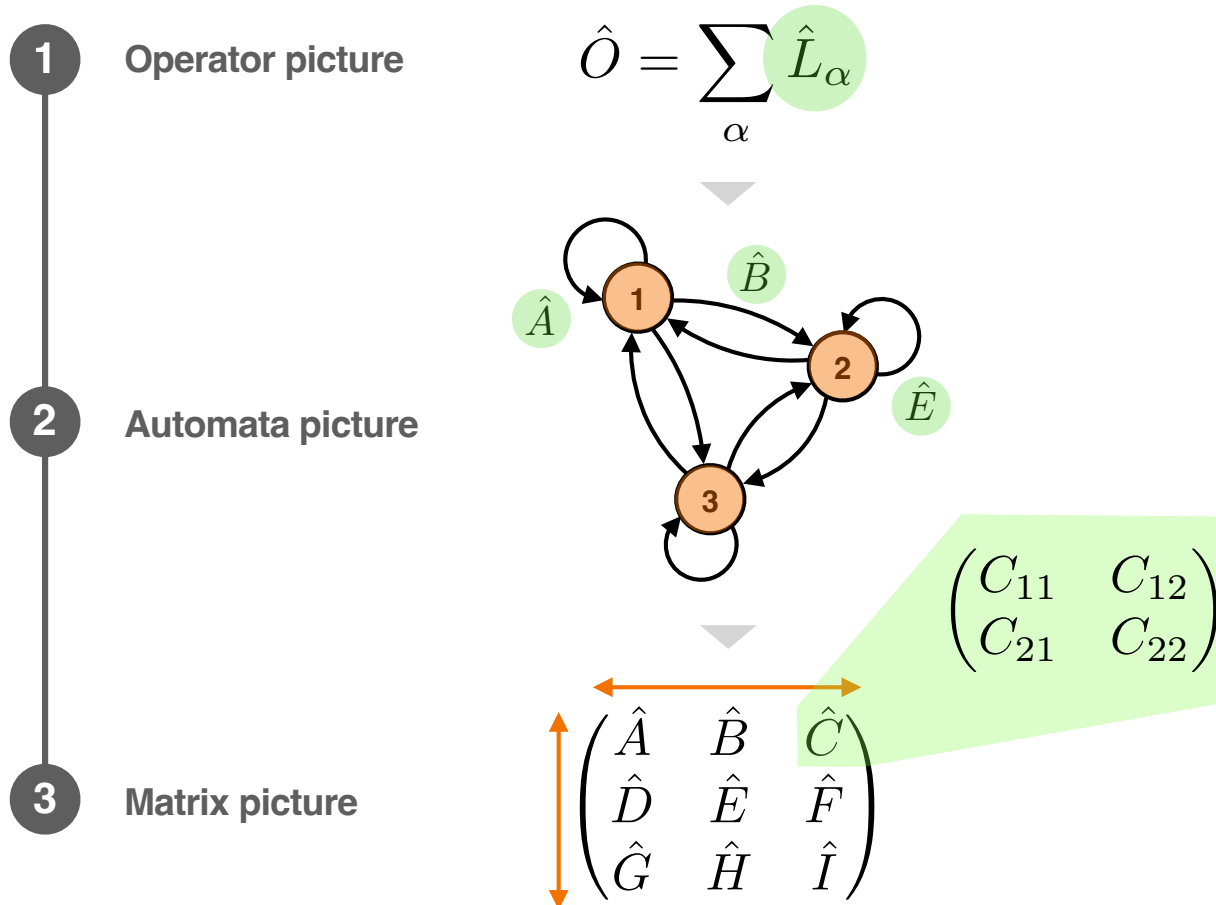
## Automata procedure





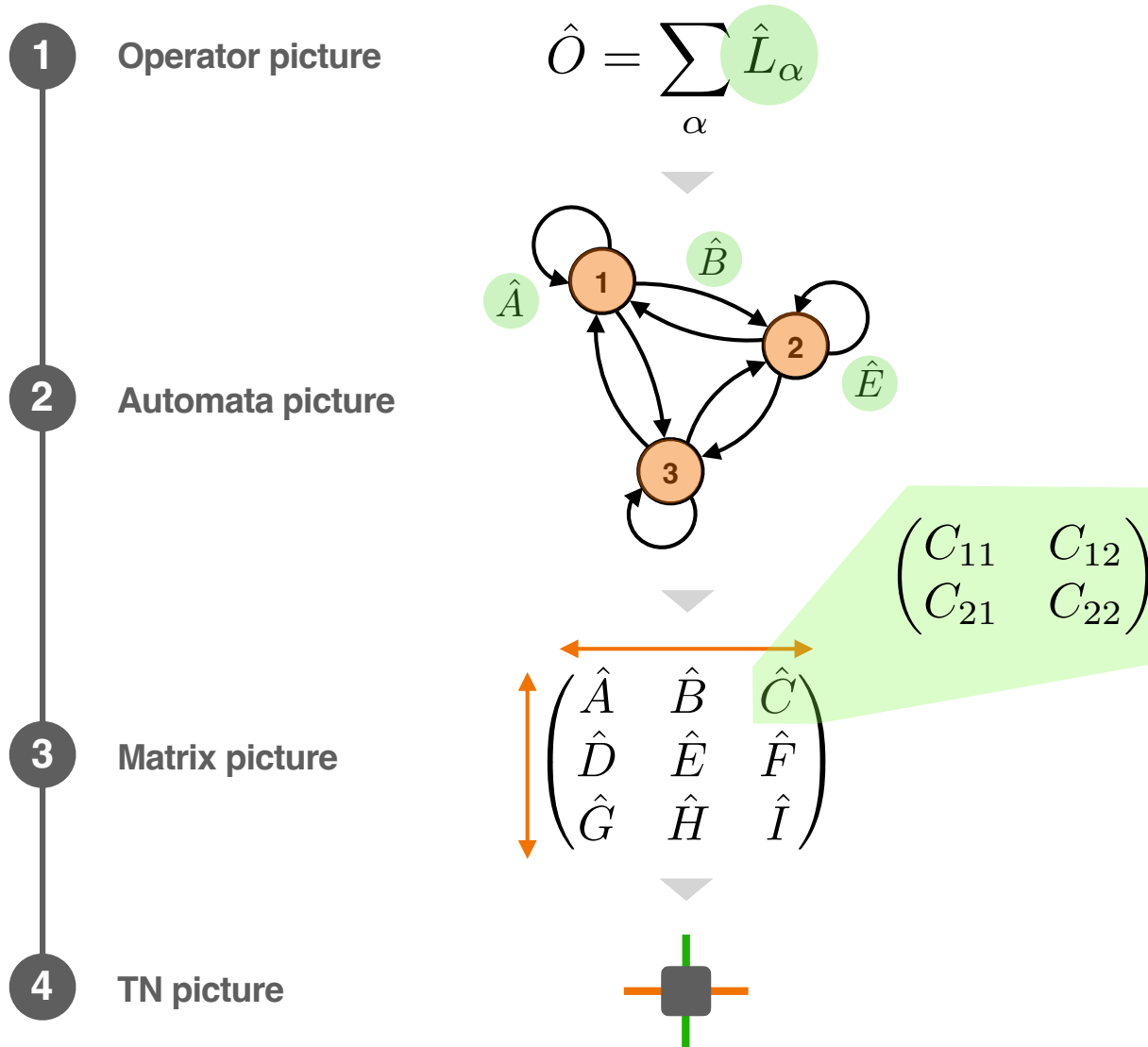
# 4. Tensor Network methods in a nutshell

## Automata procedure



# 4. Tensor Network methods in a nutshell

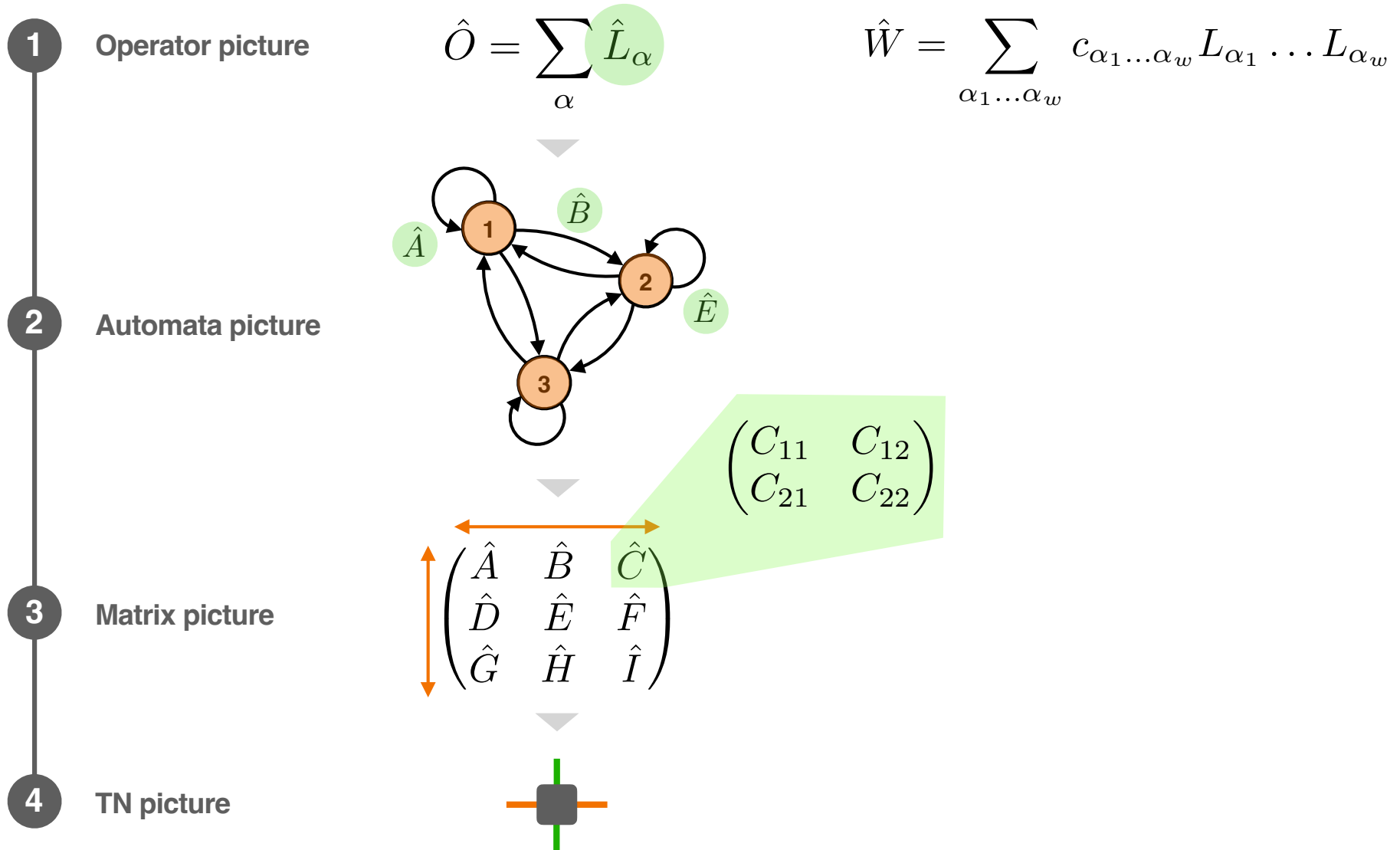
## Automata procedure



# 4. Tensor Network methods in a nutshell

## Automata procedure

## Wannier creation operator



# 4. Tensor Network methods in a nutshell

## Automata procedure

## Wannier creation operator

1

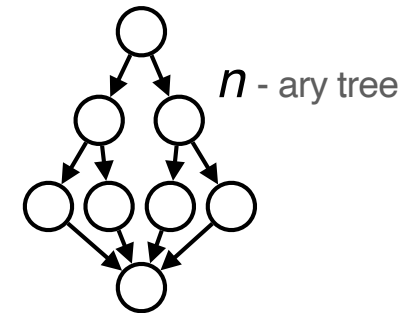
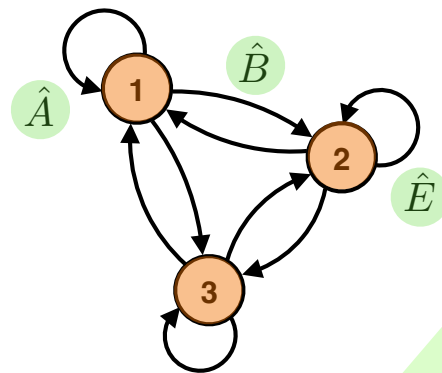
Operator picture

$$\hat{O} = \sum_{\alpha} \hat{L}_{\alpha}$$

$$\hat{W} = \sum_{\alpha_1 \dots \alpha_w} c_{\alpha_1 \dots \alpha_w} L_{\alpha_1} \dots L_{\alpha_w}$$

2

Automata picture



3

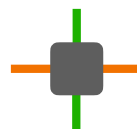
Matrix picture

$$\begin{pmatrix} \hat{A} & \hat{B} & \hat{C} \\ \hat{D} & \hat{E} & \hat{F} \\ \hat{G} & \hat{H} & \hat{I} \end{pmatrix}$$

A 3x3 matrix of operators. A green callout box points to the  $\hat{C}$  element, containing the matrix  $\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$ .

4

TN picture



# 4. Tensor Network methods in a nutshell

## Automata procedure

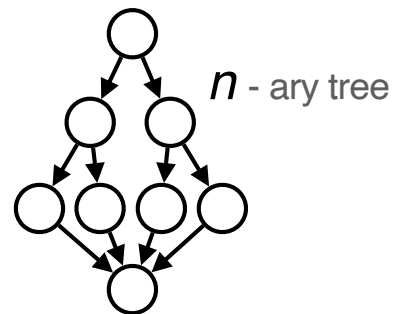
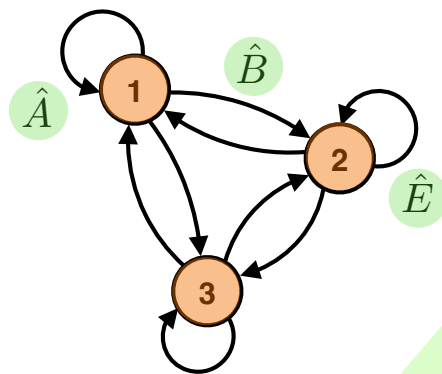
## Wannier creation operator

1 Operator picture

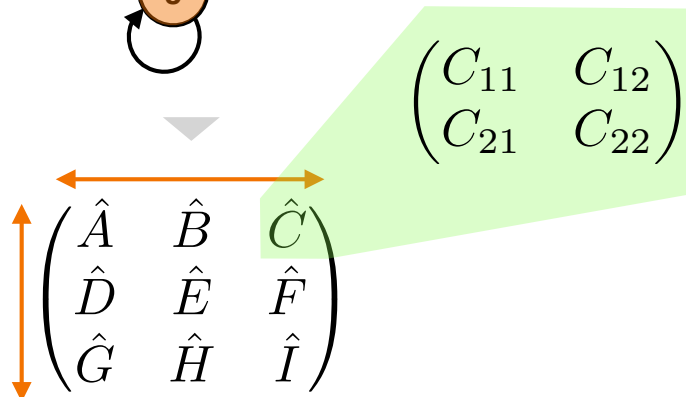
$$\hat{O} = \sum_{\alpha} \hat{L}_{\alpha}$$

$$\hat{W} = \sum_{\alpha_1 \dots \alpha_w} c_{\alpha_1 \dots \alpha_w} L_{\alpha_1} \dots L_{\alpha_w}$$

2 Automata picture

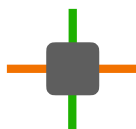


3 Matrix picture



$$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \mathcal{O}(e^w)$$

4 TN picture



# 4. Tensor Network methods in a nutshell

## Automata procedure

## Wannier creation operator

1

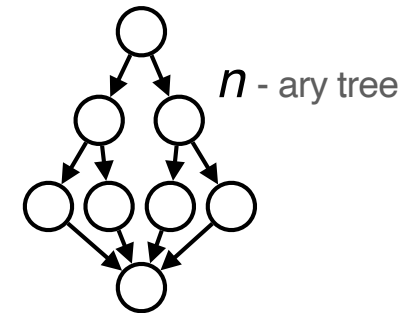
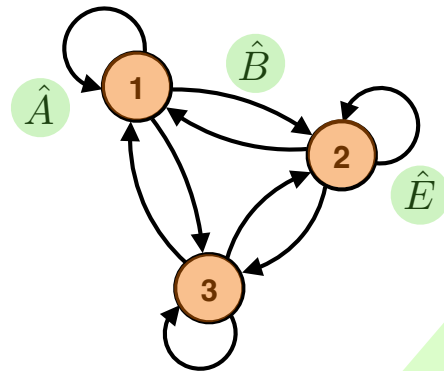
Operator picture

$$\hat{O} = \sum_{\alpha} \hat{L}_{\alpha}$$

$$\hat{W} = \sum_{\alpha_1 \dots \alpha_w} c_{\alpha_1 \dots \alpha_w} L_{\alpha_1} \dots L_{\alpha_w}$$

2

Automata picture



3

Matrix picture

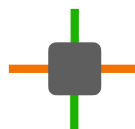
$$\begin{pmatrix} \hat{A} & \hat{B} & \hat{C} \\ \hat{D} & \hat{E} & \hat{F} \\ \hat{G} & \hat{H} & \hat{I} \end{pmatrix}$$

A green callout box contains the matrix  $\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$ .

$$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \mathcal{O}(e^w)$$

4

TN picture



## 5. Back to Wavepackets



“Wannier Ansätze”

## 5. Back to Wavepackets

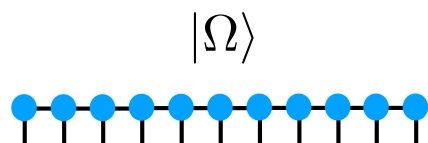
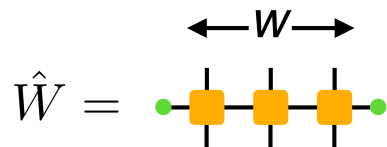
Wannier creation  
operator Ansätze

$$\hat{W} = \text{---} \begin{array}{c} \leftarrow W \rightarrow \\ | \quad | \quad | \\ \bullet \text{---} \square \text{---} \square \text{---} \square \text{---} \bullet \\ | \quad | \quad | \end{array} \text{---}$$



# 5. Back to Wavepackets

Wannier creation  
operator Ansatz

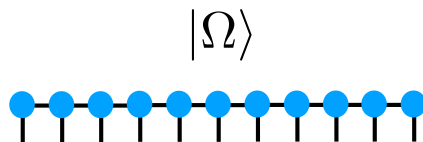
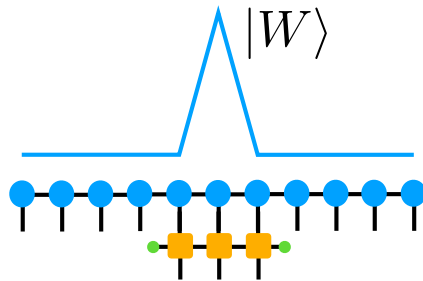


Large  $L$  vacuum state  
found with DMRG

# 5. Back to Wavepackets

Wannier creation operator Ansatz

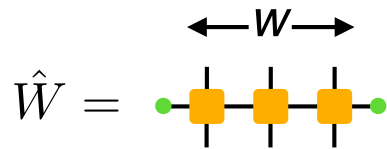
$$\hat{W} = \text{---} \overset{\leftarrow W \rightarrow}{\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array}} \text{---}$$



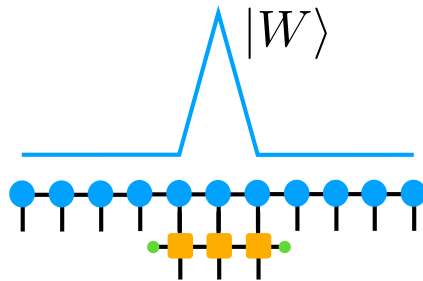
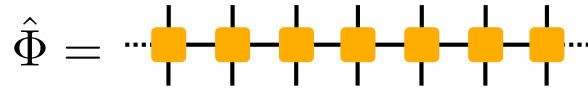
Large  $L$  vacuum state found with DMRG

# 5. Back to Wavepackets

Wannier creation operator Ansatz



Wavepacket Ansatz



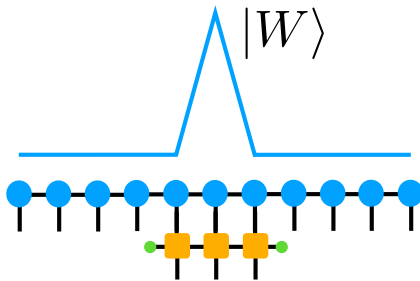
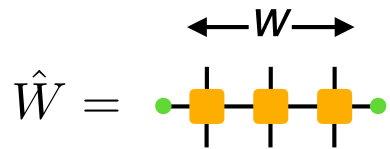
$|\Omega\rangle$



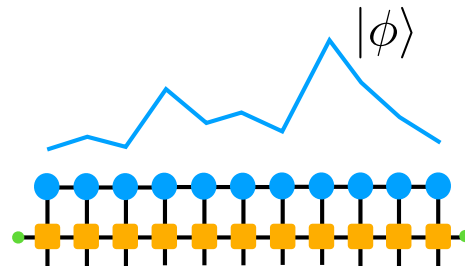
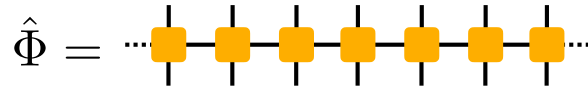
Large  $L$  vacuum state  
found with DMRG

# 5. Back to Wavepackets

Wannier creation operator Ansatz



Wavepacket Ansatz



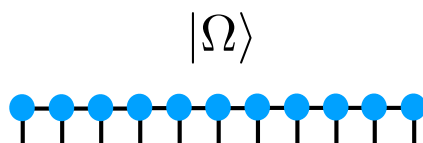
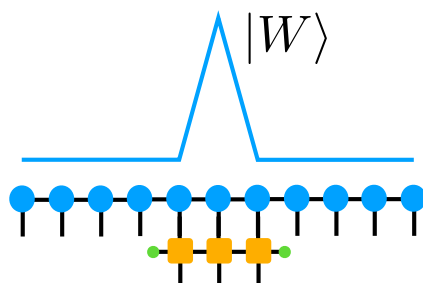
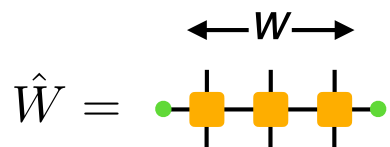
$|\Omega\rangle$



Large  $L$  vacuum state found with DMRG

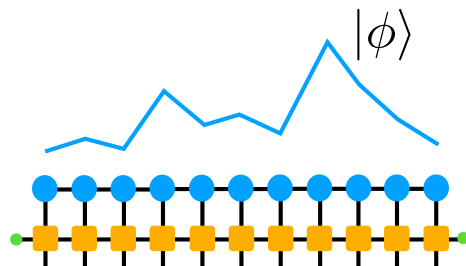
# 5. Back to Wavepackets

Wannier creation operator Ansatz



Large  $L$  vacuum state found with DMRG

Wavepacket Ansatz

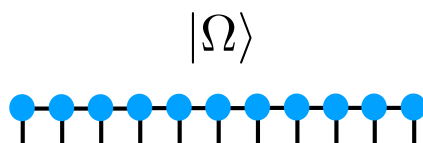
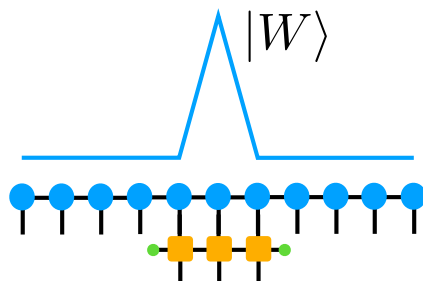
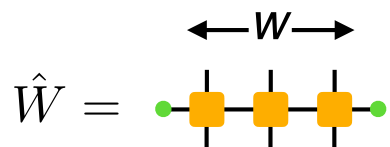


No scaling of  $\chi$  with size!

$$\chi = \mathcal{O}(e^w, \cancel{L})$$

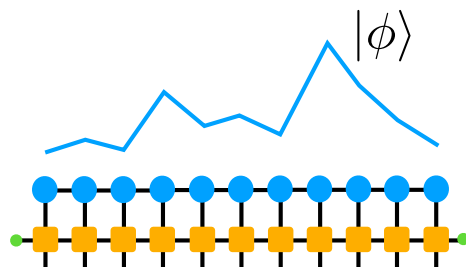
# 5. Back to Wavepackets

Wannier creation operator Ansatz



Large  $L$  vacuum state found with DMRG

Wavepacket Ansatz



No scaling of  $\chi$  with size!

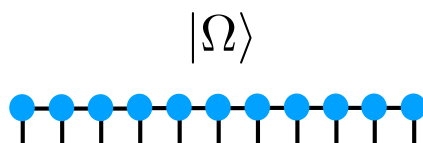
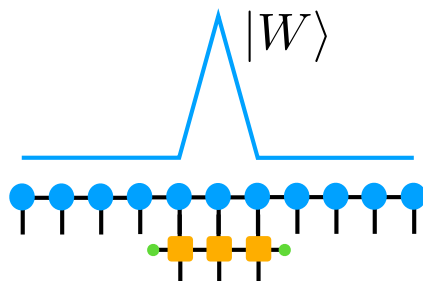
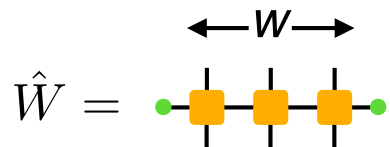
$$\chi = \mathcal{O}(e^w, \mathbf{L})$$

Gaussian wavepacket

$$\frac{1}{\mathcal{N}} e^{-\frac{(j-j_0)^2}{2\sigma}} e^{ijk_0}$$

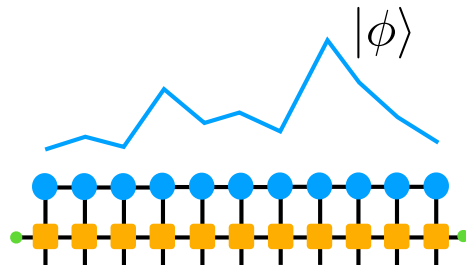
# 5. Back to Wavepackets

Wannier creation operator Ansatz



Large  $L$  vacuum state found with DMRG

Wavepacket Ansatz



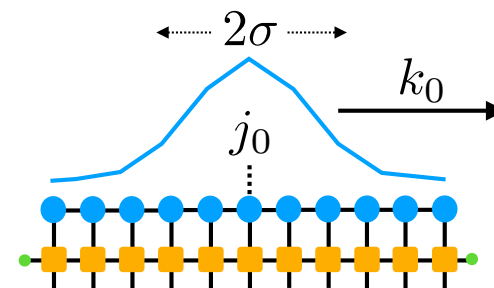
No scaling of  $\chi$  with size!

$$\chi = \mathcal{O}(e^w, \mathbf{L})$$

(Real space)

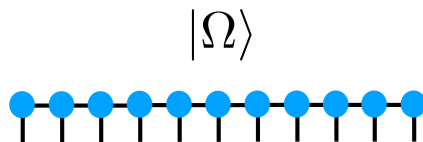
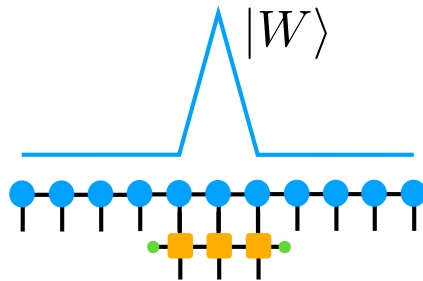
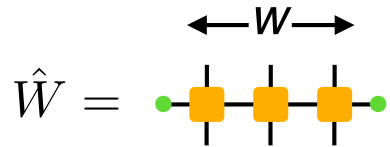
Gaussian wavepacket

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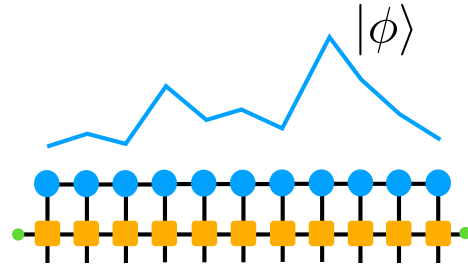
# 5. Back to Wavepackets

Wannier creation operator Ansatz



Large  $L$  vacuum state found with DMRG

Wavepacket Ansatz



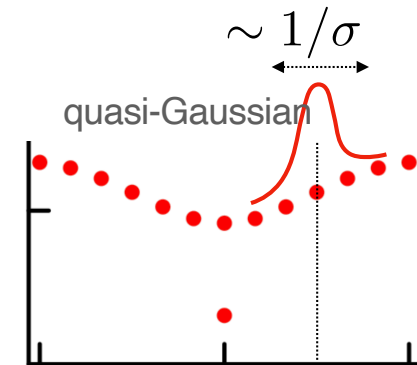
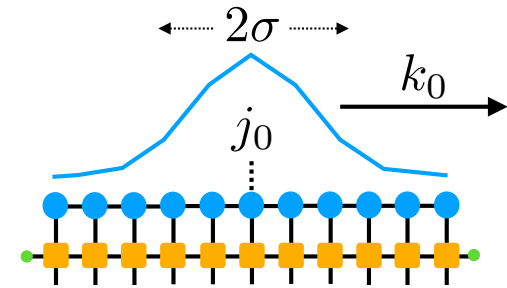
No scaling of  $\chi$  with size!

$$\chi = \mathcal{O}(e^w, \mathbf{L})$$

(Real space)

Gaussian wavepacket

$$\frac{1}{\mathcal{N}} e^{-\frac{(j-j_0)^2}{2\sigma}} e^{ijk_0}$$



Momentum space



## 6. Numerical simulations

### System parameters

$$a = 1$$

$$L = 100$$

$$g^4 = 0.1$$

(Dirichlet OBC)

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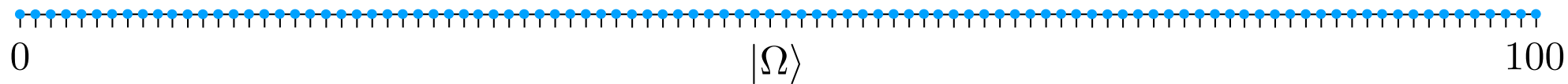
(Dirichlet OBC)

### DMRG parameters

$$\chi_{\max} = 200$$

$$n_{\text{sweeps}} = 50$$

$$\epsilon_{\text{SVD}} = 10^{-13}$$



## 6. Numerical simulations

### System parameters

$$a = 1$$
$$L = 100$$
$$g^4 = 0.1$$

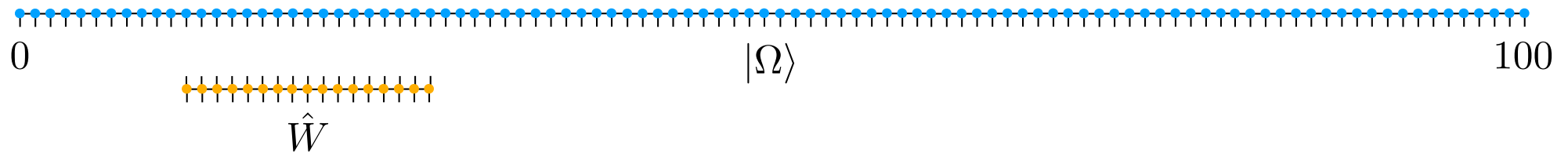
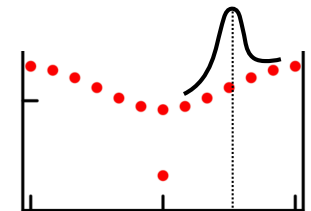
(Dirichlet OBC)

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### Wavepacket parameters

$$\sigma = 3a$$
$$k = \pi/2a$$
$$j_0 = 20$$



## 6. Numerical simulations

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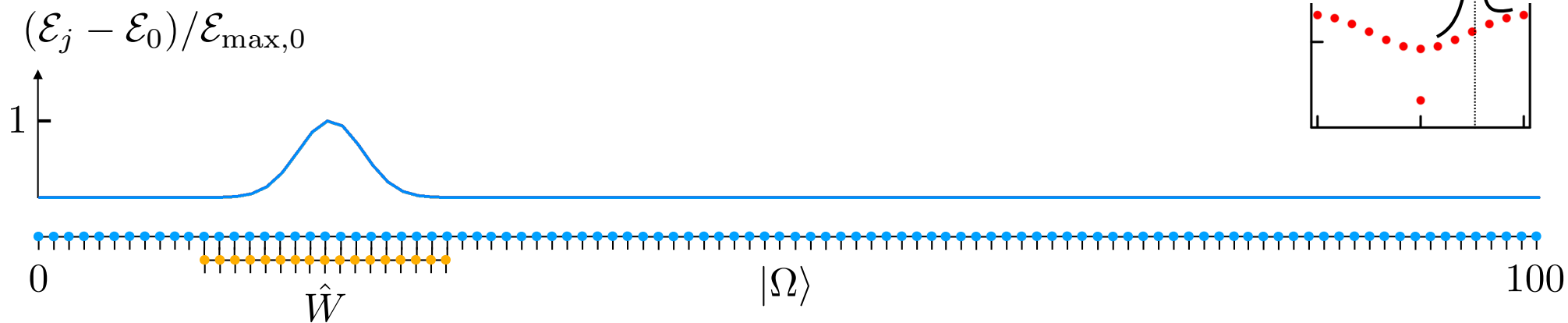
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# 6. Numerical simulations

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 (Dirichlet OBC)

## DMRG parameters

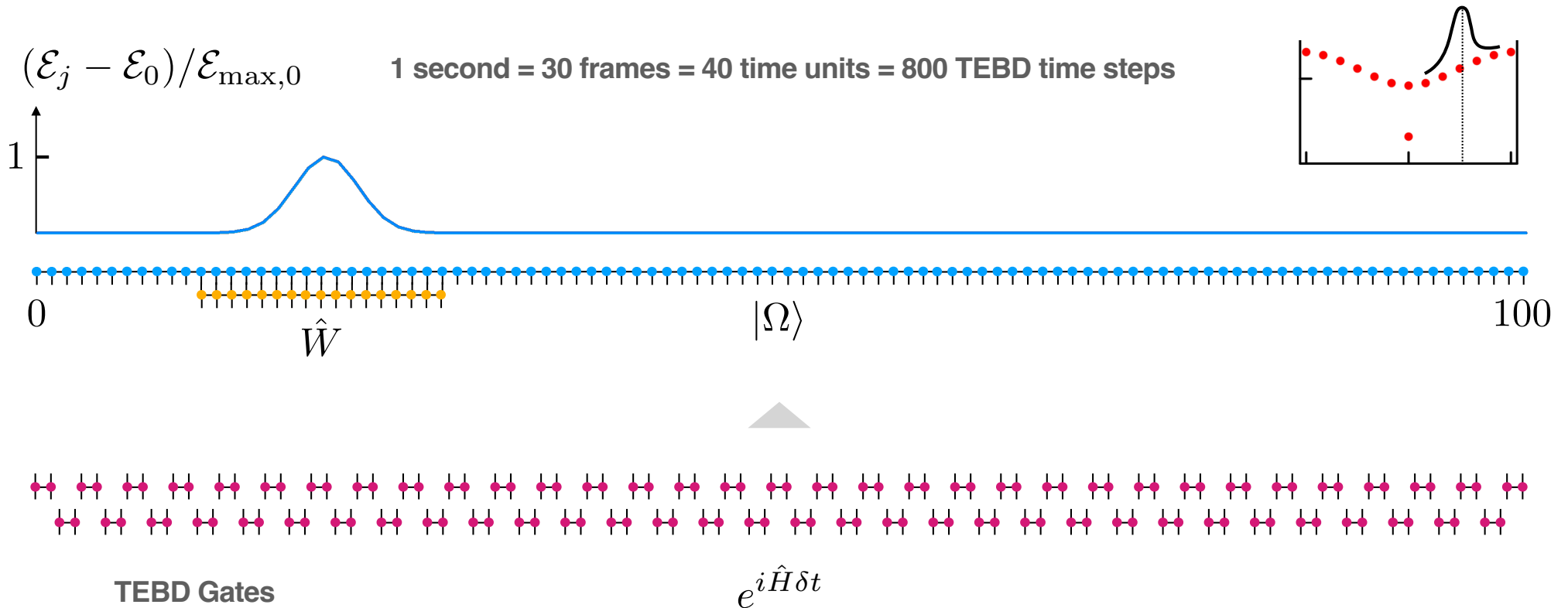
$\chi_{\max} = 200$   
 $n_{\text{sweeps}} = 50$   
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## Wavepacket parameters

$\sigma = 3a$   
 $k = \pi/2a$   
 $j_0 = 20$

## TEBD parameters

$\delta t = 0.05$   
 $\Delta t = 400$   
 $\epsilon_{\text{SVD}} = 10^{-10}$   
 $\chi_{\max} = 50$



## 6. Numerical simulations

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(Dirichlet OBC)

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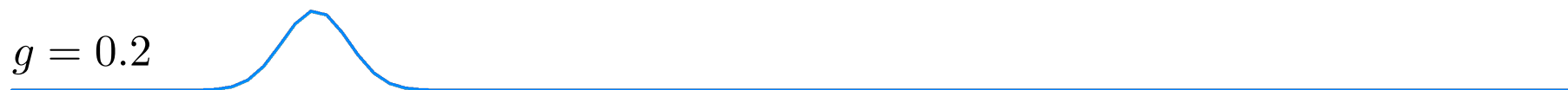
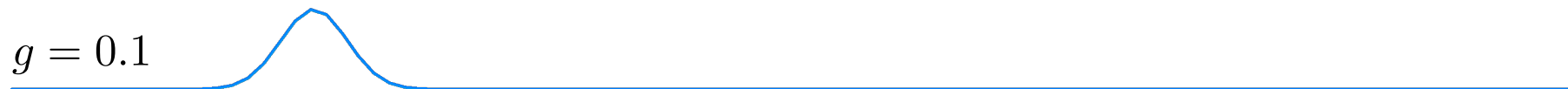
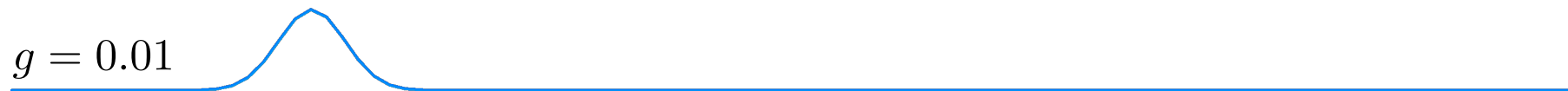
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## 6. Numerical simulations

### System parameters

$$a = 1$$
$$L = 100$$
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(Dirichlet OBC)

### DMRG parameters

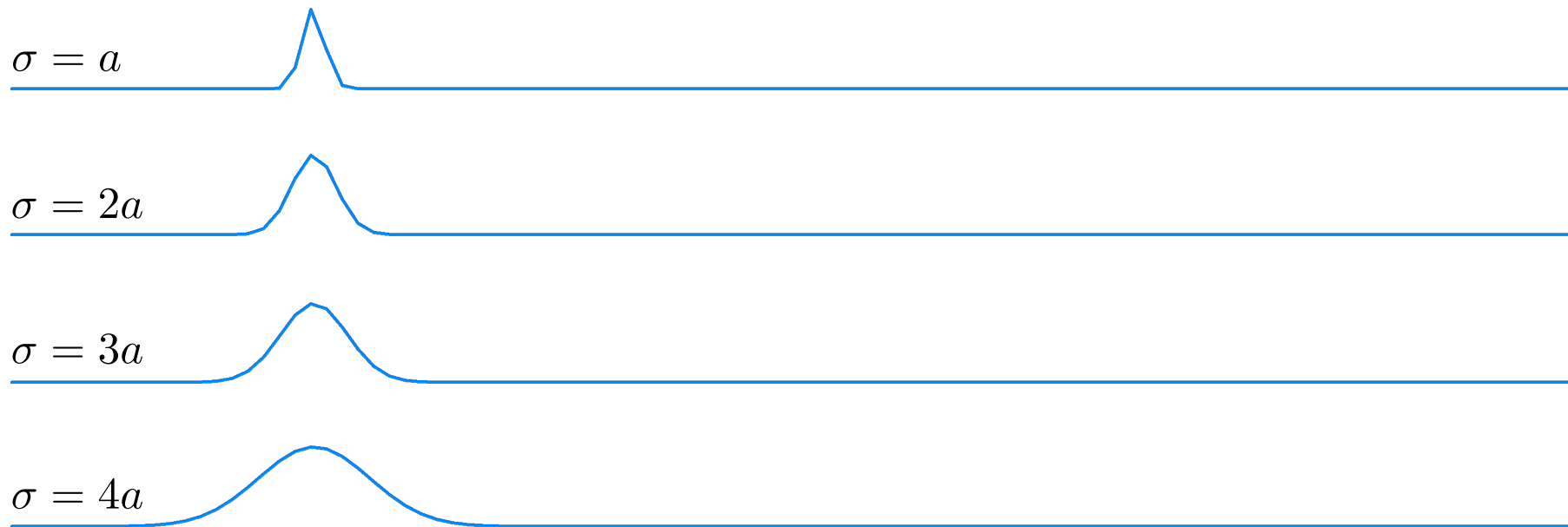
$$\chi_{\max} = 200$$
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$$\sigma = 3a$$
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### TEBD parameters

$$\delta t = 0.05$$
$$\Delta t = 400$$
$$\epsilon_{\text{SVD}} = 10^{-10}$$
$$\chi_{\max} = 50$$



## 6. Numerical simulations

### System parameters

$$\begin{aligned} a &= 1 \\ L &= 100 \\ g^4 &= 0.1 \\ &\text{(Dirichlet OBC)} \end{aligned}$$

### DMRG parameters

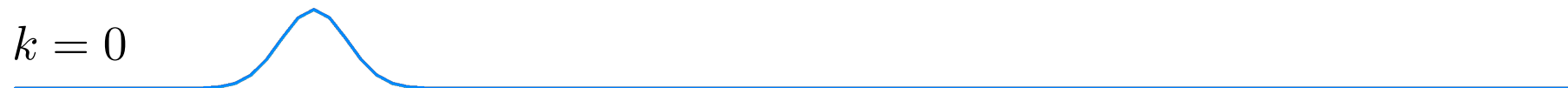
$$\begin{aligned} \chi_{\max} &= 200 \\ n_{\text{sweeps}} &= 50 \\ \epsilon_{\text{SVD}} &= 10^{-13} \end{aligned}$$

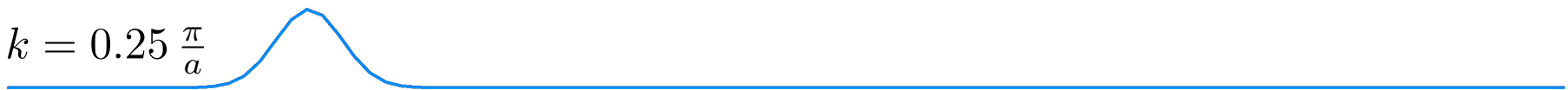
### Wavepacket parameters

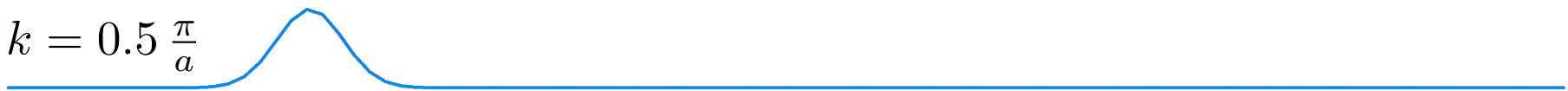
$$\begin{aligned} \sigma &= 3a \\ k &= \pi/2a \\ j_0 &= 20 \end{aligned}$$

### TEBD parameters

$$\begin{aligned} \delta t &= 0.05 \\ \Delta t &= 400 \\ \epsilon_{\text{SVD}} &= 10^{-10} \\ \chi_{\max} &= 50 \end{aligned}$$

$$k = 0$$


$$k = 0.25 \frac{\pi}{a}$$


$$k = 0.5 \frac{\pi}{a}$$




# 6. Numerical simulations

## System parameters

$$a = 1$$
$$L = 100$$
$$g^4 = 0.1$$

(Dirichlet OBC)

## DMRG parameters

$$\chi_{\max} = 200$$
$$n_{\text{sweeps}} = 50$$
$$\epsilon_{\text{SVD}} = 10^{-13}$$

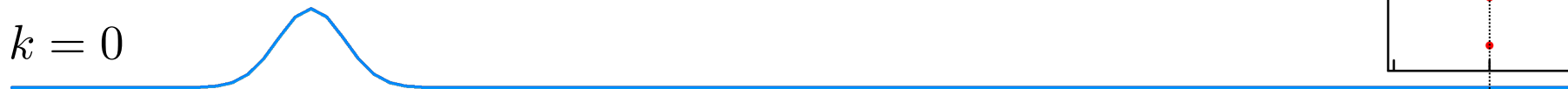
## Wavepacket parameters

$$\sigma = 3a$$
$$k = \pi/2a$$
$$j_0 = 20$$

## TEBD parameters

$$\delta t = 0.05$$
$$\Delta t = 400$$
$$\epsilon_{\text{SVD}} = 10^{-10}$$
$$\chi_{\max} = 50$$

$$k = 0$$

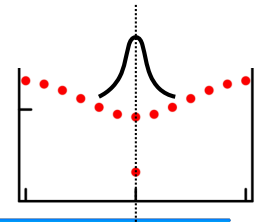
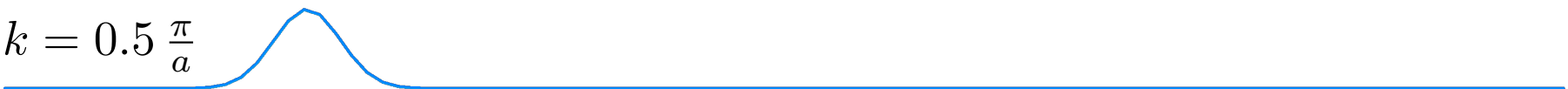


maximum dispersion (curvature), null group velocity

$$k = 0.25 \frac{\pi}{a}$$



$$k = 0.5 \frac{\pi}{a}$$



# 6. Numerical simulations

## System parameters

$$a = 1$$
$$L = 100$$
$$g^4 = 0.1$$

(Dirichlet OBC)

## DMRG parameters

$$\chi_{\max} = 200$$
$$n_{\text{sweeps}} = 50$$
$$\epsilon_{\text{SVD}} = 10^{-13}$$

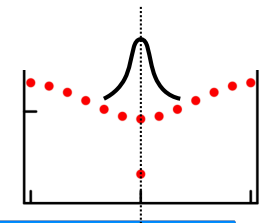
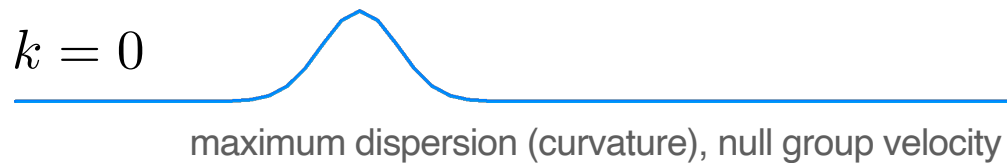
## Wavepacket parameters

$$\sigma = 3a$$
$$k = \pi/2a$$
$$j_0 = 20$$

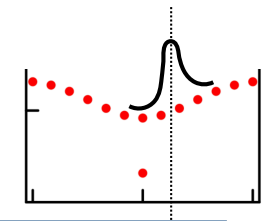
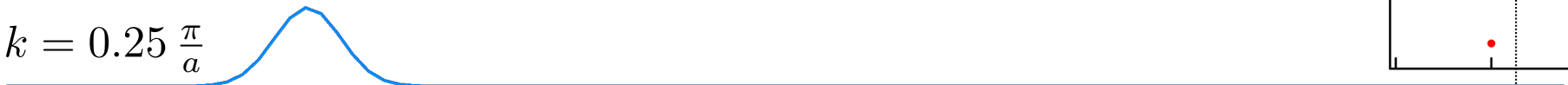
## TEBD parameters

$$\delta t = 0.05$$
$$\Delta t = 400$$
$$\epsilon_{\text{SVD}} = 10^{-10}$$
$$\chi_{\max} = 50$$

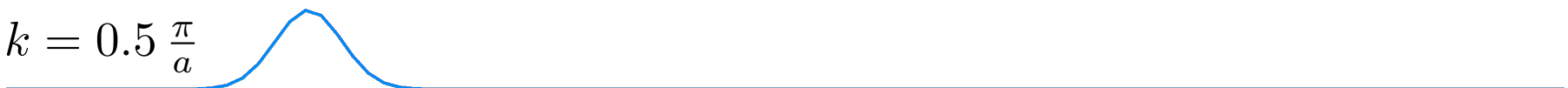
$$k = 0$$



$$k = 0.25 \frac{\pi}{a}$$



$$k = 0.5 \frac{\pi}{a}$$



# 6. Numerical simulations

## System parameters

$$a = 1$$

$$L = 100$$

$$g^4 = 0.1$$

(Dirichlet OBC)

## DMRG parameters

$$\chi_{\max} = 200$$

$$n_{\text{sweeps}} = 50$$

$$\epsilon_{\text{SVD}} = 10^{-13}$$

## Wavepacket parameters

$$\sigma = 3a$$

$$k = \pi/2a$$

$$j_0 = 20$$

## TEBD parameters

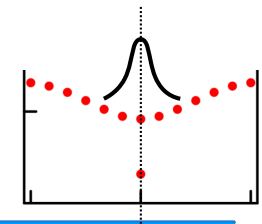
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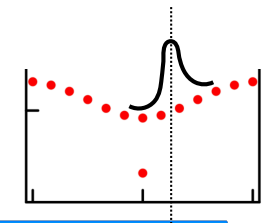
$$\epsilon_{\text{SVD}} = 10^{-10}$$

$$\chi_{\max} = 50$$

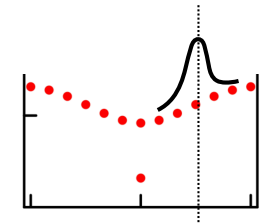
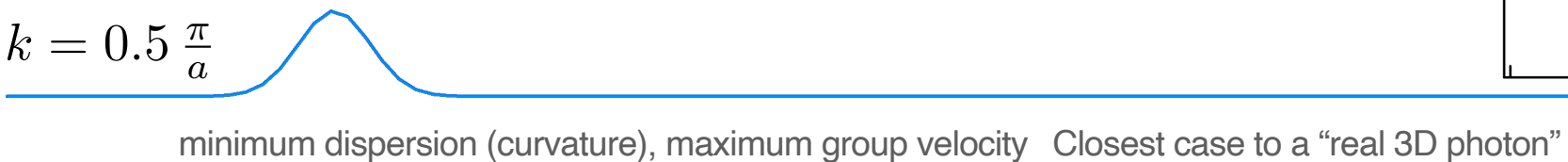
$$k = 0$$



$$k = 0.25 \frac{\pi}{a}$$

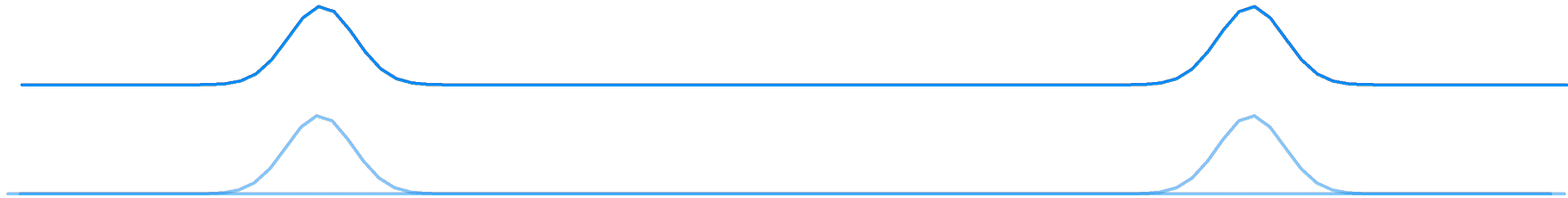


$$k = 0.5 \frac{\pi}{a}$$



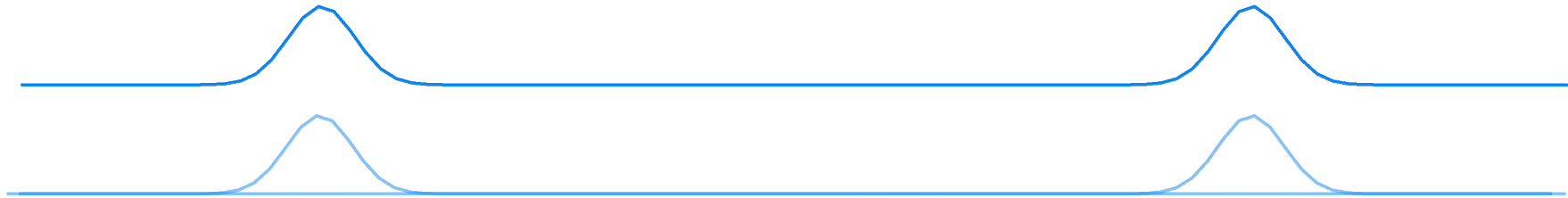
## 6. Numerical simulations

$$\sigma = 3a \quad k = \pi/2a$$



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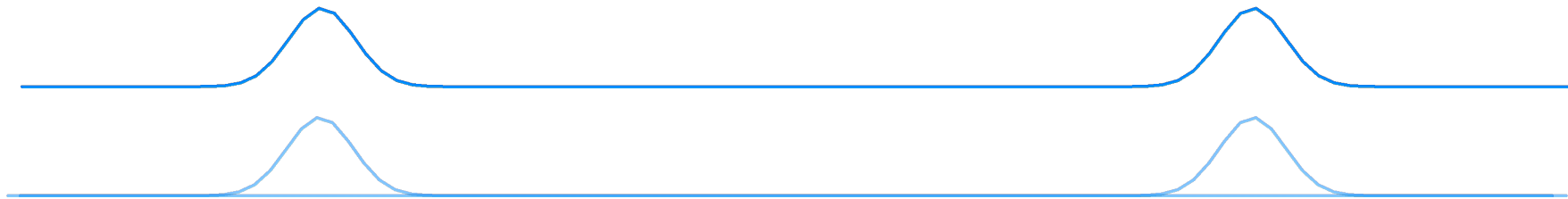
$$\sigma = 3a \quad k = \pi/2a$$



Nothing happens: **good**, they are like photons, but **bad**, it's boring like this!

## 6. Numerical simulations

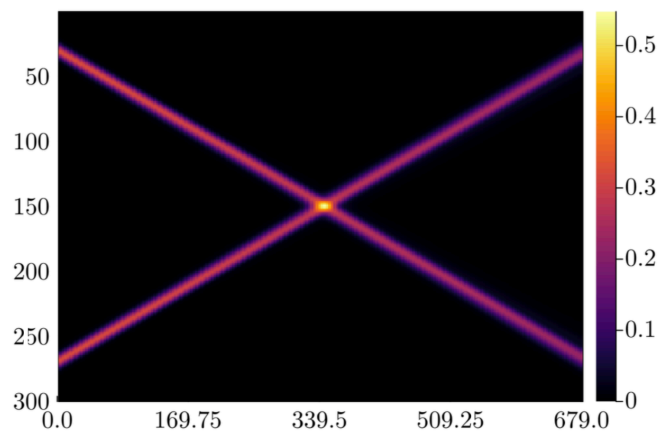
$$\sigma = 3a \quad k = \pi/2a$$



Nothing happens: **good**, they are like photons, but **bad**, it's boring like this!

It becomes less and less interacting as we approach the continuum limit:

Energy density

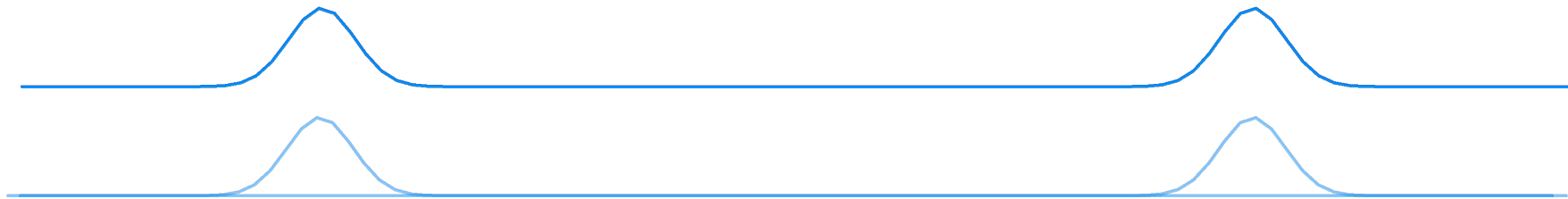


$$L = 300$$

$$\sigma = 5a$$

## 6. Numerical simulations

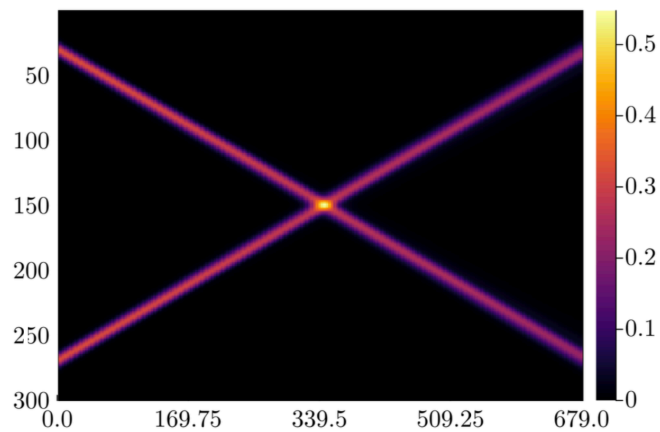
$$\sigma = 3a \quad k = \pi/2a$$



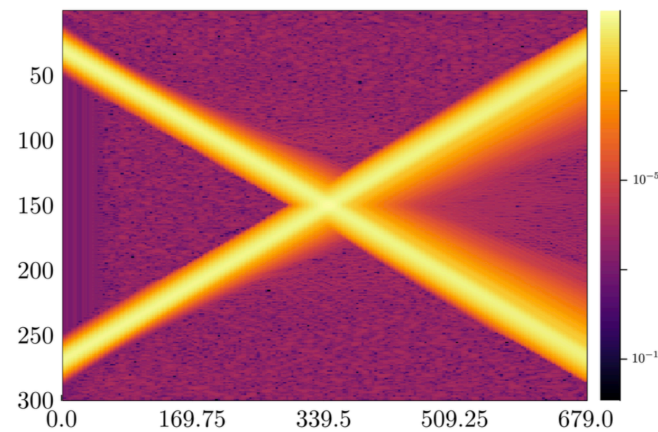
Nothing happens: **good**, they are like photons, but **bad**, it's boring like this!

It becomes less and less interacting as we approach the continuum limit:

Energy density



Energy density in log



$$L = 300$$

$$\sigma = 5a$$

**Interaction effects:**

- **Lattice** artifacts
- **Finite size** effects
- **1D** lattice geometry

## | 7. Conclusions

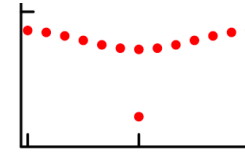


## 7. Conclusions

- Inputs  $\hat{H}, \hat{T}$  plus **few assumptions** (model independent)

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# 7. Conclusions

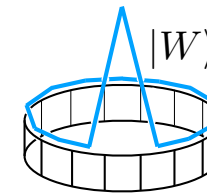
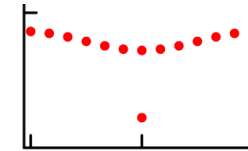
● Inputs  $\hat{H}, \hat{T}$  plus **few assumptions** (model independent)

1 Simultaneous exact diagonalization, finding the Bloch states

$$[\hat{H}, \hat{T}] = 0 \quad \text{Computationally expensive step: intermediate system size}$$

2 Computation of the maximally localized Wannier states

$$|W(\theta_k)\rangle = \frac{1}{\sqrt{L}} \sum_k e^{i\theta_k} |k\rangle$$



# 7. Conclusions

Inputs  $\hat{H}, \hat{T}$  plus **few assumptions** (model independent)

**1** Simultaneous exact diagonalization, finding the Bloch states

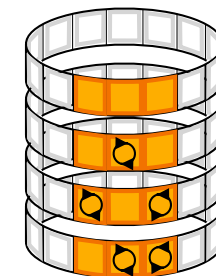
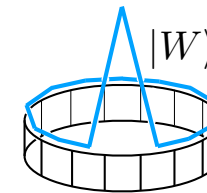
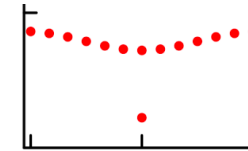
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**3** Construction of the Wannier creation operator

$$\hat{W}|\Omega\rangle = |W\rangle \quad \text{From the interacting vacuum}$$



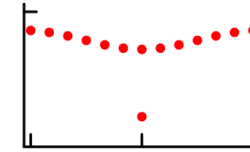
$$\begin{aligned} & c_1 \mathbb{I} \\ & + c_2 \hat{U}_{\square,2}^\dagger \\ & + c_3 \hat{U}_{\square,1}^\dagger \hat{U}_{\square,3} \\ & + c_3 \hat{U}_{\square,2}^\dagger \hat{U}_{\square,3} \end{aligned}$$

# 7. Conclusions

Inputs  $\hat{H}, \hat{T}$  plus **few assumptions** (model independent)

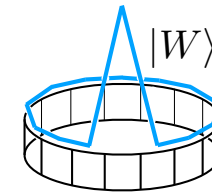
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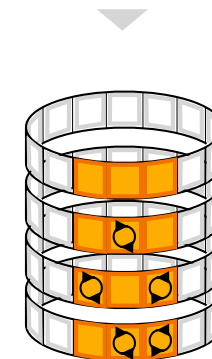
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**4 Construction of the Wavepacket creation operator**

$$\hat{\Phi} = \sum_j \phi_j \hat{W}_j \quad \text{We mostly choose a gaussian wavepacket}$$

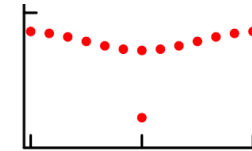
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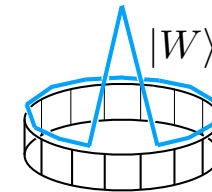
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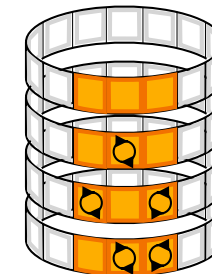
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$$c_1 \mathbb{I} + c_2 \hat{U}_{\square,2}^\dagger + c_3 \hat{U}_{\square,1}^\dagger \hat{U}_{\square,3} + c_3 \hat{U}_{\square,2}^\dagger \hat{U}_{\square,3}$$

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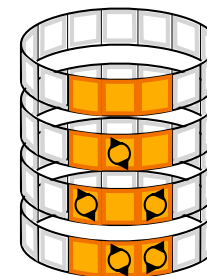
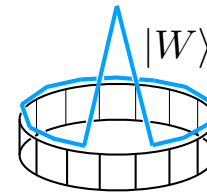
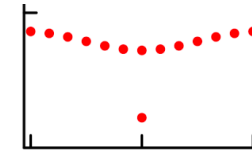


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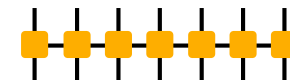
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- 5 Conversion of the Wavepacket creation operator to an MPO
- Output: the MPO



$$\begin{aligned}
 &c_1 \mathbb{I} \\
 &+ c_2 \hat{U}_{\square,2}^\dagger \\
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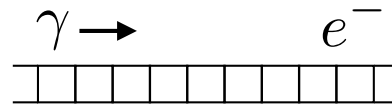
## | 8. Outlook



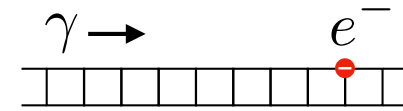
## 8. Outlook

$(1, 1), (\frac{3}{2}, 2), \dots$

**Higher spin  
representations**



**Adding matter d.o.f**



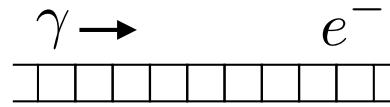
**Background charge**



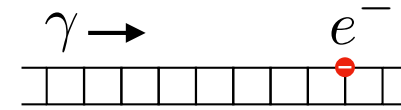
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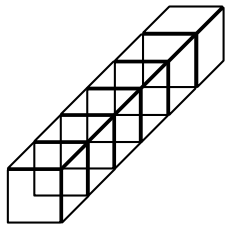
**Higher spin representations**



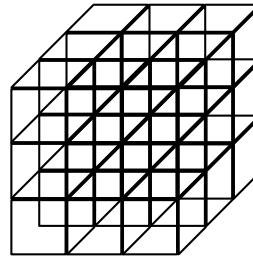
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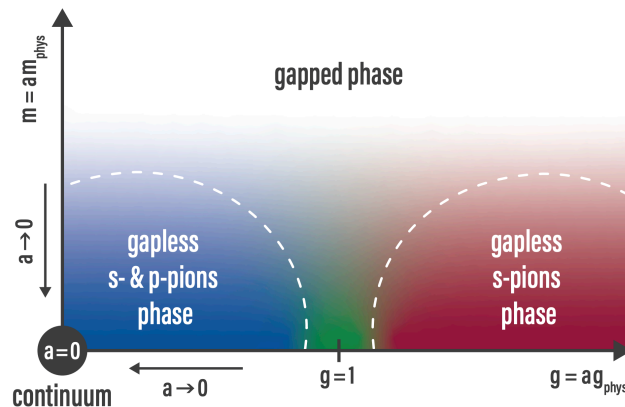
**Different geometries**



**Higher dimension**

$$\begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$$

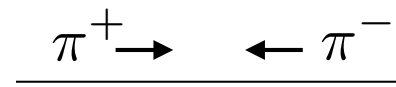
**Try to overcome exact diagonalization**



arXiv:2308.04488

**Last but not least**

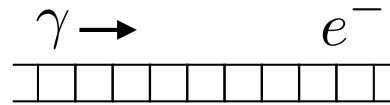
moving to **1D QCD with two flavors**,  
simulating **pion-pion scattering**



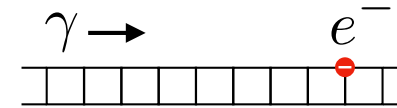
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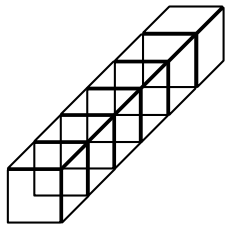
**Higher spin representations**



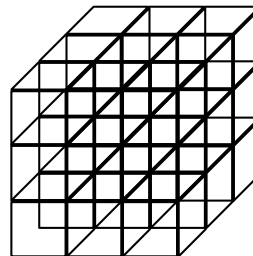
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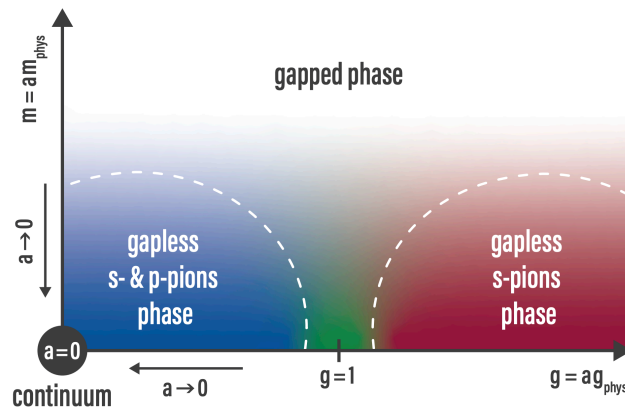
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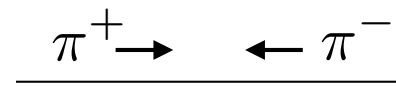
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moving to **1D QCD with two flavors**,  
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**Challenge:  $d = 54$  local dimension**



UNIVERSITÀ  
DEGLI STUDI  
DI PADOVA



Dipartimento  
di Fisica  
e Astronomia  
Galileo Galilei



QUANTUM  
Information and Matter



QUANTUM  
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ICSC

Centro Nazionale di Ricerca in HPC,  
Big Data and Quantum Computing



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COMPUTING  
AND  
SIMULATION  
CENTER



QuantHEP

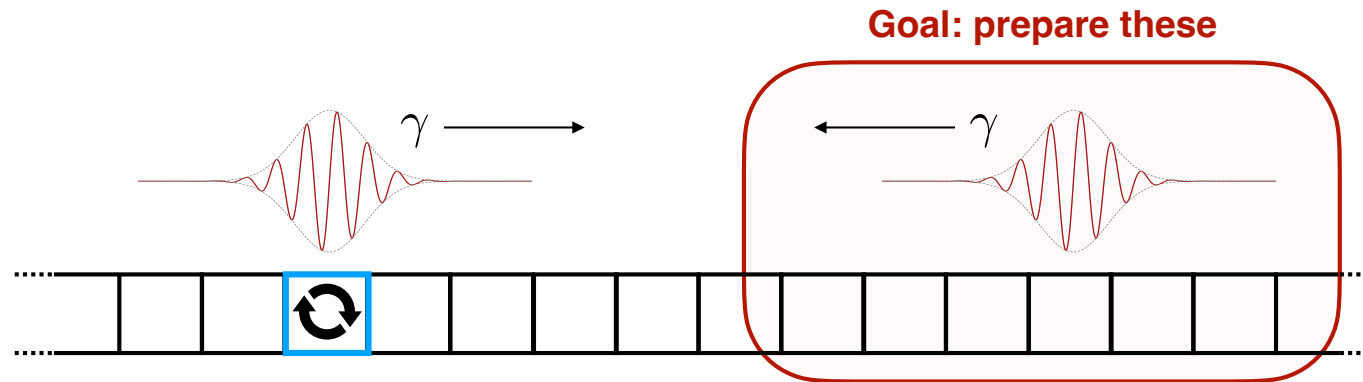
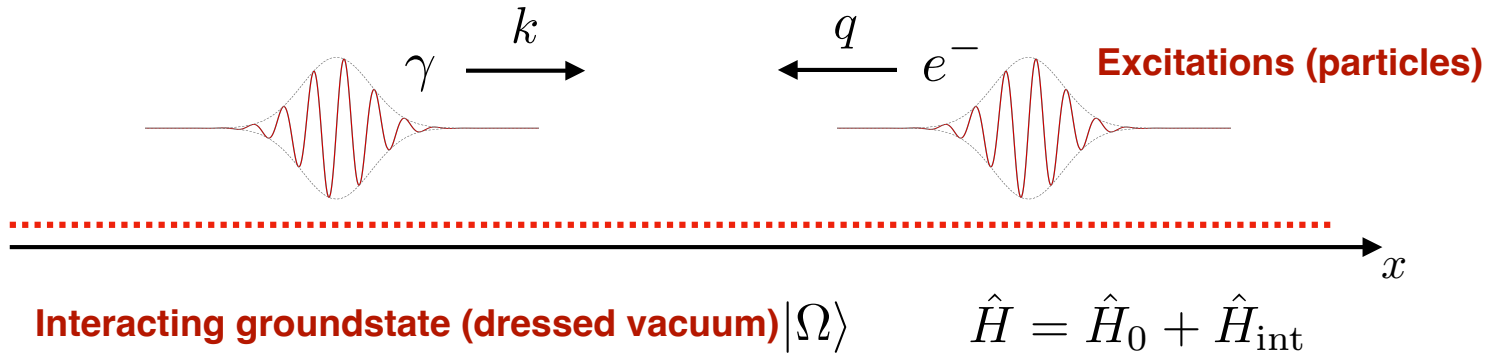


T-NISQ

Tensor Networks in Simulation of Quantum Matter



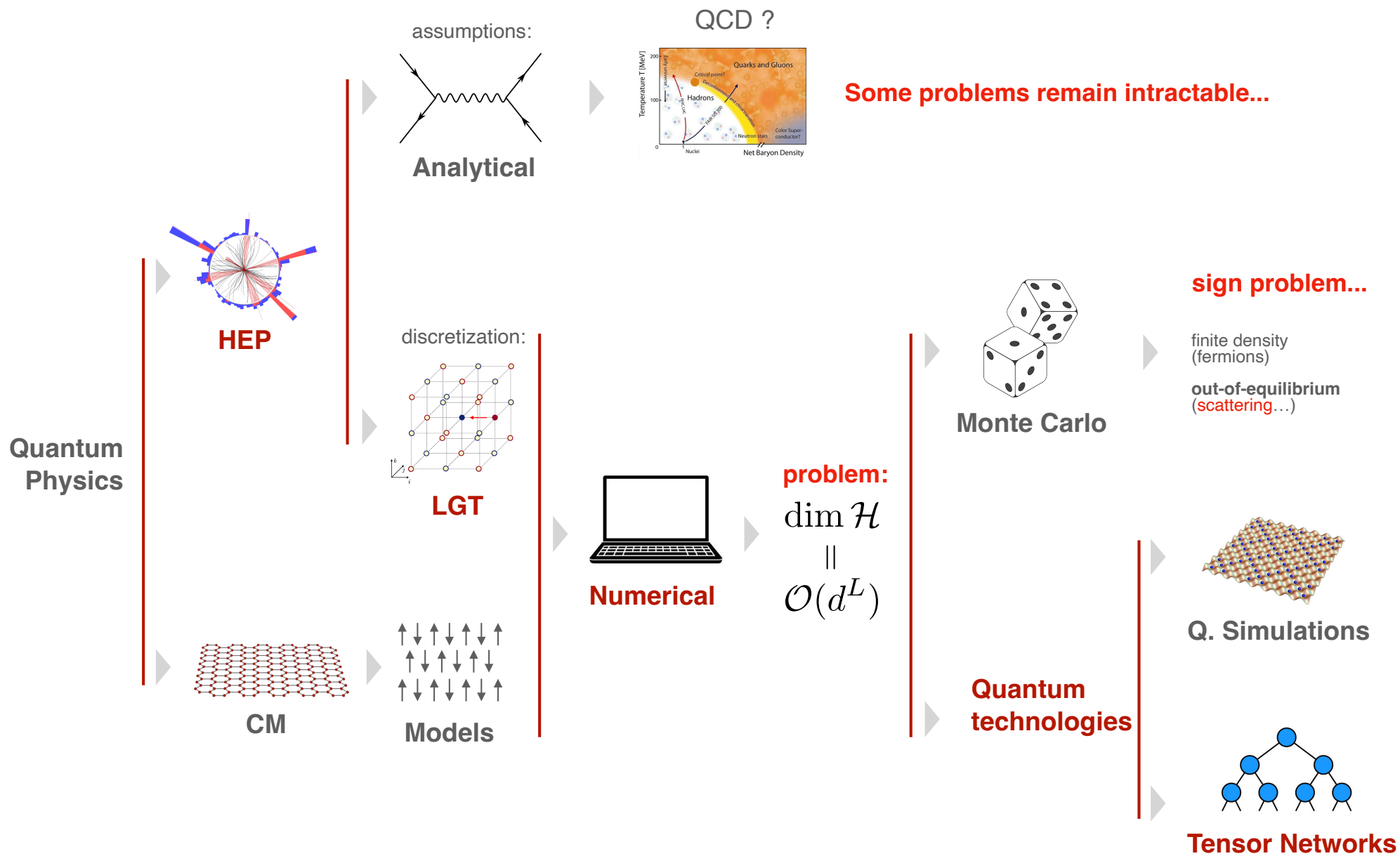
# Introduction



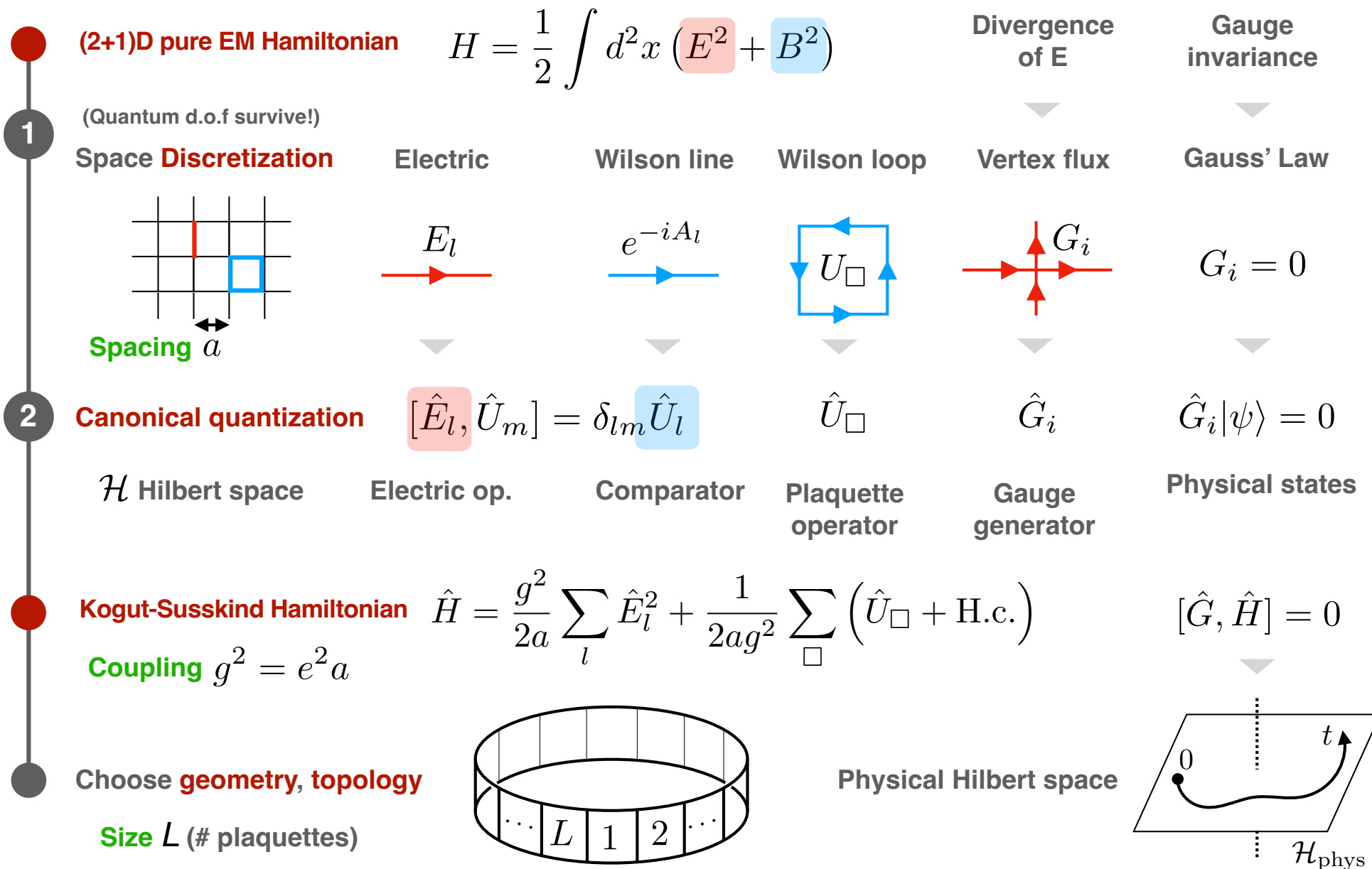
Toy Model: (quasi)-1D Hamiltonian Lattice Pure Quantum Electro Dynamics on Ladder Geometries



# Motivation: problems and solutions



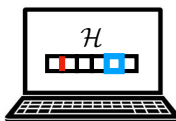
# 1. Theoretical background





# 1. Theoretical background

To simulate  $\mathcal{H}$  



We want  $\mathcal{H}$  **finite**-dimensional!

**U(1) Lattice QED**

**U(1) Quantum Link Model (QLM)**

$\forall$  link Hilbert space  $\mathcal{H}_{\text{link}}$

SU(2) irreducible representations  $s \in \mathbb{N}/2$

Operators  $\left\{ \begin{array}{l} \hat{E} \\ \hat{U} \\ \hat{U}^\dagger \end{array} \right.$

$\hat{S}^z$

$\hat{S}^+ / s$

$\hat{S}^- / s$

Arrow notation

$\longrightarrow$   $s_z = 1/2$

$\longrightarrow\longrightarrow$   $s_z = 1$

$\longrightarrow\longrightarrow\longrightarrow$   $s_z = 3/2$

$\vdots$

$\sigma(\hat{E})$

$\sigma(\hat{S}^z) = \{-s, \dots, s\}$  **finite!** ✓

CCR  $[\hat{E}, \hat{U}] = \hat{U}$

$[\hat{S}^z, \hat{S}^+] = \hat{S}^+$  ✓

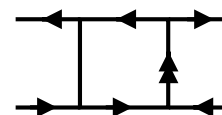
Unitarity  $\hat{U}\hat{U}^\dagger = \mathbb{I}$

$\hat{S}^+ \hat{S}^- / s^2 \rightarrow \mathbb{I}$  ✓

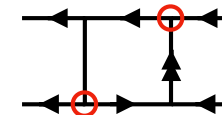
**Kogut - Susskind limit**  $s \rightarrow \infty$

Gauge generator  $\hat{G}$

$\hat{S}_i^z + \hat{S}_k^z - \hat{S}_j^z$



Allowed ✓



Not allowed ✗

## 2. The pure Lattice QED on ladder geometry

### Spin representation

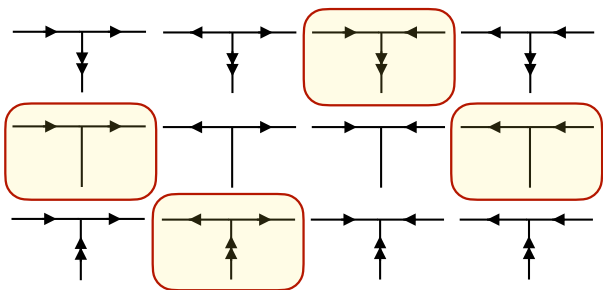
Translation and reflection inv.



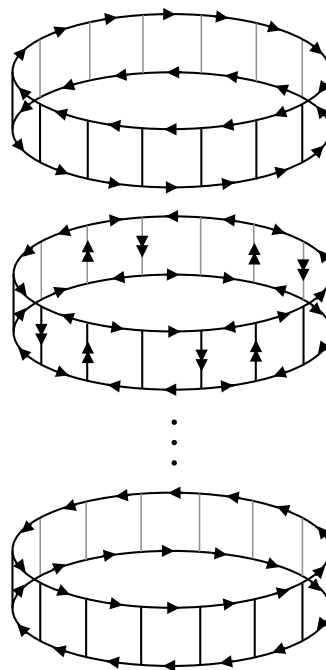
Lowest spin irrep assignments which admits gauge inv. configs:



### Gauss' Law on vertices



### $L$ plaquettes ladder in PBC

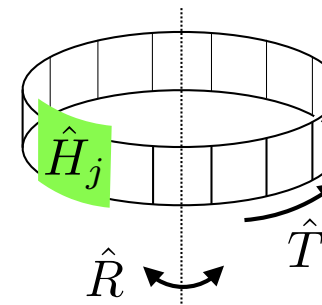


$$\dim \mathcal{H} = 2^L + 2$$

↑  
Exp scaling

### Construct operators

Computational basis

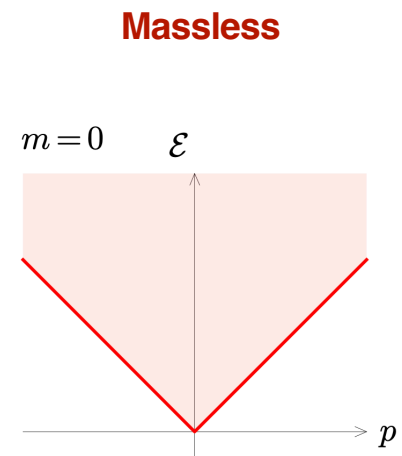
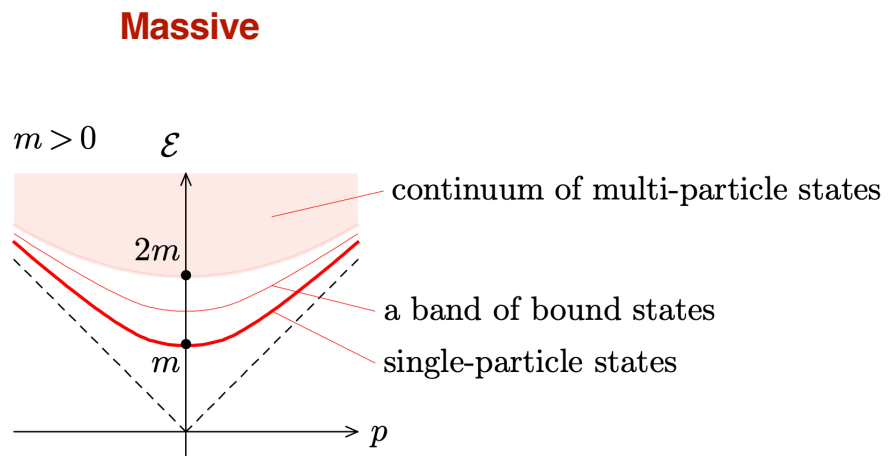


$$[\hat{H}, \hat{T}] = 0$$

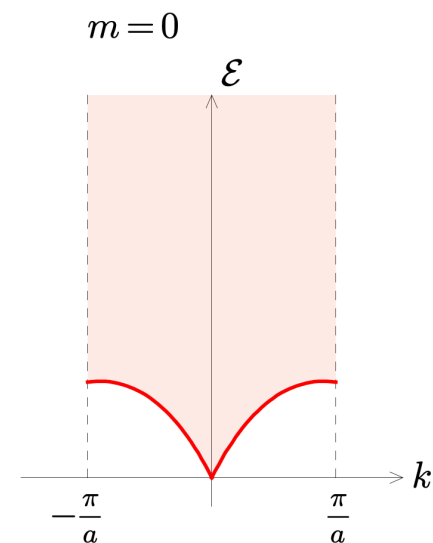
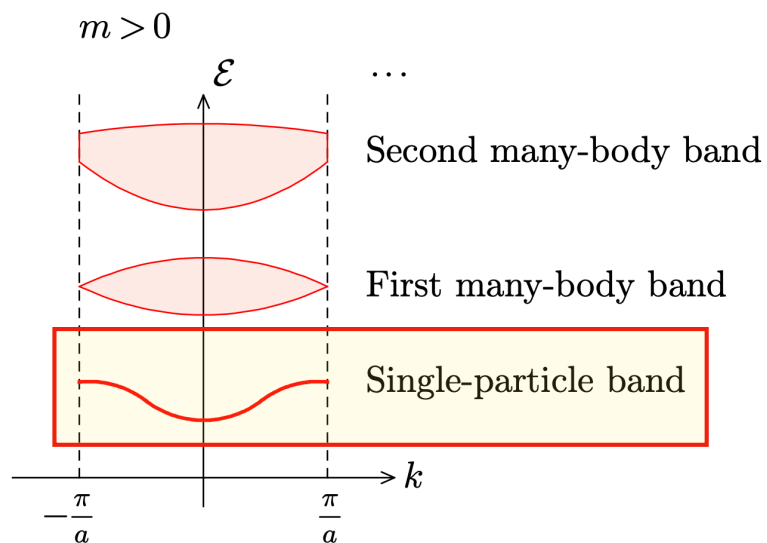
**Dispersion relation!**

## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$

**Continuum**



**Lattice**



## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$

**Assuming**

$[\hat{H}, \hat{T}] = 0$  Translational invar. (PBC)

$L = 13$  Intermediate system size

$\frac{1}{2} \square 1$  Lowest spin rep.

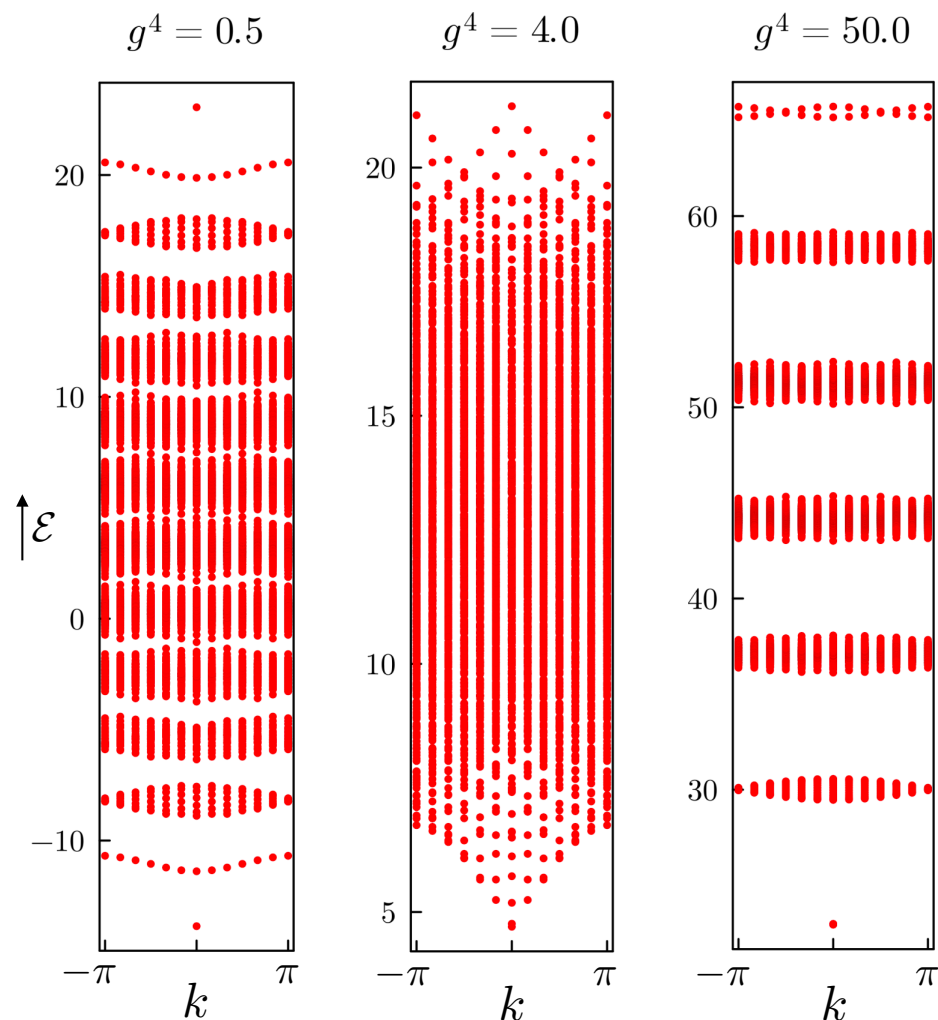
$a = 1$  Unit lattice spacing

(varying the coupling  $g$ )

**Simultaneous *exact* diagonalization  
(computationally difficult step)**

$\dim \mathcal{H} = 8194$

**Dispersion relation  
in our (interacting!) model:**

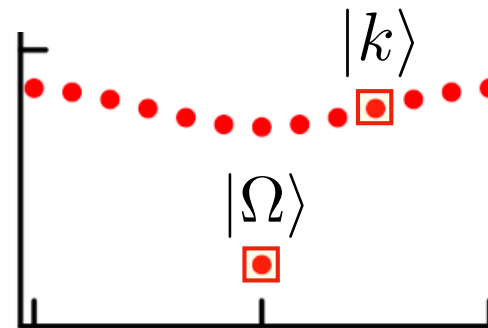
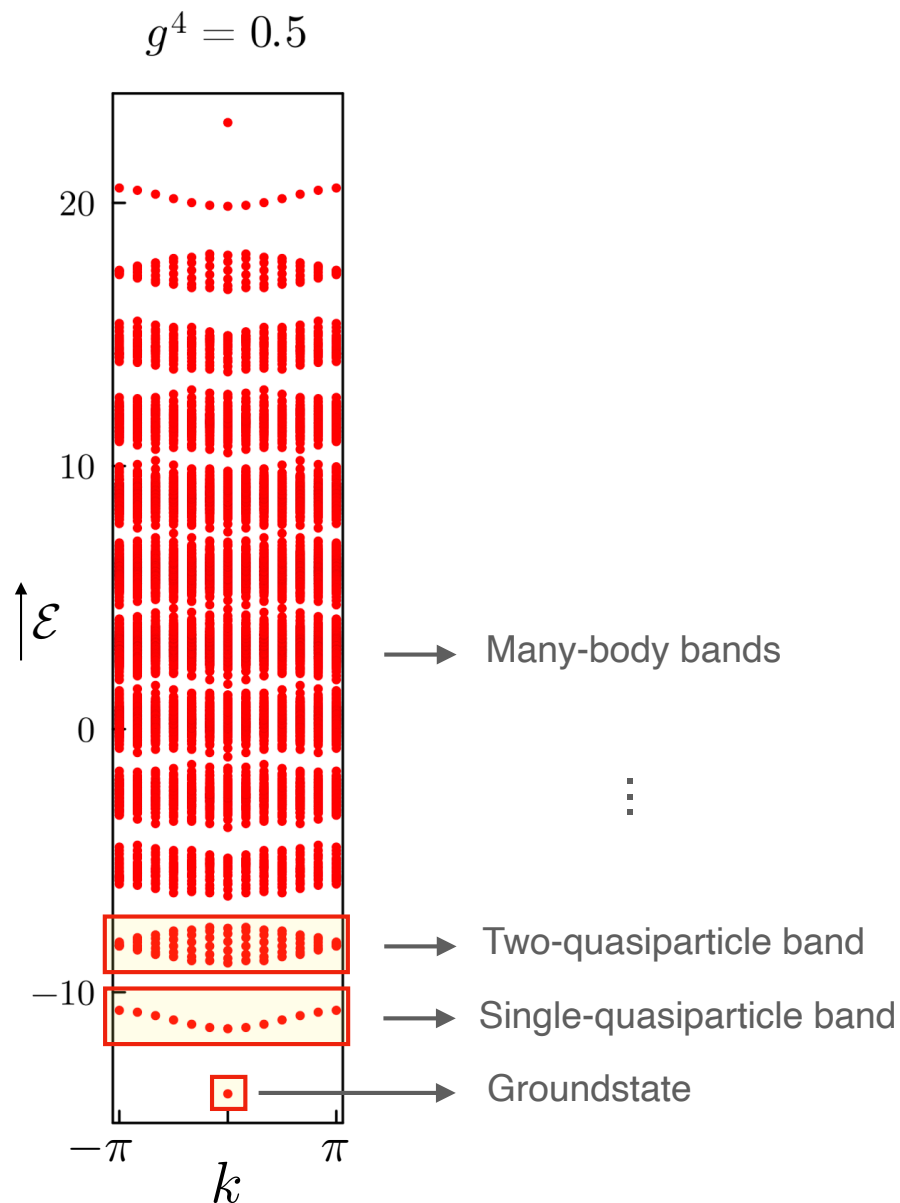


Gapped phase  
(massive photon)

Critical point  
(massless photon)

Gapped SSB phase  
(degenerate g.s.)

## 2. The pure Lattice QED on ladder geometry $(\frac{1}{2}, 1)$



**Program**

$$|\phi\rangle = \sum a_k |k\rangle$$

Single-particle state  
(Bloch basis)

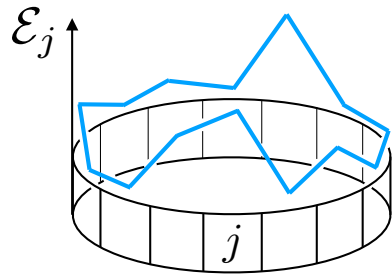
Wannier Functions  
(real-space basis)

Wave-packet state

# 3. Construction of the wavepackets

## Wannier states

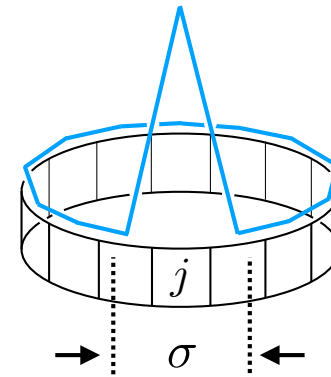
$$|W(\theta_k)\rangle = \frac{1}{\sqrt{L}} \sum_k e^{i\theta_k} |k\rangle$$



## Maximally localized Wannier states

$$|W_j\rangle \equiv |W_j(\bar{\theta})\rangle$$

$\theta \rightarrow \bar{\theta}$   
Minimize  $\sigma^2$



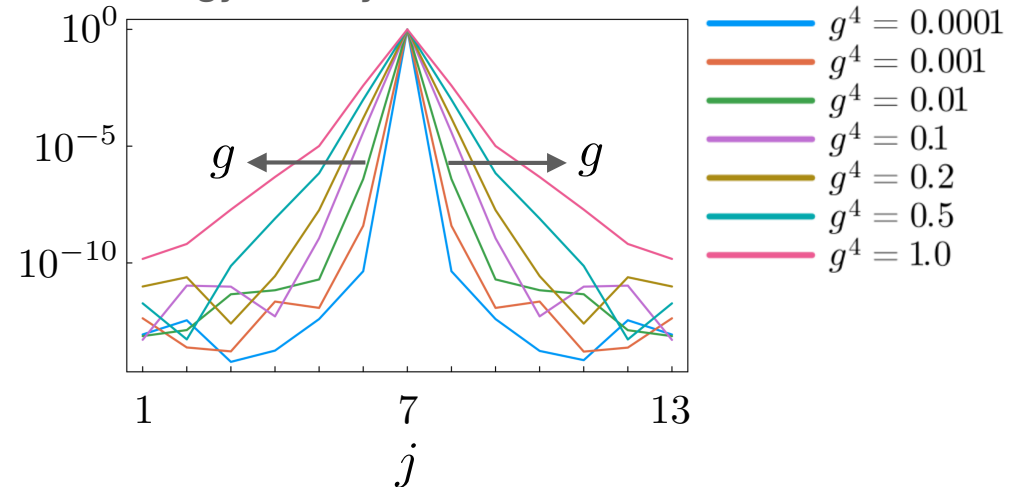
## Energy density

$$\mathcal{E}_j[\phi] = \langle \phi | \hat{H}_j | \phi \rangle$$

## Spread functional

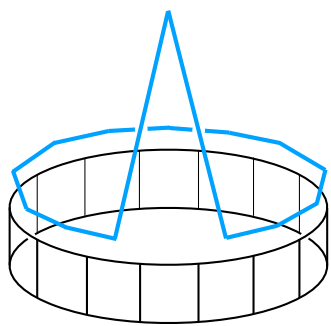
$$\sigma^2[\phi] \equiv \frac{\sum_j j^2 \mathcal{E}_j[\phi]}{\sum_j \mathcal{E}_j[\phi]} - \left( \frac{\sum_j j \mathcal{E}_j[\phi]}{\sum_j \mathcal{E}_j[\phi]} \right)^2$$

## Energy density after minimization



# 3. Construction of the wavepackets

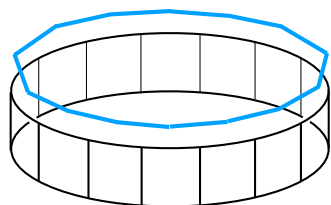
Wannier creation operator



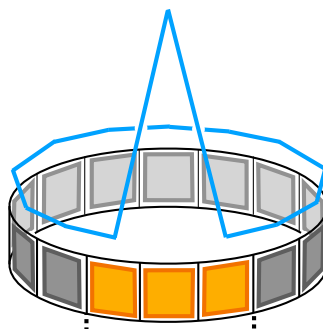
$$\hat{W}|\Omega\rangle = |W\rangle$$

||

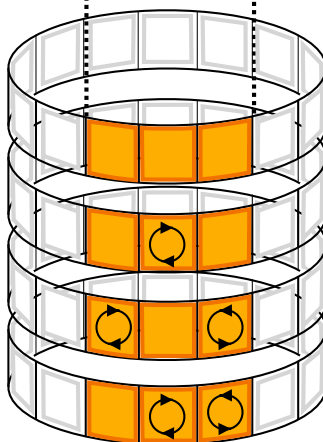
$|\Omega\rangle$  Interacting!



Wannier creation ansatz



$W$

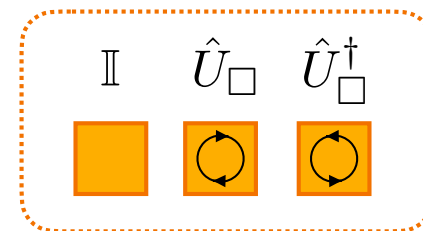


$$\begin{aligned}
 & c_1 \mathbb{I} \\
 & + c_2 \hat{U}_{\square,2}^\dagger \\
 & + c_3 \hat{U}_{\square,1}^\dagger \hat{U}_{\square,3} \\
 & + c_3 \hat{U}_{\square,2}^\dagger \hat{U}_{\square,3}
 \end{aligned}$$

$$\hat{W} = \sum_{\alpha_1 \dots \alpha_w} c_{\alpha_1 \dots \alpha_w} L_{\alpha_1} \dots L_{\alpha_w}$$

Interpolation

choose  $L_\alpha$



Minimize

$$\left| \hat{W}(c)|\Omega\rangle - |W\rangle \right|^2$$

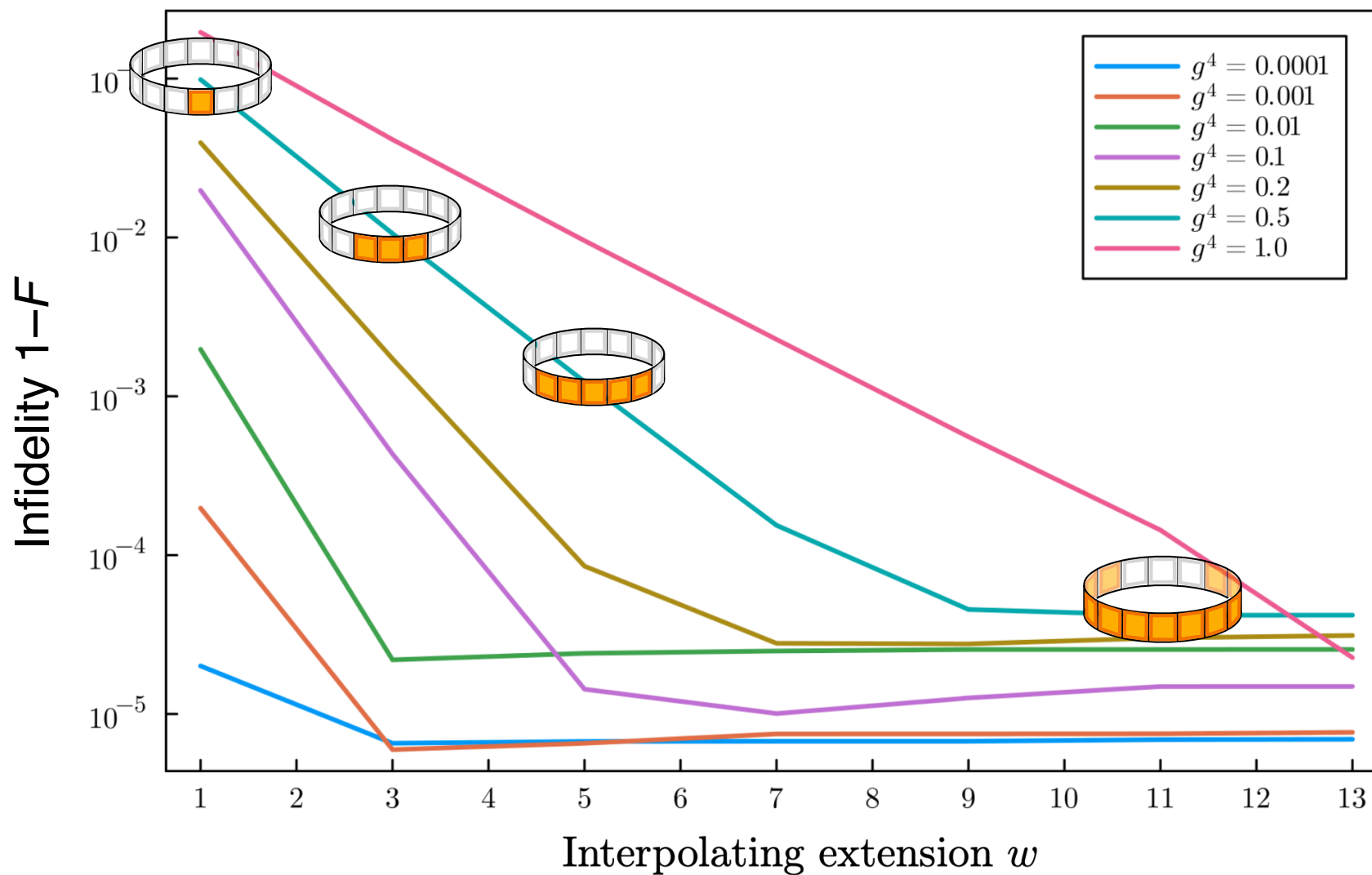


Linear system

$$Ac = b$$

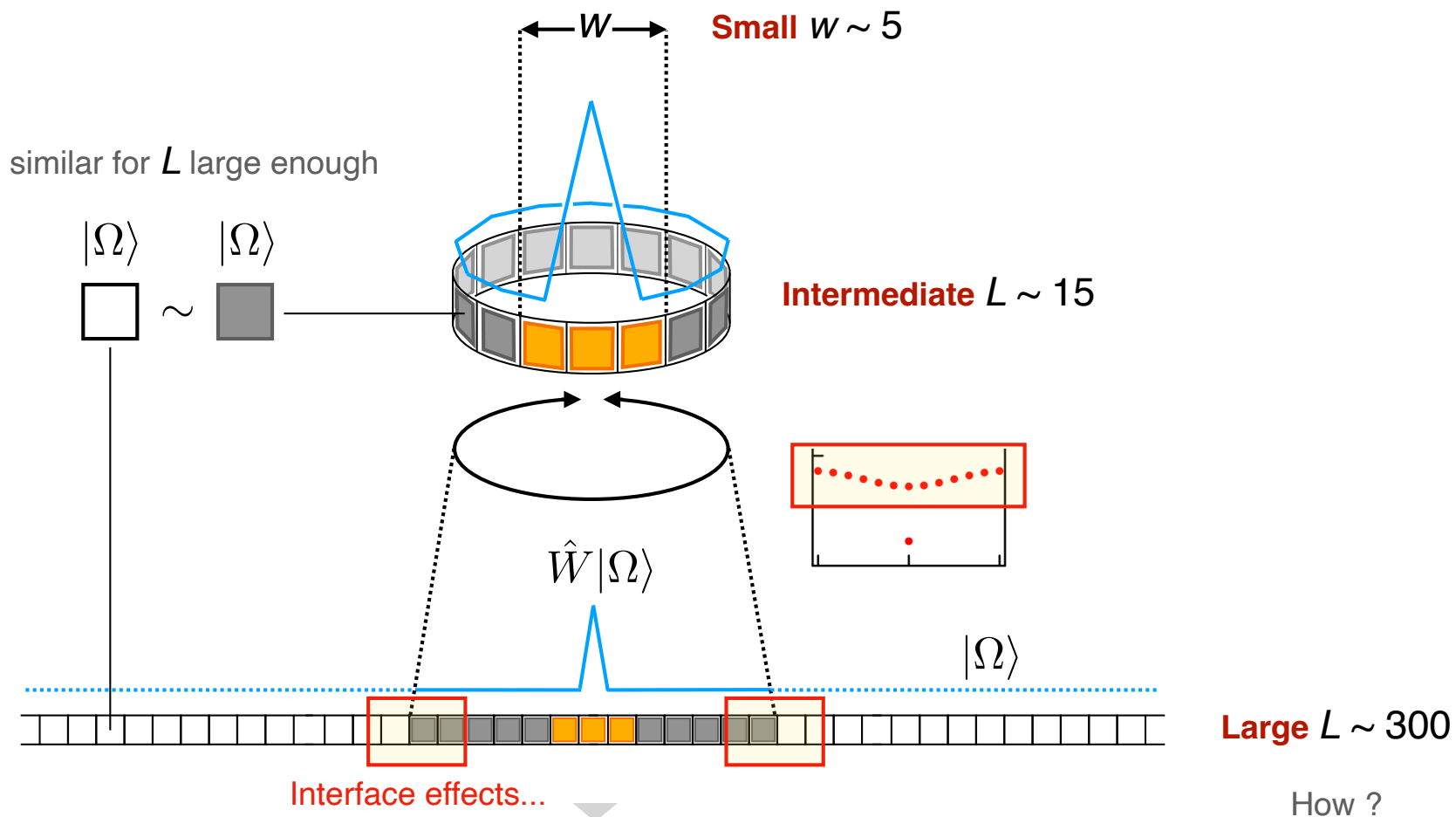
### 3. Construction of the wavepackets

Infidelity of the interpolation of the Wannier state  $|W_7\rangle$ ,  $L = 13$





### 3. Construction of the wavepackets



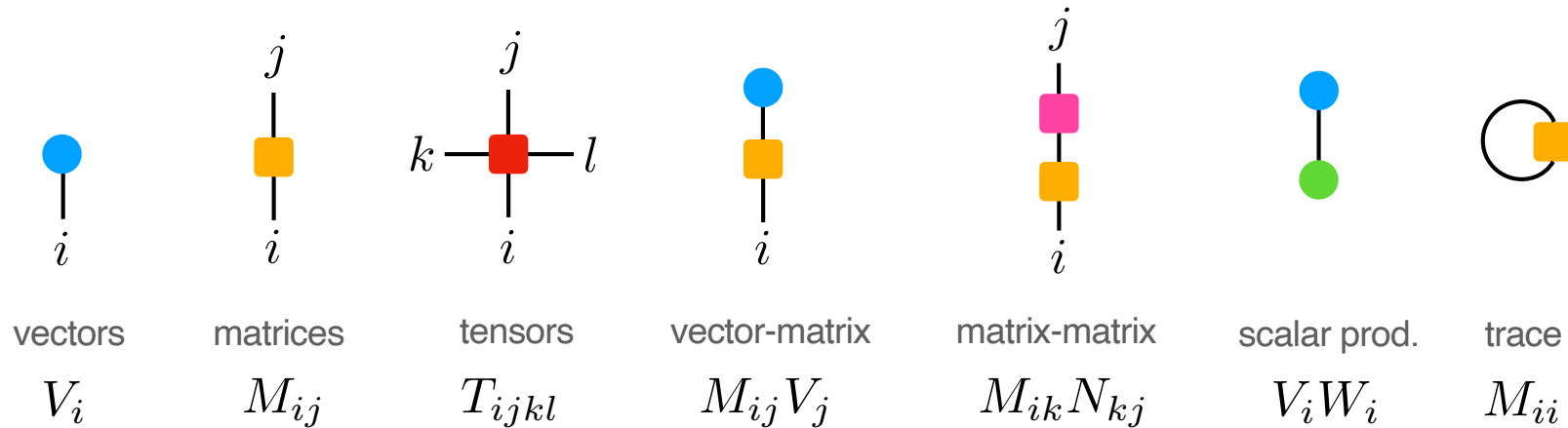
(On top of the interacting vacuum)

$$|W_j\rangle = T^j |W_0\rangle$$

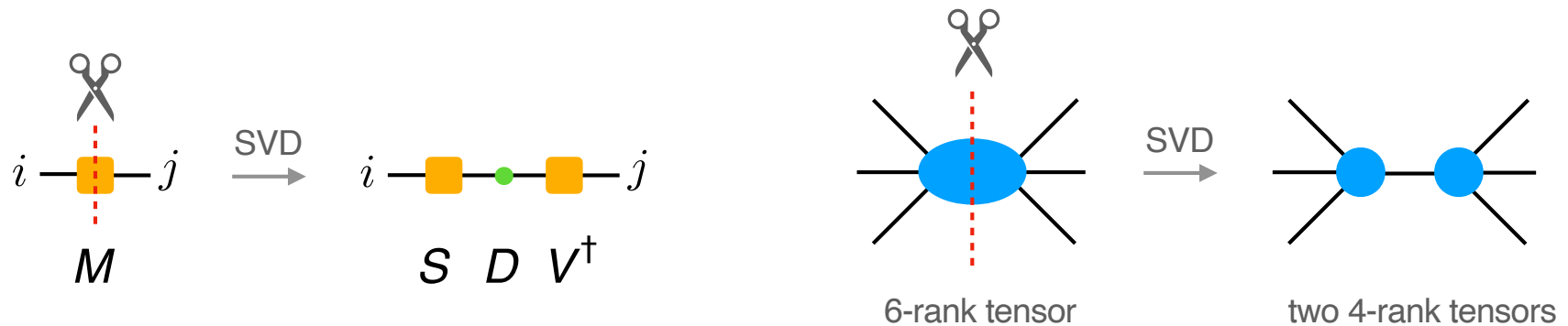
Wannier function  $\rightarrow$  **building blocks** to construct any single-(quasi)particle state.

# 4. Tensor Network methods in a nutshell

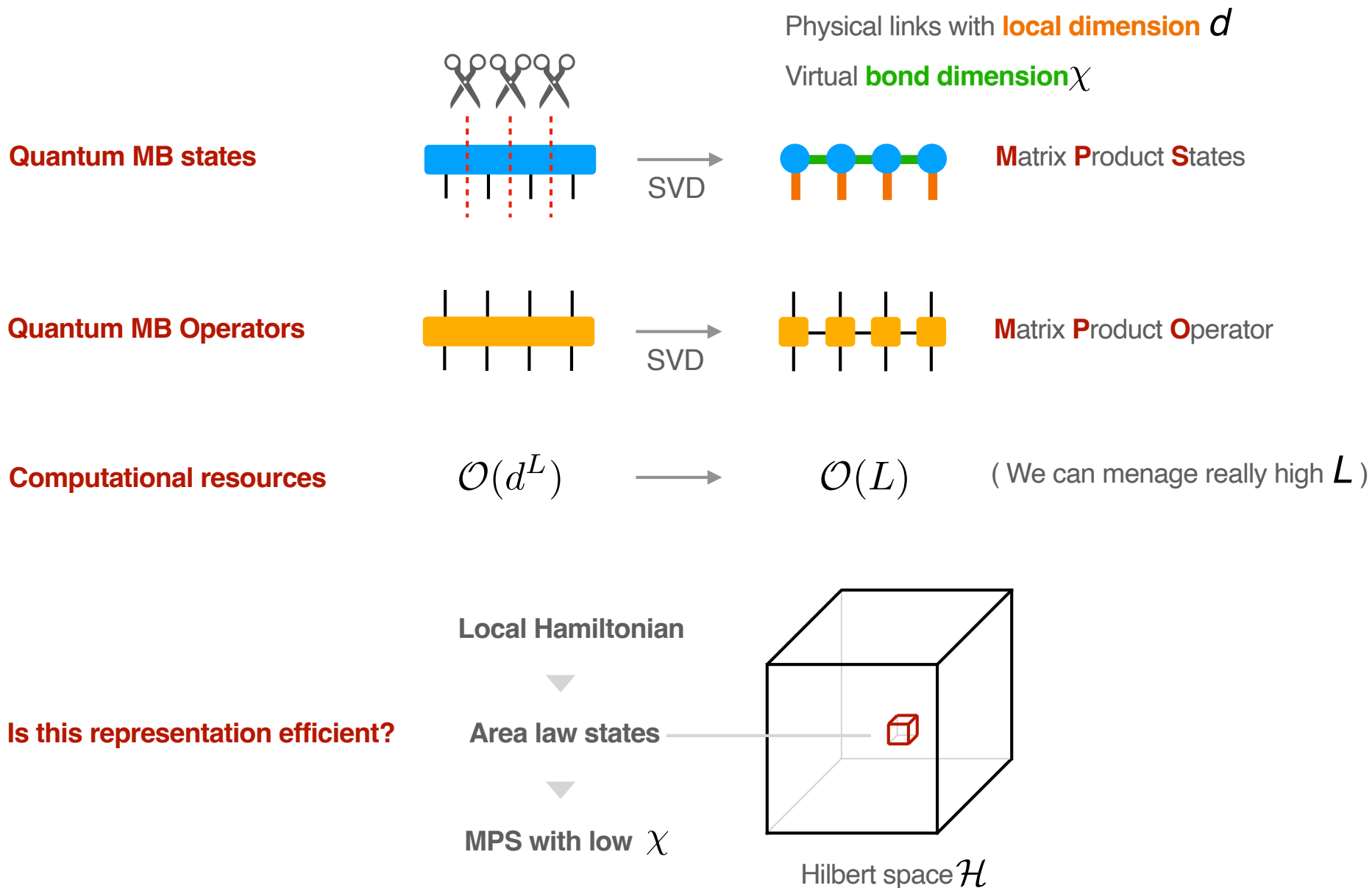
**Tensor Networks notation:** each tensor  $T$  (node) has  $n$  indices  $i$  (links). Each index has a dimension  $d$  (size).



## Singular Value Decomposition (SVD)



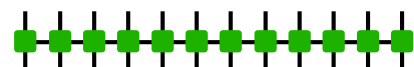
# 4. Tensor Network methods in a nutshell



# 4. Tensor Network methods in a nutshell

## Useful MPS and MPO Algorithms

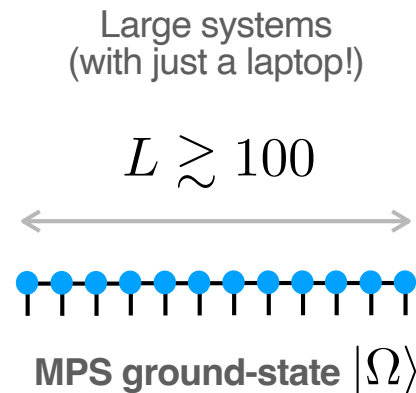
**Ground-state search** Density Matrix Renormalization Group



MPO Hamiltonian



DMRG



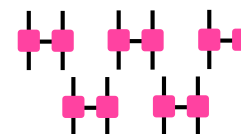
**Time evolution for MPS** Time Evolving Block Decimation (...but also TDVP)



Time evolution operator



Suzuki-Trotter  $\delta t$



Iteration of gates

**Operator to MPO conversion**

$$\sum_{\alpha} \hat{L}_{\alpha} = \sum \text{[Diagram of yellow squares with lines]}$$

The diagram shows a sum over  $\alpha$  of  $\hat{L}_{\alpha}$  equals a sum over configurations of yellow squares. Each yellow square has four vertical lines extending from its top and bottom, representing the conversion of local operators to an MPO.

Sum of compositions of local operators



Automata procedure



Matrix Product Operator

# 4. Tensor Network methods in a nutshell

## Automata procedure

## Wannier creation operator

1

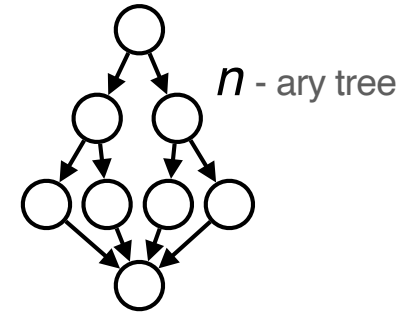
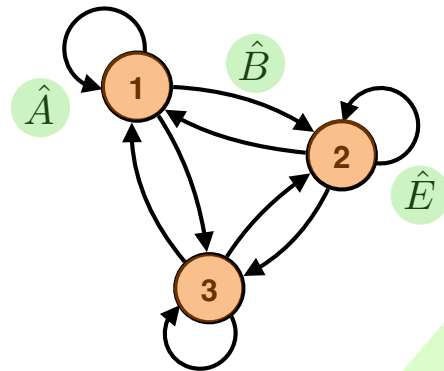
Operator picture

$$\hat{O} = \sum_{\alpha} \hat{L}_{\alpha}$$

$$\hat{W} = \sum_{\alpha_1 \dots \alpha_w} c_{\alpha_1 \dots \alpha_w} L_{\alpha_1} \dots L_{\alpha_w}$$

2

Automata picture



3

Matrix picture

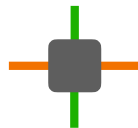
$$\begin{pmatrix} \hat{A} & \hat{B} & \hat{C} \\ \hat{D} & \hat{E} & \hat{F} \\ \hat{G} & \hat{H} & \hat{I} \end{pmatrix}$$

A green callout box highlights the submatrix  $\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$ .

$$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \mathcal{O}(e^w)$$

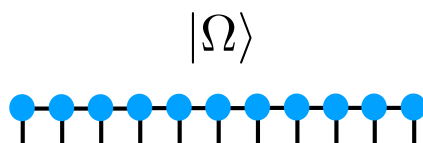
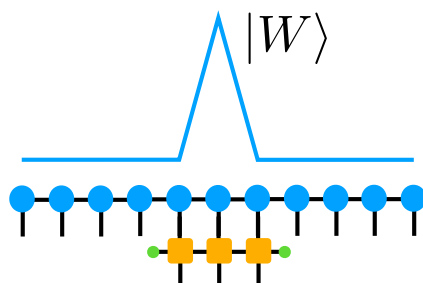
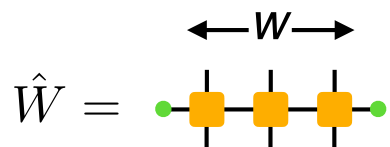
4

TN picture



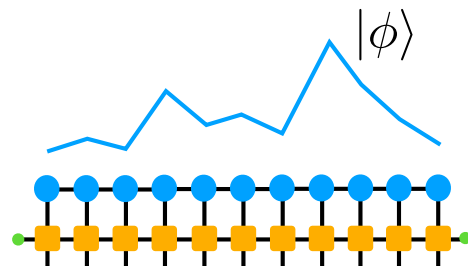
# 5. Back to Wavepackets

Wannier creation operator Ansatz



Large  $L$  vacuum state found with DMRG

Wavepacket Ansatz



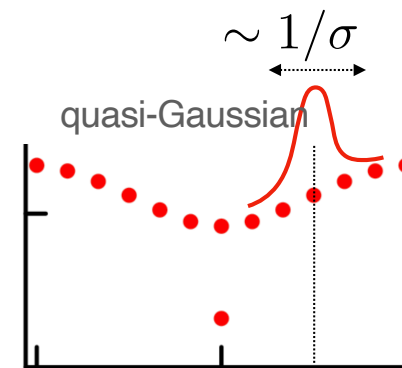
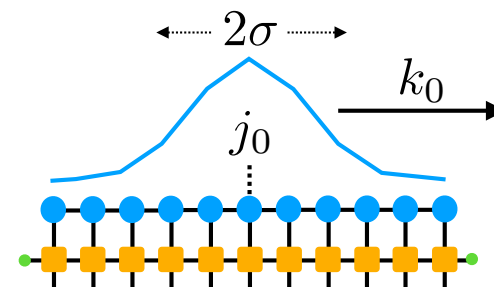
No scaling of  $\chi$  with size!

$$\chi = \mathcal{O}(e^w, \mathbf{L})$$

(Real space)

Gaussian wavepacket

$$\frac{1}{\mathcal{N}} e^{-\frac{(j-j_0)^2}{2\sigma}} e^{ijk_0}$$



Momentum space

# 6. Numerical simulations

## System parameters

$a = 1$   
 $L = 100$   
 $g^4 = 0.1$   
 (Dirichlet OBC)

## DMRG parameters

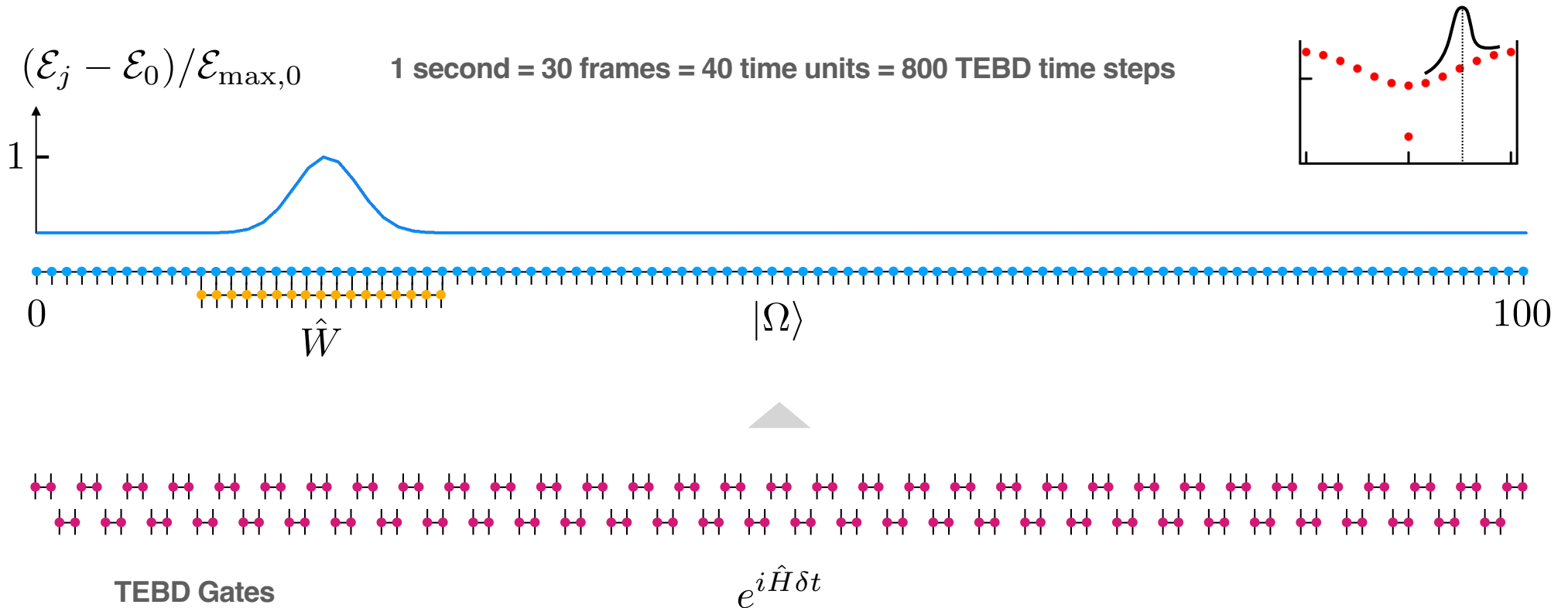
$\chi_{\max} = 200$   
 $n_{\text{sweeps}} = 50$   
 $\epsilon_{\text{SVD}} = 10^{-13}$

## Wavepacket parameters

$\sigma = 3a$   
 $k = \pi/2a$   
 $j_0 = 20$

## TEBD parameters

$\delta t = 0.05$   
 $\Delta t = 400$   
 $\epsilon_{\text{SVD}} = 10^{-10}$   
 $\chi_{\max} = 50$



## 6. Numerical simulations

### System parameters

$$a = 1$$
$$L = 100$$
$$g^4 = 0.1$$

(Dirichlet OBC)

### DMRG parameters

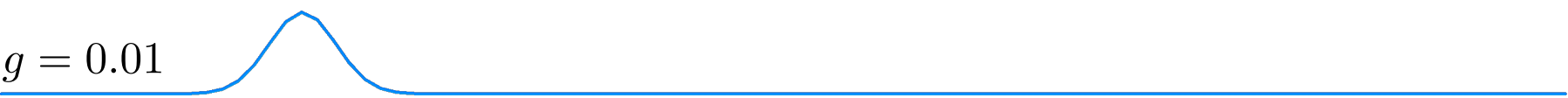
$$\chi_{\max} = 200$$
$$n_{\text{sweeps}} = 50$$
$$\epsilon_{\text{SVD}} = 10^{-13}$$


### Wavepacket parameters


$$\sigma = 3a$$
$$k = \pi/2a$$
$$j_0 = 20$$

### TEBD parameters

$$\delta t = 0.05$$
$$\Delta t = 400$$
$$\epsilon_{\text{SVD}} = 10^{-10}$$
$$\chi_{\max} = 50$$

$$g = 0.01$$
A blue line plot showing a wavepacket centered at  $x=20$  for  $g=0.01$ . The wavepacket is a smooth, bell-shaped curve with a peak height of approximately 1. The x-axis ranges from 0 to 100.

$$g = 0.1$$
A blue line plot showing a wavepacket centered at  $x=20$  for  $g=0.1$ . The wavepacket is a smooth, bell-shaped curve with a peak height of approximately 1. The x-axis ranges from 0 to 100.

$$g = 0.2$$
A blue line plot showing a wavepacket centered at  $x=20$  for  $g=0.2$ . The wavepacket is a smooth, bell-shaped curve with a peak height of approximately 1. The x-axis ranges from 0 to 100.



## 6. Numerical simulations

### System parameters

$$a = 1$$
$$L = 100$$
$$g^4 = 0.1$$

(Dirichlet OBC)

### DMRG parameters

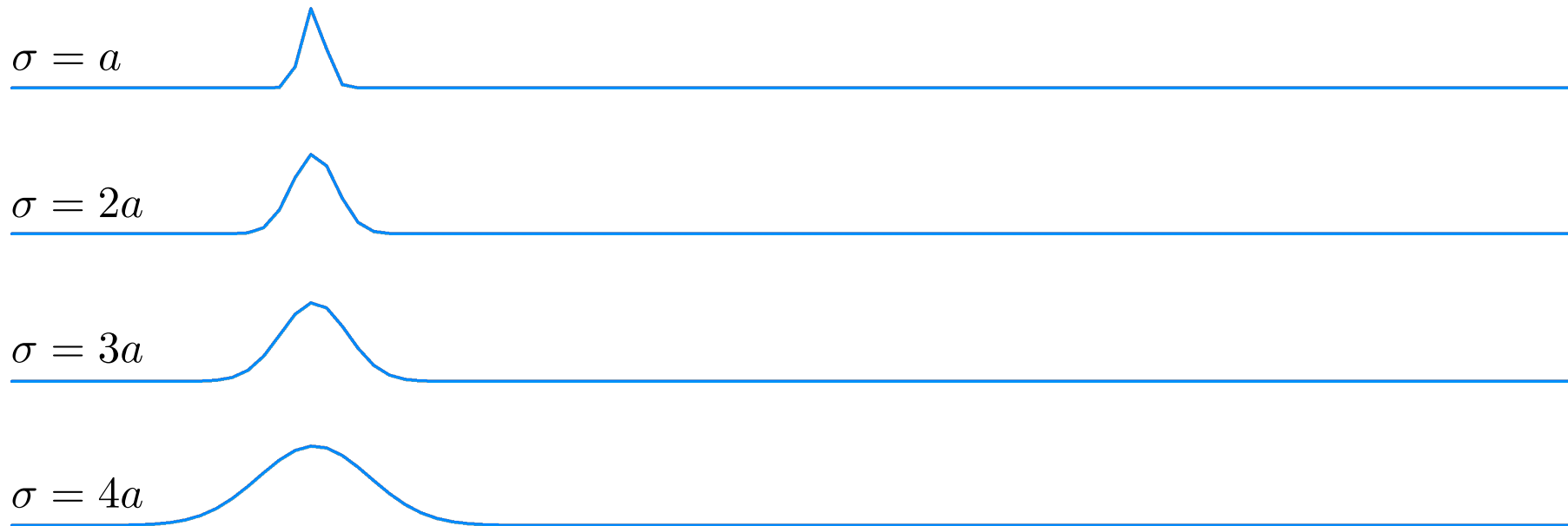
$$\chi_{\max} = 200$$
$$n_{\text{sweeps}} = 50$$
$$\epsilon_{\text{SVD}} = 10^{-13}$$

### Wavepacket parameters

$$\sigma = 3a$$
$$k = \pi/2a$$
$$j_0 = 20$$

### TEBD parameters

$$\delta t = 0.05$$
$$\Delta t = 400$$
$$\epsilon_{\text{SVD}} = 10^{-10}$$
$$\chi_{\max} = 50$$



# 6. Numerical simulations

## System parameters

$$a = 1$$

$$L = 100$$

$$g^4 = 0.1$$

(Dirichlet OBC)

## DMRG parameters

$$\chi_{\max} = 200$$

$$n_{\text{sweeps}} = 50$$

$$\epsilon_{\text{SVD}} = 10^{-13}$$

## Wavepacket parameters

$$\sigma = 3a$$

$$k = \pi/2a$$

$$j_0 = 20$$

## TEBD parameters

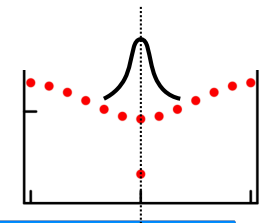
$$\delta t = 0.05$$

$$\Delta t = 400$$

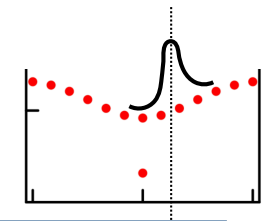
$$\epsilon_{\text{SVD}} = 10^{-10}$$

$$\chi_{\max} = 50$$

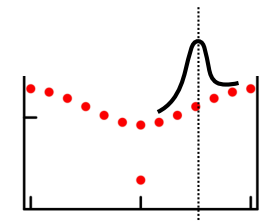
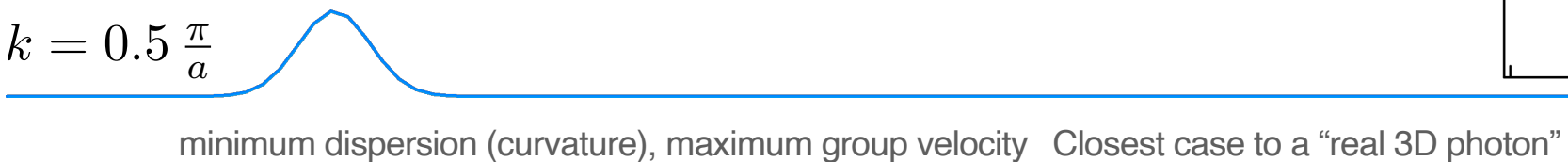
$$k = 0$$



$$k = 0.25 \frac{\pi}{a}$$

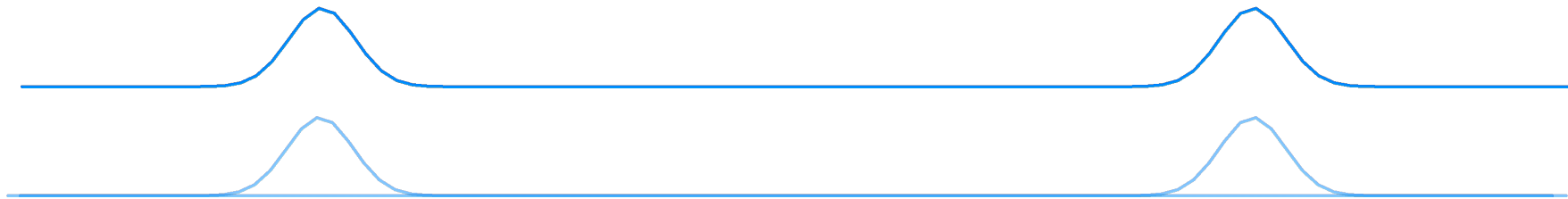


$$k = 0.5 \frac{\pi}{a}$$



## 6. Numerical simulations

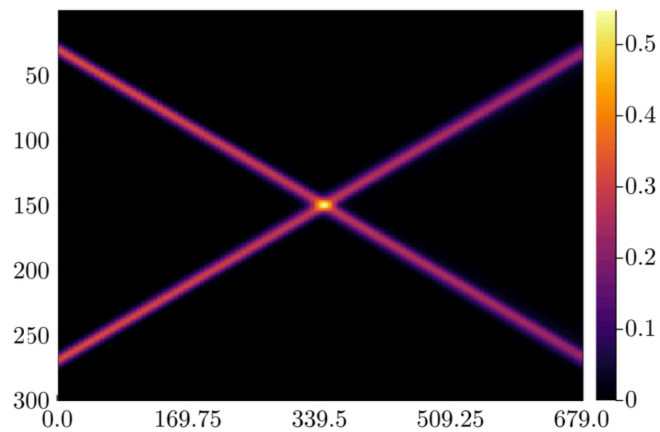
$$\sigma = 3a \quad k = \pi/2a$$



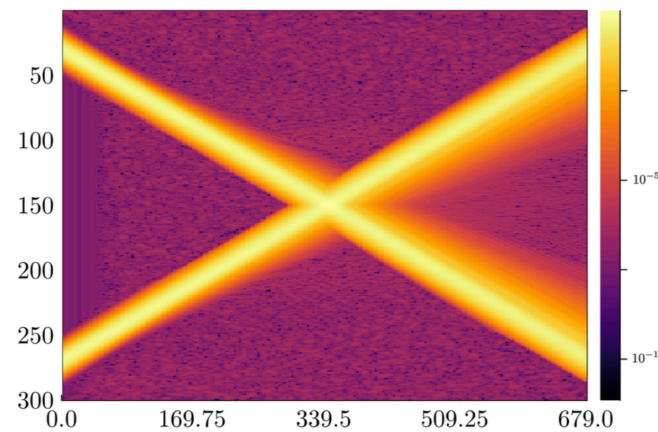
Nothing happens: **good**, they are like photons, but **bad**, it's boring like this!

It becomes less and less interacting as we approach the continuum limit:

Energy density



Energy density in log



$$L = 300$$

$$\sigma = 5a$$

**Interaction effects:**

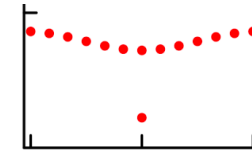
- **Lattice** artifacts
- **Finite size** effects
- **1D** lattice geometry

# 7. Conclusions

● Inputs  $\hat{H}, \hat{T}$  plus **few assumptions** (model independent)

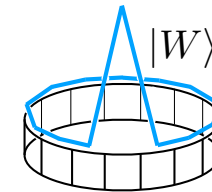
1 Simultaneous exact diagonalization, finding the Bloch states

$$[\hat{H}, \hat{T}] = 0 \quad \text{Computationally expensive step: intermediate system size}$$



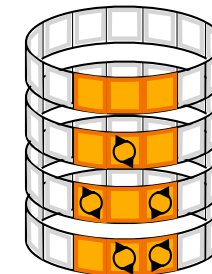
2 Computation of the maximally localized Wannier states

$$|W(\theta_k)\rangle = \frac{1}{\sqrt{L}} \sum_k e^{i\theta_k} |k\rangle$$



3 Construction of the Wannier creation operator

$$\hat{W}|\Omega\rangle = |W\rangle \quad \text{From the interacting vacuum}$$



4 Construction of the Wavepacket creation operator

$$\hat{\Phi} = \sum_j \phi_j \hat{W}_j \quad \text{We mostly choose a gaussian wavepacket}$$

$$\begin{aligned} & c_1 \mathbb{I} \\ & + c_2 \hat{U}_{\square,2}^\dagger \\ & + c_3 \hat{U}_{\square,1}^\dagger \hat{U}_{\square,3} \\ & + c_3 \hat{U}_{\square,2}^\dagger \hat{U}_{\square,3} \end{aligned}$$

5 Conversion of the Wavepacket creation operator to an MPO

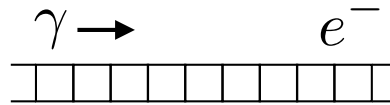


● Output: the MPO

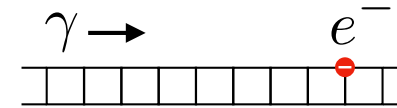
# 8. Outlook

$(1, 1), (\frac{3}{2}, 2), \dots$

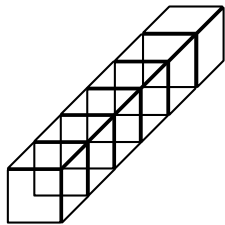
**Higher spin representations**



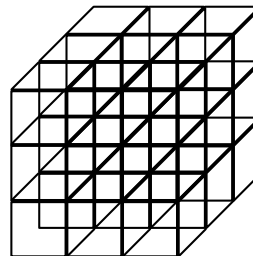
**Adding matter d.o.f**



**Background charge**



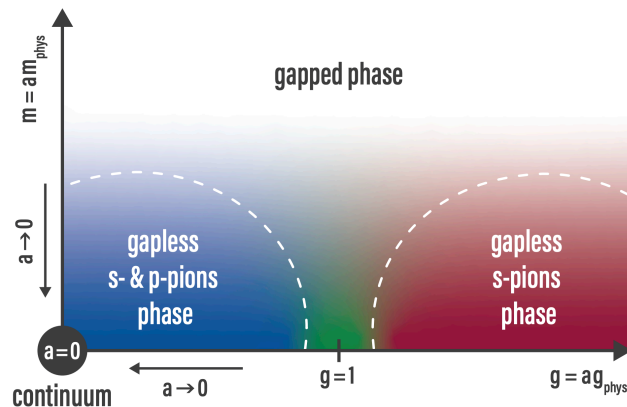
**Different geometries**



**Higher dimension**

$$\begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$$

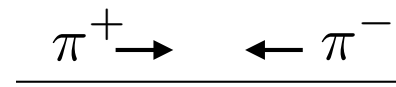
**Try to overcome exact diagonalization**



arXiv:2308.04488

**Last but not least**

moving to **1D QCD with two flavors**,  
simulating **pion-pion scattering**



**Challenge:  $d = 54$  local dimension**