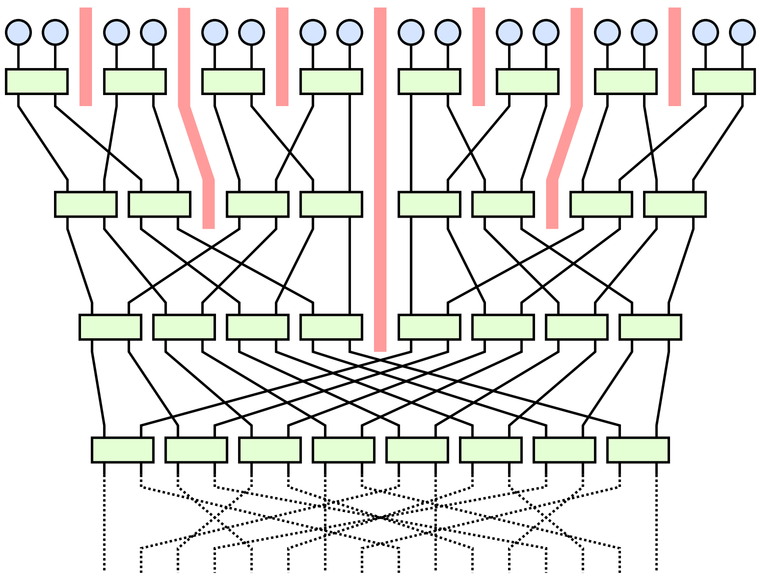
Generalized Fourier transforms with the Spectral Tensor Network



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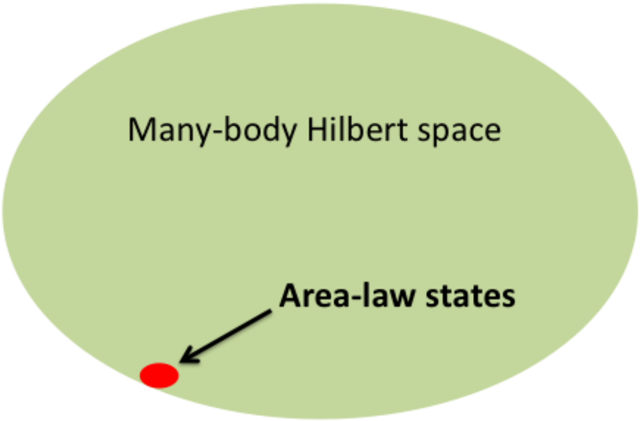
Recently jointly with:

Max Planck Institute for Quantum Optics

What am I talking about today?

- Overall goal: use tensor networks to study fermionic models in 2D and beyond
- Introduce a ***generalized*** Fourier transform for bosons and fermions (and more!)
- This suggests a new tensor network ansatz to use variationally with interacting systems

Tensor networks and area law

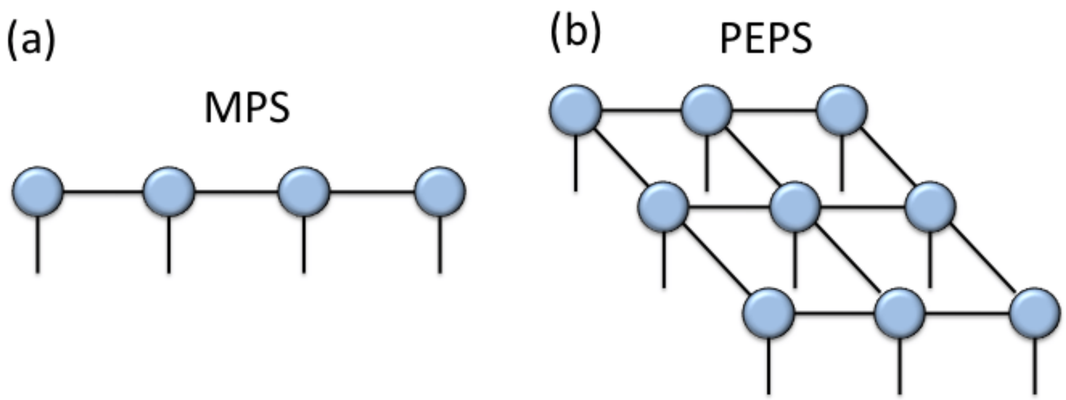


Many low-energy systems have entanglement bounded by boundary area, not volume. E.g. in 2D, $S \propto L$

Can use tensor networks to accurately and efficiently describe such states

But: some "critical" 2D systems obey:

$$S \propto L \log L$$



R. Orus, arXiv:1306.2164 (2013)

Free-fermions

- Simple quadratic / bi-linear Hamiltonian

$$\hat{H} = \sum_i t \hat{c}_i^\dagger \hat{c}_{i+1} + \mathrm{h.c.}$$

- Represents metals, band insulators, etc

- Could be more complicated
  - Spins/orbitals, longer range interactions, etc
  - Anamolous pair terms $\hat{c}_i^\dagger \hat{c}_j^\dagger + h.c.$

Entanglement in free-fermion systems

- Free-fermions exactly diagonalized by Fourier transform

$$\hat{c}_k^\dagger = \frac{1}{\sqrt{n}} \sum_x \hat{c}_x^\dagger e^{ikx}$$

- No entanglement in momentum space!
- Lots of entanglement in real space, more than area law (depending on Fermi surface)

<u>1D:</u>

$$S \propto \log L$$

<u>2D:</u>

$$S \propto L \log L$$

Where to?

- Given the large amount of entanglement in relatively simple systems, tensor networks like PEPS might not offer very efficient description of the state

- Here we make use of the fact that the state has no entanglement in momentum space

The rest of this talk…

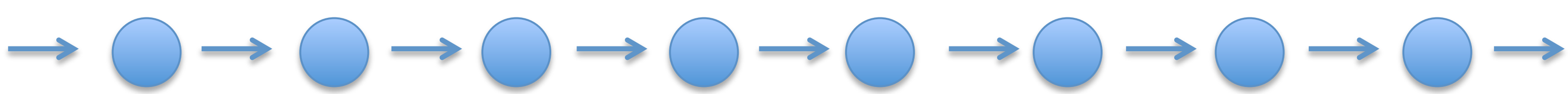
Fourier transform for quantum many-body systems

Translation invariance

Translationally invariant states don't change under translation:

$$\hat{T}_1|\Psi\rangle = e^{ik}|\Psi\rangle$$

The Fourier transform is a unitary that diagonalizes $\hat{T}_1$. Eigenvalues of $\hat{T}_1$ are e^{ik}.



Fast Fourier transform

Fourier transform of vector of numbers, x_j.

$$\tilde{a}_k = \sum_x a_x e^{ikx}$$

Linear transformation represented by matrix:

$$F_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{bmatrix}$$

Fast Fourier transform

Matrix can be decomposed into product of sparse matrices (prime factors).

$$\left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{array}\right] = (F_2 \otimes I_2)W(I \otimes F_2)P$$

Diagonal phases "twiddle factors"

Permutation matrix

$$F_2 = \left[\begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array}\right]$$

Classical Fourier decomposition

The Fourier transform can be re-written as a sum of two smaller Fourier transforms:

$$\underbrace{\sum_{x=0}^{N-1} e^{\frac{2\pi i k x}{N}} a_x}_{\text{FT over all N sites}} = \underbrace{\sum_{x'=0}^{N/2-1} e^{\frac{2\pi i k x'}{N/2}} \overset{\text{Even sites}}{a_{2x'}}}_{\text{FT over N/2 even sites}} + \overset{\text{Phase factor}}{e^{\frac{2\pi i k}{N}}} \underbrace{\sum_{x'=0}^{N/2-1} e^{\frac{2\pi i k x}{N/2}} \overset{\text{Odd sites}}{a_{2x'+1}}}_{\text{FT over N/2 odd sites}}$$

Can be applied iteratively for 2^N sites

Quantum ~~Classical~~ Fourier decomposition

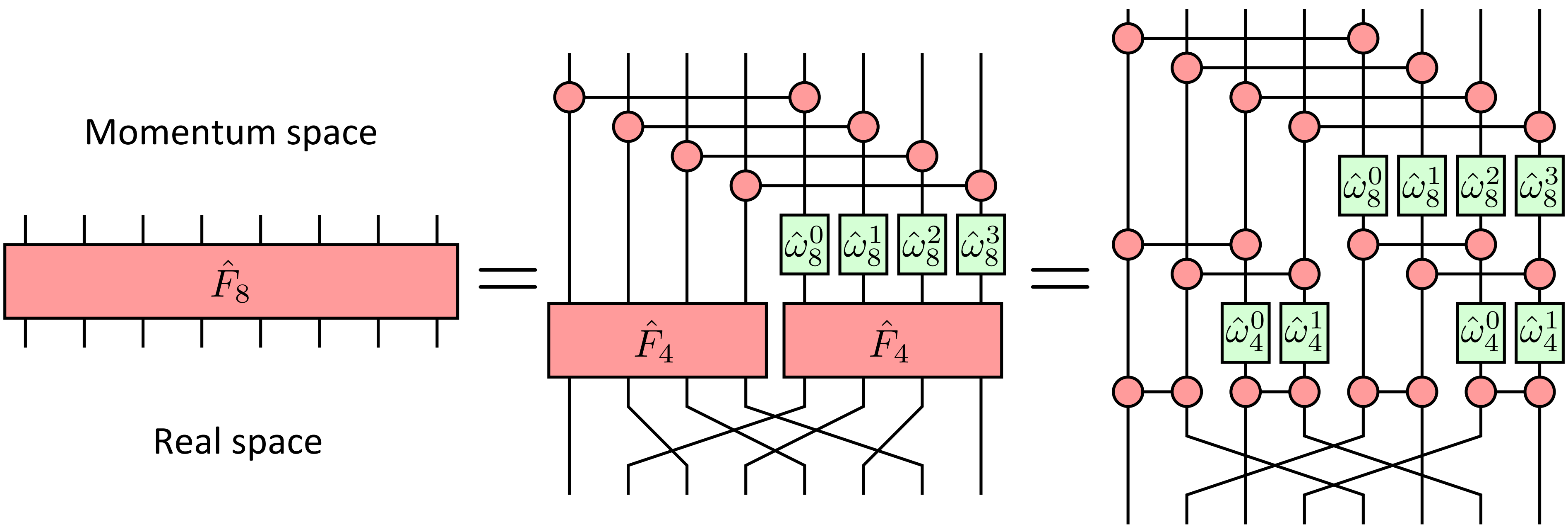
The Fourier transform can be re-written as a sum of two smaller Fourier transforms:

$$\underbrace{\sum_{x=0}^{N-1} e^{\frac{2\pi i k x}{N}} \hat{a}_x}_{\text{FT over all N sites}} = \underbrace{\sum_{x'=0}^{N/2-1} e^{\frac{2\pi i k x'}{N/2}} \overset{\text{Even sites}}{\hat{a}_{2x'}}}_{\text{FT over N/2 even sites}} + \overset{\text{Phase factor}}{e^{\frac{2\pi i k}{N}}} \underbrace{\sum_{x'=0}^{N/2-1} e^{\frac{2\pi i k x}{N/2}} \overset{\text{Odd sites}}{\hat{a}_{2x'+1}}}_{\text{FT over N/2 odd sites}}$$

Can be applied iteratively for 2^N sites

Apply decomposition successively

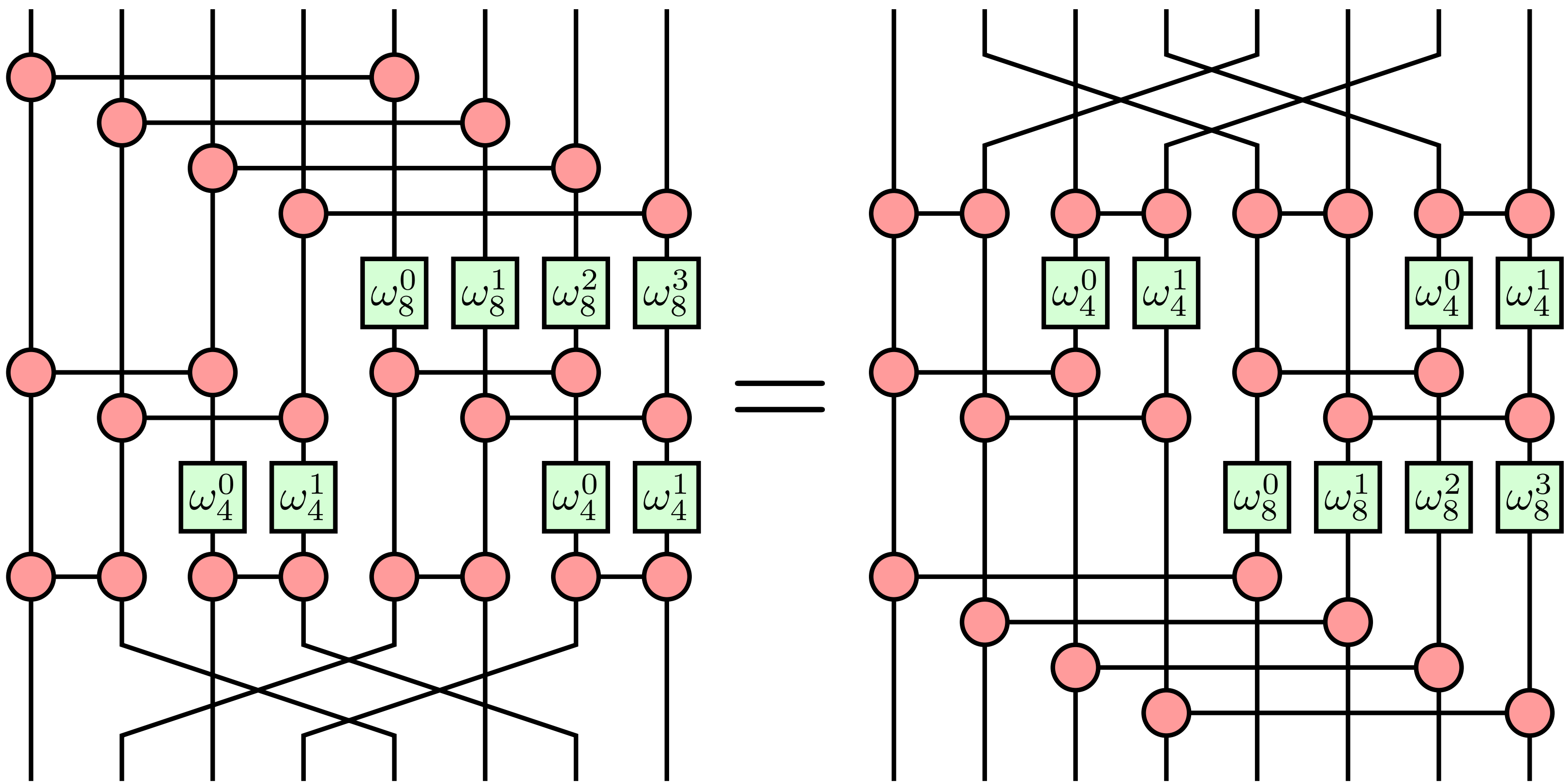
The trick: use one- and two-body linear elements



$$\omega_b^a = -1^{2a/b}$$

Quantum unitary circuit for Fourier transform

Can use graphical identities to manipulate it, in addition to $\hat{F}_n^T = \hat{F}_n$. (Similar freedom in FFT)



Gates for fermions, bosons…

- Gates are linear: $\boxed{\hat{c}'^{\dagger} = \hat{c}^{\dagger} e^{i\phi}}$

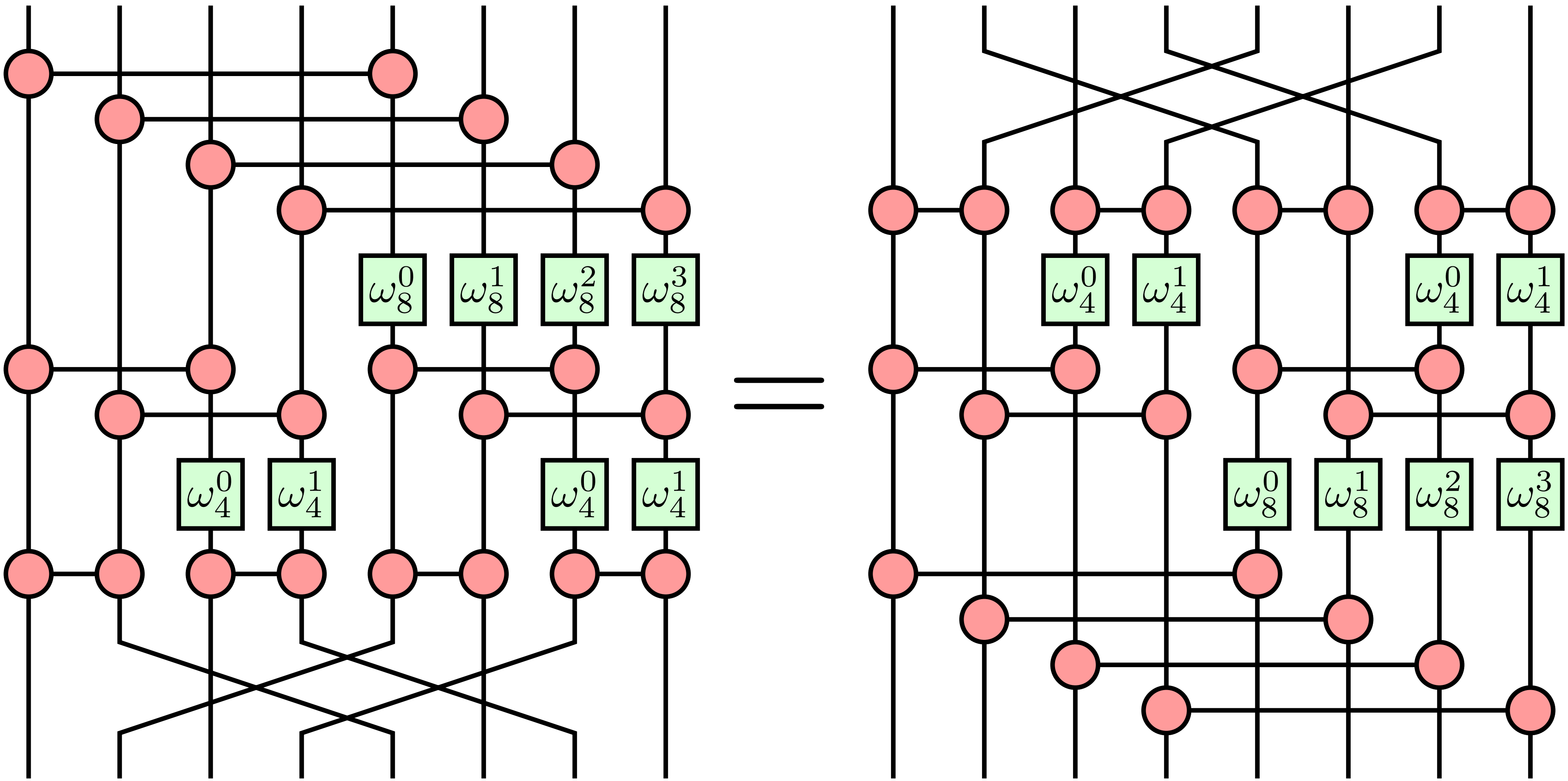
$$\boxed{\begin{aligned} \hat{c}_1' &= \frac{\hat{c}_1 + \hat{c}_2}{\sqrt{2}} \\ \hat{c}_2' &= \frac{\hat{c}_1 - \hat{c}_2}{\sqrt{2}} \end{aligned}}$$

- For fermions these are 4 x 4

$$\hat{U} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

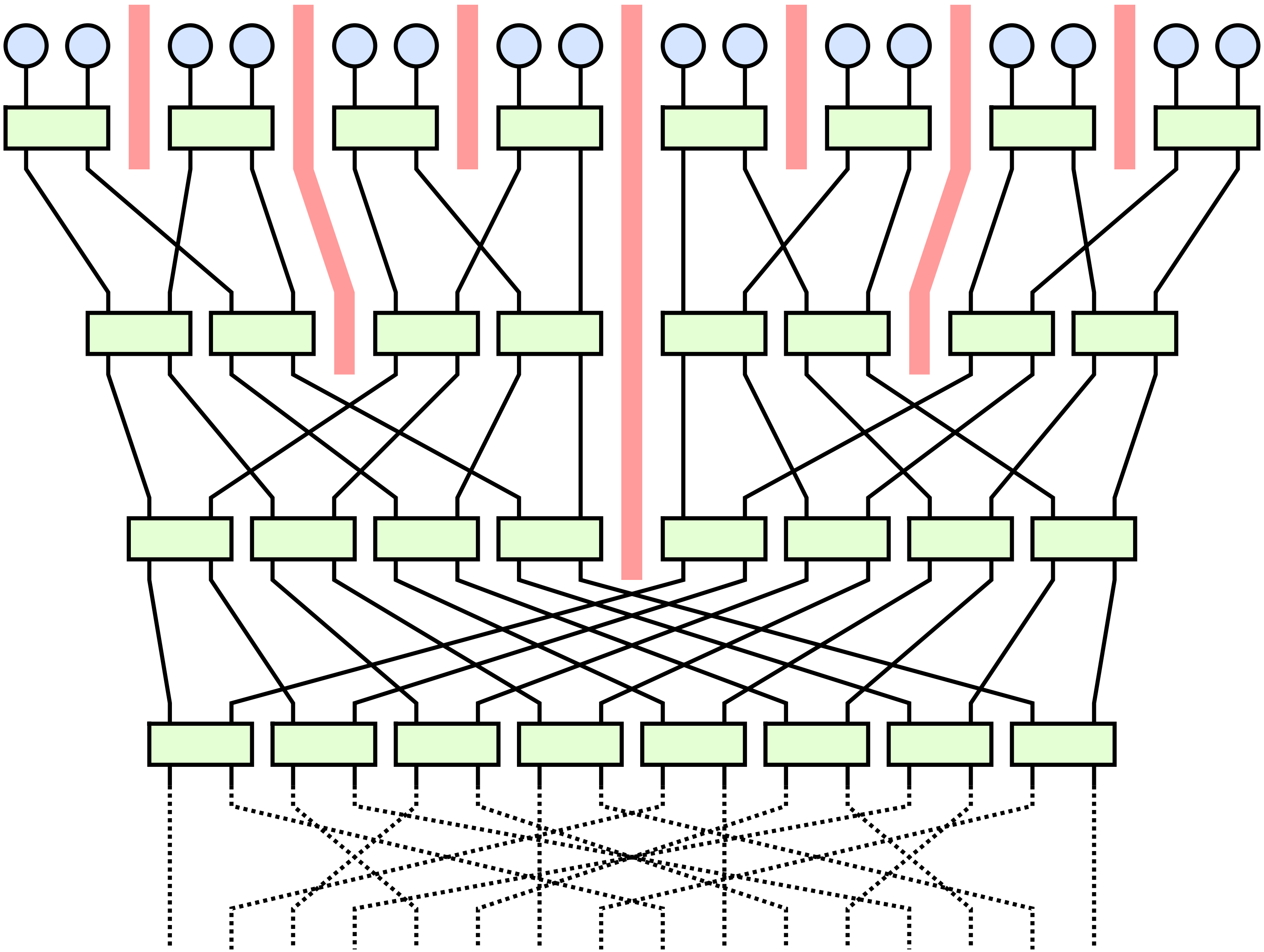
- When wires cross, multiply by -1 when two fermions are exchanged.

Fourier transform quantum circuit

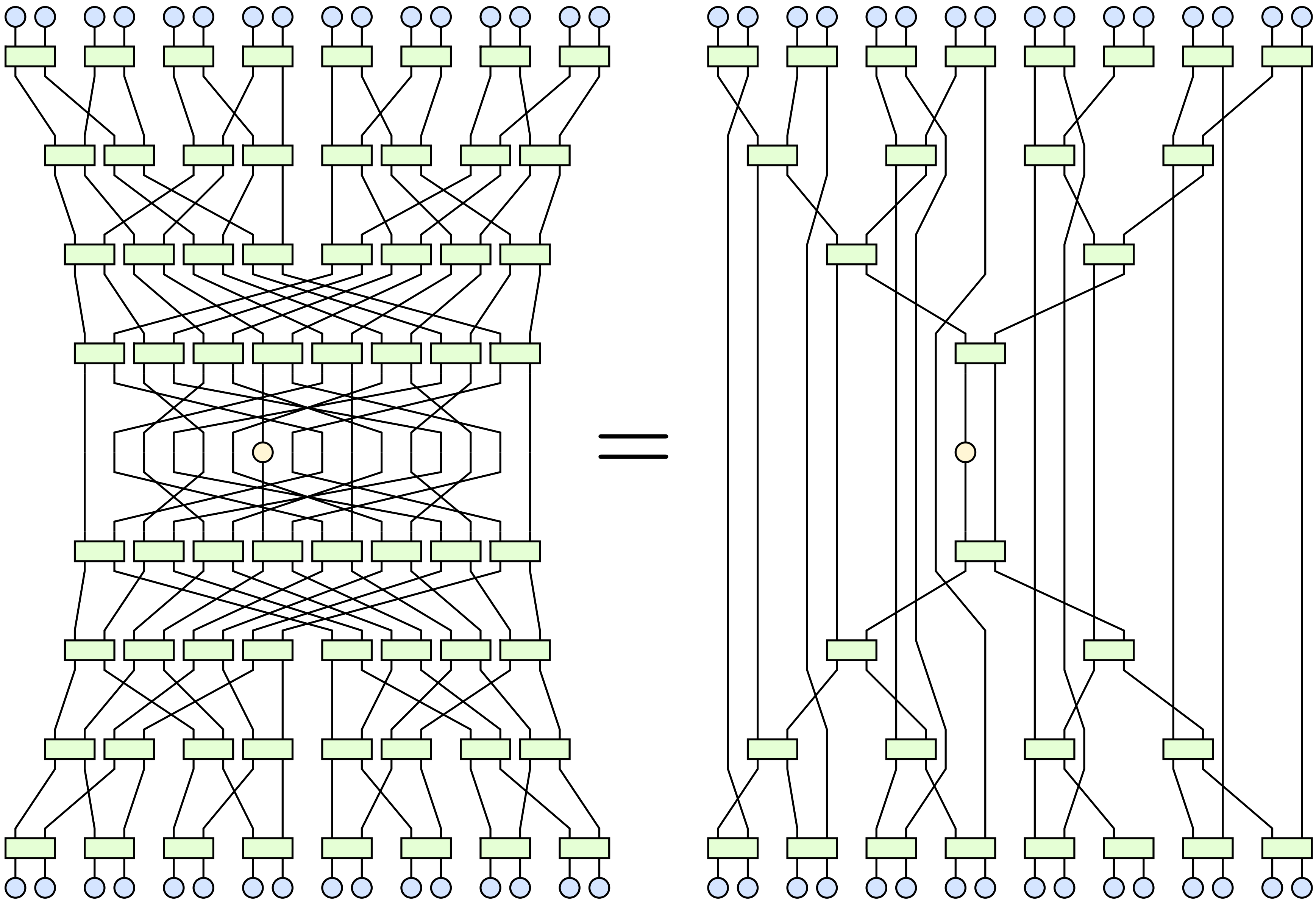


$$\omega_b^a = -1^{2a/b}$$

Spectral tensor network

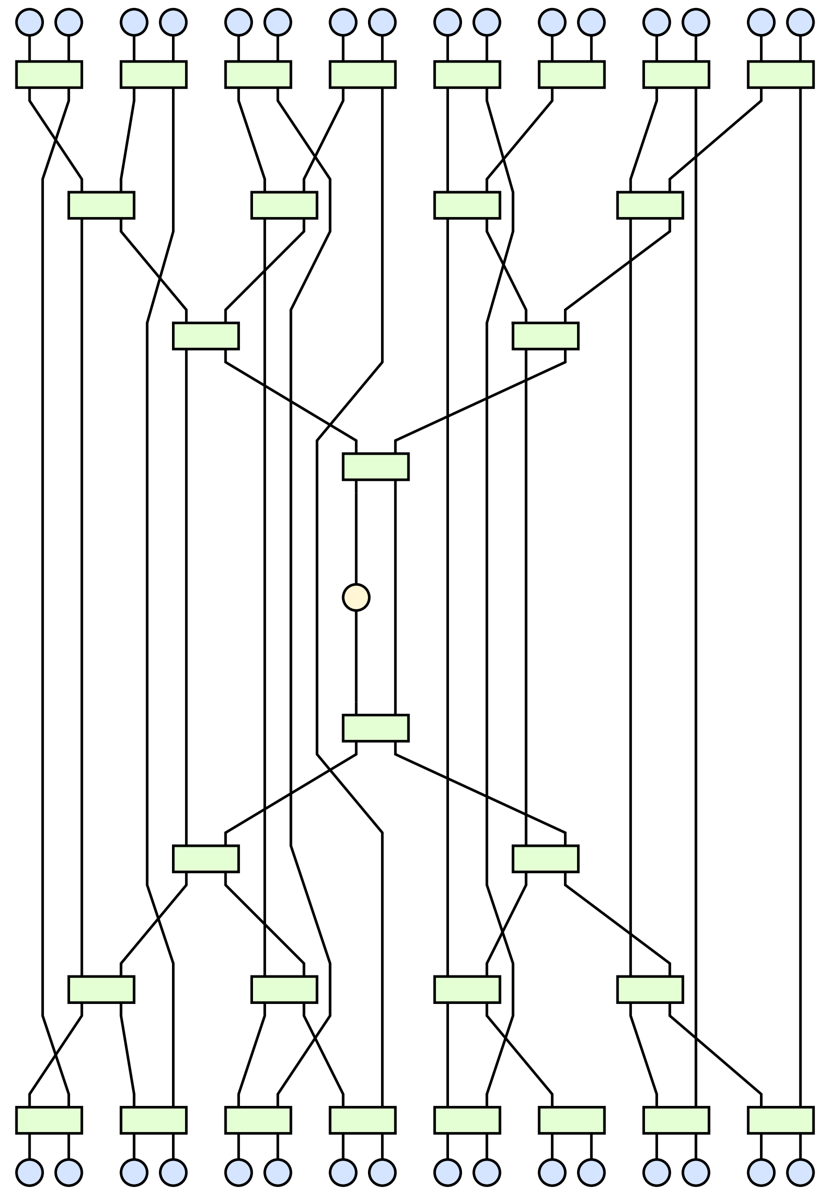


Expectation values



Tensor contractions

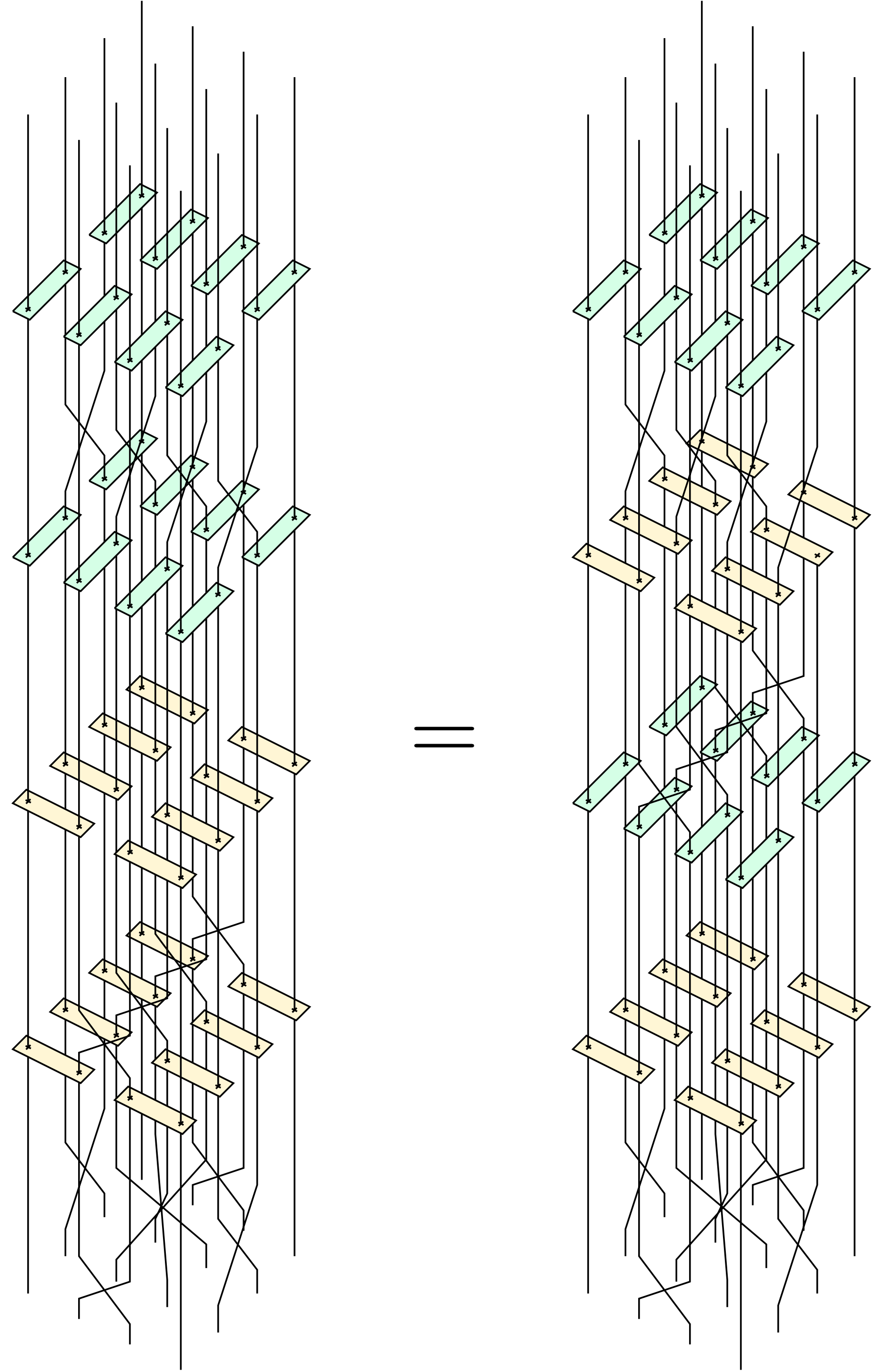
- The remaining tensor network isomorphic to a tree
  - Fold through middle
- Can be contracted with cost $\mathcal{O}(\chi^5\ n)$.
- Everything with $\mathcal{O}(\chi^8\ n \log n)$
- Two body $\mathcal{O}(\chi^8)$



2D Fourier transform

Actually, the structure of the Fourier transform is very similar in 2D, 3D, etc…

No change in cost.



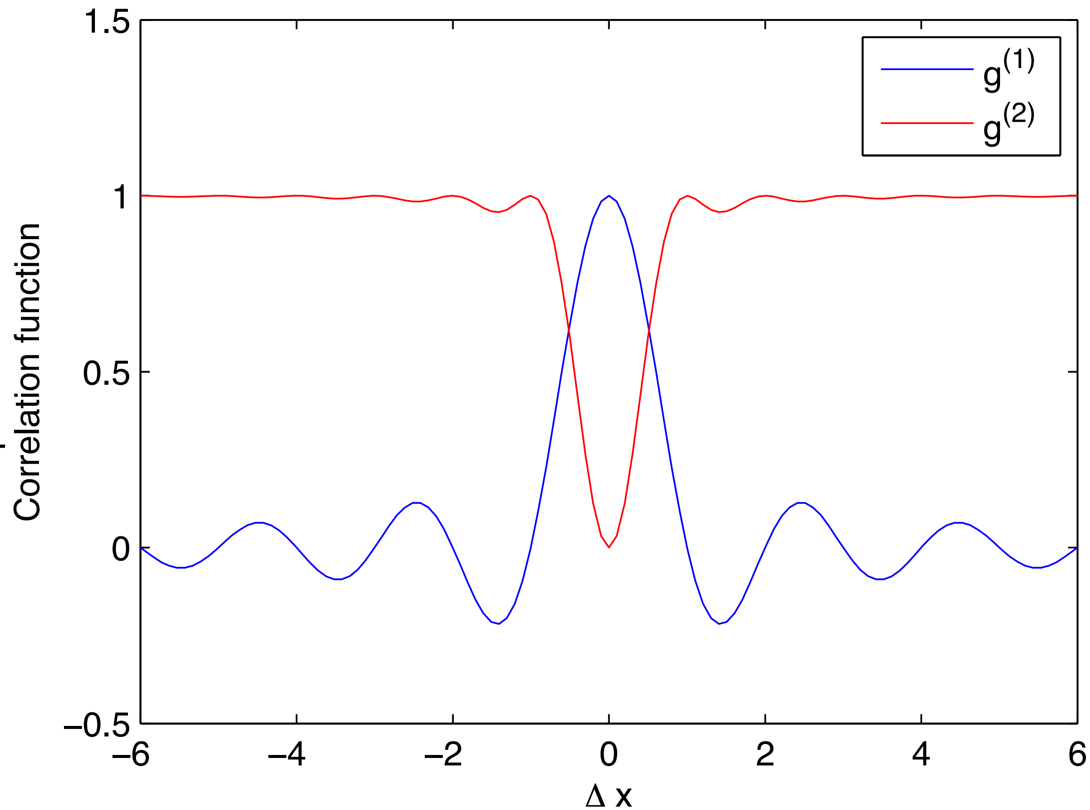
Results: 1D

$$\hat{H} = \sum_i t\hat{c}_i^\dagger \hat{c}_{i+1} + \text{h.c.}$$

Filling the lowest momentum states.

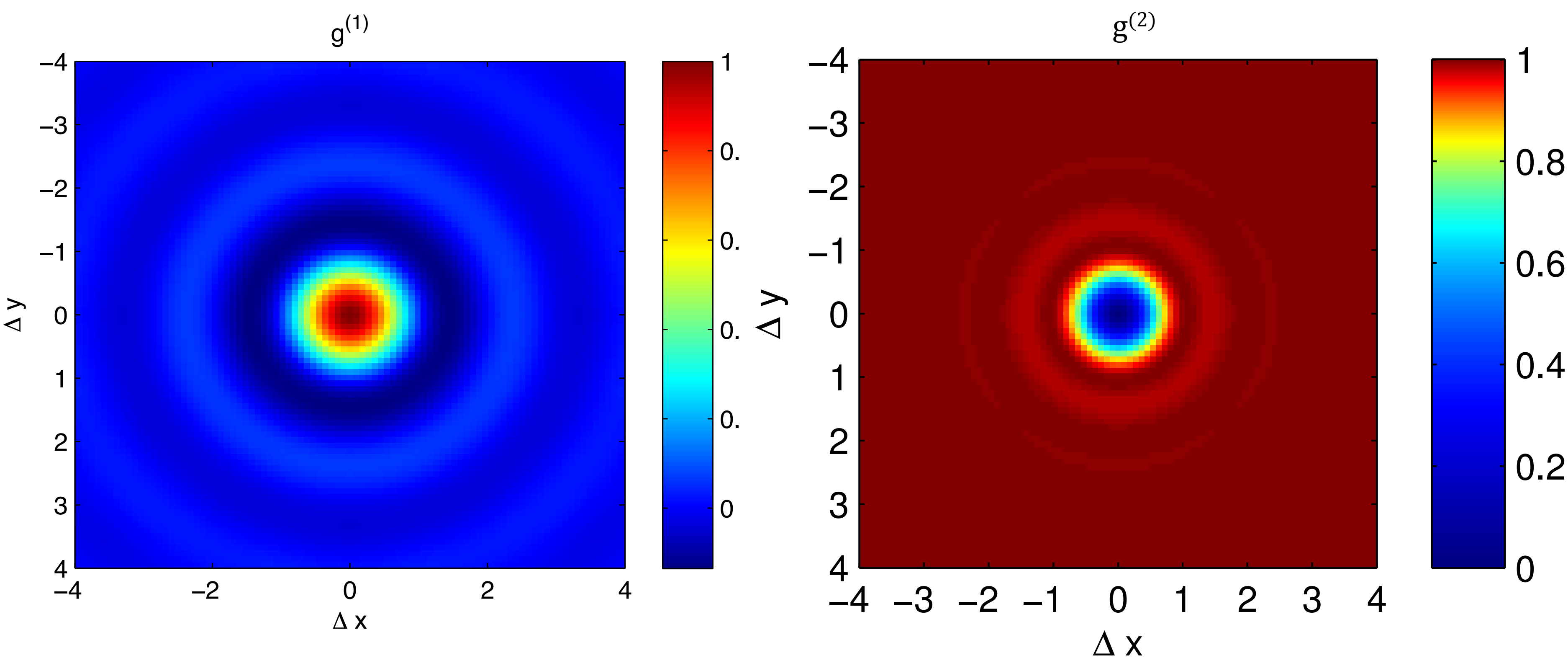
$$g^{(1)}(\Delta x) = \frac{\langle \hat{c}_i^\dagger \hat{c}_{i+\Delta x} \rangle}{\langle \hat{n} \rangle}$$

$$g^{(2)}(\Delta x) = \frac{\langle \hat{n}_i \hat{n}_{i+\Delta x} \rangle}{\langle \hat{n} \rangle^2}$$



Results: 2D

- Start with 512 x 512 lattice (1/4 million sites)
- Low filling factor (approximates free space)



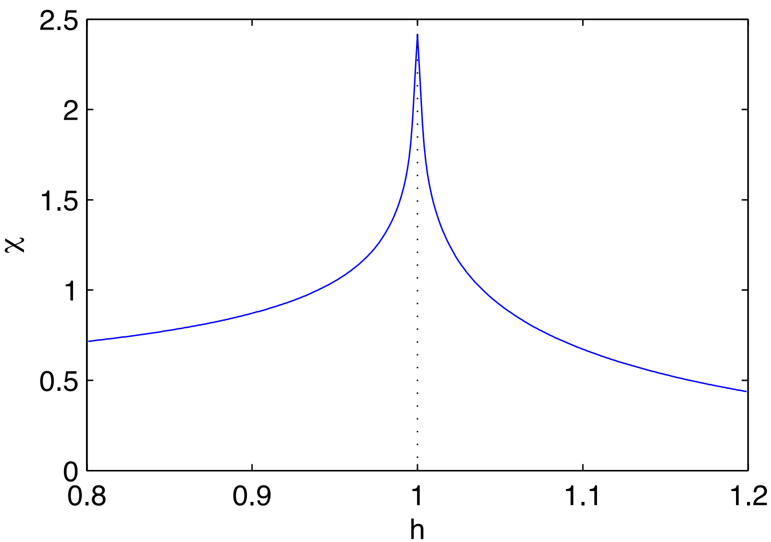
Bogoliubov transformations

$$\hat{H} = \sum_i t\hat{c}_i^\dagger \hat{c}_{i+1} + \Delta \hat{c}_i^\dagger \hat{c}_{i+1}^\dagger + \text{h.c.}$$

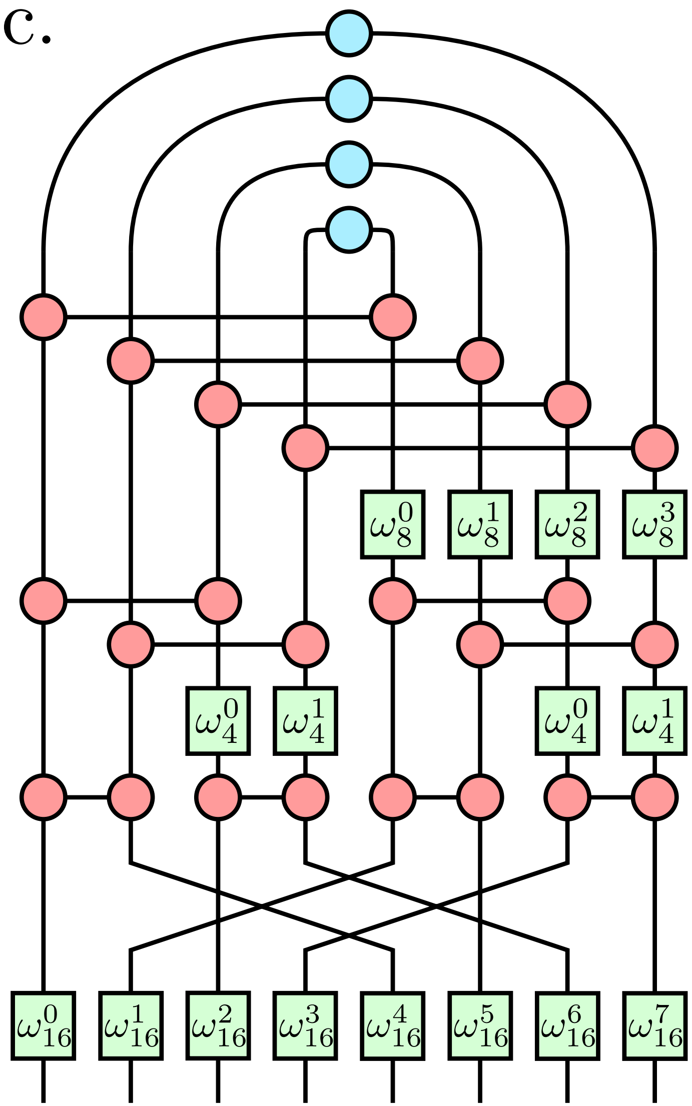
$$\hat{H} = \sum_i \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + h\hat{\sigma}_i^z$$

Correlations between $\pm k$ modes

$$\hat{\eta}_k = u_k \hat{c}_k + v_k \hat{c}_{-k}^\dagger$$



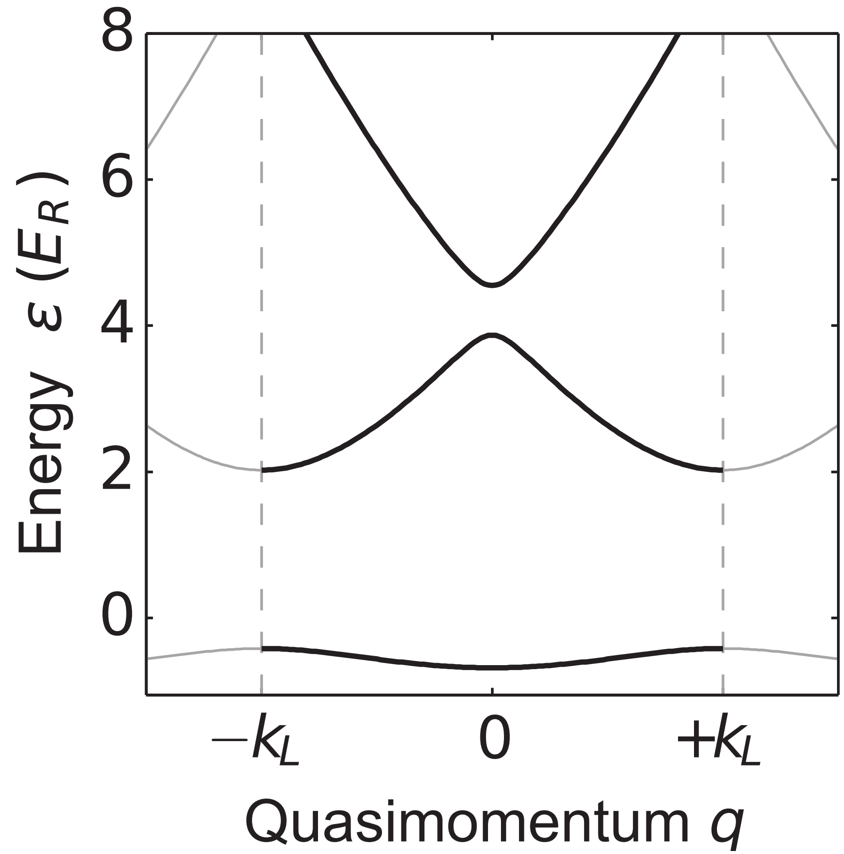
1024 sites (c-cyclic approximation)



Free fermions: Other things to calculate

- Few-site correlations, finite temperature, 3D systems, entanglement entropy of blocks

- Multiple bands or species per site
  - Conductors (metals) with arbitrary Fermi-surface or Dirac points
  - Band-insulators
  - Topological phases (chiral, Majorana, SPTO…)

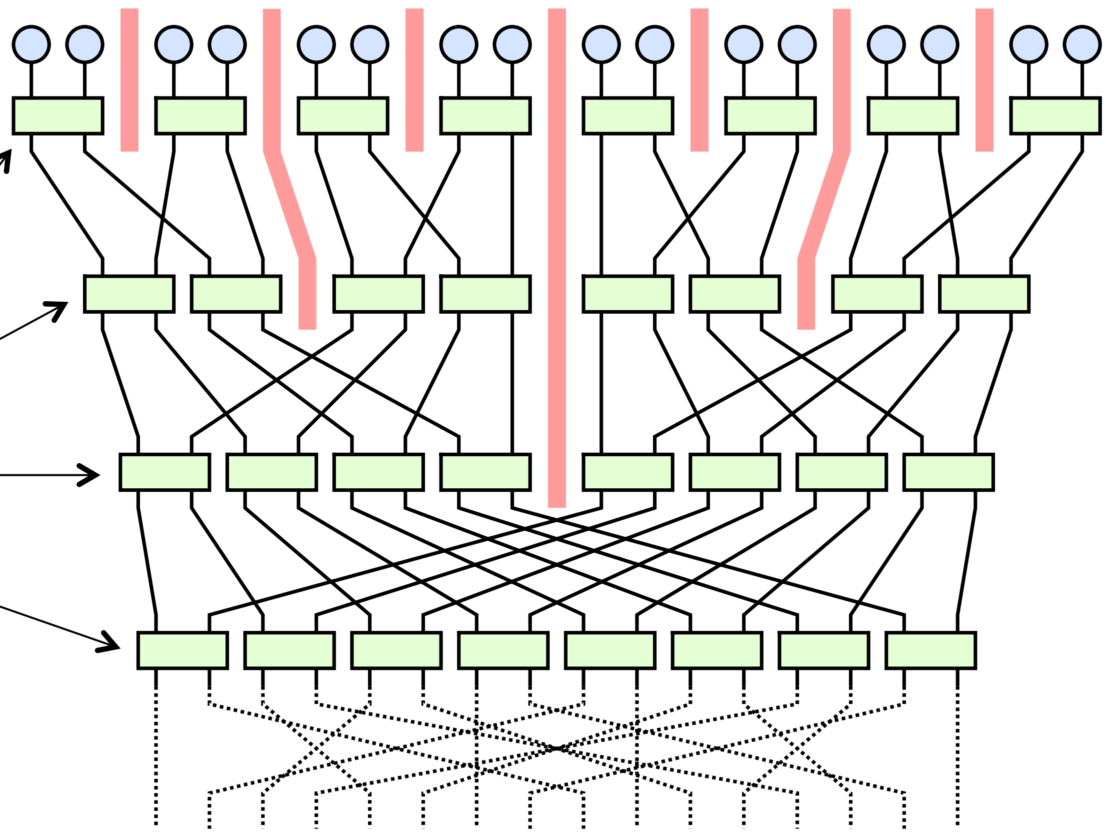


Interacting systems?

Variational approach

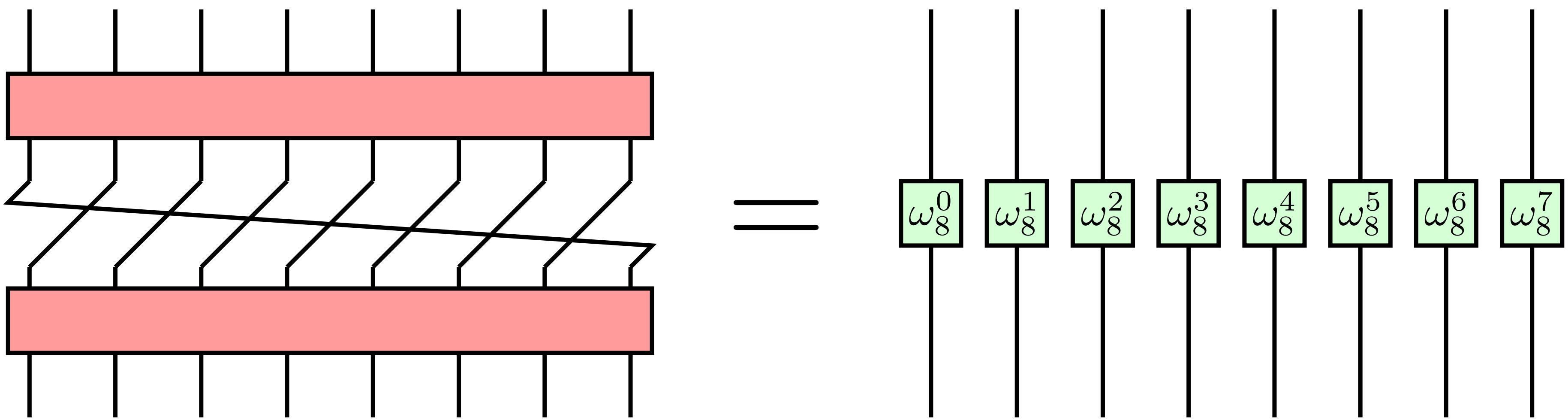
The "spectral tensor network" can be used as a wave-function ansatz

Fill with arbitrary unitary



Generalized Fourier transform

The operator that diagonalizes the shift operator is not unique

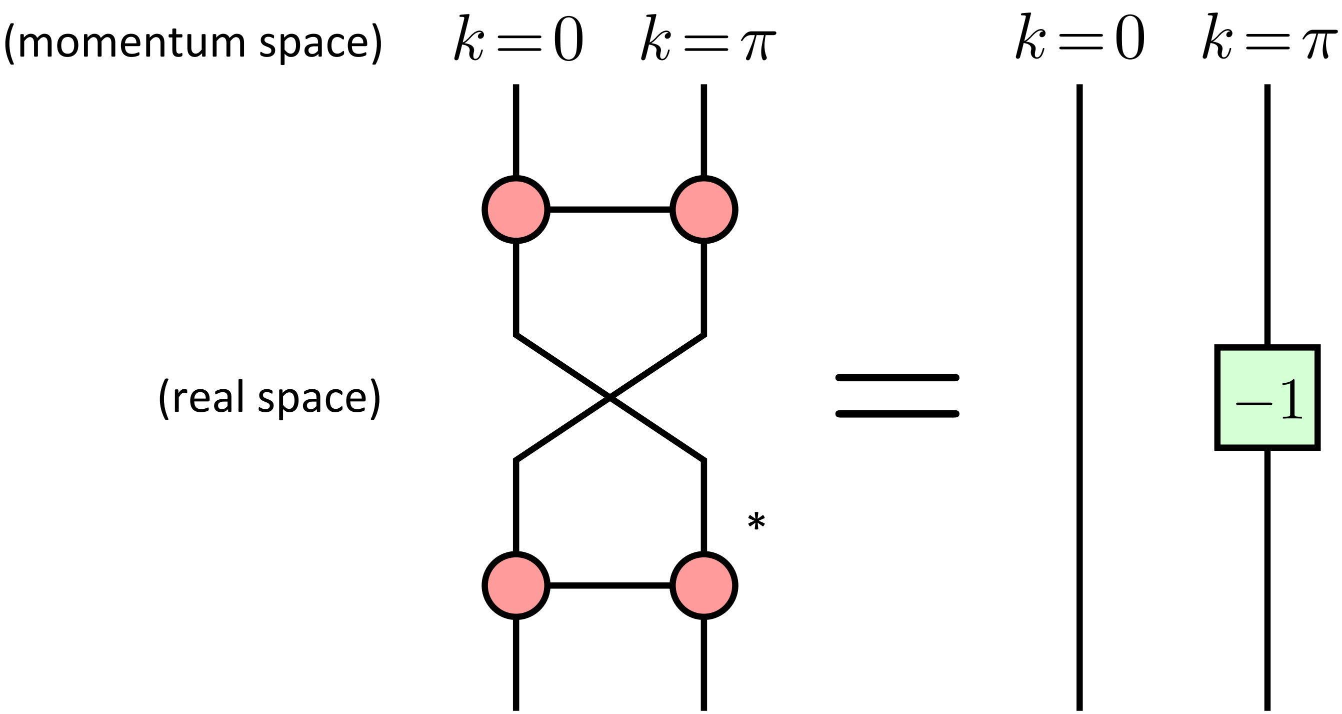


Notably: a simple constraint on the gates leads to the same decomposition as standard FFT.

2-site Fourier transform

The gate must diagonalize $\hat{T}_1 = \hat{\mathrm{SWAP}}$

– Eigenvalues ± 1 (symmetric or antisymmetric)

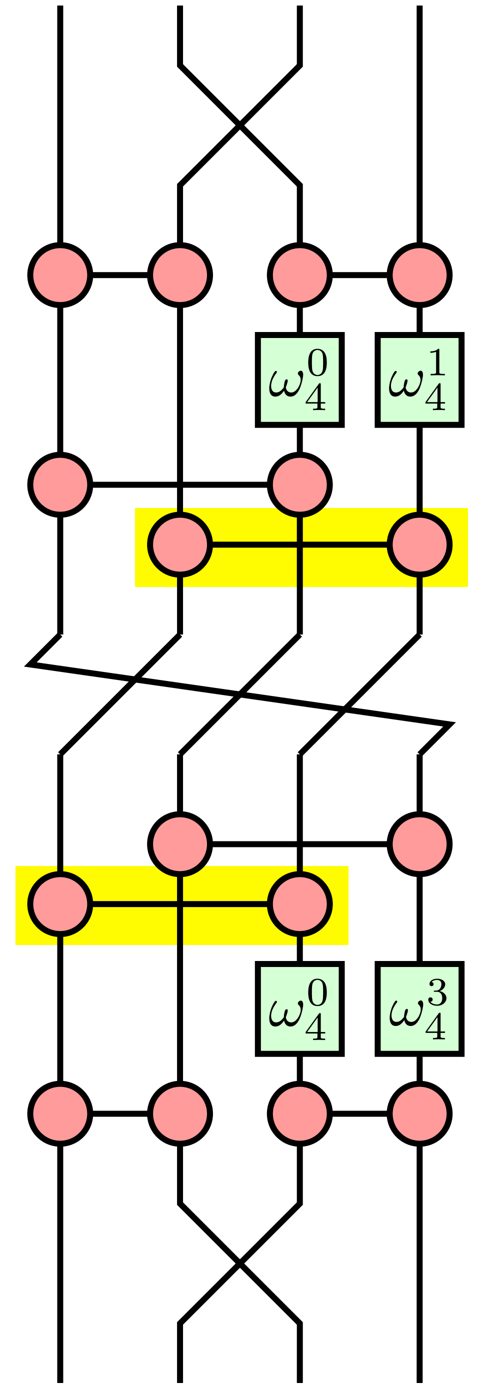


Parity of state in real space = number parity of π-momentum state

4-site Fourier transform

Using ***any*** such a gate we can ***construct*** a Fourier transform!

$$\omega_4^0 = 1$$
$$\omega_4^1 = i$$
$$\omega_4^2 = -1$$
$$\omega_4^3 = -i$$



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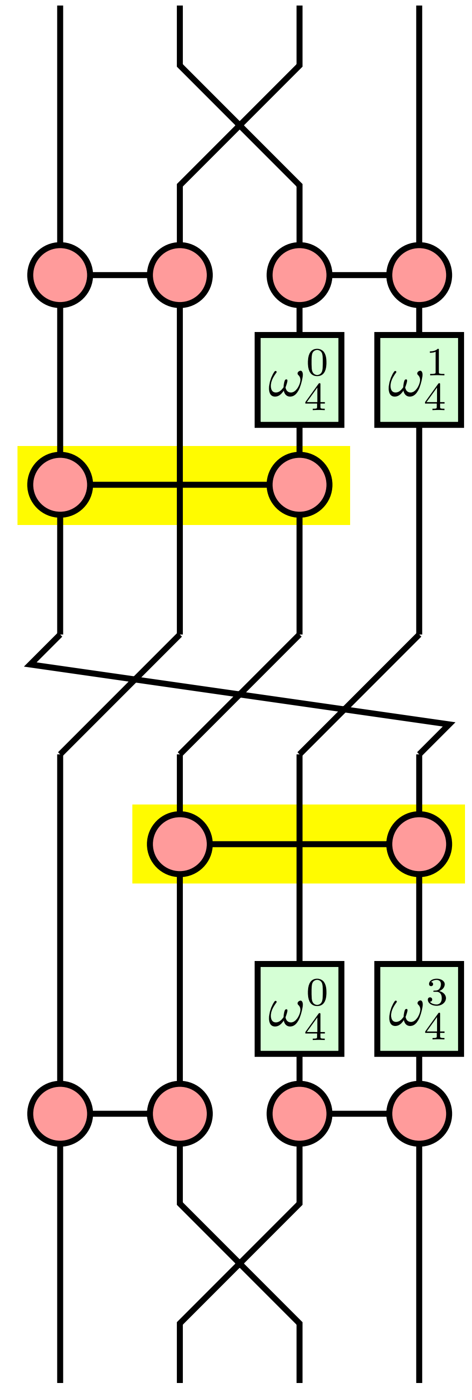

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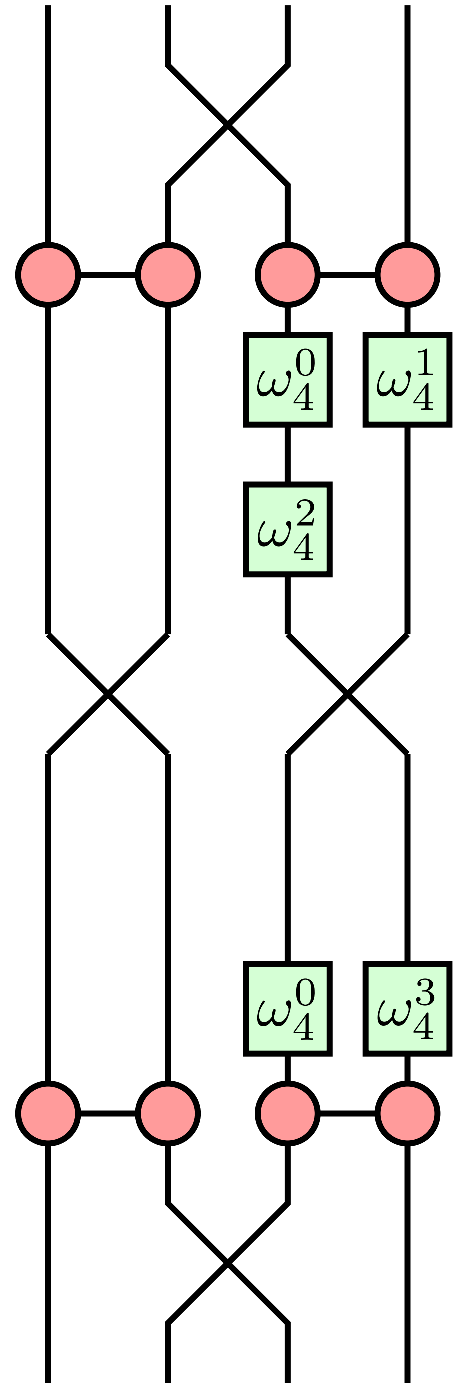

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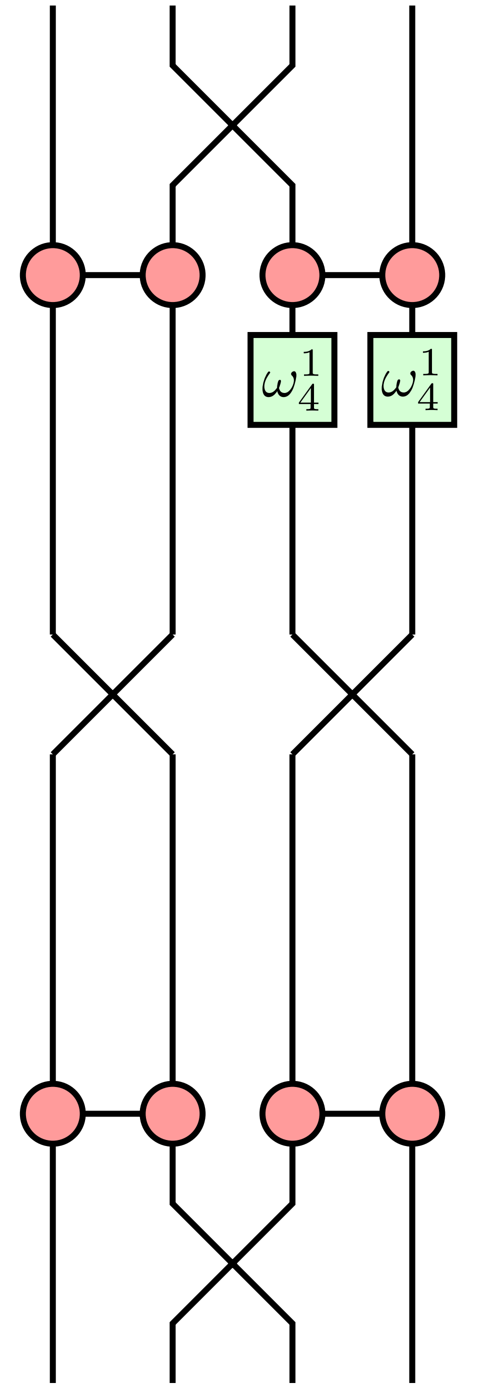

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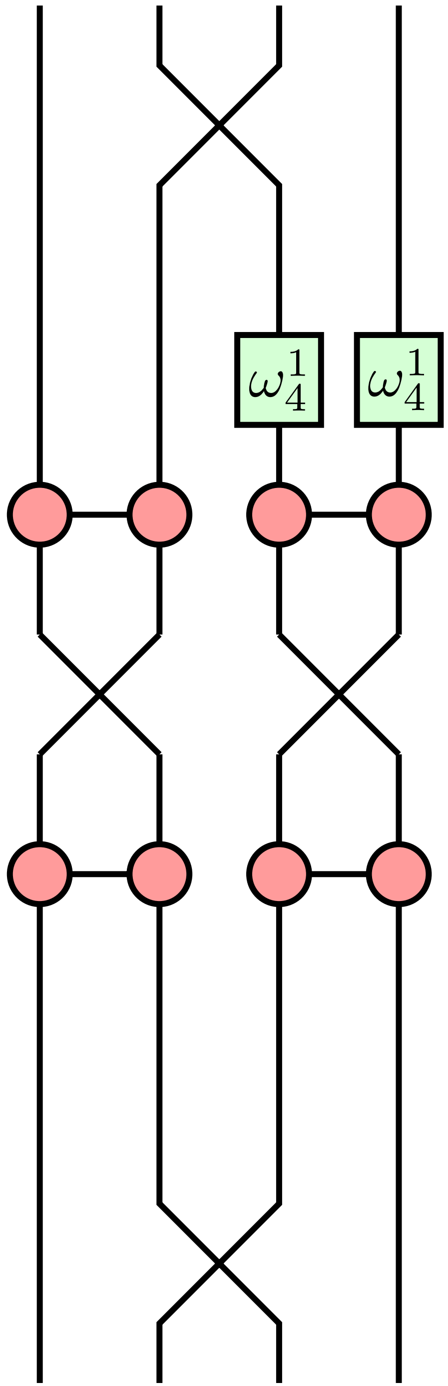

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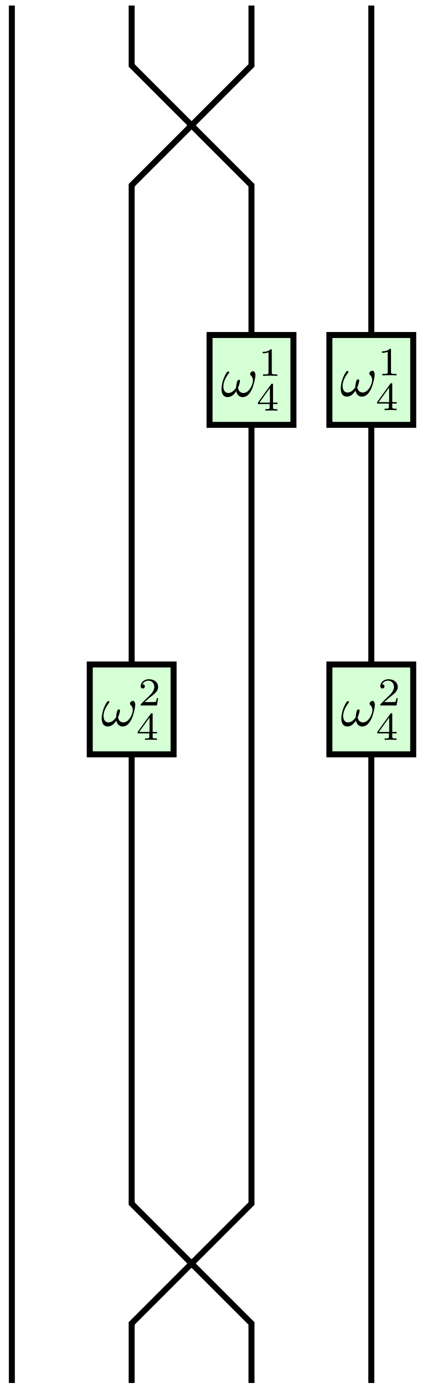

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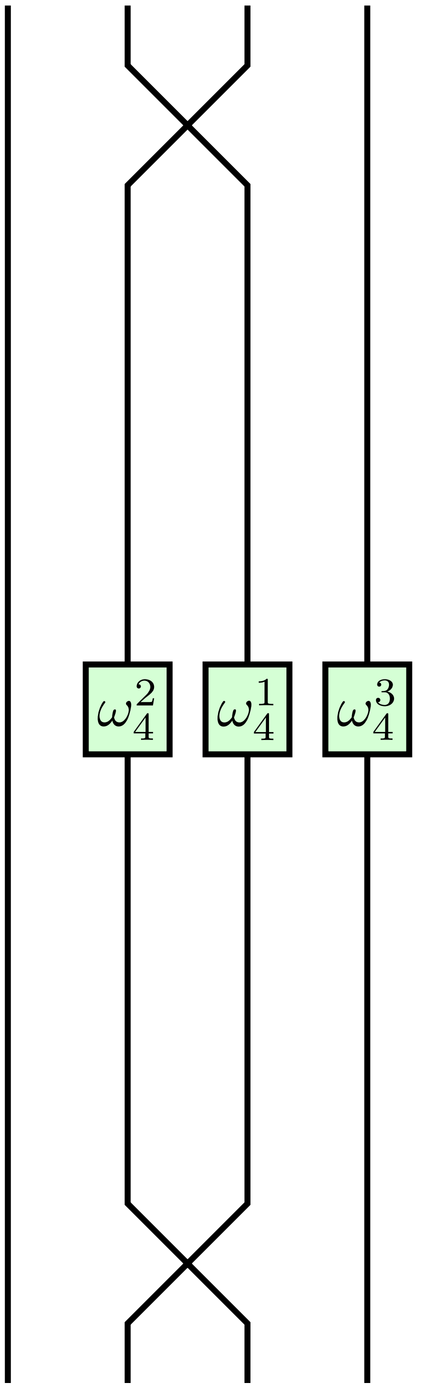

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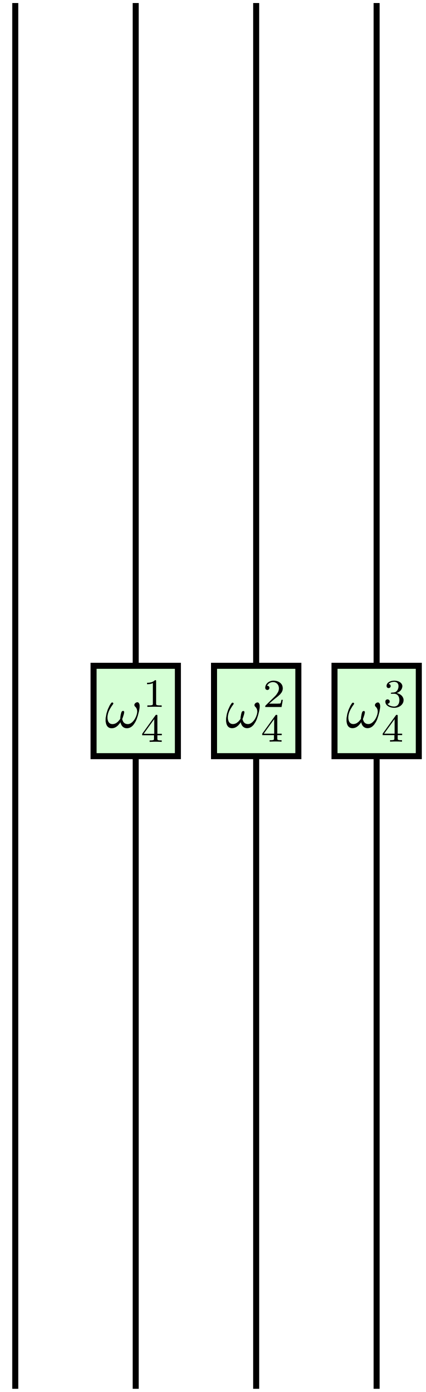
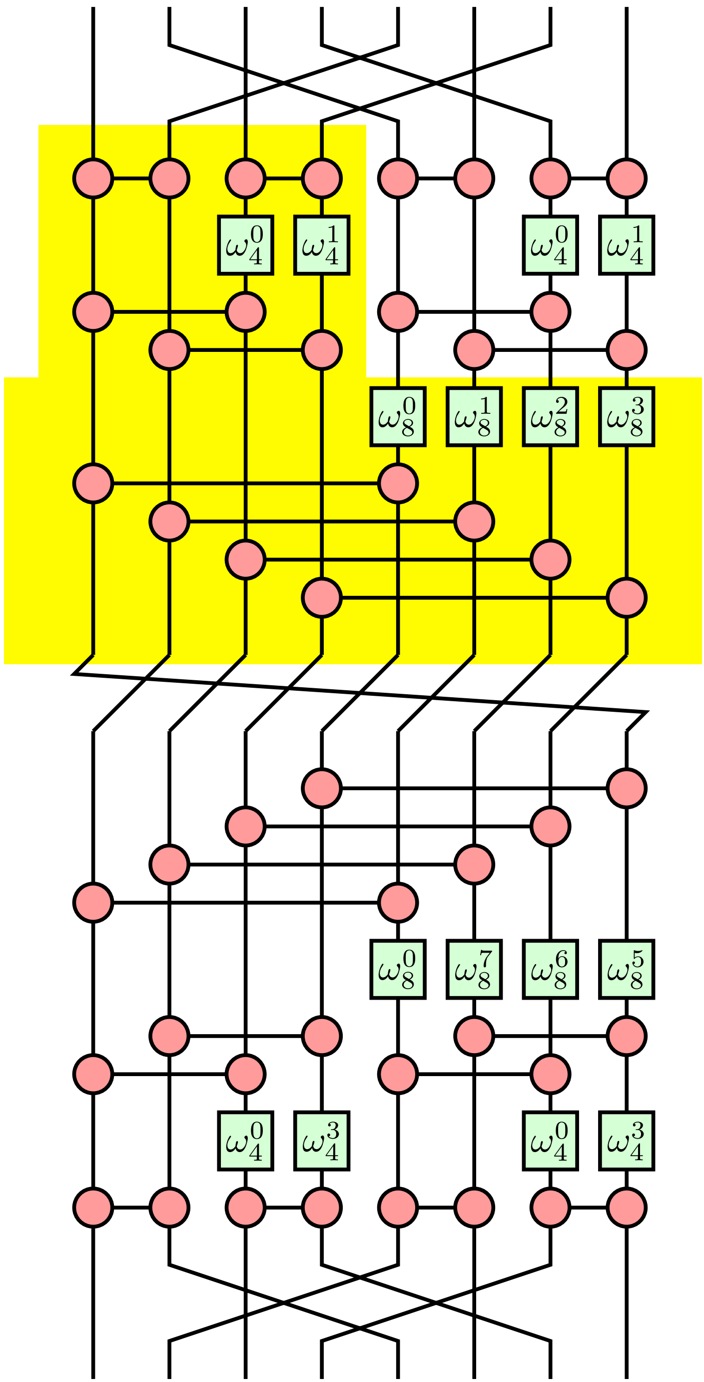
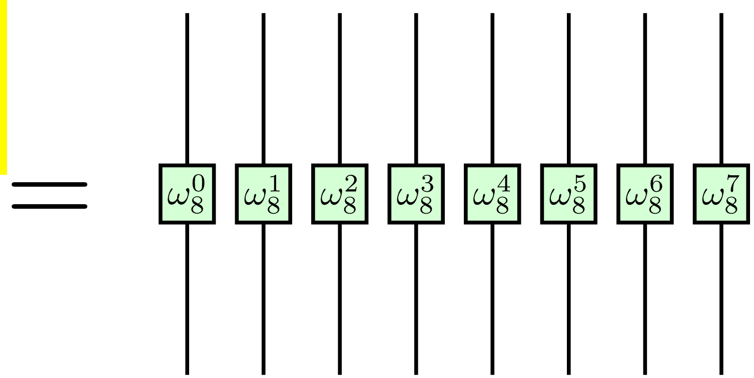


Larger systems



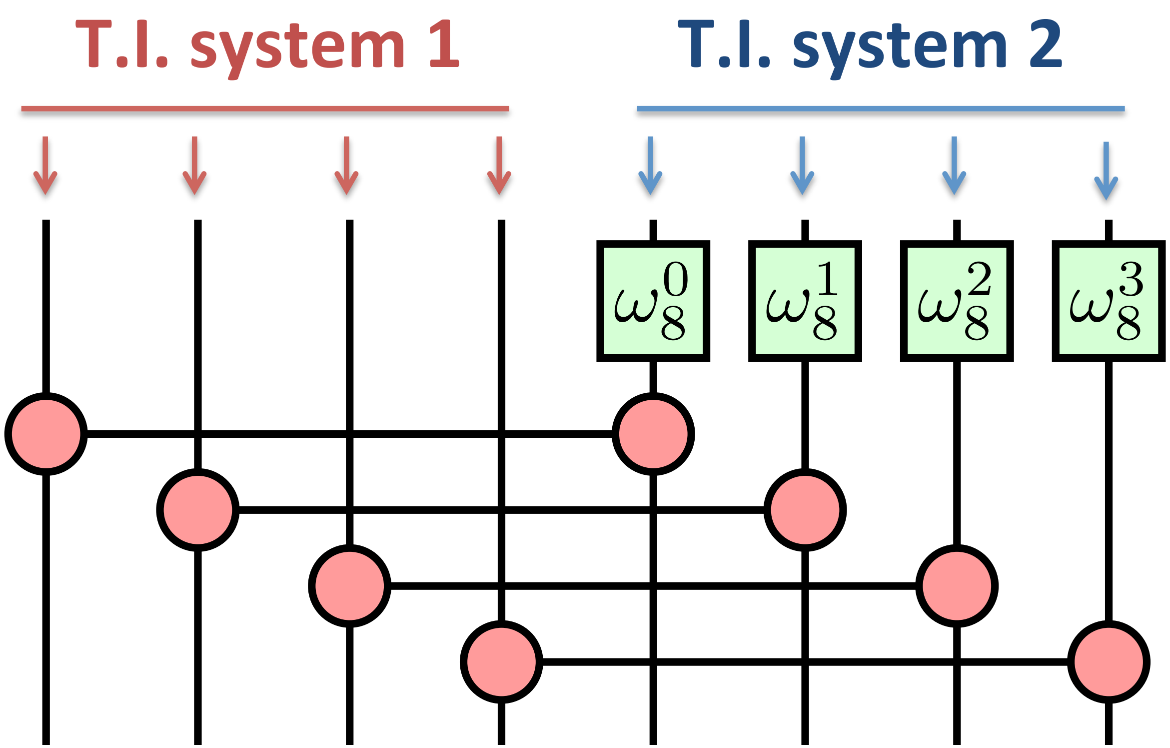
The pattern continues...



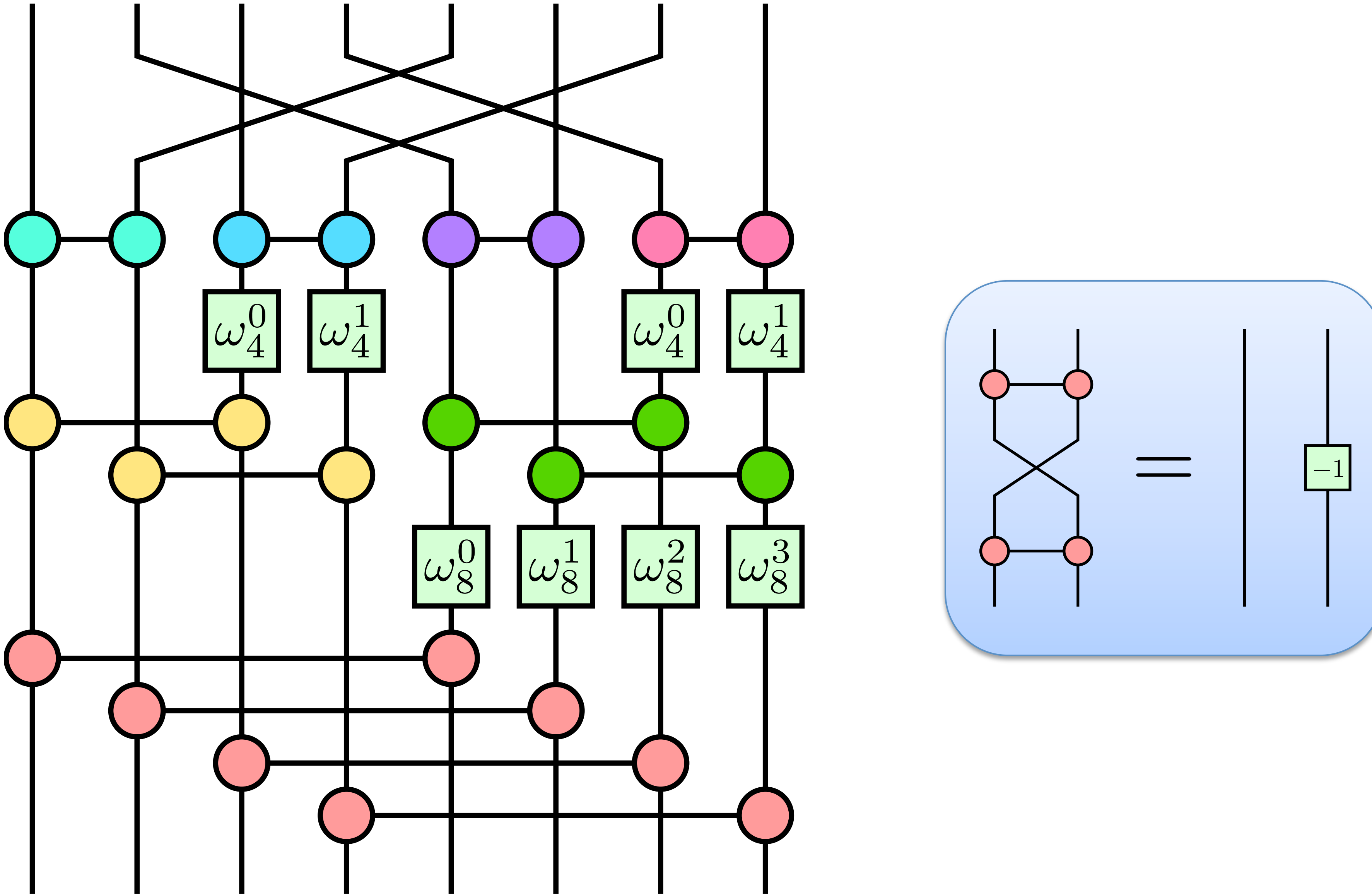
Generally, can decompose any non-prime system size.

The meaning of the phase factors

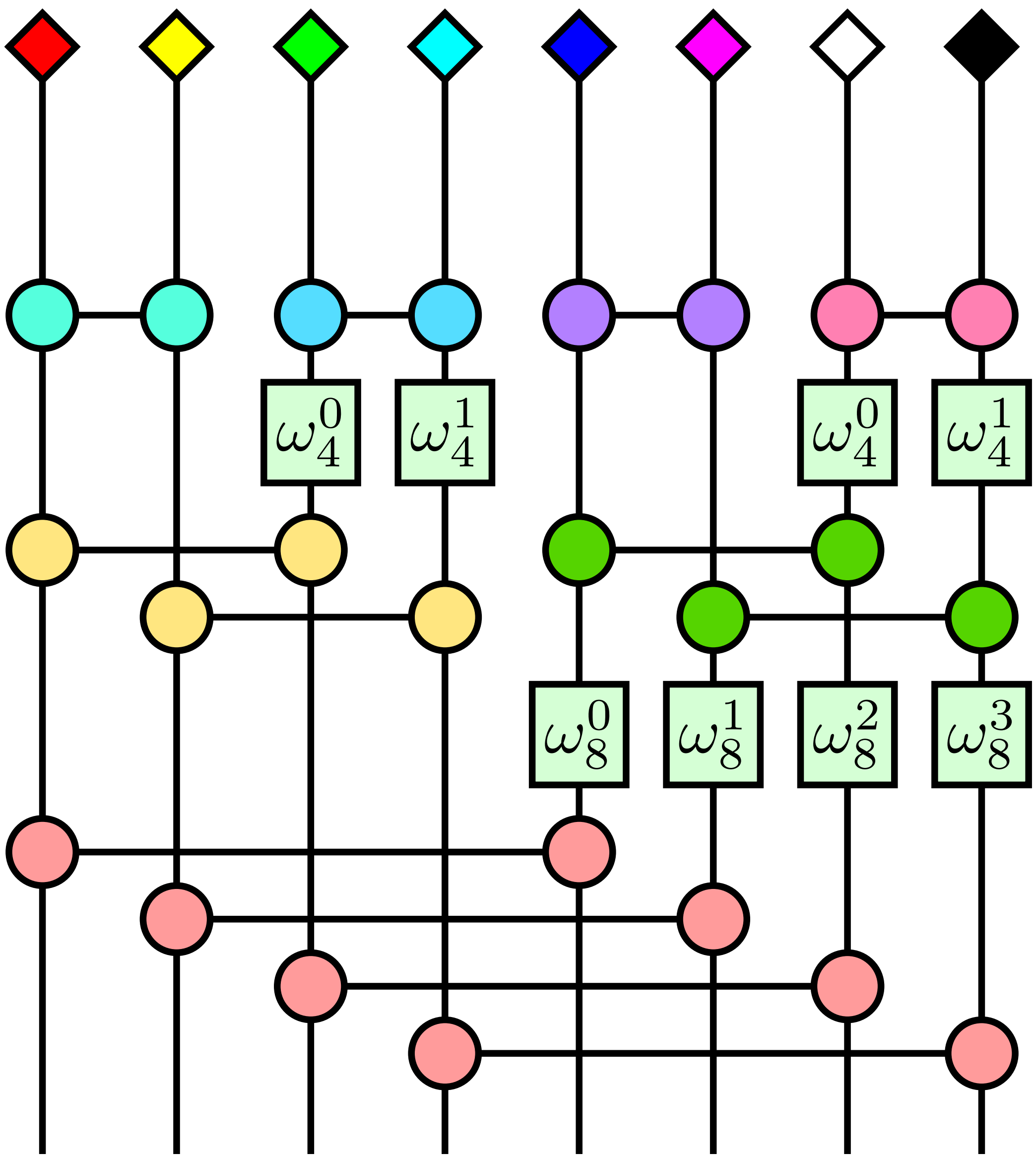
We can interpret the phase factors as applying a half-quanta momentum-boost to the right system

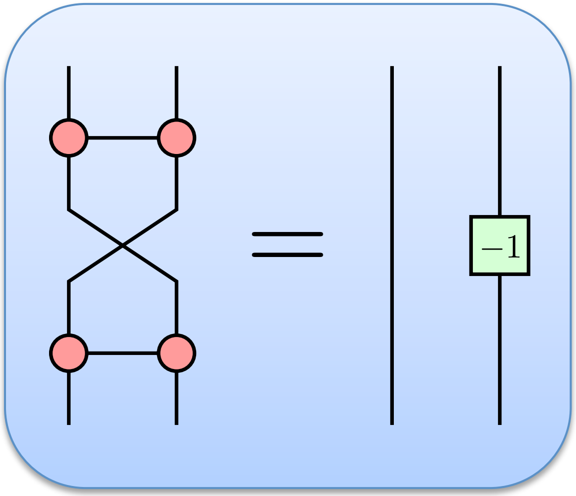


Generalized fast Fourier transform



Spectral tensor network (1D)





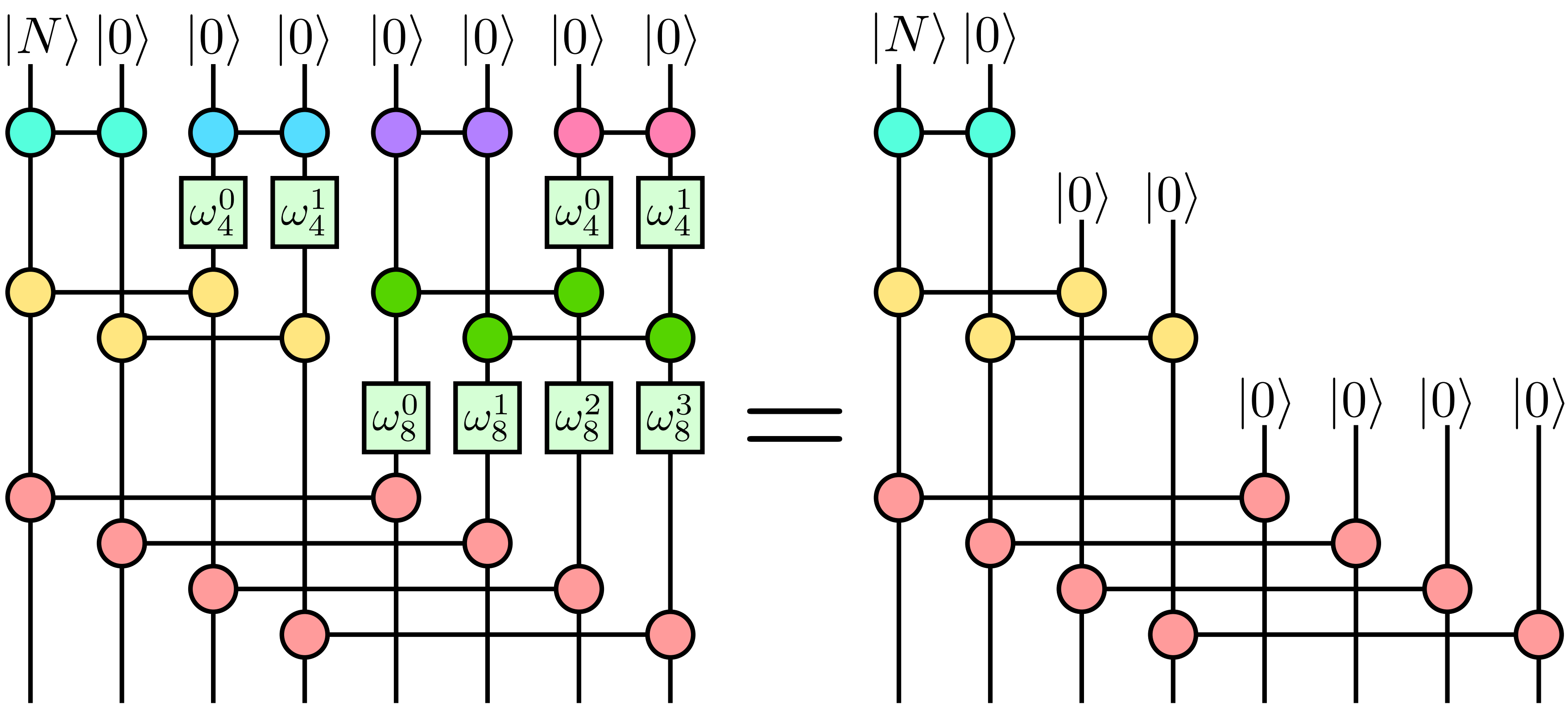
The possibilities

- We now have a tool for creating a wide variety of translationally invariant states. Known cases:

- Bosons: problem - large bond dimension
- Fermions: small Fock space
  - Free fermions include beyond area-law, chiral states, Majorana/SPTO, etc…
  - Interacting fermions?
- Abelian anyons: E.g. parafermions

A ~~simple~~ stupid example

Generalized Bose "condensate"



A ~~simple~~ stupid example

Ger

$|N\rangle$ $|($

Coherent state

$$|\Psi\rangle = |\alpha\rangle|\alpha\rangle \ldots$$

Ma

$|010101\ldots\rangle$

$|0\rangle$ $|0\rangle$

sed state/"Bosanova" (attractive)

$$|\Psi\rangle = |N00\ldots\rangle + |0N0\ldots\rangle + \ldots$$

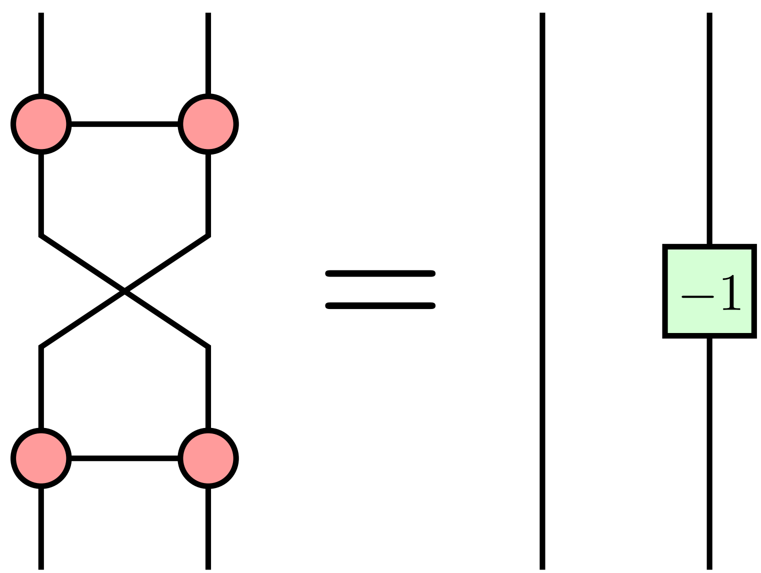
Bad ansatz otherwise

Better example: Hubbard model

Each site has two fermion orbitals (spin up/down).

$$\hat{H} = \sum_{i,s} -t\hat{a}^{\dagger}_{i,s}\hat{a}_{i+1,s} + h.c. + U\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}$$

Unitary has significant freedom.



Better example: Hubbard model

Unitary must preserve number & sort momenta:

	$k = 0$	$k = \pi$
$n = 0$	$\|00\rangle$	
$n = 1$	$\|\uparrow 0\rangle + \|0 \uparrow\rangle$ $\|\downarrow 0\rangle + \|0 \downarrow\rangle$	$\|\uparrow 0\rangle - \|0 \uparrow\rangle$ $\|\downarrow 0\rangle - \|0 \downarrow\rangle$
$n = 2$	$\|\uparrow\downarrow\rangle + \|\downarrow\uparrow\rangle$ $\|20\rangle + \|02\rangle$	$\|\downarrow\downarrow\rangle, \quad \|\uparrow\uparrow\rangle$ $\|\uparrow\downarrow\rangle - \|\downarrow\uparrow\rangle$ $\|20\rangle - \|02\rangle$ Arbitary unitary
$n = 3$	$\|2 \downarrow\rangle + \|\downarrow 2\rangle$ $\|2 \uparrow\rangle + \|\uparrow 2\rangle$	$\|2 \uparrow\rangle - \|\uparrow 2\rangle$ $\|2 \downarrow\rangle - \|\downarrow 2\rangle$
$n = 4$	$\|22\rangle$	

Better example: Hubbard model

Unitary must preserve number & sort momenta:

	$k = 0$	$k =$
$n = 0$	$\lvert 00\rangle$	
$n = 1$		
		itary itary
n		$- \lvert \uparrow 2\rangle$ $\lvert 2 \downarrow\rangle - \lvert \downarrow 2\rangle$
$n =$	$\lvert 22\rangle$	

Simulations in progress

Z_3 parafermions

- Non-interacting parafermions. No more than two particles per site. $\hat{a}_i^{\dagger\,3} = 0$
- Operators get phase when commuted:
$$\hat{a}_i \hat{a}_j = e^{2\pi i/3} \hat{a}_j \hat{a}_i \quad (i < j)$$
$$\hat{a}_i^\dagger \hat{a}_j = e^{2\pi i/3} \hat{a}_j \hat{a}_i^\dagger \quad (i < j)$$
- Local representation of operator:

$$\hat{a}_i^\dagger = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{bmatrix}$$

Like bosons with truncated Fock space

Z_3 parafermions

- Can find a two-body gate such that

$$\hat{U}\hat{a}_1\hat{U}^\dagger = \frac{\hat{a}_1 + \hat{a}_2}{\sqrt{2}} \qquad \hat{U}\hat{a}_2\hat{U}^\dagger = \frac{\hat{a}_1 - \hat{a}_2}{\sqrt{2}}$$

- This gate satisfies the conditions for the spectral tensor network. Implications:
  - Can easily perform (linear) Fourier transform on these parafermions
  - Exactly solve translationally invariant, quadratic Hamiltonians (1D, 2D, long-range hopping + chemical potential)

Parafermion "Jordan-Wigner" transformation

- Can perform a more general Jordan-Wigner transformation to a spin-1 chain.

$$\hat{a}_i = \exp(2\pi i/3 \sum_{j<i} (\hat{Z}_j + 1)) \hat{M}_i$$

- Doesn't work for anomalous terms.
- Gives a very messy spin-1 Hamiltonian
  – I won't even write it here!
- (previously known result)

Discussion

- We are just scratching the surface of what is possible
- Many ways to implement / extend the ansatz
  - TN geometry, system type, Bogoliubov, MPS…
- Many open questions
  - Efficient for interacting models? Fermi liquids?
  - Open boundary conditions? (DST/DCT)
  - Impurity problems or other non-translationally invariant systems?

Thank you!