Universal Computation by Quantum Scattering

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Outline

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Problem Setup

1. Free particles are easy to solve.
2. Particles in potential fields are usually hard to solve.
3. If the initial state and the final state are free, the potential shows up as a perturbation.

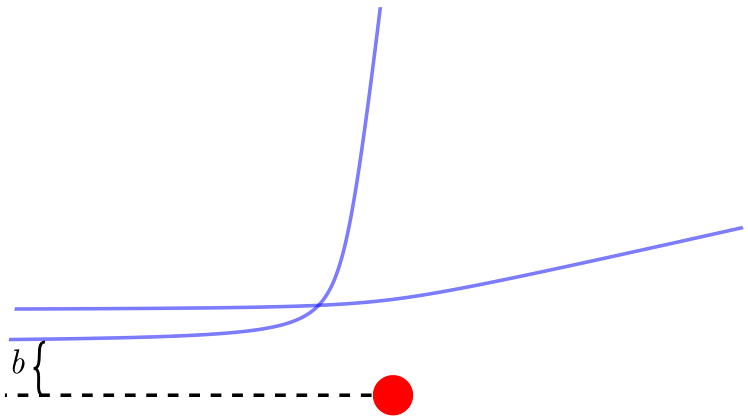
Rutherford Scattering

The trajectory is determined by energy and angular momentum.

$$T = T(L, E), L = pb, E = \frac{p^2}{2m}$$

The scattered state, described by the scattered angle, is determined by the impact parameter b and momentum p.

$$\theta = \theta(p, b)$$



Quantum Scattering

Due to superposition principle, the scattered state may be a superposition of states on different "trajectories".

$$\psi_{\mathrm{in}}(k) = e^{-i\omega t} e^{-ikx}, \psi_{\mathrm{out}}(k) = e^{-i\omega t} \sum_{k'} S_{kk'} e^{ik'x},$$

$$\psi_{\mathrm{sc}}(k) = e^{-i\omega t} \left(\delta_{kk'} e^{-ikx} + \sum_{k'} S_{kk'} e^{ik'x} \right)$$

The S-matrix is vital to scattering problem. The orthonormality of $\psi_{\mathrm{sc}}(k)$ proves the unitarity of S-matrix.

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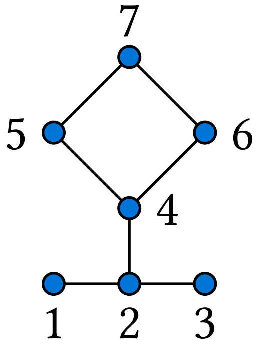
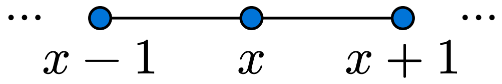
Quantum Evolution on Graphs (Quantum Walk)

For a given graph G, its vertices correspond to states of a system, its adjacency matrix corresponds to Hamiltonian of the system.



$$H = \sum_{(i,j)\in E(G)} |i\rangle\langle j| = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

Free Particles on Graphs



For an infinite path graph, its Hamiltonian is $H = \sum_{x\in\mathbb{Z}} |x\rangle\langle x+1| + |x+1\rangle\langle x|$.

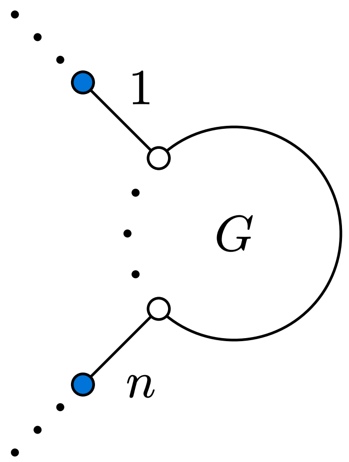
Consider a plane wave $|\mathrm{pl}(k)\rangle = \sum_{x\in\mathbb{Z}} e^{ikx}\,|x\rangle$ and we have

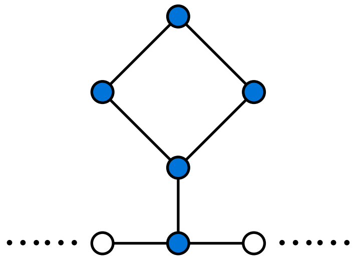
$$\begin{aligned}
H|\mathrm{pl}(k)\rangle &= \sum_{x\in\mathbb{Z}} e^{ikx}(|x-1\rangle + |x+1\rangle) \\
&= \sum_{x\in\mathbb{Z}} \left(e^{ik(x+1)} + e^{-ik(x-1)}\right)|x\rangle \\
&= 2\cos k|\mathrm{pl}(k)\rangle
\end{aligned}$$

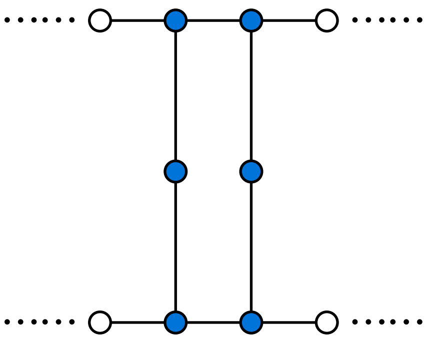
So a particle is “free” when it is on an infinite path graph.

Scattering Problem on Graphs

As defined in "normal" QM, scattering process should take a set of plane wave eigen-states to another. So the scattering process corresponds to a graph shown below.







Solve the S-Matrix

Suppose a graph G is the scattering center. The sites on tails are denoted as $|x, j\rangle$, where $x \in \mathbb{R}^+, 1 \leq j \leq n$. For the vertices with attachments, they can also be denoted as $|0, j\rangle$. The Hamiltonian should be sum of three terms

$$H = H_G + \sum_{1 \leq j \leq n} \left(T_j + |0, j\rangle\langle 1, j| + |1, j\rangle\langle 0, j| \right)$$

The solution of time-independent Schrödinger equation gives

$$H|\mathrm{sc}_q(k)\rangle = 2\cos k\ |\mathrm{sc}_q(k)\rangle \Rightarrow \boxed{S_{qj} = (1 - z^2)\langle 0, q|\ \mathbb{A}^{-1}(z)|0, q\rangle - \delta_{qj},}$$

$$z = e^{ik}, \mathbb{A}(z) = \mathbb{I} - zH_G + z^2\mathbb{Q}, \mathbb{Q} = \mathbb{I} - \sum_{1 \leq j \leq n} |0, j\rangle\langle 0, j|.$$

For detailed proof, see Appendix A.

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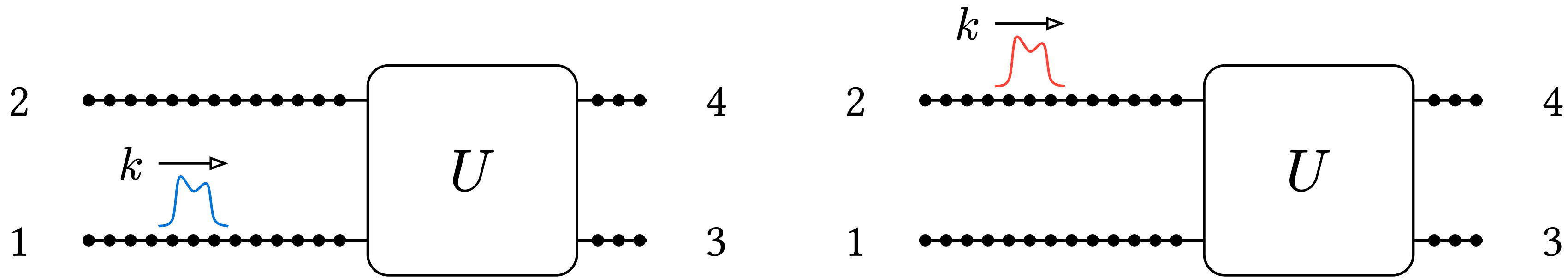
Dual-Rail Encode

For a scattering device with 4 tails. Two of the tails are chosen as input, the other two are chosen as output.

$|0\rangle$ intput: $|1\rangle$ intput:



If there is no scattered component between input tails/output tails, then the device can be served as a single-qubit gate.

S-Matrix and Unitary Operator

Under the above mentioned condition,

$$S = \begin{pmatrix} 0 & 0 & a^* & c^* \\ 0 & 0 & b^* & d^* \\ a & b & 0 & 0 \\ c & d & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & U^\dagger \\ U & 0 \end{pmatrix}$$

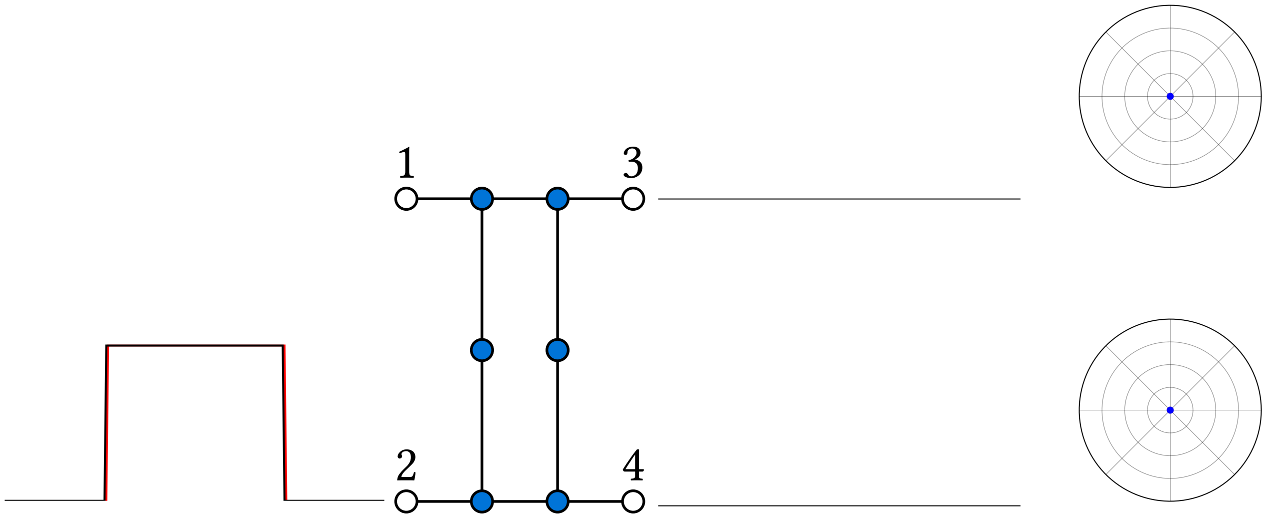
By definition of S-matrix, the state after scattering is

$$\begin{pmatrix} \bar{\psi}_1 \\ \bar{\psi}_2 \\ \bar{\psi}_3 \\ \bar{\psi}_4 \end{pmatrix} = \begin{pmatrix} 0 & 0 & a^* & c^* \\ 0 & 0 & b^* & d^* \\ a & b & 0 & 0 \\ c & d & 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 = 0 \\ \psi_4 = 0 \end{pmatrix} \Rightarrow \boxed{\begin{pmatrix} \bar{\psi}_3 \\ \bar{\psi}_4 \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}}, \begin{pmatrix} \bar{\psi}_1 \\ \bar{\psi}_2 \end{pmatrix} = 0$$

Basis Change Gate

$$k = \frac{\pi}{4}$$

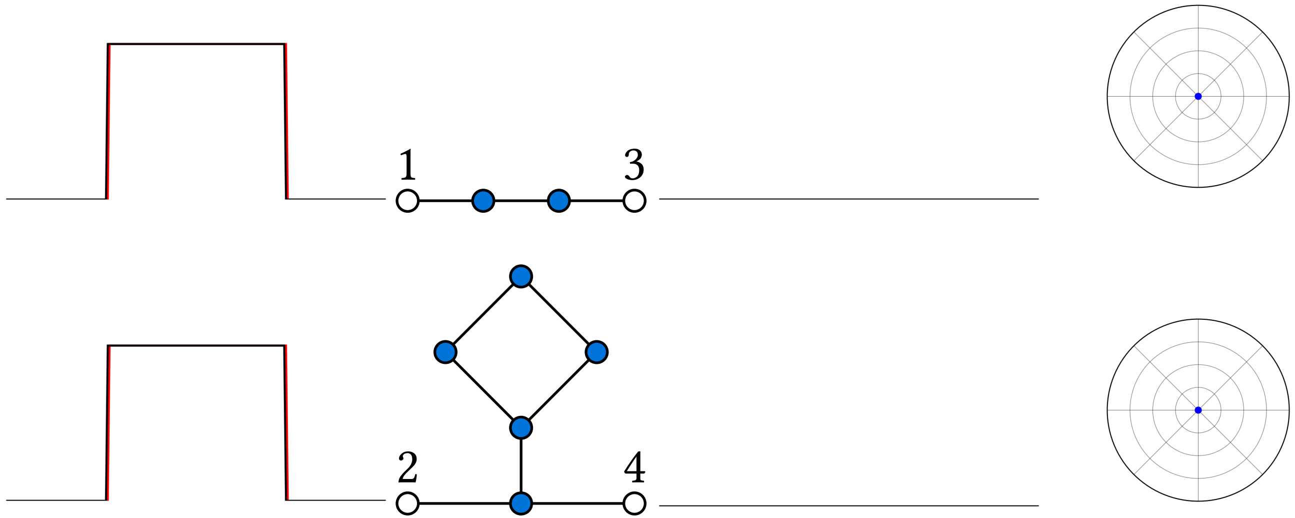
$$S = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 & -\frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}$$



Phase Gate

$$k = \frac{\pi}{4}$$

$$S = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{-i\frac{\pi}{4}} \\ 1 & 0 & 0 & 0 \\ 0 & e^{i\frac{\pi}{4}} & 0 & 0 \end{pmatrix}$$



Two Qubit Gate: Controlled Phase Gate

Introduce one ancilla qubit (mediator qubit).

$$
\begin{aligned}
\mathrm{CP}_{ij}|a_i, b_j, 0_m\rangle &= \mathrm{CNOT}_{im}\mathrm{CP}_{jm}\mathrm{CNOT}_{im}|a_i, b_j, 0_m\rangle \\
&= H_m \mathrm{CP}^2_{im} H_m \mathrm{CP}_{jm} H_m \mathrm{CP}^2_{im} H_m \; |a_i, b_j, 0_m\rangle
\end{aligned}
$$

Thus, gates needed to build universal computer are:

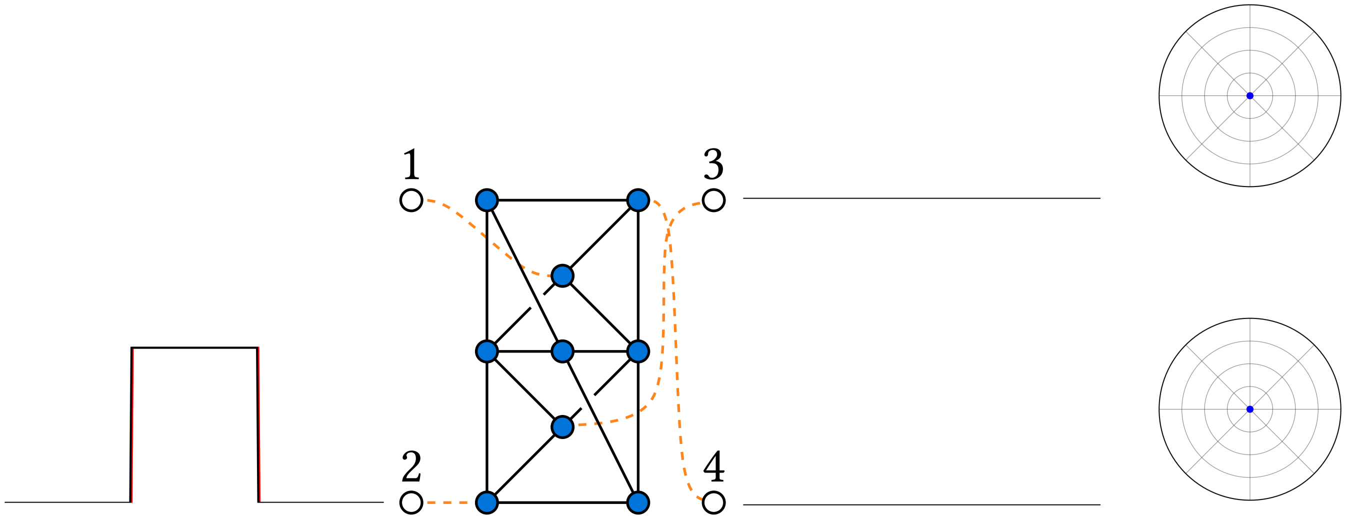
1. single-qubit gates on computational qubits (✓) ,
2. controlled phase gate between computational qubit and mediator qubit,
3. Hadamard gate on mediator qubit.

Note: only when the mediator qubit and computational qubit have different momentum, can they gain non-trivial phase after interaction.

Hadamard Gate

$$k = \frac{\pi}{2}$$

$$S = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}$$



1. single-qubit gates on computational qubits (✓) ,
2. controlled phase gate between computational qubit and mediator qubit,
3. Hadamard gate on mediator qubit (✓) .

Two Interacting Bosonic Walker on Infinite Chain

For Bose-Hubbard interaction

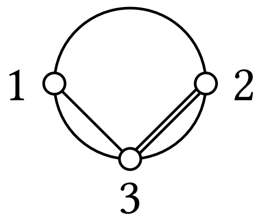
$$U(r) = u\delta_{r,0},$$

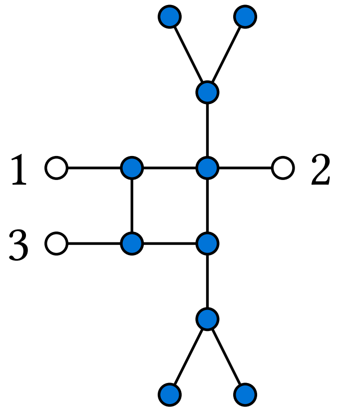
the phase gained is

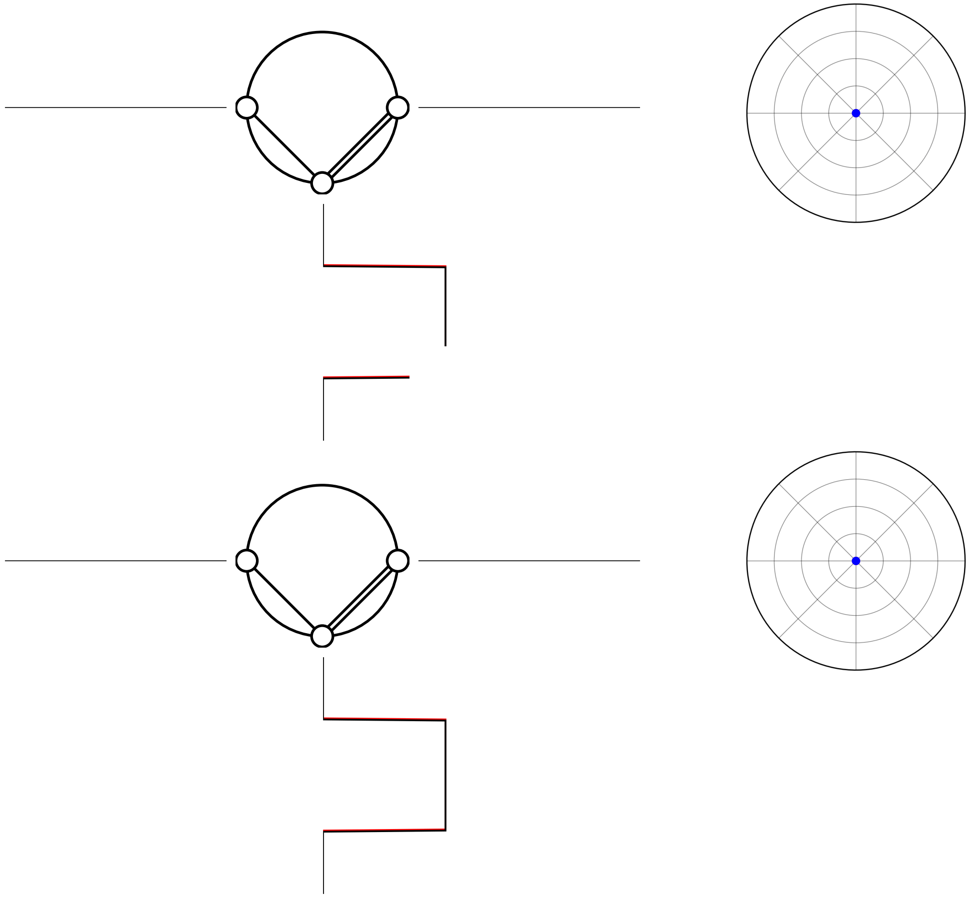
$$e^{i\theta} = -\frac{u + 4i\cos\ell\sin k}{u - 4i\cos\ell\sin k}, \ell = \frac{p_1 + p_2}{2}, k = \frac{p_1 - p_2}{2}$$

For detailed proof, see Appendix B.

Momentum Switch





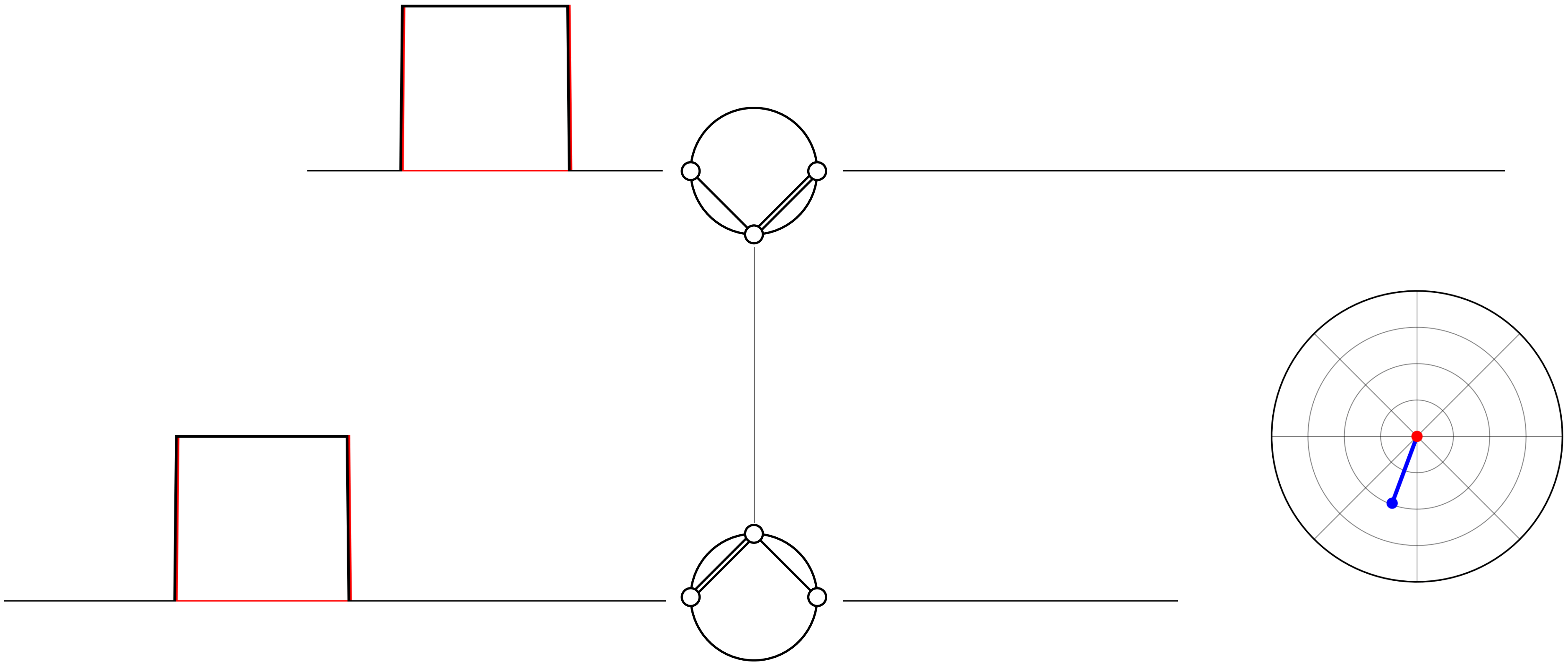


Momentum switch is a gadget that leads wave with different momentum to different rail.

For $k = \frac{\pi}{4}$, perfect transmission happens only between 1 and 3.

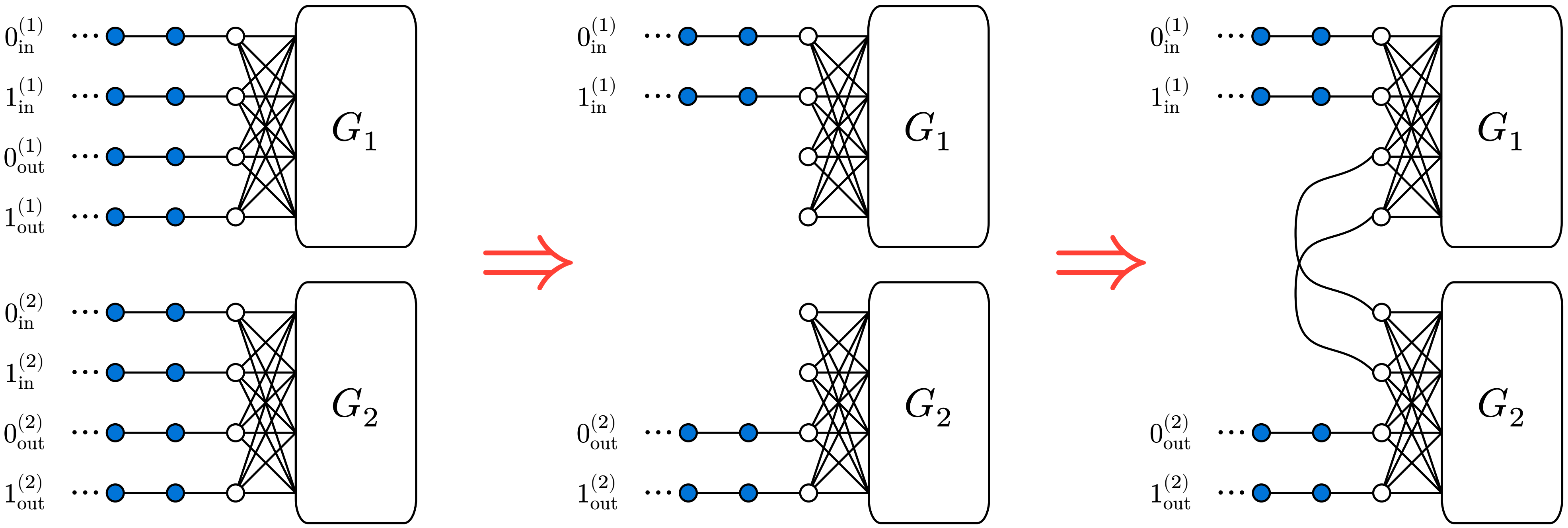
For $k = \frac{\pi}{2}$, perfect transmission happens only between 2 and 3.

C-Phase Gate

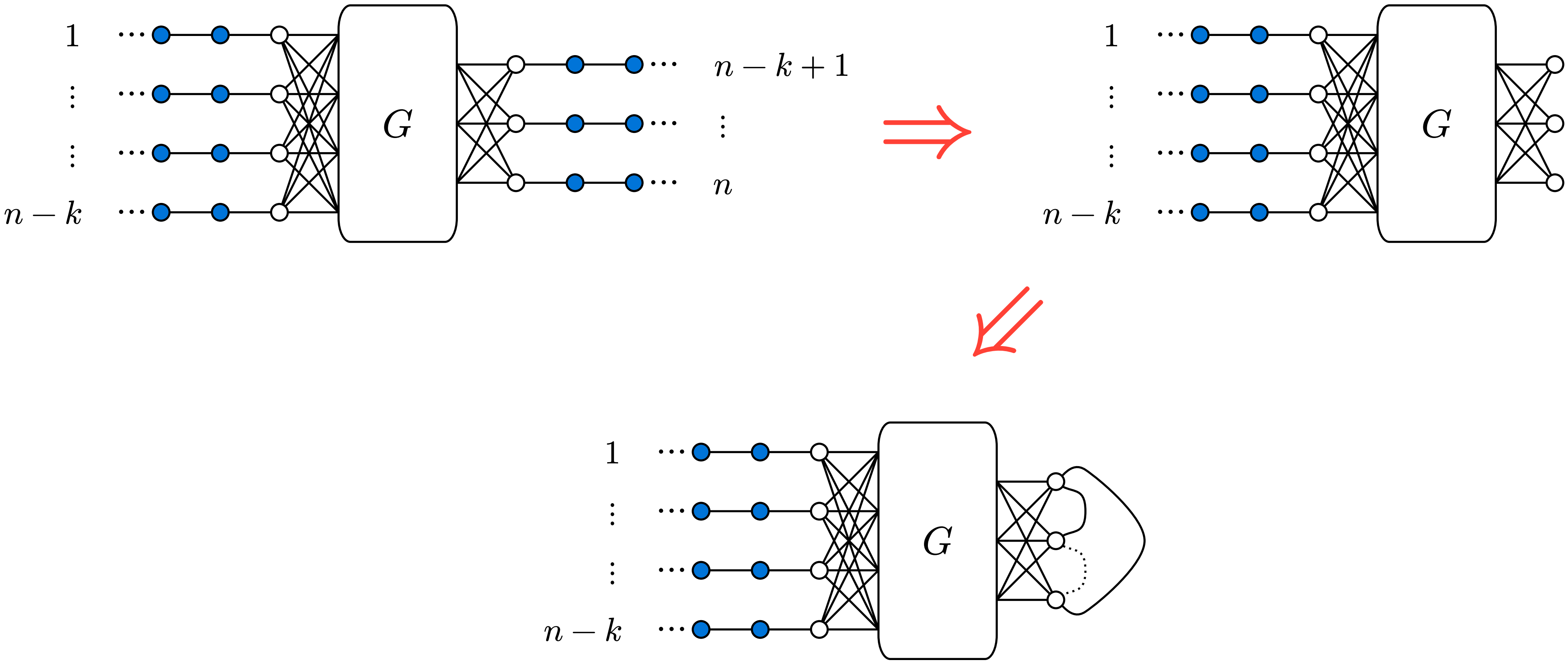


Outline

Link Two Gadget



Link Two Gadget: Abstraction



Link Two Gadget: Calculation

The above operation results in the change of Hamiltonian H_G and $\mathbb{Q}$ matrix.

$$\tilde{H}_G = H_G + \sum_{(\alpha,\beta)\in\tilde{E}} |\alpha\rangle\langle\beta| + |\beta\rangle\langle\alpha| =: H_G + h_G$$

$$\tilde{\mathbb{Q}} = \mathbb{I} - \sum_{j\in \text{ remained}} |0,j\rangle\langle 0,j| = \mathbb{Q} + \sum_{j\in \text{ cutted}} |0,j\rangle\langle 0,j| =: \mathbb{Q} + Q$$

$$\Rightarrow \tilde{\mathbb{A}}(z) = \mathbb{I} - z\tilde{H}_G + z^2\tilde{\mathbb{Q}} = \mathbb{A}(z) + z^2 Q - z h_G =: \mathbb{A}(z) + P$$

Link Two Gadget: Result

Suppose the original S-matrix, in block form, is

$$S = \begin{pmatrix} T_{(n-k)\times(n-k)} & U_{(n-k)\times k} \\ V_{k\times(n-k)} & W_{k\times k} \end{pmatrix}$$

$$\begin{aligned} \tilde{S} &= (1-z^2)(\mathbb{I}_n 0)\tilde{\mathbb{A}}^{-1}(z)\begin{pmatrix} \mathbb{I}_n \\ 0 \end{pmatrix} - \mathbb{I}_n \\ &= T - UP\left[(1-z^2)\mathbb{I} + P + WP\right]^{-1} V \end{aligned}$$

For two scattering gates, the above formula gives

$$S_1 = \begin{pmatrix} 0 & U_1^\dagger \\ U_1 & 0 \end{pmatrix}, S_2 = \begin{pmatrix} 0 & U_2^\dagger \\ U_2 & 0 \end{pmatrix} \Rightarrow S = \begin{pmatrix} 0 & z^* U_2^\dagger U_1^\dagger \\ z U_1 U_2 & 0 \end{pmatrix}$$

Outline

Summary

About A.M. Childs' construction:

1. no time-dependent quantum controll
2. error bound $\sim O\left(L^{-\frac{1}{4}}\right)$
3. numerous sites

Future work:

1. delay gadget
2. gadget cascade
3. realization in bio-systems (polymers)

Thank you

Outline

Solve the S-Matrix: take a guess!

The eigen-state of Hamiltonian can be expressed as

$$|\mathrm{sc}_q(k)\rangle = \sum_v \alpha_{q,v} \, |v\rangle + \sum_{1\leq j\leq n} \sum_{x\geq 1} \beta_{x,q,j} \, |x,j\rangle.$$

Recall the quantum scattering page, here we take

$$\beta_{x,q,j} = \langle x,j| \, \mathrm{sc}_q(k)\rangle = \delta_{qj} e^{-ikx} + S_{qj} e^{ikx}$$

(Actually, suppose this relation holds for all $x \geq 0$. Because $|0,j\rangle$ is also a part of path graph.)

Quantum Scattering (Re-visit)

Due to superposition principle, the scattered state may be a superposition of states on different "trajectories".

$$\psi_{\text{in}}(k) = e^{-i\omega t} e^{-ikx}, \psi_{\text{out}}(k) = e^{-i\omega t} \sum_{k'} S_{kk'} e^{ik'x},$$

$$\psi_{\text{sc}}(k) = e^{-i\omega t} \left(\delta_{kk'} e^{-ikx} + \sum_{k'} S_{kk'} e^{ik'x} \right)$$

The S-matrix is vital to scattering problem. The orthonormality of $\psi_{\text{sc}}(k)$ proves the unitarity of S-matrix.

Solve the S-Matrix: for sites on tails

$$
\begin{aligned}
|\mathrm{sc}_q(k)\rangle &= \sum_v \alpha_{q,v}\, |v\rangle + \sum_{1\le j\le n} \sum_{x\ge 1} \left(\delta_{qj} e^{-ikx} |x, j\rangle + S_{qj} e^{ikx}\, |x, j\rangle\right) \\
&= |\mathrm{sc}_q(k)\rangle^G + \sum_{1\le j\le n} \sum_{x\ge 1} \left(\delta_{qj} e^{-ikx} + S_{qj} e^{ikx}\right) |x, j\rangle
\end{aligned}
$$

Use the result of free propagation, we have

$$
\begin{aligned}
\langle x', q' | H | \mathrm{sc}_q(k)\rangle &= \langle x', q' | T_{q'} | \mathrm{sc}_q(k)\rangle \\
&= \langle x', q' | 2\cos k | \mathrm{sc}_q(k)\rangle.
\end{aligned}
$$

Since $|\mathrm{sc}_q(k)\rangle$ is an energy eigen-state,

$$
\boxed{H|\mathrm{sc}_q(k)\rangle = 2\cos k |\mathrm{sc}_q(k)\rangle}
$$

Solve the S-Matrix

$$H = H_G + \sum_{1\le j\le n} \left(T_j + |0,j\rangle\langle 1,j| + |1,j\rangle\langle 0,j|\right)$$

$$|\mathrm{sc}_q(k)\rangle = |\mathrm{sc}_q(k)\rangle^G + \sum_{1\le j\le n}\sum_{x\ge 1}(\delta_{qj}e^{-ikx} + S_{qj}e^{ikx})|x,j\rangle$$

$$H|\mathrm{sc}_q(k)\rangle = 2\cos k|\mathrm{sc}_q(k)\rangle$$

$$\begin{aligned} H|\mathrm{sc}_q(k)\rangle = H_G|\mathrm{sc}_q(k)\rangle^G &+ \\ &\sum_{1\le j\le n}\left(2\cos k\sum_{x\ge 1}(\delta_{qj}e^{-ikx} + S_{qj}e^{ikx})|x,j\rangle - (\delta_{qj} + S_{qj})|1,j\rangle\right) \\ &+ \sum_{1\le j\le n}\left(|1,j\rangle\langle 0,j|\mathrm{sc}_q(k)\rangle^G + |0,j\rangle\langle 1,j|(\delta_{qj}e^{-ik} + S_{qj}e^{ik})|1,j\rangle\right) = 2\cos k|\mathrm{sc}_q(k)\rangle \end{aligned}$$

Solve the S-Matrix

$$(H_G - 2\cos k)|\mathrm{sc}_q(k)\rangle^G + \sum_{1\le j\le n} \left(\delta_{qj}e^{-ik} + S_{qj}e^{ik}\right)|0,j\rangle = \sum_{1\le j\le n} \left(\delta_{qj} + S_{qj} - \langle 0,j|\mathrm{sc}_q(k)\rangle^G\right)|1,j\rangle$$

$$\Rightarrow S_{qj} = \langle 0,j|\mathrm{sc}_q(k)\rangle^G - \delta_{qj}$$

$$(H_G - 2\cos k)|\mathrm{sc}_q(k)\rangle^G + \sum_{1\le j\le n} \left(\delta_{qj}e^{-ik} - \delta_{qj}e^{ik} + e^{ik}\langle 0,j|\mathrm{sc}_q(k)\rangle\right)|0,j\rangle = 0$$

$$(H_G - 2\cos k)|\mathrm{sc}_q(k)\rangle^G + \left(e^{-ik} - e^{ik}\right)|0,q\rangle + \sum_{1\le j\le n} e^{ik}|0,j\rangle\langle 0,j|\mathrm{sc}_q(k)\rangle = 0$$

$$\left(H_G - 2\cos k + e^{ik}\sum_{1\le j\le n}|0,j\rangle\langle 0,j|\right)|\mathrm{sc}_q(k)\rangle^G = \left(e^{ik} - e^{-ik}\right)|0,q\rangle$$

Solve the S-Matrix

Denote $z = e^{ik}$ and get

$$\mathbb{A}(z)|\mathrm{sc}_q(k)\rangle^G = (\mathbb{I} - zH_G + z^2\mathbb{Q})|\mathrm{sc}_q(k)\rangle^G = (1 - z^2)|0, q\rangle, \mathbb{Q} = \mathbb{I} - \sum_{1\leq j\leq n} |0, j\rangle\langle 0, j|.$$

Then

$$S_{qj} = (1 - z^2)\langle 0, q|\ \mathbb{A}^{-1}(z)|0, q\rangle - \delta_{qj}$$

Outline

Two Interacting Walkers in Free Space

The coordinates of two bosons are denoted as x, y.

Then the sites of the system are

$$|x, y\rangle = |x\rangle \otimes |y\rangle.$$

Note that exchange symmetry is not considered here.
But it will be considered are the very end of the proof.

The Hamiltonian is, under this “basis”,

$$H = \sum_{x,y} (|x+1, y\rangle\langle x, y| + |x, y\rangle\langle x+1, y| + \\ |x, y+1\rangle\langle x, y| + |x, y\rangle\langle x, y+1| + U(|x-y|)|x, y\rangle\langle x, y|)$$

Basis Transformation

Consider a set of new coordinates $s = x + y, r = x - y$, the Hamiltonian can be expressed as

$$
\begin{aligned}
H = \sum_{s,r} (&|s+1, r+1\rangle\langle s, r| + |s, r\rangle\langle s+1, r+1| + \\
&|s+1, r-1\rangle\langle s, r| + |s, r\rangle\langle s+1, r-1| + U(|r|)|s, r\rangle\langle s, r|) \\
= \sum_{s,r} (&|s+1\rangle\langle s| \otimes |r+1\rangle\langle r| + |s\rangle\langle s+1| \otimes |r\rangle\langle r+1| + \\
&|s+1\rangle\langle s| \otimes |r-1\rangle\langle r| + |s\rangle\langle s+1| \otimes |r\rangle\langle r-1| + U(|r|)|s\rangle\langle s| \otimes |r\rangle\langle r|) \\
= H^{(s)}_{\text{free}} &\otimes H^{(r)}_{\text{free}} + \mathbb{I}^{(s)} \otimes \sum_r U(|r|)|r\rangle\langle r| \\
=: F_s &\otimes F_r + \mathbb{I}_s \otimes U_r
\end{aligned}
$$

Eigen-State

Notice that s-part Hamiltonian is just free particle.

$$\langle s, r|\mathrm{cr}(\ell, k)\rangle = e^{-i\ell s}\langle r|\ \psi_r(\ell, k)\rangle$$

Assume the interaction $U(|r|)$ is of range C, i.e., $U(|r|) = 0$ for $|r| > C$.

So for $|r| > C$, the r-part Hamiltonian is also free particle.

$$\langle r|\psi_r(\ell, k)\rangle = e^{-ikr} + \alpha(\ell, k)e^{ikr},\ \text{ for } r < -C$$
$$\langle r|\psi_r(\ell, k)\rangle = \beta(\ell, k)e^{-ikr},\ \text{ for } r > C$$

Again, for $|r| > C$

$$\begin{aligned}\langle s, r|H|\mathrm{cr}(\ell, k)\rangle &= \langle s, r|F_s \otimes F_r|\mathrm{cr}(\ell, k)\rangle \\ &= 4\cos\ell\cos k\langle s, r|\mathrm{cr}(\ell, k)\rangle\end{aligned}$$

Time-Independent Schrödinger Equation

The eigen-state, plugged in konwn information, is of the form

$$|\psi_r(\ell,k)\rangle = \sum_{-C\le r\le C} \varphi_r\, |r\rangle + \sum_{r<-C} \left(e^{-ikr} + \alpha(\ell,k)e^{ikr}\right)|r\rangle + \sum_{r>C} \beta(\ell,k)e^{-ikr}|r\rangle$$

$$|\mathrm{cr}(\ell,k)\rangle = |\mathrm{pl}(\ell)\rangle \otimes |\psi_r(\ell,k)\rangle$$

Consider the Schrödinger equation for eigen-state $|\mathrm{cr}(\ell,k)\rangle$,

$$H|\mathrm{cr}(\ell,k)\rangle = 2\cos\ell|\mathrm{pl}(\ell)\rangle \otimes F_r|\psi_r(\ell,k)\rangle + |\mathrm{pl}(\ell)\rangle \otimes U_r|\psi_r(\ell,k)\rangle = 4\cos\ell\cos k|\mathrm{cr}(\ell,k)\rangle$$

$$\Rightarrow 2\cos\ell F_r|\psi_r(\ell,k)\rangle + U_r|\psi_r(\ell,k)\rangle = 4\cos\ell\cos k|\psi_k(\ell,k)\rangle$$

Exchange Symmetry

By swapping the particle coordinates x and y, we have

$$\begin{aligned}\mathrm{Sym}(|x,y\rangle) &= \frac{1}{\sqrt{2}}(|x,y\rangle \pm |y,x\rangle)\\ &= \frac{1}{\sqrt{2}}(|s,r\rangle \pm |s,-r\rangle)\\ &= |s\rangle \otimes \mathrm{Sym}(|r\rangle).\end{aligned}$$

As for the eigen-state, we have

$$|\psi_{-r}(\ell,k)\rangle = \sum_{-C\le r\le C} \varphi_{-r}\,|r\rangle + \sum_{r>C}\left(e^{ikr} + \alpha(\ell,k)e^{-ikr}\right)|r\rangle + \sum_{r<-C} \beta(\ell,k)e^{ikr}|r\rangle = |\psi_r(\ell,-k)\rangle$$

is another eigen-state with same energy ($E = 4\cos\ell\cos k$ is even in k).

Exchange Symmetry: Continued

The "true" eigen-state that satisfies exchange symmetry is

$$\mathrm{Sym}(|\psi_r(\ell,k)\rangle) = \frac{1}{\sqrt{2}} \sum_{-C\leq r\leq C} (\varphi_r \pm \varphi_{-r})\ |r\rangle + \frac{1}{\sqrt{2}} \sum_{r>C} [e^{ikr} + (\alpha \pm \beta) e^{-ikr}] |r\rangle + \frac{1}{\sqrt{2}} \sum_{r<-C} [e^{-ikr} + (\alpha \pm \beta) e^{ikr}] |r\rangle.$$

Clearly, the phase gained through interaction is

$$e^{i\theta} = \alpha(\ell,k) \pm \beta(\ell,k).$$

Bose-Hubbard Model

For Bose-Hubbard model, $U(r) = u\delta_{r,0}$, $C = 0$.

$$|\psi_r(\ell, k)\rangle = \varphi_0 \; |0\rangle + \sum_{r<0} \left(e^{-ikr} + \alpha(\ell, k) e^{ikr}\right) |r\rangle + \sum_{r>0} \beta(\ell, k) e^{-ikr} |r\rangle$$

And the Schrödinger equation gives

$$2\cos\ell \left[\varphi_0 |1\rangle + \varphi_0 |-1\rangle + \left(e^{ik} + \alpha(\ell, k) e^{ik}\right) |0\rangle - (1+\alpha)|-1\rangle + \beta e^{-ik} |0\rangle - \beta \; |1\rangle\right]$$
$$+ u\varphi_0 |0\rangle = 4\cos\ell \cos k \varphi_0 \; |0\rangle$$

$$\varphi_0 = 1 + \alpha$$
$$\varphi_0 = \beta$$
$$u\varphi_0 = 4i\cos\ell \sin k(\varphi_0 - 1)$$

$$\Rightarrow e^{i\theta} = \frac{4i\cos\ell \sin k + u}{4i\cos\ell \sin k - u}$$