Chapter 1

Universality of single-particle scattering

1.1 Finite truncation

I think I should include theorem 1 here (maybe)

Theorem 1. *Let $\widehat{G}$ be an $(N+m)$-vertex graph. Let G be the graph obtained from $\widetilde{G}$ by attaching semi-infinite paths to the first N of its vertices, and let S be the corresponding S-matrix. Let H_G be the quantum walk Hamiltonian of equation [**CITE:** correct equation] . Let $k \in (-\pi, 0)$, $M, L \in \mathbb{N}$, $j \in [N]$, and*

$$|\psi^j(0)\rangle = \frac{1}{\sqrt{L}} \sum_{x=M+1}^{M4L} e^{-ikx}|x, j\rangle. \tag{1.1}$$

Let c_0 be a constant independent of L. Then, for all $0 \le t \le c_0 L$,

$$\left\| e^{-iH_G t}|\psi^j(0)\rangle - |\alpha^j(t)\rangle \right\| = \mathcal{O}(L^{-1/4}) \tag{1.2}$$

where

$$|\alpha^j(t)\rangle = \frac{1}{\sqrt{L}} e^{-2it\cos k} \sum_{x=1}^{\infty} \sum_{q=1}^{N} (\delta_{qj} e^{-ikx} R(x - \lfloor 2t \sin k \rfloor) + S_{qj}(k) e^{ikx} R(-x - \lfloor 2t \sin k \rfloor))|x, q\rangle \tag{1.3}$$

with

$$R(l) = \begin{cases} 1 & \text{if } l - M \in [L] \\ 0 & \text{otherwise.} \end{cases} \tag{1.4}$$

n this section we prove Theorem **??**. The proof is based on (and follows closely) the calculation from the appendix of reference [**?**].

Recall from (**??**) that the scattering eigenstates of $H_G^{(1)}$ have the form

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

for each $k \in (-\pi, 0)$.

Before delving into the proof, we first establish that the state $|\alpha^j(t)\rangle$ is approximately normalized. This state is not normalized at all times t. However, $\langle\alpha^j(t)|\alpha^j(t)\rangle = 1+\mathcal{O}(L^{-1})$, as we now show:

$$\begin{aligned}
\langle\alpha^j(t)|\alpha^j(t)\rangle &= \frac{1}{L}\sum_{x=1}^{\infty}\left|e^{-ikx}R(x-\lfloor 2t\sin k\rfloor)+S_{jj}(k)e^{ikx}R(-x-\lfloor 2t\sin k\rfloor)\right|^2 \\
&\quad+\frac{1}{L}\sum_{q\neq j}\sum_{x=1}^{\infty}|S_{qj}(k)|^2R(-x-\lfloor 2t\sin k\rfloor) \\
&=\frac{1}{L}\sum_{x=1}^{\infty}\left[R(x-\lfloor 2t\sin k\rfloor)+R(-x-\lfloor 2t\sin k\rfloor)\right] \\
&\quad+\frac{1}{L}\sum_{x=1}^{\infty}\left(e^{-2ikx}S_{jj}^*(k)+e^{2ikx}S_{jj}(k)\right)R(x-\lfloor 2t\sin k\rfloor)R(-x-\lfloor 2t\sin k\rfloor) \\
&=1+\frac{1}{L}\sum_{x=1}^{\infty}\left(e^{-2ikx}S_{jj}^*(k)+e^{2ikx}S_{jj}(k)\right)R(x-\lfloor 2t\sin k\rfloor)R(-x-\lfloor 2t\sin k\rfloor)+\mathcal{O}(L^{-1})
\end{aligned}$$

where we have used unitarity of S in the second step. When it is nonzero, the second term can be written as

$$\frac{1}{L}\sum_{x=1}^{b}\left(e^{-2ikx}S_{jj}^*(k)+e^{2ikx}S_{jj}(k)\right)$$

where b is the maximum positive integer such that $\{-b,b\}\subset\{M+1+\lfloor 2t\sin k\rfloor,\ldots,M+L+\lfloor 2t\sin k\rfloor\}$. Performing the sums, we get

$$\begin{aligned}
\left|\frac{1}{L}\sum_{x=1}^{b}\left(e^{-2ikx}S_{jj}^*(k)+e^{2ikx}S_{jj}(k)\right)\right| &= \frac{1}{L}\left|S_{jj}^*(k)e^{-2ik}\frac{e^{-2ikb}-1}{e^{-2ik}-1}+S_{jj}(k)e^{2ik}\frac{e^{2ikb}-1}{e^{2ik}-1}\right| \\
&\leq \frac{2}{L|\sin k|}.
\end{aligned}$$

Thus we have $\langle\alpha^j(t)|\alpha^j(t)\rangle = 1+\mathcal{O}(L^{-1})$.

Proof of Theorem **??**. Define

$$|\psi^j(t)\rangle = e^{-iH_G^{(1)}t}|\psi^j(0)\rangle$$

and write

$$|\psi^j(t)\rangle = |w^j(t)\rangle + |v^j(t)\rangle$$

where

$$|w^j(t)\rangle = \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}e^{-2it\cos(k+\phi)}\sum_{q=1}^{N}|\mathrm{sc}_q(k+\phi)\rangle\langle\mathrm{sc}_q(k+\phi)|\psi^j(0)\rangle$$

and $\langle w^j(t)|v^j(t)\rangle = 0$. We take $\epsilon = \frac{|\sin k|}{2\sqrt{L}}$. Now

$$\langle\mathrm{sc}_q(k+\phi)|\psi^j(0)\rangle = \frac{1}{\sqrt{L}}\sum_{x=M+1}^{M+L}\left(e^{i\phi x}\delta_{qj}+e^{-i(2k+\phi)x}S_{qj}^*(k+\phi)\right),$$

so

$$|w^j(t)\rangle = |w_A^j(t)\rangle + \sum_{q=1}^{N} |w_B^{q,j}(t)\rangle$$

where

$$\begin{aligned}
|w_A^j(t)\rangle &= \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{-2it\cos(k+\phi)} f(\phi) |\mathrm{sc}_j(k+\phi)\rangle \\
|w_B^{q,j}(t)\rangle &= \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{-2it\cos(k+\phi)} g_{qj}(\phi) |\mathrm{sc}_q(k+\phi)\rangle
\end{aligned}$$

with

$$\begin{aligned}
f(\phi) &= \frac{1}{\sqrt{L}} \sum_{x=M+1}^{M+L} e^{i\phi x} \\
g_{qj}(\phi) &= \frac{1}{\sqrt{L}} \sum_{x=M+1}^{M+L} e^{-i(2k+\phi)x} S_{qj}^*(k+\phi).
\end{aligned}$$

We will see that $|\,\psi^j(t)\,\rangle \approx |\,w^j(t)\,\rangle \approx |\,w_A^j(t)\,\rangle \approx |\,\alpha^j(t)\,\rangle$.

Now

$$\langle w_A^j(t)|w_A^j(t)\rangle = \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \left|f(\phi)\right|^2 = \frac{1}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)}$$

but

$$\frac{1}{L}\int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} = 1$$

and

$$\begin{aligned}
\frac{1}{L}\left(\int_{\epsilon}^{\pi} + \int_{-\pi}^{-\epsilon}\right) \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} &= \frac{2}{L}\int_{\epsilon}^{\pi} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)} \\
&\le \frac{2}{L}\int_{\epsilon}^{\pi} \frac{d\phi}{2\pi} \frac{\pi^2}{\phi^2} \\
&\le \frac{\pi}{L\epsilon}.
\end{aligned} \tag{1.5}$$

Therefore

$$1 \ge \langle w_A^j(t)|w_A^j(t)\rangle \ge 1 - \frac{\pi}{L\epsilon}.$$

Similarly,

$$\langle w_B^{qj}(t)|w_B^{qj}(t)\rangle = \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \frac{\left|S_{qj}(k+\phi)\right|^2}{L} \frac{\sin^2(\frac{1}{2}L(2k+\phi))}{\sin^2(\frac{1}{2}(2k+\phi))},$$

and, using the unitarity of S,

$$\begin{aligned}
\sum_{q=1}^{N} \langle w_B^{qj}(t)|w_B^{qj}(t)\rangle &= \frac{1}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \frac{\sin^2(\frac{1}{2}L(2k+\phi))}{\sin^2(\frac{1}{2}(2k+\phi))} \\
&\le \frac{1}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \frac{1}{\sin^2(\frac{1}{2}(2k+\phi))}.
\end{aligned}$$

Now $|\sin(k+\phi/2)-\sin k| \le |\phi|/2$ (by the mean value theorem). So

$$\sin^2\left(k+\frac{\phi}{2}\right) \ge \left(|\sin k| - \left|\frac{\phi}{2}\right|\right)^2.$$

Since $\epsilon = \frac{|\sin k|}{2\sqrt{L}} < |\sin k|$ we then have

$$\begin{aligned}\sum_{q=1}^{N}\langle w_B^{qj}(t)|w_B^{qj}(t)\rangle &\le \frac{1}{L}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\frac{4}{\sin^2 k}\\ &= \frac{4\epsilon}{\pi L\sin^2 k}.\end{aligned}$$

Hence

$$\begin{aligned}\langle w^j(t)|w^j(t)\rangle &\ge \langle w_A^j(t)|w_A^j(t)\rangle - 2\left|\sum_{q=1}^{N}\langle w_A^j(t)|w_B^{qj}(t)\rangle\right|\\ &\ge 1-\frac{\pi}{L\epsilon} - 2\left\|\sum_{q=1}^{n}|w_B^{qj}(t)\rangle\right\|\\ &\ge 1-\frac{\pi}{L\epsilon} - 2\sum_{q=1}^{n}\left\||w_B^{qj}(t)\rangle\right\|\\ &\ge 1-\frac{\pi}{L\epsilon} - 4\sqrt{\frac{\epsilon N}{\pi L\sin^2 k}},\end{aligned}$$

so

$$\langle v^j(t)|v^j(t)\rangle \le \frac{\pi}{L\epsilon} + 4\sqrt{\frac{\epsilon N}{\pi L\sin^2 k}}$$

since $\langle v^j(t)|v^j(t)\rangle + \langle w^j(t)|w^j(t)\rangle = 1$. Thus

$$\begin{aligned}\left\||\psi^j(t)\rangle - |w_A^j(t)\rangle\right\| &= \left\||v^j(t)\rangle + \sum_{q=1}^{N}|w_B^{qj}(t)\rangle\right\|\\ &\le \left(\frac{\pi}{L\epsilon} + 4\sqrt{\frac{\epsilon N}{\pi L\sin^2 k}}\right)^{\frac{1}{2}} + 2\sqrt{\frac{\epsilon N}{\pi L\sin^2 k}}.\end{aligned}$$

With our choice $\epsilon = \frac{|\sin k|}{2\sqrt{L}}$, we have $\left\||\psi^j(t)\rangle - |w_A^j(t)\rangle\right\| = \emptyset(L^{-1/4})$.

We now show that

$$\left\||w_A^j(t)\rangle - |\alpha^j(t)\rangle\right\| = \emptyset(L^{-1/8}). \tag{1.6}$$

Letting

$$P = \sum_{q=1}^{N}\sum_{x=1}^{\infty}|x,q\rangle\langle x,q|$$

be the projector onto the semi-infinite paths, to show equation (1.6) it is sufficient to show that

$$\left\| P|w_A^j(t)\rangle - |\alpha^j(t)\rangle \right\| = \mathcal{O}(L^{-1/4}) \tag{1.7}$$

since this implies that

$$\begin{aligned}\left\| P|w_A^j(t)\rangle \right\| &= \left\| |\alpha^j(t)\rangle \right\| + \mathcal{O}(L^{-1/4}) \\ &= 1 + \mathcal{O}(L^{-1/4})\end{aligned}$$

and hence

$$\begin{aligned}\left\| (1-P)\, |w_A^j(t)\rangle \right\|^2 &= \left\| |w_A^j(t)\rangle \right\|^2 - \left\| P|w_A^j(t)\rangle \right\|^2 \\ &\leq 1 - \left(1 + \mathcal{O}(L^{-1/4})\right) \\ &= \mathcal{O}(L^{-1/4}).\end{aligned} \tag{1.8}$$

From the above formula we now see that inequality (1.7) implies (1.6).

Noting that

$$\frac{1}{\sqrt{L}} R(l) = \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi l} f(\phi),$$

we write

$$\begin{aligned}\langle x, q|\alpha^j(t)\rangle = e^{-2it\cos k} \Bigg(&\delta_{qj} e^{-ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi(x - \lfloor 2t \sin k \rfloor)} f(\phi) \\ &+ S_{qj}(k) e^{ikx} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\phi(-x - \lfloor 2t \sin k \rfloor)} f(\phi) \Bigg).\end{aligned} \tag{1.9}$$

On the other hand,

$$\langle x, q|w_A^j(t)\rangle = \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} e^{-2it\cos(k+\phi)} f(\phi) \left(e^{-i(k+\phi)x} \delta_{qj} + e^{i(k+\phi)x} S_{qj}(k+\phi) \right). \tag{1.10}$$

Using equations (1.9) and (1.10) we can write

$$P|w_A^j(t)\rangle = |\alpha^j(t)\rangle + \sum_{i=1}^{7} |c_i^j(t)\rangle$$

where $P|c_i^j(t)\rangle = |c_i^j(t)\rangle$ and

$$\langle x,q|c_1^j(t)\rangle = \delta_{qj}e^{-2it\cos k}e^{-ikx}\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}e^{-i\phi x}f(\phi)\left(e^{2it\phi\sin k}-e^{i\phi\lfloor 2t\sin k\rfloor}\right)$$

$$\langle x,q|c_2^j(t)\rangle = S_{qj}(k)e^{-2it\cos k}e^{ikx}\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}e^{i\phi x}f(\phi)\left(e^{2it\phi\sin k}-e^{i\phi\lfloor 2t\sin k\rfloor}\right)$$

$$\langle x,q|c_3^j(t)\rangle = -\delta_{qj}e^{-2it\cos k}e^{-ikx}\left(\int_{\epsilon}^{\pi}+\int_{-\pi}^{-\epsilon}\right)\frac{d\phi}{2\pi}e^{-i\phi x}f(\phi)e^{2it\phi\sin k}$$

$$\langle x,q|c_4^j(t)\rangle = -S_{qj}(k)e^{-2it\cos k}e^{ikx}\left(\int_{\epsilon}^{\pi}+\int_{-\pi}^{-\epsilon}\right)\frac{d\phi}{2\pi}e^{i\phi x}f(\phi)e^{2it\phi\sin k}$$

$$\langle x,q|c_5^j(t)\rangle = \delta_{qj}e^{-ikx}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}e^{-i\phi x}f(\phi)\left(e^{-2it\cos(k+\phi)}-e^{-2it\cos k+2it\phi\sin k}\right)$$

$$\langle x,q|c_6^j(t)\rangle = S_{qj}(k)e^{ikx}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}e^{i\phi x}f(\phi)\left(e^{-2it\cos(k+\phi)}-e^{-2it\cos k+2it\phi\sin k}\right)$$

$$\langle x,q|c_7^j(t)\rangle = e^{ikx}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}e^{i\phi x}e^{-2it\cos(k+\phi)}f(\phi)\left(S_{qj}(k+\phi)-S_{qj}(k)\right).$$

We now bound the norm of each of these states:

$$\begin{aligned}
\langle c_1^j(t)|c_1^j(t)\rangle &= \sum_{q=1}^{N}\sum_{x=1}^{\infty}\left|\delta_{qj}e^{-2it\cos k}e^{-ikx}\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}e^{-i\phi x}f(\phi)\left(e^{2it\phi\sin k}-e^{i\phi\lfloor 2t\sin k\rfloor}\right)\right|^2\\
&\le \sum_{q=1}^{N}\sum_{x=-\infty}^{\infty}\left|\delta_{qj}e^{-2it\cos k}e^{-ikx}\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}e^{-i\phi x}f(\phi)\left(e^{2it\phi\sin k}-e^{i\phi\lfloor 2t\sin k\rfloor}\right)\right|^2\\
&= \int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\left|e^{2it\phi\sin k}-e^{i\phi\lfloor 2t\sin k\rfloor}\right|^2\\
&\le \int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\left(2t\phi\sin k-\lfloor 2t\sin k\rfloor\phi\right)^2\\
&\le \int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\phi^2
\end{aligned}$$

where we have used the facts that $|e^{is}-1|^2\le s^2$ for $s\in\mathbb{R}$ and $|2t\sin k-\lfloor 2t\sin k\rfloor|<1$. In the above we performed the sum over x using the identity

$$\sum_{x=-\infty}^{\infty}e^{i(\phi-\tilde{\phi})x} = 2\pi\delta(\phi-\tilde{\phi}) \text{ for } \phi,\tilde{\phi}\in(-\pi,\pi).$$

We use this fact repeatedly in the following calculations. Continuing, we get

$$\begin{aligned}
\langle c_1^j(t)|c_1^j(t)\rangle &\le \frac{1}{L}\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)}\phi^2\\
&\le \frac{1}{L}\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\frac{1}{\sin^2(\frac{1}{2}\phi)}\phi^2\\
&\le \frac{\pi^2}{L}
\end{aligned}$$

using the fact that $\sin^2(\phi/2) \geq \phi^2/\pi^2$ for $\phi \in [-\pi, \pi]$. Similarly we bound $\langle c_2^j(t)|c_2^j(t)\rangle \leq \pi^2/L$.

Using equation (1.5) we get

$$\begin{aligned}\langle c_3^j(t)|c_3^j(t)\rangle &\leq \left(\int_{\epsilon}^{\pi} + \int_{-\pi}^{-\epsilon}\right)\frac{d\phi}{2\pi}\left|f(\phi)\right|^2 \\ &\leq \frac{\pi}{L\epsilon}\end{aligned}$$

and similarly for $\langle c_4^j(t)|c_4^j(t)\rangle$. Next, we have

$$\begin{aligned}\langle c_5^j(t)|c_5^j(t)\rangle &\leq \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\left|e^{-2it\cos(k+\phi)} - e^{-2it\cos k + 2it\phi\sin k}\right|^2 \\ &\leq \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\left(2t\cos\left(k+\phi\right) - 2t\cos k + 2t\phi\sin k\right)^2 \\ &= \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\left(2t\cos k\left(\cos\phi - 1\right) + 2t\sin k\left(\phi - \sin\phi\right)\right)^2 \\ &\leq \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2 4t^2\phi^4 \\ &= \frac{4t^2}{L}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)}\phi^4 \\ &\leq \frac{4t^2}{L}\int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\pi^2\phi^2 \\ &= \frac{4\pi}{3L}t^2\epsilon^3\end{aligned}$$

and we have the same bound for $|c_6^j(t)\rangle$. Finally,

$$\langle c_7^j(t)|c_7^j(t)\rangle \leq \int_{-\epsilon}^{\epsilon}\frac{d\phi}{2\pi}\left|f(\phi)\right|^2\sum_{q=1}^{N}\left|S_{qj}(k+\phi) - S_{qj}(k)\right|^2.$$

Now, for each $q \in \{1, \ldots, N\}$,

$$|S_{qj}(k+\phi) - S_{qj}(k)| \leq \Gamma|\phi|$$

where the Lipschitz constant

$$\Gamma = \max_{q,j\in\{1,\ldots,N\}}\max_{k'\in[-\pi,\pi]}\left|\frac{d}{dk'}S_{qj}(k')\right|$$

is well defined since each matrix element $S_{qj}(k')$ is a bounded rational function of $e^{ik'}$, as can be seen from equation (??). Hence

$$\begin{aligned}
\langle c_7^j(t)|c_7^j(t)\rangle &\le \int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi} \left|f(\phi)\right|^2 N\Gamma^2\phi^2 \\
&= \frac{N\Gamma^2}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi}\frac{\sin^2(\frac{1}{2}L\phi)}{\sin^2(\frac{1}{2}\phi)}\phi^2 \\
&\le \frac{N\Gamma^2}{L}\int_{-\epsilon}^{\epsilon} \frac{d\phi}{2\pi}\pi^2 \\
&= N\Gamma^2\frac{\pi\epsilon}{L}.
\end{aligned}$$

Now using the bounds on the norms of each of these states we get

$$\begin{aligned}
\left\|P|w_A^j(t)\rangle - |\alpha^j(t)\rangle\right\| &\le 2\frac{\pi}{\sqrt{L}} + 2\sqrt{\frac{\pi}{L\epsilon}} + 2\sqrt{\frac{4\pi}{3L}t^2\epsilon^3} + \sqrt{N\Gamma^2\frac{\pi\epsilon}{L}} \\
&= \emptyset(L^{-1/4})
\end{aligned}$$

using the choice $\epsilon = \frac{|\sin p|}{2\sqrt{L}}$ and the fact that $t = \emptyset(L)$. □

Note that this analysis assumes that $N = \emptyset(1)$, which is the case in our applications of Theorem ??.

1.2 Using scattering for simple computation

1.3 Encoded two-qubit gates

1.4 Single-qubit blocks

1.5 Combining blocks

It might be worthwhile to include a new proof of universal computation of single-particle scattering in this model.