Isometry of $\hat{\Omega}_\pm$

i) Scalar product preservation:

$$\boxed{\langle\psi_i^\pm|\psi_j^\pm\rangle = \langle\psi_i|\psi_j\rangle}$$

Proof:

$$\langle\psi_i^+|\psi_j^+\rangle = \langle\psi_i|1+\hat V\frac{1}{E_i-\hat{H}-i0}|\psi_j^+\rangle = \langle\psi_i|\psi_j^+\rangle + \frac{\langle\psi_i|\hat V|\psi_j^+\rangle}{E_i-E_j-i0}$$

$$=\langle\psi_i|\psi_j\rangle + \langle\psi_i|\frac{1}{E_j-\hat H_0+i0}\hat T_j|\psi_j\rangle + \frac{\langle\psi_i|\hat V|\psi_j^+\rangle}{E_i-E_j-i0}$$

$$= \langle\psi_i|\psi_j\rangle + \frac{1}{E_i-E_j-i0}\overbrace{\left[\langle\psi_i|\hat V|\psi_j^+\rangle - \langle\psi_i|\hat T_j|\psi_j\rangle\right]}^{0}$$

since $\hat V\hat\Omega_j = \hat T_j$

$$\langle\psi_i|\hat\Omega_\pm^+(E_i)\,\hat\Omega_\pm(E_j)|\psi_j\rangle = \langle\psi_i|\psi_j\rangle$$

$$\hat\Omega_\pm = \sum_i \hat\Omega_\pm(E_i)|\psi_i\rangle\langle\psi_j| = \sum|\psi_i^\pm\rangle\langle\psi_i|$$

$$\hat\Omega_\pm^+\hat\Omega_\pm = \sum_i|\psi_i\rangle\langle\psi_i| = 1$$ - isometric (not unitary if not reversible!)

$$\hat\Omega_\pm\hat\Omega_\pm^+ = \sum_i|\psi_i^\pm\rangle\langle\psi_i^\pm| = 1-\hat P_B$$

Projector onto bound states (if any)

S-matrix

Reminder
$$\begin{cases} |\psi(0)\rangle = \hat{\Omega}_+ |in\rangle \\ |\psi(0)\rangle = \hat{\Omega}_- |out\rangle \end{cases}$$

Isometry of $\hat{\Omega}_\pm$: $\quad |out\rangle = \hat{\Omega}_-^+ \hat{\Omega}_+ |in\rangle$

$$\boxed{\hat{S} = \hat{\Omega}_-^+ \hat{\Omega}_+}$$

Unitarity of the $\hat{S}$-matrix:

$$\left.\begin{aligned} \hat{S}^+\hat{S} &= \hat{\Omega}_+^+ (1-\hat{P}_B)\hat{\Omega}_+ = 1 \\ \hat{S}\hat{S}^+ &= \hat{\Omega}_-^+ (1-\hat{P}_B)\hat{\Omega}_- = 1 \end{aligned}\right\} \begin{array}{l} \text{Orthogonality} \\ \langle\psi_i^\pm|bound\rangle = 0 \end{array}$$

Since $[\hat{S}, \hat{H}_0] = 0 \Rightarrow$ "diagonal" in free wave basis

$$\langle\psi_i^-|\psi_j^+\rangle = \langle\psi_i|\hat{S}|\psi_j\rangle$$

$$= \langle\psi_i|\psi_j\rangle - 2\pi i\,\delta(E_i - E_j)\langle\psi_i|\hat{T}|\psi_j\rangle$$

on-shell

$$\boxed{\hat{S} = 1 - i\hat{\mathbb{T}}} \text{ - S-matrix}$$

$\hat{S}$-matrix elements

$$\langle \psi_i^- | \psi_j^+ \rangle = \langle i | \hat{\Omega}_-^+ \hat{\Omega}_+ | j \rangle = \langle i | \hat{S} | j \rangle \quad , \quad \hat{\mathcal{H}}_0 | i \rangle = E_i | i \rangle$$

$$\parallel$$

$$\langle \psi_i^- | j \rangle + \langle \psi_i^- | \frac{1}{E_j - \hat{\mathcal{H}} + i0} \hat{V} | j \rangle$$

$$= \langle i | j \rangle + \langle i | \hat{T}_-^+(E_i) \frac{1}{E_i - \hat{\mathcal{H}}_0 + i0} | j \rangle + \frac{\langle \psi_i^- | \hat{V} | j \rangle}{E_j - E_i + i0}$$

$$= \langle i | j \rangle + \frac{\langle i | \hat{T}_-^+(E_i) | j \rangle}{E_i - E_j + i0} - \frac{\langle i | \hat{\Omega}_-^+(E_i) \hat{V} | j \rangle}{E_i - E_j - i0}$$

since $\hat{T}_- = \hat{V} \hat{\Omega}_-$

$$= \langle i | j \rangle - 2\pi i \, \delta(E_i - E_j) \langle i | \hat{T}_+(E_i) | j \rangle$$

$$\boxed{\langle i | \hat{S} | j \rangle = \langle i | j \rangle - 2\pi i \, \delta(E_i - E_j) \langle i | \hat{T}_+(E_i) | j \rangle}$$

On-shell: initial and final energies are equal to each other!

Transition rate

Some initial state $|j\rangle$ becomes the final state $\hat{S}|j\rangle$. Their overlap for $i=j$ $\langle i|\hat{S}|j\rangle = -2\pi i\,\delta(E_i-E_j)\langle i|\hat{T}|j\rangle$ should give (being squared module) the probability to find a system in $|i\rangle$ at $t\to+\infty$.

The origin of the energy conservation

$$\Delta p\cdot\Delta r \geq \hbar \Rightarrow \Delta E\cdot\Delta t \geq \hbar \Rightarrow \Delta E \geq \frac{\hbar}{T} \leftarrow \text{observation time}$$

$$2\pi\delta(E_i-E_j) = \int_{-\infty}^{\infty} dt\, e^{-i(E_i-E_j)t} \to \int_{-T/2}^{T/2} dt\, e^{-i(E_i-E_j)t}$$

Then the probability

$$P_{ij}(T) = \underbrace{\left|\int_{-T/2}^{T/2} dt\, e^{-i(E_i-E_j)t}\right|^2}_{\simeq T\frac{2\pi}{\hbar}\delta(E_i-E_j)} \cdot |\langle i|\hat{T}|j\rangle|^2 \quad \text{as } T\to+\infty$$

Transition rate $\boxed{\Gamma_{ij} = \frac{2\pi}{\hbar}\delta(E_i-E_j)|\langle i|\hat{T}|j\rangle|^2}$

Perturbation $\hat{T}\approx\hat{V}$ – Fermi Golden rule!

1-particle scattering (in 3D)

$$|\psi^+_{\vec p}\rangle = \hat{\Omega}_+(\varepsilon_p)|\vec p\rangle, \quad \hat{\mathcal{H}}_0|\vec p\rangle = \varepsilon_p|\vec p\rangle, \quad \varepsilon_p = \frac{p^2}{2m}$$

Projecting onto $|\vec r\rangle$-basis

$$\psi^+_{\vec p}(\vec r) = e^{i\vec p\vec r} + \int d^3r'\, G_0(\vec r-\vec r';\varepsilon_p)\, T(\vec r',\vec p)$$

where $\langle\vec r|\vec p\rangle = e^{i\vec p\vec r}$, $\langle\vec r'|\hat T|\vec p\rangle \equiv T(\vec r',\vec p)$

$$\langle\vec r|\frac{1}{\varepsilon_p-\hat{\mathcal{H}}_0+i0}|\vec r'\rangle = \int\frac{d^3k}{(2\pi)^3}\frac{e^{i\vec k(\vec r-\vec r')}}{\varepsilon_p-\varepsilon_k+i0} = -\frac{m}{2\pi}\frac{e^{ip|\vec r-\vec r'|}}{|\vec r-\vec r'|}$$

It is useful to define DoS (density of states)

$$\nu(\varepsilon) = \int\frac{d^3p}{(2\pi)^3}\delta(\varepsilon-\varepsilon_p) = -\frac{1}{\pi}\,\mathrm{Im}\, G(0,\varepsilon)$$

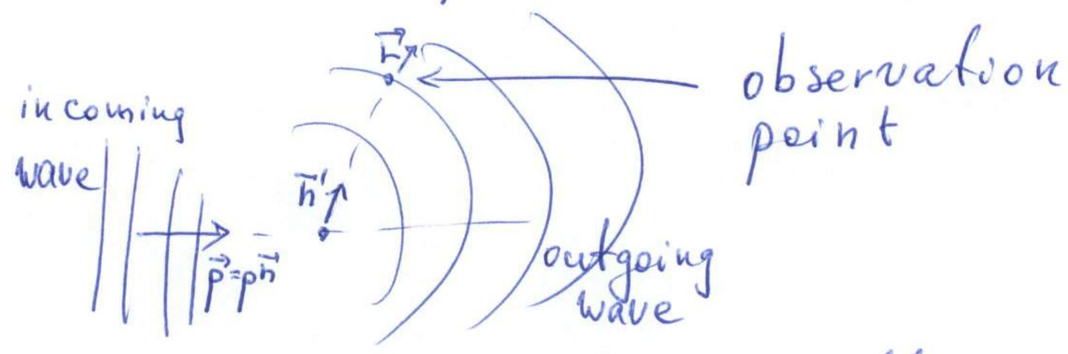
Taking into account that

$$G_0(\vec r,\varepsilon_p) = -\pi\nu_0(\varepsilon)\frac{e^{ipr}}{pr}$$

Asymptote $G_0(\vec r-\vec r';\varepsilon) \underset{r\to\infty}{\sim} -\pi\nu_0\frac{e^{ipr}}{pr}e^{-ip\vec n\vec r'}$

$$\psi^+_{\vec p}(\vec r\to\infty) = e^{ipr\vec n\vec n'} - \pi\nu\,\frac{e^{ipr}}{pr}\underbrace{\int d^3r'\, e^{-ip\vec n'\vec r'}\langle \vec r'|}_{=\langle p\vec n'|}\hat T|\vec p\rangle$$

$$\psi^+_{p}(\vec r\to\infty) = e^{ipr\vec n\vec n'} - \pi\nu\,\frac{e^{ipr}}{pr}\langle p\vec n'|\hat T|p\vec n\rangle$$



$$f(\vec n',\vec n) = -\frac{\pi\nu}{p}\langle \vec n'|\hat T(\varepsilon)|\vec n\rangle$$ – scattering amplitude

All directions of $\vec n$ correspond to eigenfunctions with the same energy ε_p.

General eigenstate

$$\psi^+_{\varepsilon}(\vec r\to\infty) = \int d\Omega_{\vec n}\, a(\vec n)\, e^{ipr\vec n\vec n'} - \frac{\pi\nu}{p}\frac{e^{ipr}}{r}\int d\Omega_{\vec n}\langle \vec n'|\hat T|\vec n\rangle a(\vec n)$$

(by parts) $\sim -\dfrac{e^{-ipr}}{r}a(-\vec n') + \dfrac{e^{ipr}}{r}\left[a(\vec n') - 2\pi i\nu(\hat T a)(\vec n')\right]$

Out going amplitude $b(\vec n') = a(\vec n') - 2\pi i\nu(\hat T a)(\vec n')$

On-shell $\longrightarrow$ $\boxed{S(\vec n',\vec n) = \delta^2(\vec n'-\vec n) - 2\pi i\nu\, T(\vec n',\vec n)}$

On-shell S-matrix

$$\langle i|S|j\rangle = \langle i|j\rangle - 2\pi i\,\delta(E_i - E_j)\langle i|\hat{T}_+(E_i)|j\rangle$$

Energy (cont.)

$$|i\rangle = |E, \alpha\rangle$$

Degeneracy quantum number ("channels") (cont. or discrete)

$$\langle \vec{p}|\vec{p}'\rangle = (2\pi\hbar)^3\delta(\vec{p}-\vec{p}') \qquad \boxed{\langle E,\alpha|E',\alpha'\rangle = \frac{\delta_{\alpha\alpha'}}{\nu_\alpha(E)}\delta(E-E')}$$

$$\int\frac{d^3p}{(2\pi\hbar)^3}\langle\vec{p}|\vec{p}'\rangle = 1 \qquad \text{Test: } \sum_\alpha\int dE\,\nu_\alpha(E)\cdot\langle E,\alpha|E',\alpha'\rangle = 1$$

$$\langle E,\alpha|\hat{S}|E',\alpha'\rangle = \frac{\delta(E-E')}{\sqrt{\nu_\alpha(E)\nu_{\alpha'}(E')}}\Big[\underbrace{\delta_{\alpha\alpha'} - i2\pi\sqrt{\nu_\alpha}\,T_{\alpha\alpha'}(E)\sqrt{\nu_{\alpha'}}}_{\text{On-shell S-matrix}\ \to\ S_{\alpha\alpha'}(E)}\Big]$$

$$\hat{S}^+\hat{S} = 1, \text{ i.e. } \langle E,\alpha|\hat{S}^+\hat{S}|E',\alpha'\rangle = \langle E,\alpha|E',\alpha'\rangle$$

$$\sum_{\alpha_1}\int dE_1\,\nu_{\alpha_1}(E_1)\cdot\langle E,\alpha|\hat{S}^+|E_1,\alpha_1\rangle\langle E_1,\alpha_1|S|E',\alpha'\rangle = \langle E,\alpha|E',\alpha'\rangle$$

$$\Downarrow$$

$$\boxed{\hat{S}^+(E)\hat{S}(E) = 1}$$

unity in channels space

$$S_{\alpha\alpha'}(E) = \delta_{\alpha\alpha'} - i2\pi\,\nu_\alpha^{1/2}(E)\,T_{\alpha\alpha'}(E)\,\nu_{\alpha'}^{1/2}(E)$$