defined in terms of resolvent of $\hat{H}$.

Relation of transition operator $\hat{t}(\lambda)$ to $\hat{S}$-matrix

Consider the S-matrix element for the normalizable wavepackets $|\phi_{\vec{k}}\rangle$ and $|\phi_{\vec{k}'}\rangle$

$$\langle \phi_{\vec{k}'} | \hat{S} | \phi_{\vec{k}} \rangle = \langle \phi_{\vec{k}'} | \hat{\Omega}_-^{\dagger} \hat{\Omega}_+ | \phi_{\vec{k}} \rangle \qquad \Omega \equiv \text{Møller operators.}$$

Wave packets

$$= \lim_{\substack{t \to \infty \\ t' \to -\infty}} \langle \phi_{\vec{k}'} | \left(e^{i\hat{H}_0 t} e^{-i\hat{H} t} \right) \left(e^{i\hat{H} t'} e^{-i\hat{H}_0 t'} \right) | \phi_{\vec{k}} \rangle$$

Result indep. of order of limits; take symmetric limit: $t = -t'$, $t \to +\infty$.

$$= \lim_{t \to \infty} \langle \phi_{\vec{k}'} | \left(e^{i\hat{H}_0 t} e^{-i\hat{H} t} \right) \left(e^{-i\hat{H} t} e^{i\hat{H}_0 t} \right) | \phi_{\vec{k}} \rangle$$

$$= \lim_{t \to \infty} \langle \phi_{\vec{k}'} | \left(e^{i\hat{H}_0 t} e^{-2i\hat{H} t} e^{i\hat{H}_0 t} \right) | \phi_{\vec{k}} \rangle \qquad (*)$$

Write $(\ldots)$ as integral of derivative:

$$\frac{d}{dt}(\ldots) = \left(iH_0 e^{iH_0 t} \right) e^{-2iHt} e^{iH_0 t}$$
$$+ e^{iH_0 t} \left(-i\hat{H} e^{-2iHt} \right) e^{iH_0 t} + e^{iH_0 t} e^{-2iHt} (-i\hat{H}) e^{iH_0 t}$$
$$+ e^{iH_0 t} e^{-2i\hat{H}t} \left(iH_0 e^{iH_0 t} \right)$$

In middle two terms, write $\hat{H} = \hat{H}_0 + \hat{V}$, so that $\hat{H}_0$ part cancels against first and last terms leaving

$$\frac{d}{dt}(\ldots) = -i \left(e^{i\hat{H}_0 t} \hat{V} e^{-2i\hat{H}t} e^{i\hat{H}_0 t} + e^{i\hat{H}_0 t} e^{-2i\hat{H}t} \hat{V} e^{i\hat{H}_0 t} \right)$$

The integral of this gives:

$$\int_0^{\infty} dt \left[\text{this} \right] = \left[(\ldots) \Big|_{t \to \infty} - (\ldots) \Big|_{t \to 0} \right] = \lim_{t \to \infty} (\ldots) - 1$$

Then, moving -1 to left hand side gives, and inserting into $(*)$ gives:

$$\langle \phi_{\vec{k}'} | \hat{S} | \phi_{\vec{k}} \rangle = \langle \phi_{\vec{k}'} | 1 | \phi_{\vec{k}} \rangle - i \int_0^{\infty} dt \, \langle \phi_{\vec{k}'} | e^{i\hat{H}_0 t} \left\{ \hat{V}, e^{-2i\hat{H}t} \right\} e^{i\hat{H}_0 t} | \phi_{\vec{k}} \rangle$$

written as an anticommutator for brevity — not meant to suggest deep algebraic structure.

Integral in RHS is absolutely convergent for wavepackets.

To ensure convergence for plane-wave states (of definite momenta), insert $e^{-\epsilon t}$

$$\langle \phi_{\vec k'} | \hat S | \phi_{\vec k} \rangle = \langle \phi_{\vec k'} | \phi_{\vec k} \rangle - i \lim_{\epsilon \to 0^+} \int_0^\infty dt\, e^{-\epsilon t} \langle \phi_{\vec k'} | e^{i\hat H_0 t} \{ \hat V, e^{-2i\hat H t} \} e^{i\hat H_0 t} | \phi_{\vec k} \rangle$$

Now replace $|\phi_{\vec k}\rangle \longrightarrow |\vec k\rangle$ and $|\phi_{\vec k'}\rangle \longrightarrow |\vec k'\rangle$ $\Longrightarrow$ $\langle \phi_{\vec k'}| e^{i\hat H_0 t} \longrightarrow \langle \vec k' | e^{iE_{\vec k'} t}$, $e^{i\hat H_0 t} |\phi_{\vec k}\rangle \longrightarrow e^{i\hat H_0 t} |\vec k\rangle$

$$\langle \vec k' | \hat S | \vec k \rangle = \delta^{(3)}(\vec k' - \vec k) - i \lim_{\epsilon \to 0^+} \int_0^\infty dt\, e^{-\epsilon t} \langle \vec k' | e^{iE_{\vec k'} t} \{ \hat V, e^{-2i\hat H t} \} e^{iE_{\vec k} t} | \vec k \rangle$$

combine exponentials:

$$= \delta^{(3)}(\vec k' - \vec k) - i \lim_{\epsilon \to 0^+} \int_0^\infty dt\, \langle \vec k' | \left\{ \hat V, e^{i(E_{\vec k'} + E_{\vec k} + i\epsilon - 2i\hat H t)} \right\} | \vec k \rangle$$

Use Schwinger proper-time integral identity: $\displaystyle\int_0^\infty dt\, e^{-i(\lambda - \hat H)t - \epsilon t} = -i\, G(\lambda - i\epsilon)$

(convergence guaranteed by $e^{-\epsilon t}$, $\epsilon > 0$)

$$\langle \vec k' | \hat S | \vec k \rangle = \delta^{(3)}(\vec k' - \vec k) - i \lim_{\epsilon \to 0} \langle \vec k' | \left\{ \hat V, \frac{i}{2} \hat G\left(\frac{E_{\vec k'} + E_{\vec k} + i\epsilon}{2} \right) \right\} | \vec k \rangle$$

Use $\hat V \hat G(\lambda) = \hat t(\lambda) \hat G_0(\lambda)$ on first term

and $\hat G(\lambda) \hat V = \hat G_0(\lambda) \hat t(\lambda)$ on second term.

$$\langle \vec k' | \hat S | \vec k \rangle = \delta^{(3)}(\vec k' - \vec k) + \frac{1}{2} \lim_{\epsilon \to 0^+} \langle \vec k' | \hat t\left(\frac{E_{\vec k'} + E_{\vec k} + i\epsilon}{2} \right) \hat G_0\left(\frac{E_{\vec k'} + E_{\vec k} + i\epsilon}{2} \right)$$
$$+ \hat G_0\left(\frac{E_{\vec k'} + E_{\vec k} + i\epsilon}{2} \right) \hat t\left(\frac{E_{\vec k'} + E_{\vec k} + i\epsilon}{2} \right) | \vec k \rangle$$

Then use $\hat G_0(\lambda) |\vec k\rangle = \dfrac{1}{\lambda - \hat H} |\vec k\rangle = \dfrac{1}{\lambda - E_{\vec k}}$ to replace

$$\hat G_0\left(\frac{E_{\vec k'} + E_{\vec k} + i\epsilon}{2} \right) \longrightarrow \frac{1}{\frac{E_{\vec k'} + E_{\vec k} + i\epsilon}{2} - E_{\vec k(')}} = \frac{2}{\pm E_{\vec k'} \mp E_{\vec k} + i\epsilon}$$

upper sign for 1st term

lower sign for 2nd term.

$\lim_{\epsilon\to 0} \frac{\epsilon}{2} \approx \epsilon$

$$\langle \vec{k}' | \hat{S} | \vec{k} \rangle = \delta^{(3)}(\vec{k}' - \vec{k}) + \frac{1}{2} \lim_{\epsilon \to 0^+} \left(\frac{2}{E_{\vec{k}'} - E_{\vec{k}} + i\epsilon} + \frac{2}{-E_{\vec{k}'} + E_{\vec{k}} + i\epsilon} \right) \langle \vec{k}' | \hat{t}\left(\frac{E_{\vec{k}'} + E_{\vec{k}}}{2} + i\epsilon \right) | \vec{k} \rangle$$

Then the $\epsilon \to 0$ limit of $(\cdots)$ gives its imaginary part: $-2\pi i\, \delta(E_{\vec{k}'} - E_{\vec{k}})$

$$\boxed{\langle \vec{k}' | \hat{S} | \vec{k} \rangle = \delta^{(3)}(\vec{k}' - \vec{k}) - 2\pi i\, \delta(E_{\vec{k}'} - E_{\vec{k}}) \lim_{\epsilon \to 0^+} \langle \vec{k}' | \hat{t}(E_{\vec{k}} + i\epsilon) | \vec{k} \rangle}$$

<u>Connecting formulae:</u>

$$\hat{S} = \mathbb{1} + i\hat{T}$$

$$\langle \vec{k}' | \hat{S} | \vec{k} \rangle = \delta^{(3)}(\vec{k}' - \vec{k}) + i \langle \vec{k}' | \hat{T} | \vec{k} \rangle$$

$$= \delta^{(3)}(\vec{k}' - \vec{k}) + \frac{i\hbar^2}{2\pi m} \delta(E_{\vec{k}'} - E_{\vec{k}})\, f(\vec{k}' \leftarrow \vec{k})$$

Match to above result:

$$\lim_{\epsilon \to 0} \langle \vec{k}' | \hat{t}(E_{\vec{k}} + i\epsilon) | \vec{k} \rangle = \frac{-\hbar^2}{(2\pi)^2 m} f(\vec{k}' \leftarrow \vec{k})$$

so that

$$\langle \vec{k}' | \hat{T} | \vec{k} \rangle = -2\pi i\, \delta(E_{\vec{k}'} - E_{\vec{k}}) \lim_{\epsilon \to 0} \langle \vec{k}' | \hat{t}(E_{\vec{k}} + i\epsilon) | \vec{k} \rangle$$

On-shell T-matrix (defined for states connected by energy conservation)

Transition matrix operator. (defined for any external states)

lends itself to an off-shell def^{n} of the T-matrix.