If the atom can decay to many states we must sum over these to find the total rate, then

$$dN = -N \sum_f^{i} \Gamma_{fi}^{Dipole}\, dt$$

So (to lowest order in α) $\Rightarrow$

$$N = N_0\, e^{-\left(\sum_f^{i} \Gamma_{fi}^{Dip.}\right)t} \equiv N_0\, e^{-\frac{t}{\tau}}$$

$$\Rightarrow \quad \boxed{\tau = \frac{1}{\sum_f^{i} \Gamma_{fi}^{Dip.}}}$$

add transition rates to find lifetime.

8.4. The Formal Theory of Scattering

So far we have been working to lowest order in time-dependent perturbation theory. Many times it's necessary to determine the transition probability in higher orders. As well, it is often useful to have a formal expression for the exact solution, as in the case of potential scattering with the L-S equation, so that symmetry principles and conservation laws may be directly applied to it. Our first order formalism was just obtained by approximating the solution to Schrödinger's equation in the interaction picture. Let us return to this abstract formulation and introduce the idea of the time evolution operator. On page -1135- and following we introduced the interaction picture states $|\psi(t)\rangle_{IP}$ corresponding to the Schrödinger picture state $|\psi(t)\rangle$. The SP states evolved in time according to the Schrödinger equation with the full Hamiltonian, now possibly time dependent,

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle .$$

If, however, H is time independent then Schrödinger's equation is easily solved

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar} H (t-t_0)} |\psi(t_0)\rangle .$$

Further, it proves convenient, as we have seen, to break the Hamiltonian into a sum of two parts $H = H_0 + H'$ where H_0 is the <u>free</u> or non-interacting Hamiltonian and H' is the <u>interaction</u> Hamiltonian. The time evolution resulting from the <u>time independent</u> H_0 can be removed from the states $|\psi(t)\rangle$ by a unitary transformation to define the interaction picture states

$$|\psi(t)\rangle_{IP} \equiv e^{+\frac{i}{\hbar}H_0 t}\,|\psi(t)\rangle .$$

As we showed on page -1138-, $|\psi(t)\rangle_{IP}$ obeys the Schrödinger equation with the interaction Hamiltonian in the IP

$$i\hbar \frac{d}{dt}|\psi(t)\rangle_{IP} = H'_{IP}(t)\,|\psi(t)\rangle_{IP},$$

with the IP interaction Hamiltonian defined by

$$H'_{IP}(t) \equiv e^{+\frac{i}{\hbar}H_0 t}\,H'(t)\,e^{-\frac{i}{\hbar}H_0 t} .$$

Since the transformation from the SP to the IP is <u>unitary</u>, probability amplitudes are unchanged.

Thus $\langle \varphi(t)|\psi(t)\rangle = \underbrace{\langle \varphi(t)| e^{-\frac{i}{\hbar}H_0 t}}_{= {}_{IP}\langle \varphi(t)|} \underbrace{e^{+\frac{i}{\hbar}H_0 t}|\psi(t)\rangle}_{=|\psi(t)\rangle_{IP}}$

$$= {}_{IP}\langle \varphi(t)|\psi(t)\rangle_{IP} .$$

Indeed, given any operator $O(t)$ in the SP we can define the corresponding operator in the IP so that its matrix elements are unchanged

$$\langle \varphi(t)|O(t)|\psi(t)\rangle \equiv {}_{IP}\langle \varphi(t)|O_{IP}(t)|\psi(t)\rangle_{IP}$$

$$= \langle \varphi(t)| e^{-\frac{i}{\hbar}H_0 t} O_{IP}(t) e^{+\frac{i}{\hbar}H_0 t} |\psi(t)\rangle$$

$$\Rightarrow \boxed{O_{IP}(t) \equiv e^{+\frac{i}{\hbar}H_0 t} O(t) e^{-\frac{i}{\hbar}H_0 t}}$$

just as $H'_{IP}(t)$ was given. Note that $O_{IP}(t)$ evolves in time according to the Heisenberg equations of motion with H_0 as ~~the~~ Hamiltonian. They obey free or unperturbed time evolution.

$$-i\hbar \frac{d}{dt} O_{IP}(t) = H_0 e^{\frac{i}{\hbar}H_0 t} O(t) e^{-\frac{i}{\hbar}H_0 t} + e^{\frac{i}{\hbar}H_0 t}\left(-i\hbar \frac{\partial}{\partial t} O(t)\right) e^{-\frac{i}{\hbar}H_0 t} - e^{\frac{i}{\hbar}H_0 t} O(t) H_0 e^{-\frac{i}{\hbar}H_0 t}$$

$$= [H_0, O_{IP}(t)] + e^{\frac{i}{\hbar}H_0 t}\left(-i\hbar \frac{\partial}{\partial t} O(t)\right) e^{-\frac{i}{\hbar}H_0 t}$$

Now in the Schrödinger picture the observables have only explicit time dependence or none at all. So wlog $O(t) = O$ = indep. of t thus $\frac{\partial}{\partial t} O(t) = 0$,

and

$$\boxed{-i\hbar \frac{d}{dt} O_{IP}(t) = [H_0, O_{IP}(t)]}$$

The Heisenberg equations of motion with H_0 as the Hamiltonian. Hence in the IP the states evolve according to H_{IP} the interaction while the observables $O_{IP}(t)$ carry the free H_0 time evolution.

Recall

$$H_{0IP} = e^{\frac{i}{\hbar}H_0 t} H_0 e^{-\frac{i}{\hbar}H_0 t}$$

$$= H_0 \; .$$

Back to the state evolution, since we are interested in the transition probability after some finite (long) time interval we would like to solve, at least formally the IP Schrödinger equation.

As before if H, the full Hamiltonian, is time independent H = const., we can formally solve the IP Schrödinger equation

$$|\psi(t)\rangle_{IP} = e^{\frac{i}{\hbar}H_0 t} |\psi(t)\rangle$$

$$= e^{\frac{i}{\hbar}H_0 t} e^{-\frac{i}{\hbar}H(t-t_0)} |\psi(t_0)\rangle$$

$$= e^{\frac{i}{\hbar}H_0 t} e^{-\frac{i}{\hbar}H(t-t_0)} e^{-\frac{i}{\hbar}H_0 t_0} |\psi(t_0)\rangle_{I}$$

Thus we find

$$|\psi(t)\rangle_{IP} = U(t,t_0)\,|\psi(t_0)\rangle_{IP}$$

with the <u>time evolution operator</u> $U(t,t_0)$ given by

$$U(t,t_0) = e^{\frac{i}{\hbar}H_0 t}\, e^{-\frac{i}{\hbar}H(t-t_0)}\, e^{-\frac{i}{\hbar}H_0 t_0}.$$

In this case let's note some general properties of the time evolution operator.

1) $U(t,t_0)$ is the time evolution operator in the IP. We have surpressed the "IP" subscript. In the Schrödinger picture $U_S(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}$, recall.

2) $U(t_0,t_0) = 1$ is the initial condition obeyed by U.

3) Since $[H, H_0] = [H', H_0] \neq 0$ in general, we must be careful about the order of operators, i.e. we cannot simply combine exponents

of the exponentials [Baker-Campbell-Hausdorf)

4) $U(t,t_0)$ is unitary

$$U^\dagger(t,t_0) = e^{+\frac{i}{\hbar}H_0 t_0} e^{-\frac{i}{\hbar}H(t_0-t)} e^{-\frac{i}{\hbar}H_0 t}$$

$$= U(t_0,t)$$

and $U^\dagger(t,t_0)U(t,t_0) = 1 = U(t,t_0)U^\dagger(t,t_0)$

Thus $U^{-1}(t,t_0) = U(t_0,t)$.

5) $U(t,t_0)$ obeys a group multiplication law

$$U(t_1,t_2)U(t_2,t_3) = U(t_1,t_3).$$

So $U(t,t_0)U(t_0,t) = U(t,t) = 1$.

Even in the case where $H=H(t)$ is time dependent we can introduce the time evolution operator $U(t,t_0)$ with the above properties (pages -318- to -327-). In general then define $U(t,t_0)$ as the

Unitary operator that determines the finite (or infinite) time evolution of the IP states

$$|\psi(t)\rangle_{IP} \equiv \mathcal{U}(t,t_0)\,|\psi(t_0)\rangle_{IP}$$

with $\mathcal{U}(t_0,t_0)=1$. Substituting into the IP Schrödinger equation, we find a differential equation for $\mathcal{U}(t,t_0)$

$$i\hbar \frac{d}{dt}|\psi(t)\rangle_{IP} = H'_{IP}(t)\,|\psi(t)\rangle_{IP}$$

$\Rightarrow$

$$i\hbar \frac{\partial \mathcal{U}(t,t_0)}{\partial t}|\psi(t_0)\rangle_{IP} = H'_{IP}(t)\,\mathcal{U}(t,t_0)\,|\psi(t_0)\rangle_{IP}$$

$\Rightarrow$

$$\boxed{i\hbar \frac{\partial \mathcal{U}(t,t_0)}{\partial t} = H'_{IP}(t)\,\mathcal{U}(t,t_0)}$$

with the i.c.

$$\boxed{\mathcal{U}(t_0,t_0) = 1}\;.$$

As usual the differential equation plus initial condition can be converted to an integral equation for $U(t,t_0)$

$$\boxed{U(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\, H'_{IP}(t_1)\, U(t_1,t_0)}\ .$$

Clearly
$$U(t_0,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t_0} \cancelto{0}{dt_1\, H'_{IP}(t_1)\, U(t_1,t_0)}$$
$$= 1 \quad \text{as required}$$

and
$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = \frac{\partial}{\partial t}\int_{t_0}^{t} dt_1\, H'_{IP}(t_1)\, U(t_1,t_0)$$
$$= H'_{IP}(t)\, U(t,t_0)$$

the Schrödinger equation for $U(t,t_0)$.

We can solve the above integral equation by iteration starting with $U = 1$ and so on.

$$U(t,t_0) = 1 + \left(\frac{-i}{\hbar}\right)\int_{t_0}^{t} dt_1\, H'_{IP}(t_1)$$

$$+ \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1\, H'_{IP}(t_1) \int_{t_0}^{t_1} dt_2\, H'_{IP}(t_2)$$

$$+ \left(\frac{-i}{\hbar}\right)^3 \int_{t_0}^{t} dt_1\, H'_{IP}(t_1) \int_{t_0}^{t_1} dt_2\, H'_{IP}(t_2) \int_{t_0}^{t_2} dt_3\, H'_{IP}(t_3)$$

$$+ \cdots + \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1\, H'_{IP}(t_1) \int_{t_0}^{t} dt_2\, H'_{IP}(t_2) \cdots \int_{t_0}^{t_{n-1}} dt_n\, H'_{IP}(t_n)$$

$$+ \cdots .$$

Thus we find

$$\boxed{U(t,t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \times H'_{IP}(t_1) \cdots H'_{IP}(t_n)}$$

To see this consider $H'_{IP}(t)$ to be written as $\lambda \hat{H}'_{IP}(t) = H'_{IP}(t)$, and $U(t,t_0)$ to be a power series in λ

$$U(t,t_0) = \sum_{n=0}^{\infty} U_n(t)\lambda^n .$$

The integral equation for $U(t,t_0)$ becomes

$$U(t,t_0) = \sum_{n=0}^{\infty} \lambda^n U_n(t)$$

$$= 1 - \frac{i}{\hbar}\sum_{n=1}^{\infty} \lambda^n \int_{t_0}^{t} dt_1\, \hat{H}'_{IP}(t_1) U_{n-1}(t_1) .$$

Equating like powers of λ, we find for $n=0$

$$U_0(t) = 1$$

and for $n \geq 1$

$$U_n(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt_1\, \hat{H}'_{IP}(t_1) U_{n-1}(t_1) .$$

Hence we obtain

$$U_0(t) = 1$$

$$U_1(t) = -\frac{i}{\hbar}\int_{t_0}^{t} dt_1\, \hat{H}'_{IP}(t_1)$$

$$U_2(t) = \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt_1\, \hat{H}'_{IP}(t_1) \int_{t_0}^{t_1} dt_2\, \hat{H}'_{IP}(t_2)$$

$$\vdots$$

$$U_n(t) = \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, \hat{H}'_{IP}(t_1) \cdots \hat{H}'_{IP}(t_n)$$

and so on, securing the above iterative solution. Noticed that in each term U_n the integration interval is such that the Hamiltonians are ordered by decreasing time; the time of each Hamiltonian is later than the one to its right, $t_1 > t_2 > t_3 > \dots > t_n$. They are said to be time ordered.

We can introduce a time ordering operator T such that for arbitrary operators $A_1(t_1)\cdots A_n(t_n)$ it orders the operators chronologically with later times to the left, and earlier times to the right. Specifically we have first the trivial case

$$TA(t) = A(t). \tag{01}$$

Then for products of two operators we have

$$TA_1(t_1)A_2(t_2) = \begin{cases} A_1(t_1)A_2(t_2), & \text{if } t_1 > t_2; \\ A_2(t_2)A_1(t_1), & \text{if } t_2 > t_1. \end{cases} \tag{02}$$

These are the 2! ways to order (t_1, t_2). With the help of the step function $\theta(t_1 - t_2)$

$$\theta(t_1 - t_2) = \begin{cases} 1, & \text{if } t_1 > t_2; \\ 0, & \text{if } t_2 > t_1, \end{cases}$$

we write these cases as

$$TA_1(t_1)A_2(t_2) = \theta(t_1 - t_2)A_1(t_1)A_2(t_2) + \theta(t_2 - t_1)A_2(t_2)A_1(t_1). \tag{03}$$

We can more compactly write the time ordered product as a sum over these two permutations of the times

$$TA_1(t_1)A_2(t_2) = \sum_{(1,2)\xrightarrow{P}(i_1,i_2)} \theta(t_{i_1} - t_{i_2})A_{i_1}(t_{i_1})A_{i_2}(t_{i_2}). \tag{04}$$

Next for products of three operators we define

$$TA_1(t_1)A_2(t_2)A_3(t_3) = \begin{cases} A_1(t_1)A_2(t_2)A_3(t_3), & \text{if } t_1 > t_2 > t_3; \\ A_1(t_1)A_3(t_3)A_2(t_2), & \text{if } t_1 > t_3 > t_2; \\ A_2(t_2)A_1(t_1)A_3(t_3), & \text{if } t_2 > t_1 > t_3; \\ A_2(t_2)A_3(t_3)A_1(t_1), & \text{if } t_2 > t_3 > t_1; \\ A_3(t_3)A_1(t_1)A_2(t_2), & \text{if } t_3 > t_1 > t_2; \\ A_3(t_3)A_2(t_2)A_1(t_1), & \text{if } t_3 > t_2 > t_1. \end{cases} \tag{05}$$

These are the 3! ways to order (t_1, t_2, t_3), again we can use the step function to write this as

$$\begin{aligned} &TA_1(t_1)A_2(t_2)A_3(t_3) \\ &= \theta(t_1 - t_2)\theta(t_2 - t_3)A_1(t_1)A_2(t_2)A_3(t_3) \\ &+\theta(t_1 - t_3)\theta(t_3 - t_2)A_1(t_1)A_3(t_3)A_2(t_2) + \cdots. \end{aligned} \tag{06}$$

We can more compactly write this by summing over the six permutations of the times

$$TA_1(t_1)A_2(t_2)A_3(t_3)$$

$$= \sum_{(1,2,3)\xrightarrow{P}(i_1,i_2,i_3)} \theta(t_{i_1} - t_{i_2})\theta(t_{i_2} - t_{i_3})A_{i_1}(t_{i_1})A_{i_2}(t_{i_2})A_{i_3}(t_{i_3}). \tag{07}$$

And in general we define the time ordering operator to yield

$$TA_1(t_1)....A_n(t_n)$$

$$= \sum_{(1,...,n)\xrightarrow{P}(i_1,...i_n)} \theta(t_{i_1} - t_{i_2})\theta(t_{i_2} - t_{i_3})\cdots\theta(t_{i_n-1} - t_{i_n})\ A_{i_1}(t_{i_1})......A_{i_n}(t_{i_n}), \tag{08}$$

where the sum is over all n! ways to order $t_1, ..., t_n$. That is $\sum_P$ is the sum over all permutations P of the n integers $(1, \cdots, n)$ into the order $(i_1, \cdots, i_n)$, each i_j being one of the n integers from 1 through n.

Hence, we can apply the time ordering operator to our product of Hamiltonians

$$TH'_{IP}(t_1)\cdots H'_{IP}(t_n) = \sum_P \theta(t_{i_1} - t_{i_2})\cdots\theta(t_{i_n-1} - t_{i_n})H'_{IP}(t_{i_1})\cdots H'_{IP}(t_{i_n})$$

$$= H'_{IP}(t_{a_1})\cdots H'_{IP}(t_{a_n}), \qquad \text{for } t_{a_1} > t_{a_2} > t_{a_3} > \cdots > t_{a_n}. \tag{09}$$

Thus, we can use the T operator to extend our region of integration on each integral in U_n from $t_0 < t_i < t_{i-1}$ to the whole time interval $t_0 < t_i < t$ since T automatically chronologically orders the Hamiltonian factors

$$U_n(t) = (-i)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n H'_{IP}(t_1)\cdots H'_{IP}(t_n)$$

$$= (-i)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_n-1} dt_n T H'_{IP}(t_1)\cdots H'_{IP}(t_n)$$

$$= \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n\ TH'_{IP}(t_1)\cdots H'_{IP}(t_n). \tag{010}$$

The $\frac{1}{n!}$ arises from the fact that by integrating from $t_0 < t_i < t$ we are just doing the original integral n! times, just relabeling the dummy integration variables each time we have one of the n! permutations of the times from the definition of T. To make this perfectly clear let's do the U_2 case in detail

$$U_2(t) = \frac{(-i)^2}{2!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 T H'_{IP}(t_1) H'_{IP}(t_2)$$

$$= \frac{(-i)^2}{2!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 [\theta(t_1 - t_2) H'_{IP}(t_1) H'_{IP}(t_2) + \theta(t_2 - t_1) H'_{IP}(t_2) H'_{IP}(t_1)]. \quad (011)$$

Now in the second term let $t_1 = u_2$ and $t_2 = u_1$ and interchange the order of integration so that

$$U_2(t) = \frac{(-i)^2}{2!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \theta(t_1 - t_2) H'_{IP}(t_1) H'_{IP}(t_2)$$

$$+ \frac{(-i)^2}{2!} \int_{t_0}^{t} du_1 \int_{t_0}^{t} du_2 \theta(u_1 - u_2) H'_{IP}(u_1) H'_{IP}(u_2). \quad (012)$$

Relabel $u_1 \to t_1$ and $u_2 \to t_2$ to obtain

$$U_2(t) = \frac{(-i)^2}{2!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \theta(t_1 - t_2) H'_{IP}(t_1) H'_{IP}(t_2)$$

$$+ \frac{(-i)^2}{2!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \theta(t_1 - t_2) H'_{IP}(t_1) H'_{IP}(t_2)$$

$$= (-i)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \theta(t_1 - t_2) H'_{IP}(t_1) H'_{IP}(t_2). \quad (013)$$

Since

$$\theta(t_1 - t_2) = \begin{cases} 1, & \text{if } t_1 > t_2; \\ 0, & \text{if } t_2 > t_1, \end{cases}$$

we obtain

$$U_2(t) = (-i)^2 \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 H'_{IP}(t_1) H'_{IP}(t_2) \tag{014}$$

as desired. Similar arguments apply to $U_n(t)$.

Hence, the time evolution operator in the interaction representation can be written as

$$U(t,t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n T H'_{IP}(t_1) \cdots H'_{IP}(t_n). \tag{015}$$

Formally, we write the sum as an exponential

$$U(t,t_0) = T e^{-i\int_{t_0}^{t} dt' H'_{IP}(t')} \tag{016}$$

where again the exponential is understood to stand for the above series expansion equation (15).

The utility of the interaction representation is realized when we consider scattering experiments. Given any state $|\psi(t_0)>_{iP}$, we can now calculate to any order in the interaction its time evolution

$$|\psi(t)>_{iP} = U(t,t_0)|\psi(t_0)>_{iP} . \tag{017}$$

In scattering experiments the initial states are prepared in the remote past (as $t_0 \to -\infty$). For instance, two beams of particles of specified momenta and spins can be prepared spatially separate (opposite ends of the lab) so that initially they are not interacting. We imagine, according to the formal theory of scattering, that the interaction Hamiltonian $H'_{IP}(t)$ is adiabatically, that is very slowly compared to the characteristic interaction times to avoid any energy absorption or emission during the process, switched off in the remote past. A complete set of initial states are then the eigenstates of the free Hamiltonian H_0 since $|\psi>_{IP}$ is time independent if $H'_{IP} = 0$ and the interaction picture states coincide with the Heisenberg picture states for a system described by H_0 . As time proceeds the interaction is slowly turned on and eventually the particles collide. As time runs foward the collision products start to separate and after a sufficiently long time the interaction adiabatically turns off so that in the remote future $(t \to +\infty)$ the final states are again eigenstates of the free Hamiltonian H_0 . This slow switching on and off of the interaction without disturbing the results of the particle collisions is called the adiabatic hypothesis. Initially the particles are well separated and noninteracting (eigenstates of H_0). They approach each other and interact, producing new particles , scattering(and QFT annihilating) The reaction products then separate again into noninteracting final states (also eigenstates of H_0). We shall denote these special non-interacting initial and final states in the interaction representation, which are described by the eigenstates of H_0, by rounded brackets with no subscripts, $|i \supset$ and $|f \supset$, respectively. The transition probabilty amplitude for the system to go from the initial state $|i \supset$ at time $t = -\infty$ to the final state $|f \supset$ at time $t = +\infty$ is given by the scalar product

$$S_{fi} = \subset f|U(+\infty, -\infty)|i \supset . \tag{018}$$

That is, $U(t, -\infty)$ takes the initial state $|i \supset = |i(-\infty) >_{iP}$ from time $t = -\infty$ to the time t

$$|i(t) \supset = U(t, -\infty)|i(-\infty) >_{iP} . \tag{019}$$

Hence the probability amplitude for the initial state $|i \supset$ to evolve from $t = -\infty$ into the final state $|f \supset$ at $t = +\infty$ is just

$$S_{fi} = \lim_{t \to +\infty} \subset f|i(t) \supset = \subset f|i(+\infty) \supset$$

$$= \subset f|U(+\infty, -\infty)|i \supset . \tag{020}$$

S_{fi} is called the scattering matrix element or simply the S-matrix element.

$$S \equiv U(+\infty, -\infty) \tag{021}$$

is known as the scattering or S-operator. From the perturbation expansion for the time evolution operator $U(t, t_0,)$ we have that

$$S = Te^{-i\int_{-\infty}^{+\infty} dt H'_{IP}(t)}$$

$$= 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{+\infty} dt_1 \cdots \int_{-\infty}^{+\infty} dt_n T H'_{IP}(t_1) \cdots H'_{IP}(t_n). \tag{022}$$

Hence the S-matrix element is given by

$$S_{fi} = \subset f|Te^{-i\int_{-\infty}^{+\infty} dt H'_{IP}(t)}|i \supset . \tag{023}$$

Recall that the operators in the interaction picture have time dependence determined by the free Hamiltonian H_0 . Hence, we can calculate the transition probability amplitude for the process $i \to f$ by using states and operators determined in terms of the free dynamical variables appearing in H_0 . The price we pay for using noninteracting or free quantities is the insertion of the term $Te^{-i\int dt H'_{Ir}}$ in the transition amplitude. Further, $|S_{fi}|^2$ is a measurable quantity for any reaction. However, it depends upon the details of the initial state preparation, for example it depends on the flux of incoming particles, and on the target particle density. A more intrinsic quantity derived from $|S_{fi}|^2$ is the cross section for a process $\sigma_{fi} \propto |S_{fi}|^2$.

So to repeat, using our more conventional notation, in the remote past the system is in the eigenstate of H_0, $|\psi_i(-\infty)\rangle$. In the distant future we ask for the probability that this state has evolved into another eigenstate of the free Hamiltonian H_0, $|\psi_f(+\infty)\rangle$. In order to guarantee that $H'(t)$ vanishes for early and late times so that the system can be described by eigenstates of H_0 we introduce an explicit time dependence for H' by $\lambda \to \lambda(t) = \lambda e^{-\epsilon|t|}$. Then H' turns on and off very slowly, $H' = e^{-\epsilon|t|} \lambda \hat{H}'(t)$. $0 < \epsilon \ll 1$, and $\epsilon \to 0^+$ at the end of the calculation, providing convergence for all intermediate calculations.

Since $H'=0$ for $t \to \pm\infty$, the initial and final states evolve in the SP according to H_0, that is for stationary states

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Et}|\varphi\rangle$$

where $H_0|\varphi\rangle = E|\varphi\rangle$. Hence in the IP

$$|\psi(t)\rangle_{IP} = e^{\frac{i}{\hbar}H_0 t}|\psi(t)\rangle$$
$$= e^{+\frac{i}{\hbar}H_0 t}\, e^{-\frac{i}{\hbar}Et}|\varphi\rangle$$
$$= |\varphi\rangle,$$

the IP state is just the eigenstate of H_0.

So at $t \to -\infty$ the state of the system is given in the IP by

$$|\psi_i(-\infty)\rangle_{IP} = |\varphi_i\rangle,$$

the initial eigenstate of H_0

$$H_0|\psi_i(-\infty)\rangle_{IP} = H_0|\varphi_i\rangle = E_i|\varphi_i\rangle$$
$$= E_i|\psi_i(-\infty)\rangle_{IP}$$

As time increases the system evolves, interacts and scatters according to $H'(t)$. As the particles separate again $H'(t) \to 0$ and at $t \to +\infty$ $H = H_0$ and the system is in state

$$|\psi_i(+\infty)\rangle_{IP} = U(+\infty,-\infty)|\psi_i(-\infty)\rangle_{IP}$$

$$= U(+\infty,-\infty)\,|\varphi_i\rangle .$$

The probability that the system is in the eigenstate $|\varphi_f\rangle$ of H_0 at $t\to\infty$ is given by the transition probability

$$P_{fi} = |\langle\varphi_f|\psi_i(+\infty)\rangle_{IP}|^2$$

$$= |\langle\varphi_f|U(+\infty,-\infty)|\varphi_i\rangle|^2$$

$$\equiv |\langle\varphi_f|S|\varphi_i\rangle|^2$$

where $S \equiv U(+\infty,-\infty)$ is the S-operator.

Hence the S-matrix elements are just the initial $\to$ final state transition ~~probabilities~~ amplitudes. According to the adiabatic hypothesis we have, in the IP,

$$S = U(+\infty, -\infty)$$
$$= \lim_{\epsilon \to 0^+} T\, e^{-\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt\, e^{-\epsilon|t|} H'(t)_{IP}}$$

where recall $H'_{IP}(t) \equiv e^{\frac{i}{\hbar}H_0 t} H'(t)\, e^{-\frac{i}{\hbar}H_0 t}$.

Hence the S-matrix elements become

$$\langle\varphi_f|S|\varphi_i\rangle = \lim_{\epsilon \to 0^+} \sum_{n=0}^{\infty} \langle\varphi_f|S_n^{(\epsilon)}|\varphi_i\rangle$$

where

$$S_n^{(\epsilon)} = \left(\frac{-i}{\hbar}\right)^n \int_{-\infty}^{+\infty} dt_1\, e^{-\epsilon|t_1|} \int_{-\infty}^{t_1} dt_2\, e^{-\epsilon|t_2|} \cdots \int_{-\infty}^{t_{n-1}} dt_n\, e^{-\epsilon|t_n|} \times$$
$$\times \left(e^{\frac{i}{\hbar}H_0 t_1} H'(t_1)\, e^{-\frac{i}{\hbar}H_0 t_1}\right) \cdots \left(e^{\frac{i}{\hbar}H_0 t_n} H'(t_n)\, e^{-\frac{i}{\hbar}H_0 t_n}\right).$$

But we can exploit the H_0 eigenstates using

$$e^{-\frac{i}{\hbar}H_0 t_n}|\varphi_i\rangle = e^{-\frac{i}{\hbar}E_i t_n}|\varphi_i\rangle$$
$$\langle\varphi_f|e^{+\frac{i}{\hbar}H_0 t_1} = e^{+\frac{i}{\hbar}E_f t_1}\langle\varphi_f|$$

to find

$$\langle\varphi_f|S_n^{(\epsilon)}|\varphi_i\rangle = \langle\varphi_f|\left(\frac{-i}{\hbar}\right)^n\int_{-\infty}^{+\infty}dt_1\, e^{\frac{i}{\hbar}E_f t_1 - \epsilon|t_1|}\times$$

$$\times\int_{-\infty}^{t_1}dt_2\, e^{-\epsilon|t_2|}\cdots\int_{-\infty}^{t_{n-1}}dt_n\, e^{-\epsilon|t_n|-\frac{i}{\hbar}E_i t_n}\times$$

$$\times H'(t_1)\, e^{+\frac{i}{\hbar}H_0(t_2-t_1)}\, H'(t_2)\, e^{+\frac{i}{\hbar}H_0(t_3-t_2)}\cdots$$

$$\cdots H'(t_{n-1})\, e^{+\frac{i}{\hbar}H_0(t_n-t_{n-1})}\, H'(t_n)|\varphi_i\rangle .$$

To proceed further we make the change of variables

$$\begin{aligned}\tau_1 &= t_1 \\ \tau_2 &= t_2-t_1 \\ \tau_3 &= t_3-t_2 \\ &\vdots \\ \tau_n &= t_n-t_{n-1}\end{aligned}\qquad \text{or inverting}\qquad \begin{aligned}t_1 &= \tau_1 \\ t_2 &= \tau_1+\tau_2 \\ t_3 &= \tau_1+\tau_2+\tau_3 \\ &\vdots \\ t_n &= \tau_1+\tau_2+\cdots+\tau_n\end{aligned}$$

The Jacobian for such a transformation is just 1

$$1 = J = \left\|\left(\frac{\partial t}{\partial \tau}\right)\right\| = \begin{array}{c|c} & \tau \\ \hline t & \begin{vmatrix} 1 & 0 & 0 & 0 & \cdots \\ 1 & 1 & 0 & 0 & \cdots \\ 1 & 1 & 1 & 0 & \cdots \\ \vdots & & & \ddots & \end{vmatrix}\end{array} = \begin{vmatrix} 1 & & 0 \\ & \ddots & \\ 1 & & 1\end{vmatrix}$$

As well the limits of integration now become

$$\int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n = \int_{-\infty}^{+\infty} d\tau_1 \int_{-\infty}^{0} d\tau_2 \cdots \int_{-\infty}^{0} d\tau_n \; .$$

To go further let's assume H' is time independent, only the exponential damping $e^{-\epsilon|t|}$ turned it on and off. Then we can pull it out of the integrals to obtain

$$\langle \varphi_f | S_n^{(\epsilon)} | \varphi_i \rangle = \left(\frac{-i}{\hbar} \int_{-\infty}^{+\infty} d\tau_1 \, e^{\frac{-i}{\hbar}(E_i - E_f)\tau_1 - \epsilon|\tau_1|} \right)$$

$$\langle \varphi_f | H' \left(\frac{-i}{\hbar} \int_{-\infty}^{0} d\tau_2 \, e^{\frac{-i}{\hbar}(E_i - H_0)\tau_2} \, e^{-\epsilon|\tau_1 + \tau_2|} \right) \times$$

$$\times H' \left(\frac{-i}{\hbar} \int_{-\infty}^{0} d\tau_3 \, e^{\frac{-i}{\hbar}(E_i - H_0)\tau_3} \, e^{-\epsilon|\tau_1 + \tau_2 + \tau_3|} \right) \times$$

$$\times \cdots H' \left(\frac{-i}{\hbar} \int_{-\infty}^{0} d\tau_n \, e^{\frac{-i}{\hbar}(E_i - H_0)\tau_n} \, e^{-\epsilon|\tau_1 + \tau_2 + \cdots + \tau_n|} \right) \times$$

$$\times H' | \varphi_i \rangle .$$

Each integral is of the form

$$-\frac{i}{\hbar}\int_{-\infty}^{0} d\tau_k\, e^{-\frac{i}{\hbar}(E_i - H_0)\tau_k}\, e^{-\epsilon|\tau_1+\tau_2+\cdots+\tau_k|}$$

with $k=2,3,\ldots,n$. Note that the $\epsilon>0$ factor serves to guarantee convergence of the integrals at the $\tau_k \to -\infty$ limit. Since it is this convergence that we need we can replace

$$e^{-\epsilon|\tau_1+\tau_2+\cdots+\tau_k|} \quad \text{with simply}$$

$$e^{-\epsilon|\tau_k|} = e^{\epsilon\tau_k} \quad \text{since } \tau_k<0$$

for $k=2,3,\ldots,n$, and still have convergence! So

$$-\frac{i}{\hbar}\int_{-\infty}^{0} d\tau_k\, e^{-\frac{i}{\hbar}(E_i-H_0)\tau_k}\, e^{-\epsilon|\tau_1+\tau_2+\cdots+\tau_k|}$$

$$\longrightarrow -\frac{i}{\hbar}\int_{-\infty}^{0} d\tau_k\, e^{-\frac{i}{\hbar}(E_i-H_0)\tau_k+\epsilon\tau_k}$$

$$= -\frac{i}{\hbar}\frac{+1}{\left[-\frac{i}{\hbar}(E_i-H_0)+\epsilon\right]}$$

$$= \frac{1}{E_i-H_0+i\underbrace{\epsilon\hbar}_{\text{re-label as }\epsilon}} \quad \text{for each } k=2,3,\ldots,n$$

Substituting in the S matrix expansion yields

$$\langle\varphi_f|S_n^{(\epsilon)}|\varphi_i\rangle = \left(-\frac{i}{\hbar}\int_{-\infty}^{+\infty} d\tau_1\, e^{-\frac{i}{\hbar}(E_i-E_f)\tau_1 - \epsilon|\tau_1|}\right)$$

$$\times \langle\varphi_f|H' \frac{1}{E_i - H_0 + i\epsilon} H' \frac{1}{E_i - H_0 + i\epsilon} H' \cdots$$

$$\cdots H' \frac{1}{E_i - H_0 + i\epsilon} H' |\varphi_i\rangle$$

where we have n-factors of H' above.

At last we can perform the τ_1-integral

$$\lim_{\epsilon\to 0^+}\int_{-\infty}^{+\infty} d\tau_1\, e^{-\frac{i}{\hbar}(E_i-E_f)\tau_1 - \epsilon|\tau_1|}$$

$$= \int_{-\infty}^{+\infty} d\tau_1\, e^{-\frac{i}{\hbar}(E_i-E_f)\tau_1}$$

$$= 2\pi\,\delta\!\left(\frac{E_i-E_f}{\hbar}\right) = 2\pi\hbar\,\delta(E_i-E_f).$$

Thus we obtain

$$\boxed{\begin{aligned}\langle \varphi_f | S_n^{(\epsilon)} | \varphi_i \rangle = &-2\pi i\, \delta(E_f - E_i) \times \\ &\times \langle \varphi_f | H' \left(\frac{1}{E_i - H_0 + i\epsilon} H' \right)^{n-1} | \varphi_i \rangle\end{aligned}}$$

Substituting into the series on page -1252-

$$\langle \varphi_f | S | \varphi_i \rangle = \lim_{\epsilon \to 0^+} \sum_{n=0}^{\infty} \langle \varphi_f | S_n^{(\epsilon)} | \varphi_i \rangle$$

$$= \langle \varphi_f | \varphi_i \rangle + \sum_{n=1}^{\infty} \lim_{\epsilon \to 0^+} \langle \varphi_f | S_n^{(\epsilon)} | \varphi_i \rangle$$

$$\boxed{\begin{aligned}&= \langle \varphi_f | \varphi_i \rangle - 2\pi i\, \delta(E_f - E_i) \times \\ &\qquad \times \sum_{n=1}^{\infty} \langle \varphi_f | H' \left(\frac{1}{E_i - H_0 + i\epsilon} H' \right)^{n-1} | \varphi_i \rangle \\ &= \langle \varphi_f | S | \varphi_i \rangle\end{aligned}}$$

where the limit $\epsilon \to 0^+$ is understood.

Note that we, as earlier, can define the operator $\frac{1}{E_i - H_0 + i\epsilon}$ by allowing it to operator on the identity

$$1 = \sum_j{}' |\varphi_j\rangle\langle\varphi_j| \quad \text{since}$$

$$\frac{1}{E_i - H_0 + i\epsilon}|\varphi_j\rangle = \frac{1}{E_i - E_j + i\epsilon}|\varphi_j\rangle.$$

So the S-matrix elements become

$$\langle\varphi_f|S|\varphi_i\rangle = \langle\varphi_f|\varphi_i\rangle - 2\pi i\,\delta(E_f - E_i)\times$$

$$\times\sum_{n=1}^{\infty}{}' \sum_{j_1}{}' \sum_{j_2}{}' \cdots \sum_{j_{n-1}}{}' \frac{\langle\varphi_f|H'|\varphi_{j_1}\rangle\langle\varphi_{j_1}|H'|\varphi_{j_2}\rangle\cdots\langle\varphi_{j_{n-1}}|H'|\varphi_i\rangle}{(E_i - E_{j_1} + i\epsilon)(E_i - E_{j_2} + i\epsilon)\cdots(E_i - E_{j_{n-1}} + i\epsilon)}$$

For $n=1$ and $f \neq i$ we find Fermi's Golden Rule,

$$\langle\varphi_f|S|\varphi_i\rangle\Big|_{\substack{\text{first}\\\text{order}}} = -2\pi i\,\delta(E_f - E_i)\langle\varphi_f|H'|\varphi_i\rangle,$$

for the transition probability amplitude.

We can also use the time evolution operator to find an expression for the scattering state $|\psi_i^{(+)}\rangle$

recall we used the label $\vec{k}$ before

Recall too that this state was an eigenstate of H, as we shall recover.

The initial state at time $t=0$ is the same in the SP and IP, since (the pictures) they coincide at $t=0$

$$|\psi_i^{(+)}(0)\rangle = |\psi_i(0)\rangle_{IP}$$

$$= \mathcal{U}(0,-\infty)|\psi_i(-\infty)\rangle_{IP}$$

$$= \mathcal{U}(0,-\infty)|\varphi_i\rangle$$

$$= \lim_{\epsilon\to 0^+} T e^{-\frac{i}{\hbar}\int_{-\infty}^{0} dt\, e^{-\epsilon|t|} H'_{IP}(t)} |\varphi_i\rangle$$

$$= \lim_{\epsilon\to 0^+} \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_{-\infty}^{0} dt_1 e^{-\epsilon|t_1|} \int_{-\infty}^{t_1} dt_2 e^{-\epsilon|t_2|} \cdots \int_{-\infty}^{t_{n-1}} dt_n e^{-\epsilon|t_n|} \times$$

$$\times \left(e^{\frac{+i}{\hbar}H_0 t_1} H' e^{\frac{-i}{\hbar}H_0 t_1}\right) \cdots \left(e^{\frac{+i}{\hbar}H_0 t_n} H' \underbrace{e^{\frac{-i}{\hbar}H_0 t_n} |\varphi_i\rangle}_{e^{\frac{-i}{\hbar}E_i t_n}|\varphi_i\rangle}\right)$$

Note each $e^{-\epsilon|t_k|} = e^{+\epsilon t_k}$ since all the $t_k < 0$. Also this is exactly like the formula we had for $S = U(+\infty,-\infty)$ except the t_1 integral stops at $t_1 = 0$ instead of all the way to $+\infty$. So as before we introduce <u>relative</u> time variables

$$\begin{aligned} \tau_1 &= t_1 & \text{and the} \quad t_1 &= \tau_1 \\ \tau_2 &= t_2 - t_1 & \text{inverse} \quad t_2 &= \tau_1 + \tau_2 \\ &\vdots & &\vdots \\ \tau_n &= t_n - t_{n-1} & t_n &= \tau_1 + \tau_2 + \cdots + \tau_n . \end{aligned}$$

The expression for $U(0,-\infty)$ becomes

$$U(0,-\infty)|\varphi_i\rangle = \lim_{\epsilon\to 0^+} \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\int_{-\infty}^{0} d\tau_1\, e^{\frac{-i}{\hbar}(E_i - H_0)\tau_1 + n\epsilon\tau_1} \right)$$

$$\times H' \left(\frac{-i}{\hbar}\int_{-\infty}^{0} d\tau_2\, e^{\left[\frac{i}{\hbar}(E_i - H_0) + (n-1)\epsilon\right]\tau_2} \right) H' \times$$

$$\times \cdots H' \left(\frac{-i}{\hbar}\int_{-\infty}^{0} d\tau_n\, e^{\left[\frac{i}{\hbar}(E_i - H_0) + \epsilon\right]\tau_n} \right) H_1 |\varphi_i\rangle .$$

As $\epsilon \to 0^+$, we replace $n\epsilon$ ~~by~~ ϵ to obtain the same convergence effect ($n\epsilon \to \epsilon$, $(n-1)\epsilon \to \epsilon$ etc.), thus we have for each integral (there are n-of them)

$$-\frac{i}{\hbar}\int_{-\infty}^{0} d\tau\, e^{\left(-\frac{i}{\hbar}(E_i - H_0)+\epsilon\right)\tau} = \frac{1}{E_i - H_0 + i\epsilon}$$

as before for S. Thus we find with $\epsilon \to 0^+$ understood

$$|\Psi_i^{(+)}(0)\rangle = U(0,-\infty)|\varphi_i\rangle$$

$$= \sum_{n=0}^{\infty}\left(\frac{1}{E_i - H_0 + i\epsilon}H'\right)^n |\varphi_i\rangle$$

$$= |\varphi_i\rangle + \sum_{n=1}^{\infty}\left(\frac{1}{E_i - H_0 + i\epsilon}H'\right)^n |\varphi_i\rangle .$$

We can group the terms on the RHS as

$$= |\varphi_i\rangle + \frac{1}{E_i - H_0 + i\epsilon}H' \underbrace{\sum_{n=1}^{\infty}\left(\frac{1}{E_i - H_0 + i\epsilon}H'\right)^{n-1}|\varphi_i\rangle}$$

re-label $n \to n-1$ $$= \underbrace{\sum_{n=0}^{\infty}\left(\frac{1}{E_i - H_0 + i\epsilon}H'\right)^{n}|\varphi_i\rangle}$$

$$= |\Psi_i^{(+)}(0)\rangle \text{ again}$$

Thus

$$|\psi_i^{(+)}(0)\rangle = |\varphi_i\rangle + \frac{1}{E_i - H_0 + i\epsilon} H' |\psi_i^{(+)}(0)\rangle$$

Since all pictures coincide at $t=0$ we can drop the $|\psi_i^{(+)}(0)\rangle \equiv |\psi_i^{(+)}\rangle$ the Heisenberg state. So

$$\boxed{|\psi_i^{(+)}\rangle = |\varphi_i\rangle + \frac{1}{E_i - H_0 + i\epsilon} H' |\psi_i^{(+)}\rangle}$$

This is the Lippman-Schwinger Equation. (we found this on page -1029- in potential scattering).

Note that $|\psi_i^{(+)}\rangle$ as we had earlier, is an eigenstate of the full Hamiltonian. To see this consider

$$(H_0 - E_i)|\psi_i^{(+)}\rangle = \overbrace{(H_0 - E_i)|\varphi_i\rangle}^{=(E_i - E_i)|\varphi_i\rangle = 0}$$

$$+ \underbrace{(H_0 - E_i)\frac{1}{E_i - H_0 + i\epsilon}}_{=-1} H' |\psi_i^{(+)}\rangle$$

So

$$(H_0 - E_i)|\psi_i^{(+)}\rangle = -H'|\psi_i^{(+)}\rangle$$

$\Rightarrow$

$$\underbrace{(H_0 + H')}_{H}|\psi_i^{(+)}\rangle = E_i|\psi_i^{(+)}\rangle$$

$$H|\psi_i^{(+)}\rangle = E_i|\psi_i^{(+)}\rangle .$$

$|\psi_i^{(+)}\rangle$ is an eigenstate of the full Hamiltonian H with the initial energy E_i eigenvalue.

As before this equation is an integral equation, indeed substituting a complete set of states on the RHS of the L-S equation we find

$$|\psi_i^{(+)}\rangle = |\varphi_i\rangle + \sum_n \frac{\langle \varphi_n | H' | \psi_i^{(+)}\rangle}{E_i - E_n + i\epsilon} |\varphi_n\rangle .$$

We can use the L-S equation to write the S-Matrix elements in terms of $|\psi_i^{(+)}\rangle$, (page -1257-):

$$S_{fi} = \langle \varphi_f | S | \varphi_i \rangle$$

$$= \underbrace{\langle \varphi_f | \varphi_i \rangle}_{=\delta_{fi}} - 2\pi i\, \delta(E_f - E_i) \times$$

$$\times \underbrace{\sum_{n=1}^{\infty} \langle \varphi_f | H' \left(\frac{1}{E_i - H_0 + i\epsilon} H' \right)^{n-1} | \varphi_i \rangle}$$

let $n \to n-1$

$$= \sum_{n=0}^{\infty} \langle \varphi_f | H' \left(\frac{1}{E_i - H_0 + i\epsilon} H' \right)^{n} | \varphi_i \rangle$$

$$= \delta_{fi} - 2\pi i\, \delta(E_f - E_i) \langle \varphi_f | H' \underbrace{\sum_{n=0}^{\infty} \left(\frac{1}{E_i - H_0 + i\epsilon} H' \right)^{n} | \varphi_i \rangle}_{= |\psi_i^{(+)}\rangle}$$

(page -1261-)

So

$$\boxed{S_{fi} = \delta_{fi} - 2\pi i\, \delta(E_f - E_i) \langle \varphi_f | H' | \psi_i^{(+)} \rangle} .$$

This is an exact equation relating the S-matrix element to the scattering state $|\psi_i^{(+)}\rangle$. Since we are usually interested in "transitions" (scattering) from i to ~~f~~ $\neq i$, we define the transition matrix or T-matrix as

$$T_{fi} \equiv \langle \varphi_f | H' | \psi_i^{(+)} \rangle \quad , \text{ hence}$$

$$S_{fi} = \delta_{fi} - 2\pi i \, \delta(E_f - E_i) T_{fi} \quad .$$

Since $U(t, t_0)$ is unitary, we suspect that S is also, this we can check directly deriving an important unitarity relation for the T-matrix in the process.

If the S-matrix is unitary, we have

$$\sum_f (S^\dagger)_{if} S_{fi'} = \delta_{ii'}$$

$$\|$$

$$\sum_f S^*_{fi} S_{fi'} = \delta_{ii'} \, .$$

As follows from $S^\dagger S = 1$. To show the above we exploit the L-S equation

$$|\psi_i^{(+)}\rangle = |\varphi_i\rangle + \frac{1}{E_i - H_0 + i\epsilon} H' |\psi_i^{(+)}\rangle$$

and its hermitian conjugate

$$\langle \psi_i^{(+)}| = \langle \varphi_i| + \langle \psi_i^{(+)}| H' \frac{1}{E_i - H_0 - i\epsilon} .$$

The transition matrix element then becomes

$$T_{i'i} = \langle \varphi_{i'}| H' |\psi_i^{(+)}\rangle \quad \text{, using the L-S eq.} \Rightarrow$$

$$= \langle \psi_{i'}^{(+)}| H' |\psi_i^{(+)}\rangle$$

$$- \langle \psi_{i'}^{(+)}| H' \frac{1}{E_{i'} - H_0 - i\epsilon} H' |\psi_i^{(+)}\rangle .$$

Taking the hermitian conjugate

$$T_{ii'}^{*} = \langle \psi_i^{(+)}| H' |\psi_{i'}^{(+)}\rangle^{*}$$

$$- \langle \psi_i^{(+)}| H' \frac{1}{E_i - H_0 - i\epsilon} H' |\psi_{i'}^{(+)}\rangle^{*}$$

$$= \langle \psi_{i'}^{(+)}| H' |\psi_i^{(+)}\rangle$$

$$- \langle \psi_{i'}^{(+)}| H' \frac{1}{E_i - H_0 + i\epsilon} H' |\psi_i^{(+)}\rangle .$$

Taking the difference of the two, we get

$$T_{i'i} - T^*_{ii'} = -\langle \psi^{(+)}_{i'} | H' \Big(\frac{1}{E_{i'} - H_0 - i\epsilon}$$

$$- \frac{1}{E_i - H_0 + i\epsilon} \Big) H' | \psi^{(+)}_i \rangle .$$

Multiplying by $\delta(E_{i'} - E_i) \Rightarrow$

$$\delta(E_{i'} - E_i)(T_{i'i} - T^*_{ii'})$$

$$= -\delta(E_{i'} - E_i) \langle \psi^{(+)}_{i'} | H' \Big(\frac{1}{E_i - H_0 - i\epsilon} - \frac{1}{E_i - H_0 + i\epsilon} \Big) \times$$

$$\times H' | \psi^{(+)}_i \rangle .$$

But the difference of operators is just

$$\left(\frac{1}{A - i\epsilon} - \frac{1}{A + i\epsilon} \right) = \frac{(A + i\epsilon) - (A - i\epsilon)}{(A - i\epsilon)(A + i\epsilon)} = \frac{2i\epsilon}{A^2 + \epsilon^2}$$

Thus as $\epsilon \to 0^+$ this is just $2\pi i \delta(A)$, i.e.

$$\lim_{\epsilon \to 0^+} \frac{\epsilon}{A^2 + \epsilon^2} = \pi \delta(A)$$

So

$$\delta(E_{i'}-E_i)(T_{i'i}-T_{ii'}^{*})$$

$$=-2\pi i\,\delta(E_{i'}-E_i)\langle\psi_{i'}^{(+)}|H'\delta(E_i-H_0)H'|\psi_i^{(+)}\rangle$$

As usual we define such an operator expression by inserting a complete set of H_0-eigenstates

$$=-2\pi i\,\delta(E_{i'}-E_i)\sum_f\langle\psi_{i'}^{(+)}|H'|\varphi_f\rangle\times$$

$$\times\underbrace{\langle\varphi_f|\delta(E_i-H_0)}_{=\delta(E_i-E_f)\langle\varphi_f|}H'|\psi_i^{(+)}\rangle$$

$$=-2\pi i\,\delta(E_{i'}-E_i)\sum_f\delta(E_i-E_f)\times$$

$$\times\underbrace{\langle\psi_{i'}^{(+)}|H'|\varphi_f\rangle}_{=T_{fi'}^{*}}\underbrace{\langle\varphi_f|H'|\psi_i^{(+)}\rangle}_{=T_{fi}}$$

$$\boxed{\begin{aligned}\delta(E_{i'}-E_i)(T_{i'i}-T^*_{ii'}) \\ = -2\pi i\,\delta(E_{i'}-E_i)\sum_f \delta(E_i-E_f)\,T^*_{fi'}T_{fi}\end{aligned}}$$

This is the unitarity relation for the Transition matrix elements.

Recalling that

$$S_{fi} = \delta_{fi} - 2\pi i\,\delta(E_f-E_i)\,T_{fi}$$

and so

$$S^*_{fi} = \delta_{fi} + 2\pi i\,\delta(E_f-E_i)\,T^*_{fi}$$

leads us to consider

$$\sum_f S^*_{fi'}S_{fi} = \sum_f \left(\delta_{fi'} + 2\pi i\,\delta(E_f-E_{i'})\,T^*_{fi'}\right)\times$$

$$\times\left(\delta_{fi} - 2\pi i\,\delta(E_f-E_i)\,T_{fi}\right)$$

$$= \sum_f \Big(\delta_{fi}\delta_{fi'} - 2\pi i\, \delta_{fi'}\, \delta(E_f - E_i) T_{fi}$$
$$+ 2\pi i \delta_{fi}\, \delta(E_f - E_{i'}) T^*_{fi'}$$
$$- (2\pi i)^2 \delta(E_f - E_{i'}) \delta(E_f - E_i) T^*_{fi'} T_{fi} \Big)$$

$$= \delta_{ii'} - 2\pi i\, \delta(E_{i'} - E_i)(T_{i'i} - T^*_{ii'})$$
$$\underbrace{- (2\pi i)^2 \delta(E_i - E_{i'}) \sum_f \delta(E_f - E_i) T^*_{fi'} T_{fi}}$$

These are just the T-matrix unitarity relation terms $= 0$

$$= \delta_{ii'} .$$

Hence we obtain the S-matrix unitarity relations

$$\sum_f S^*_{fi'} S_{fi} = \delta_{ii'} .$$

That is $S^\dagger S = 1 = S S^\dagger$.

since the S-operator obeys

$$S^\dagger S = 1 \;\Rightarrow$$

$$\langle \varphi_{i'} | S^\dagger S | \varphi_i \rangle = \langle \varphi_{i'} | \varphi_i \rangle = \delta_{i'i}$$

$$\| $$

$$\sum_f \underbrace{\langle \varphi_{i'} | S^\dagger | \varphi_f \rangle}_{= \langle \varphi_f | S | \varphi_{i'} \rangle^* = S^*_{fi'}} \underbrace{\langle \varphi_f | S | \varphi_i \rangle}_{= S_{fi}}$$

$$\Rightarrow \quad \boxed{\sum_f S^*_{fi'} S_{fi} = \delta_{i'i}} \quad \text{and}$$

vice versa. This is just the conservation of probability. Recall that the transition probability for $|\varphi_i\rangle \to |\varphi_f\rangle$ is just

$$P_{fi} = |S_{fi}|^2 = S^*_{fi} S_{fi} \quad (\cancel{\Sigma}\ i, f)$$

Thus the sum over the probabilities that $|\varphi_i\rangle$ goes into some state $|\varphi_f\rangle$ must be one

$$\sum_f P_{fi} = \sum_f |S_{fi}|^2 = \sum_f S_{fi}^* S_{fi} = \delta_{ii} = 1.$$

From the transition probabilities we can, as before, determine the transition rates and hence cross-sections. Indeed, for $f \neq i$

$$S_{fi} = -2\pi i\, \delta(E_f - E_i)\, T_{fi}\,.$$

The transition probability is

$$P_{fi} = |S_{fi}|^2 = |-2\pi i\, \delta(E_f - E_i)|^2 |T_{fi}|^2.$$

As usual $|\delta(E_f - E_i)|^2 = \delta(E_f - E_i)\,\delta(0)$ is formally undefined. Recall the $\delta(E_f - E_i)$ came from the limit of the integral for long times

$$2\pi\delta(0) = \lim_{E_f \to E_i} 2\pi\delta(E_f - E_i) = \lim_{\omega_{fi} \to 0} \frac{2\pi}{\hbar}\delta(\omega_{fi})$$

$$= \lim_{\omega_{fi} \to 0} \frac{2\pi}{\hbar} \lim_{T \to \infty} \int_{-T/2}^{+T/2} \frac{dt}{2\pi}\, e^{i\omega_{fi} t}$$

Now interchange limits

$$2\pi\delta(0) = \lim_{T\to\infty} \frac{2\pi}{\hbar} \int_{-\frac{T}{2}}^{+\frac{T}{2}} \frac{dt}{2\pi} \lim_{\omega_{fi}\to 0} e^{i\omega_{fi}t}$$

$$= \lim_{T\to\infty} \frac{1}{\hbar} \int_{-\frac{T}{2}}^{+\frac{T}{2}} dt = \frac{1}{\hbar} T \;, \quad T \text{ limit understood}$$

Thus

$$P_{fi} = |S_{fi}|^2 = T \frac{2\pi}{\hbar} \delta(E_f - E_i) |T_{fi}|^2 \;, f \neq i$$

where T is the interaction time interval. Hence the transition rate is just

$$R_{fi} = \frac{P_{fi}}{T} = \frac{|S_{fi}|^2}{T}$$

$$\boxed{R_{fi} = \frac{2\pi}{\hbar} \delta(E_f - E_i) |T_{fi}|^2}$$

This is an exact expression for R_{fi}, and so this is an extension of Fermi's Golden Rule to all orders in the interaction i.e. $T_{fi} = \langle \varphi_f | H' | \psi_i^{(+)} \rangle$.

For $|\psi_i^{(+)}\rangle$ approximated by $|\varphi_i\rangle$, the L-S equation Born term,

we have that $T_{fi}^{Born} = \langle \varphi_f | H' | \varphi_i \rangle$
and
$$R_{fi}^{Born} = \frac{2\pi}{\hbar} \delta(E_f - E_i) \left| \langle \varphi_f | H' | \varphi_i \rangle \right|^2,$$
the original form of Fermi's Golden Rule.

As earlier, the cross section for the $i \to f$ transition is given by
$$d\sigma_{fi} = \frac{R_{fi}}{J_{in}}.$$

If one particle in the final state has energy E in the continuum, we must sum over the detector's resolution
$$d\sigma_{fi} = \frac{1}{J_{in}} \int dE \, \frac{\partial n(E)}{\partial E} \frac{2\pi}{\hbar} \delta(E_f - E_i) |T_{fi}|^2$$
$$= \frac{1}{J_{in}} \frac{2\pi}{\hbar} \frac{\partial n(E)}{\partial E} |T_{fi}|^2 \Big|_{E_f = E_i}.$$

Finally it is instructive to derive the formula for the transition rate directly in the SP using formal arguments. For H independent of time we had

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}\,\underbrace{|\Psi(0)\rangle}$$

$$= |\Psi(0)\rangle_{IP} = |\Psi(0)\rangle_I$$

$$= |\Psi_i^{(+)}\rangle$$

Thus the probability amplitude for $|\Psi_i^{(+)}\rangle$ being found in the H_0 eigenstate $|\varphi_f\rangle$, $H_0|\varphi_f\rangle = E_f|\varphi_f\rangle$, at time t is just

$$M_{fi}(t) \equiv \langle\varphi_f(t)|\Psi(t)\rangle$$

when $\quad |\varphi_f(t)\rangle = e^{-\frac{i}{\hbar}E_f t}|\varphi_f\rangle$.

So

$$M_{fi}(t) = \langle\varphi_f|e^{\frac{i}{\hbar}(E_f - H)t}|\Psi_i^{(+)}\rangle$$

and the transition probability is

$$P_{fi}(t) = |M_{fi}(t)|^2$$

with transition rate

$$R_{fi} = \frac{d}{dt} P_{fi}(t) .$$

So
$$R_{fi} = \frac{d}{dt}\Big((\operatorname{Re} M_{fi}(t))^2 + (\operatorname{Im} M_{fi}(t))^2 \Big)$$

$$= 2(\operatorname{Re} M_{fi}) \frac{d}{dt}(\operatorname{Re} M_{fi}) + 2(\operatorname{Im} M_{fi}) \frac{d}{dt}(\operatorname{Im} M_{fi})$$

$$= 2 \operatorname{Re}\Big(M_{fi}^* \frac{d}{dt} M_{fi}\Big)(t) .$$

However

$$\frac{d}{dt} M_{fi}(t) = \frac{d}{dt} \langle \varphi_f | e^{\frac{i}{\hbar}(E_f - H)t} | \psi_i^{(+)} \rangle$$

$$= \langle \varphi_f | \frac{i}{\hbar}(E_f - H) e^{\frac{i}{\hbar}(E_f - H)t} | \psi_i^{(+)} \rangle$$

$$= \frac{i}{\hbar} \langle \varphi_f | \underbrace{(H_0 - H)}_{= -H'} e^{\frac{i}{\hbar}(E_f - H)t} | \psi_i^{(+)} \rangle$$

but
$$H | \psi_i^{(+)} \rangle = E_i | \psi_i^{(+)} \rangle , \text{ so}$$

$$\frac{d}{dt} M_{fi}(t) = -\frac{i}{\hbar} \langle \varphi_f | H' e^{\frac{i}{\hbar}(E_f - E_i)t} | \psi_i^{(+)} \rangle$$

$$= -\frac{i}{\hbar} e^{\frac{i}{\hbar}(E_f - E_i)t} \langle \varphi_f | H' | \psi_i^{(+)} \rangle$$

Now we also have that

$$M_{fi}(t) = \langle \varphi_f | e^{\frac{i}{\hbar}(E_f - H)t} | \psi_i^{(+)} \rangle$$

$$= e^{\frac{i}{\hbar}(E_f - E_i)t} \langle \varphi_f | \psi_i^{(+)} \rangle$$

Hence we have that

$$\left(M_{fi}^* \frac{d}{dt} M_{fi}\right)(t) = -\frac{i}{\hbar} \langle \varphi_f | H' | \psi_i^{(+)} \rangle \langle \varphi_f | \psi_i^{(+)} \rangle^*$$

and so the transition rate becomes

$$R_{fi} = 2 \operatorname{Re} \left(M_{fi}^* \frac{d}{dt} M_{fi}\right)(t)$$

$$= \frac{2}{\hbar} \operatorname{Im} \left[\langle \varphi_f | H' | \psi_i^{(+)} \rangle \langle \varphi_f | \psi_i^{(+)} \rangle^* \right]$$

and we note that R_{fi} is independent of time.

Using the L-S equation for $|\psi_i^{(+)}\rangle$

$$|\psi_i^{(+)}\rangle = |\varphi_i\rangle + \frac{1}{E_i - H_0 + i\epsilon} H' |\psi_i^{(+)}\rangle$$

we find

$$\langle\varphi_f|\psi_i^{(+)}\rangle = \langle\varphi_f|\varphi_i\rangle + \langle\varphi_f|\frac{1}{E_i - H_0 + i\epsilon}H'|\psi_i^{(+)}\rangle$$

$$= \delta_{fi} + \frac{\langle\varphi_f|H'|\psi_i^{(+)}\rangle}{E_i - E_f + i\epsilon}$$

and so the complex conjugate is

$$\langle\varphi_f|\psi_i^{(+)}\rangle^* = \delta_{fi} + \frac{\langle\varphi_f|H'|\psi_i^{(+)}\rangle^*}{E_i - E_f - i\epsilon}.$$

This yields for the transition rate

$$R_{fi} = \frac{2}{\hbar}\delta_{fi}\,\mathrm{Im}\left[\langle\varphi_f|H'|\psi_i^{(+)}\rangle\right]$$

$$+ \frac{2}{\hbar}\,\mathrm{Im}\left[\frac{\langle\varphi_f|H'|\psi_i^{(+)}\rangle\langle\varphi_f|H'|\psi_i^{(+)}\rangle^*}{E_i - E_f - i\epsilon}\right]$$

$$= \frac{2}{\hbar}\delta_{fi}\,\mathrm{Im}\left[\langle\varphi_f|H'|\psi_i^{(+)}\rangle\right]$$

$$+ \frac{2}{\hbar}|\langle\varphi_f|H'|\psi_i^{(+)}\rangle|^2\,\underbrace{\mathrm{Im}\left[\frac{1}{E_i - E_f - i\epsilon}\right]}_{=\pi\delta(E_i - E_f)}$$

$\left(\frac{1}{A \mp i\epsilon} = P\left(\frac{1}{A}\right) \pm i\pi\delta(A)\right.$, Merzbacher p. 501$\left.\right)$

Thus we secure

$$R_{fi} = \frac{2}{\hbar}\delta_{fi}\,\mathrm{Im}\langle\varphi_i|H'|\psi_i^{(+)}\rangle$$
$$+\frac{2\pi}{\hbar}\delta(E_i - E_f)\,|\langle\varphi_f|H'|\psi_i^{(+)}\rangle|^2 .$$

But $T_{fi} \equiv \langle\varphi_f|H'|\psi_i^{(+)}\rangle$; thus

$$\boxed{R_{fi} = \frac{2\pi}{\hbar}\delta(E_i - E_f)\,|T_{fi}|^2 + \frac{2}{\hbar}\delta_{fi}\,\mathrm{Im}\,T_{ii}}$$

This is an exact expression of Fermi's Golden Rule allowing for the depletion of the initial state by the $\mathrm{Im}\,T_{ii}$ term. As before for $f \neq i$ and $|\psi_i^{(+)}\rangle \simeq |\varphi_i\rangle$ we obtain the Born approximation form of the Golden Rule,

$$R_{fi}^{\text{Born}} = \frac{2\pi}{\hbar}\,|\langle\varphi_f|H'|\varphi_i\rangle|^2\,\delta(E_f - E_i).$$

We can check that indeed our present approach reproduces the previous results for potential scattering.

Consider $H = H_0 + H'$ with

$$H_0 = \frac{1}{2m}\vec{P}^2 \text{ and } H' = V(\vec{R}).$$

We can write the L-S equation in the coordinate eigenbasis $\{|\vec{r}\rangle\}$ with

$$\langle \vec{r}|\varphi_i\rangle = \frac{1}{\Omega^{1/2}} e^{i\vec{k}\cdot\vec{r}}$$

$$\langle \vec{r}|\psi_i^{(+)}\rangle \equiv \frac{1}{\Omega^{1/2}} \psi_{\vec{k}}^{(+)}(\vec{r}),$$

the scattering state that evolves from the incoming $|\varphi_i\rangle$ with $\vec{k}$ state.

So the L-S equation becomes

$$|\psi_i^{(+)}\rangle = |\varphi_i\rangle + \frac{1}{E_i - H_0 + i\epsilon} H' |\psi_i^{(+)}\rangle$$

$\Rightarrow$

$$\frac{1}{\Omega^{1/2}} \psi_{\vec{k}}^{(+)}(\vec{r}) = \langle \vec{r}|\psi_i^{(+)}\rangle$$

$$= \frac{1}{\Omega^{1/2}} e^{i\vec{k}\cdot\vec{r}} + \langle \vec{r}|\frac{1}{E_i - H_0 + i\epsilon} H' |\psi_i^{(+)}\rangle$$

$$1 = \int d^3r' \, |\vec{r}'\rangle\langle\vec{r}'|$$

$$= \frac{1}{\Omega^{1/2}} e^{i\vec{k}\cdot\vec{r}} + \int d^3r' \langle \vec{r} | \frac{1}{E_i - H_0 + i\epsilon} | \vec{r}' \rangle \times$$

$$\times \underbrace{\langle \vec{r}' | H' | \psi_i^{(+)} \rangle}$$

Now we must evaluate the Green function

$$= V(\vec{r}') \langle \vec{r}' | \psi_i^{(+)} \rangle$$

$$= V(\vec{r}') \frac{1}{\Omega^{1/2}} \psi_{\vec{k}}^{(+)}(\vec{r}')$$

$\frac{1}{E_i - H_0 + i\epsilon}$ in the $\{|\vec{r}\rangle\}$ basis

$$\langle \vec{r} | \frac{1}{E_i - H_0 + i\epsilon} | \vec{r}' \rangle = \int \frac{d^3k'}{(2\pi)^3} \langle \vec{r} | \varphi_{\vec{k}'} \rangle \times$$

$$\times \langle \varphi_{\vec{k}'} | \frac{1}{E_i - H_0 + i\epsilon} | \vec{r}' \rangle$$

where $|\varphi_{\vec{k}'}\rangle$ are a complete set of H_0 eigenvectors (take $\Omega \to \infty$)

but

$$\langle \varphi_{\vec{k}'} | \frac{1}{E_i - H_0 + i\epsilon} | \vec{r}' \rangle$$

$$= \langle \varphi_{\vec{k}'} | \frac{1}{E_i - \frac{\hbar^2 \vec{k}'^2}{2m} + i\epsilon} | \vec{r}' \rangle$$

and $E_i = \frac{\hbar^2 \vec{k}^2}{2m}$, so we have

$$\langle \vec{r} | \frac{1}{E_i - H_0 + i\epsilon} | \vec{r}\,'\rangle = \int \frac{d^3k'}{(2\pi)^3} \frac{\overbrace{\langle \vec{r}|\varphi_{\vec{k}'}\rangle}^{e^{i\vec{k}'\cdot\vec{r}}} \overbrace{\langle\varphi_{\vec{k}'}|\vec{r}\,'\rangle}^{e^{-i\vec{k}'\cdot\vec{r}\,'}}}{\frac{\hbar^2}{2m}\left(\vec{k}^2 - \vec{k}'^2 + i\frac{2m\epsilon}{\hbar^2}\right)}$$

Now we just re-label $\frac{2m\epsilon}{\hbar^2} \to \epsilon$ and we find

$$\langle \vec{r} | \frac{1}{E_i - H_0 + i\epsilon} | \vec{r}\,'\rangle = \int \frac{d^3k'}{(2\pi)^3} \frac{\frac{2m}{\hbar^2} e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}}{\vec{k}^2 - \vec{k}'^2 + i\epsilon}$$

$$= \frac{+2m}{\hbar^2} G_+(\vec{r},\vec{r}\,')$$

with

$$G_+(\vec{r},\vec{r}\,') = -\int \frac{d^3k'}{(2\pi)^3} \frac{e^{i\vec{k}'\cdot(\vec{r}-\vec{r}\,')}}{\underbrace{\vec{k}'^2 - \vec{k}^2 - i\epsilon}_{= \vec{k}'^2 - (|\vec{k}| + i\epsilon)^2}}$$

(ignore ϵ^2 term, and let $2|\vec{k}|\epsilon \to \epsilon$)

as we had on page -1023-, the scattering Green function we found in the time independent potential scattering case with the correct "outgoing spherical wave" boundary condition (the $-i\epsilon$ factor).

Indeed the L-S equation becomes, cancelling the volume factors and letting $\Omega \to \infty$,

$$\psi_{\vec{k}}^{(+)}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \int d^3r' \, G_+(\vec{r},\vec{r}') \underbrace{\left(\frac{2m}{\hbar^2} V(\vec{r}')\right)}_{\equiv U(\vec{r}')} \psi_{\vec{k}}^{(+)}(\vec{r}')$$

And so we find the L-S equation on page (-1026-)

$$\boxed{\psi_{\vec{k}}^{(+)}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \int d^3r' \, G_+(\vec{r},\vec{r}') \, U(\vec{r}') \, \psi_{\vec{k}}^{(+)}(\vec{r}'),}$$

Hence the cross section is given for $f \neq i$ by

$$d\sigma = \frac{\partial R_{fi}}{J_{in}} = \frac{2\pi}{\hbar J_{in}} \frac{\partial n}{\partial E} |T_{fi}|^2 \Big|_{E_f = E,}$$

$$J_{in} = \frac{\hbar|\vec{k}|}{m}$$

by Fermi's Golden Rule (page -1274-)

but $J_{in} = \dfrac{\hbar|\vec{k}|}{m}$

$$\frac{\partial n}{\partial E} = d\Omega \frac{\Omega}{(2\pi\hbar)^3} m\hbar k$$

with $\langle \vec{r}|\varphi_f\rangle = \dfrac{1}{\Omega^{1/2}} e^{i\vec{k}'\cdot\vec{r}}$; $|\vec{k}'| = |\vec{k}| = k$

So
$$\frac{d\sigma}{d\Omega} = \left| \frac{-1}{4\pi} \int d^3r' \, e^{-i\vec{k}'\cdot\vec{r}'} U(\vec{r}') \psi_{\vec{k}}^{(+)}(\vec{r}') \right|^2$$
$$\equiv \left| f^{(+)}(\vec{k},\vec{k}') \right|^2$$
as we obtained earlier (page -1021-), with the exact result
$$f^{(+)}(\vec{k},\vec{k}') = \frac{-1}{4\pi} \int d^3r' \, e^{-i\vec{k}'\cdot\vec{r}'} U(\vec{r}') \psi_{\vec{k}}^{(+)}(\vec{r}') .$$