Perturbation theory: rate of transitions and scattering amplitude

1. The unperturbed Hamiltonian H_0 has solutions:
   $\Psi_n^0 = e^{-iE_n t}\psi_n^0(r)$, where $\int \psi_n^+ \psi_m dV = \delta_{nm}$
   and the system's initial state is Ψ_i^0.

2. Then, a small perturbation in the form of potential energy V(r) is added the free Hamiltonian: $H=H_0+V$.
   Under this perturbation, the wave function will start evolving according to $i\frac{\partial}{\partial t}\Psi = \left(\hat{H}_0 + \hat{U}\right)\Psi$.

3. We will be looking for solutions of this equation in the form
   $\Psi(t) = \Psi_i^0 + \sum c_n(t)\Psi_n^0$,
   where n describes the spectrum of states, $c_n(t)$ amplitudes are small and $c_n(0) = 0$

4. By substituting Ψ in eq.(2) with eq.(3):

   $$i\frac{\partial}{\partial t}\left(\Psi_i^0 + \sum c_n(t)\Psi_n^0\right) = \left(\hat{H}_0 + \hat{U}\right)\left(\Psi_i^0 + \sum c_n(t)\Psi_n^0\right)$$

   $$\cancel{i\dot{\Psi}_i^0} + i\sum \dot{c}_n\Psi_n^0 + \cancel{i\sum c_n(t)\dot{\Psi}_n^0} = \cancel{\hat{H}_0\Psi_i^0} + \hat{U}\Psi_i^0 + \cancel{\sum c_n(t)\hat{H}_0\Psi_n^0} + \cancel{\sum c_n(t)\hat{U}\Psi_n^0}$$

   Single lines cancel identity terms (all Ψ^0 are solutions for hamiltonian $\hat{H}_0$).
   Crossed term is the second order of smalleness, while other two kept terms are of the first order...

   $$i\sum \dot{c}_n\Psi_n^0 = \hat{V}\Psi_i^0$$

   By multiplying both sides by Ψ_f^{0+} and integrating over dV=dxdydz, we arrive to:

   $$i\sum \int \dot{c}_n\Psi_f^{0+}\Psi_n^0 dV = \int \Psi_f^{0+}\hat{U}\Psi_i^0 dV$$

   $$i\sum \dot{c}_n\delta_{fn} = \int \Psi_f^{0+}\hat{U}\Psi_i^0 dV$$

   $$\dot{c}_n = -i\int \Psi_f^{0+}\hat{U}\Psi_i^0 dV$$

5. By substituting wave functions as given in the point 1:

   $$\dot{c}_f(t) = -i\int e^{i(E_f-E_i)t}\psi_f^{0+}\hat{U}\psi_i^0 dV = -ie^{i(E_f-E_i)t}\int \psi_f^{0+}\hat{U}\psi_i^0 dV = -ie^{i(E_f-E_i)t}m_{fi},$$ where $m_{fi} = \int \psi_f^{0+}\hat{U}\psi_i^0 dV$

6. $m_{fi} = \int \psi_f^{0+}\hat{U}\psi_i^0 dV$ is called a **<u>matrix element</u>** (a.k.a. a **<u>scattering amplitude</u>**) connecting the process of scattering and the physical potential of interactions (U will not appear anywhere any more, except via this expression).

   In a typical scattering experiment, the incident and scattered particles can be represented by free waves. Therefore, the matrix element can be thought of as a simple **Fourier transformation** of the potential function *U(r):*

   $$m_{fi} = \int \psi_f^{0+}\hat{U}\psi_i^0 dV = C^2\int e^{-i\vec{p}_f\vec{r}}U(r)e^{i\vec{p}_i\vec{r}}dV = C^2\int U(r)e^{i(\vec{p}_i-\vec{p}_f)\vec{r}}dV = C^2\int U(r)e^{i\vec{q}\vec{r}}dV = m_{fi}(\vec{q}).$$

   Note that the **matrix element depends on the transferred momentum *q***.

7. After some calculus manipulations[1], the rate of transitions (probability per unit of time) from the initial *i*-state to one of the *dn* states in vicinity of the picked final state Ψ_f is

$$dw = 2\pi |m_{fi}|^2 \delta(E_f - E_i) dn ,$$

- The final eigenstates are contiguous functions of direction parameters and energy. Therefore, the probability of scattering into exactly one particular final state is obviously zero. So we need to open some range in the vicinity of parameters characterizing the picked final state, $d\Omega$ and dE. There will be *dn* final states in that range, which we will calculate further.

- Appearance of delta-function $\delta(E_f - E_i)$ signals us that the energy must be conserved.
The number of states *dn* can be re-written as

$$dn = \frac{d^2 n}{d\Omega_f dE_f} d\Omega_f dE_f \qquad \text{where} \quad \frac{d^2 n}{d\Omega_f dE_f} = \rho(\theta, \varphi, E_f)$$ is called a **density of states**.

The presence of the δ-function allows us to sum up (integrate) over all possible final energies, giving us the rate of transitions in the following form:

$$dw = 2\pi |m_{fi}|^2 \frac{d^2 n}{d\Omega_f dE_f} d\Omega_f$$

[1] See Appendix at the end of the note

Density of states

1. I will drop subscript *f* for now. The density of states can be re-written as:
$$\frac{d^2n}{d\Omega dE} = \frac{d^2n}{d\Omega dp}\cdot\frac{dp}{dE} = \frac{d^2n}{d\Omega dp}\cdot\frac{1}{v},$$ where v is a final velocity of a particle
$$\frac{dp}{dE} = \frac{1}{v}$$ holds true for non-relativistic and relativistic kinematics

2. I will now assume that the scattering experiment is carried out in the universe of cubic shape with a side L so that (x,y,z)-coordinates are constrained to be within $-L/2 < x, y, z < L/2$, where L can be very large (as we will see, this parameters cancels out in the final expressions).

3. Boundary conditions $\Psi(-L/2)=\Psi(L/2)=0$, lead to wave functions in the sine and cosine forms: $\psi = e^{ip_x x} \pm e^{-ip_x x}$ with allowed momenta $p_x=(\pi/L)n_x$, $p_y=(\pi/L)n_y$, $p_z=(\pi/L)n_z$, where n's are integral numbers.

4. Therefore, the number of possible states within dp_x equals to $dn_x=dp_x/(\pi/L)= dp_x(L/\pi)$, where interval dp_x should be considered only along positive p_x (negative values are not independent with the chosen boundary conditions). This condition can be removed by taking only a half *dn*'s per each dp_x-range; i.e., we will redefine $dn_x=dp_x(L/2\pi)$ and allow p_x be negative.

5. The total number of states in a cube $d^3\mathbf{p}=dp_x dp_y dp_z$ is, therefore,
$$dn = \left(\frac{L}{2\pi}dp_x\right)\left(\frac{L}{2\pi}dp_y\right)\left(\frac{L}{2\pi}dp_z\right) = \frac{L^3}{(2\pi)^3}d^3p = \frac{V}{(2\pi)^3}d^3p$$

6. The cubic $d^3\mathbf{p}$ element in volume in the momentum space can be redefined via absolute value of p and its stereo-angle $d\Omega$: $d^3\mathbf{p}=p^2dpd\Omega$, which leads to
$$dn = \frac{V}{(2\pi)^3}d^3p = \frac{V}{(2\pi)^3}p^2 d\Omega dp$$

7. From where:
$$\frac{d^2n}{d\Omega dp} = \frac{Vp^2}{(2\pi)^3} \quad \text{and} \quad \frac{d^2n}{d\Omega dE} = \frac{1}{v}\frac{Vp^2}{(2\pi)^3}$$

Final expression for transition rate

Normalization constants for the incident and scattered particle wave functions are $C = \frac{1}{\sqrt{V}}$ so that the probability to find a particle inside the cube is equals one.

Therefore, the final expressions for the transition rate (probability per unit of time) can be written as follows:

$$dw = 2\pi\left(|m_{fi}|^2 \frac{1}{V^2}\right)\left(\frac{V}{v_f}\frac{p_f^2}{(2\pi)^3}d\Omega\right) = \frac{1}{V}\frac{p_f^2}{v_f}\frac{|m_{fi}|^2}{4\pi^2}d\Omega,$$

where $m_{fi}(\vec{q}) = \int U(r)e^{i\vec{q}\vec{r}}dV$

Cross section: relating theory to experiment

1. To relate the experimental definition of cross section to the theory of scattering/transition, we will equalize the rates of scattering (experimental point of view, defined via a phenomenological cross section) to the rate of transitions (defined via a corresponding matrix element).

2. Experimentally, $J_{scattered} = \left(\frac{d\sigma}{d\Omega} d\Omega \right) \cdot j \cdot N$

3. We will now assume that the whole world has volume V. Furthermore, there is only a single target particle in that volume V and that the beam consists of a single particle. Therefore, the flux of incident particles in formula is $j=nv_i=(1/V)v_i$. Also, $J_{scattered}$ would mean in this case just a probability of scattering per unit of time, or dw. Putting all together, the experimental rate in such thought experiment is then

$$dw = \frac{d\sigma}{d\Omega} d\Omega \cdot j \cdot N = \frac{v_i}{V} \frac{d\sigma}{d\Omega} d\Omega$$

4. By combining the experimental rate with the rate obtained in the first-order perturbation approximation:

$$\frac{v_i}{V} \frac{d\sigma}{d\Omega} d\Omega = \frac{1}{V} \frac{p_f^{\,2}}{v_f} \frac{|m_{fi}|^2}{4\pi^2} d\Omega, \qquad \text{where} \quad m_{fi}(\vec{q}) = \int V(r) e^{i\vec{q}\vec{r}} dV$$

5. From where we obtain the expression allowing us to calculate cross sections once we know the amplitude of scattering, or scattering matrix element m_{fi}:

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2} |m_{fi}|^2 \frac{p_f^{\,2}}{v_i v_f}, \qquad \text{where} \quad m_{fi}(\vec{q}) = \int V(r) e^{i\vec{q}\vec{r}} dV$$

6. The expression is correct for non-relativistic and relativistic kinematics. In the case of relativistic kinematics for the process A($\mathbf{q}_i$) + B(-$\mathbf{q}_i$) → C($\mathbf{q}_f$) + D(-$\mathbf{q}_f$), all kinematical variables are to be defined in the center of mass frame.

7. If the outgoing particles have spins and all their projections are equally allowed, the number of possible final states is increased by the product of the number of possible spin projections for particles C and D:

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2} |m_{fi}|^2 \frac{\vec{p}_f^{\,2}}{v_i v_f} (2s_C + 1)(2s_D + 1), \qquad \text{where} \quad m_{fi}(\vec{q}) = \int V(r) e^{i\vec{q}\vec{r}} dV$$

- The only factor related to the nature of the force acting between two particles sits in the **Matrix Element** m_{fi}.
- All other factors affecting the value of the cross section are purely kinematical, and are related to the intensity of **the incoming flux** (~$1/v_i$), which is a plain constant for relativistic particles and the **Phase Space** available for the final products (~ $p_f^{\,2} / v_f$)

Cross Section ~ |Matrix Element|^2 × (Phase Space)

Multiple contributions

If there are more than just one potential contributing to the scattering process, e.g. there are two different forces acting between two particles described by two functions of potential energies $V_A(r)$ and $V_B(r)$, then

$V(r) = V_A(r) + V_B(r)$

This will result in a combined matrix being a plain sum of two contributions, i.e.

$$m_{fi} = m_{fi}^A + m_{fi}^B$$

and

$$\left|m_{fi}\right|^2 = \left|m_{fi}^A + m_{fi}^B\right|^2 = \left(m_{fi}^A + m_{fi}^B\right)^* \left(m_{fi}^A + m_{fi}^B\right) = \left|m_{fi}^A\right|^2 + \left|m_{fi}^B\right|^2 + \left\{m_{fi}^{A*} \cdot m_{fi}^B + m_{fi}^A \cdot m_{fi}^{B*}\right\}$$

This means that the total cross section is NOT a sum of two individual cross sections calculated individually for the two forces. One must first add matrix elements corresponding to all possible interactions (forces) and only then square the total matrix element.

The last contribution {*} is known as an interference term. It can be zero, positive, and negative. As the result, the total cross section can be equal, or larger, or smaller than the sum of cross sections corresponding to individual forces if calculated separately.

For the same reason, if a theorist predicts a new force/potential that would give a very small matrix element $\left|m_{fi}^{new}\right|^2 / \left|m_{fi}^{ordinary}\right|^2 \sim \varepsilon^2$, the effect on the actual overall cross section may be substantially larger than ε^2 via the presence of the interference term, whose order of smallness can be of the order of ε.

Generalization

A scattering of a projectile particle A on a target particle B, A+B $\rightarrow$ A+B, can be generalized to **non-elastic cases** when particles are allowed to be transformed and additional particles can be born, e.g.:

$e^+ + e^- \rightarrow \mu^+ + \mu^-$

$\nu + n \rightarrow e^- + p$

$e^+ + e^- \rightarrow e^+ + e^- + \gamma$

As we discussed in the previous note, the experimental notion of cross section remains a well define observable. Similarly, the quantum field theory allows for consistent introduction of scattering amplitudes for such processes and the phase space factors will need to take into account a larger multiplicity of particles in the final states.

Decay of a particle can also be formulated in terms of the matrix element corresponding to a force responsible for the decay and the phase space available for the final decay products.

Note: in future, **when for two processes the initial or final states not identical**, e.g.:

$e^- + p \rightarrow e^- + p$

$e^- + p \rightarrow \nu + n$

the scattering processes can be treated probabilistically, there will be no interference terms. One can therefore simply add cross sections corresponding to individual contributions.

Appendix covering calculus skipped between pages 1 and 2

We start from the last equation on page 1:

$$\dot{c}_f(t) = -ie^{i(E_f - E_i)t} \cdot V_{fi} = -ie^{i\omega_{fi}t} \cdot V_{fi}$$

We can set observation time to be t and the initial time t_0=-t. We assume that $c_f(t_0)$=0, i.e the final state ψ_f appeared as the result of scattering and was not present at the initial time. Time t will be later set to infinity. Integration of the above equation with these limits gives:

$$i(c_f(t) - 0) = \int_{-t}^{t} e^{i\omega_{fi}t} V_{fi}\, dt = V_{fi} \frac{e^{i\omega_{fi}t}}{i\omega_{fi}}\Bigg|_{-t}^{t} = V_{fi} \frac{2i \sin \omega_{fi} t}{i\omega_{fi}}$$

$$c_f(t) = -iV_{fi} \frac{2 \sin \omega_{fi} t}{\omega_{fi}}$$

Consider *dn* states in the vicinity of a particular final state *f*. Then, the probability of transition from the initial *i*-state to one of the *dn* states is:

$$\Delta P = |c_f(t)|^2\, dn = |V_{fi}|^2 \frac{4 \sin^2 \omega_{fi} t}{\omega_{fi}^2} dn$$

While the average rate of transition (probability per unit of time) is:

$$dw = \Delta P / \Delta t = \frac{|c_f(t)|^2\, dn}{2t} = |V_{fi}|^2 \frac{2 \sin^2 \omega_{fi} t}{\omega_{fi}^2 t} dn$$

One can see that for $\omega_{fi} \neq 0$, the average rate is zero at $t \to \infty$, while at $\omega_{fi} \to 0$, the function diverges at $t \to \infty$. It is not difficult to show that this function is proportional to the classical δ-function $\delta(\omega_{fi})$:

$$\lim_{t \to \infty} \frac{\sin^2 \omega t}{\omega^2 t} = \pi \delta(\omega)$$

Indeed, $\int \frac{\sin^2 \omega t}{\omega^2 t} d\omega = \int \frac{\sin^2 \omega t}{\omega^2 t^2} d\omega t = \int \frac{\sin^2 x}{x^2} dx = \pi$

Therefore, the equation for the average rate of transitions can be re-written as:

$$dw = |V_{fi}|^2 \frac{2 \sin^2 \omega_{fi} t}{\omega_{fi}^2 t} dn = 2\pi |V_{fi}|^2\, \delta(\omega_{fi}) dn = 2\pi |V_{fi}|^2\, \delta(E_f - E_i) dn$$