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 $i\frac{\partial}{\partial t}\Psi = \left(\hat{H}_0 + \hat{V}\right)\Psi$.

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):

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

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

   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:

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

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

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

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

   $$\dot{c}_f(t) = -i\int e^{i\left(E_f - E_i\right)t}\psi_f^{0+}\hat{V}\psi_i^0 dV = -ie^{i\left(E_f - E_i\right)t}\int \psi_f^{0+}\hat{V}\psi_i^0 dV = -ie^{i\left(E_f - E_i\right)t}V_{fi}$$

6. After some calculus manipulations which I skip here, 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

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

- 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

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

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:

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

- V_{fi} is called a scattering amplitude, or matrix element. 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 *V(r):*

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

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

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

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 called **Phase Space**

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. The last contribution is known as an interference term.