3 Quantum processes I: when the (quasi)classical consideration may be used.

3.1 Radiation transitions

In the classical electrodynamics, the radiation power of a non-relativistic particle is given by Larmor's formula. In the simplest case of circular motion, the particle radiates at the rotational frequency, ω; the power is

$$P = \frac{2}{3}\frac{e^2\omega^2 v_0^2}{c^3}. \tag{3.1}$$

Generally if the particle performs periodic motion with the period T, it radiates at the frequencies $\omega = 2\pi n/T$, where $n = 1, 2, \ldots$. The power of each harmonics is given by Eq. (3.1), where one has to substitute v_0 by the corresponding Fourier harmonics of the velocity.

In the quantum theory, the radiation implies transition between the energy levels,

$$\hbar\omega = E_j - E_i. \tag{3.2}$$

The transition rate $j \to i$ due to spontaneous emission is determined by the Einstein coefficient for spontaneous emission, A_{ji}, as

$$\frac{dN_i}{dt} = A_{ji}N_j, \tag{3.3}$$

where N_j is the population of the j-th level. The correspondence principle implies that for highly excited levels, $j, i \gg 1$, the transition rate could be found from the classical theory. Making use of Eq. (3.1), one gets

$$A = \frac{P}{\hbar\omega} = \frac{2}{3}\alpha\omega\frac{v^2}{c^2}. \tag{3.4}$$

This relation provides a good estimate even for the transitions between low levels, $j, i \sim 1$.

As an example, let us estimate the probability of the transition $2 \to 1$ in the hydrogen atom (the Lyman-α line) . The line frequency is

$$\omega_{21} = \frac{3I_H}{4\hbar} = \frac{3}{8}\alpha^2\frac{c}{\lambdabar_C} = 1.5 \cdot 10^{16}\,\mathrm{Hz}, \tag{3.5}$$

where $\lambdabar_C = \hbar/m_e c = 4 \cdot 10^{-11}$ cm is the electron Compton length. The electron velocity at the second level is $v = (1/2)\alpha c$. Now one gets

$$A_{21} = \frac{1}{6}\alpha^3\omega_{21} = 10^9\,\mathrm{s}^{-1}. \tag{3.6}$$

A precise quantum calculation yields $A_{21} = 4.7 \cdot 10^8$ s^{-1}.

In closed systems, like atoms, $v \sim \omega r_0$, where r_a is the size of the system. Therefore eq. (3.4) may be presented in the form

$$A \sim \alpha\omega^3\frac{r_0^2}{c^2}. \tag{3.7}$$

For example, radiative transitions between the fine structure levels correspond to the radiation at the frequency of orbit precession therefore v in this case is not the electron velocity but the velocity of the precession. For estimates of the transition rate, one can use eq. (3.7) substituting

r_0 by the size of the atom and ω by the transition frequency. Of course, eq. (3.7) describes only the electric dipole transitions. If such a transtion is forbidden by selection rules, one could get an estimate of the same sort by using classical formulas for magnetic dipole, quadruple etc radiation rate.

3.2 Radiative recombination (free-bound transitions)

Radiative recombination could be considered classically as the transition between a hyperbolic (but close to parabolic) to a highly elongated elliptic (also close to parabolic) orbit. We are interested in relative close encounters such that the particle approaches the ion at the minimal distance, r_0, much less than the impact parameter, b; which implies $Ze^2/b \gg m_e v^2$. This distance, as well as the corresponding velocity, v_0, could be found from the conservation of energy and angular momentum,

$$\frac{m_e v_0^2}{2} - \frac{Ze^2}{r_0} = \frac{m_e v^2}{2}; \qquad v_0 r_0 = vb. \tag{3.8}$$

Since $r_0 \ll b$ implies $v_0 \gg v$, one finds

$$r_0 = \frac{m_e v^2 b^2}{2Ze^2}; \qquad v_0 = \frac{2Ze^2}{m_e v b}. \tag{3.9}$$

When the electron closely approaches the ion, it radiates at the frequencies of the order of

$$\omega \sim \frac{v_0}{r_0}. \tag{3.10}$$

The electron remains bound to the atom if the energy of the radiated photon exceeds the electron energy,

$$\hbar\omega > E = \frac{m_e v^2}{2}. \tag{3.11}$$

Making use of Eqs. (3.9) and (3.10), one writes this condition as

$$b^3 < \frac{8Z^2 e^4 \hbar}{m_e^3 v^5}, \tag{3.12}$$

which is reduced to

$$b < 2^{1/6} \left(\frac{I_Z}{E}\right)^{5/6} a_Z; \tag{3.13}$$

where

$$a_Z = \frac{r_e}{Z\alpha^2} = \frac{\hbar^2}{Ze^2 m_e}; \qquad I_Z = \frac{Z^2}{2}\alpha^2 m_e c^2 = \frac{Z^2 e^4 m_e}{2\hbar^2} \tag{3.14}$$

are the ion radius and the binding energy, correspondingly.

The classical description of the electron motion implies $\hbar/m_e v < b$. Substituting b from eq. (3.12), one reduces this condition to $E < 8I_Z$. This condition is not very restrictive because the recombination is significant when the electron energy is less than the atom binding energy.

Note that even if the electron recombines on an excited level, it immediately falls down to the ground level because the rates of the radiation transition between the atomic levels, Eq. (3.4), are very high.

The total recombination cross section may be presented as

$$\sigma_{\rm rec}^{\rm rad} = \pi b^2 w, \tag{3.15}$$

where w is the probability of photon emission in the course of encounter. The electron radiates with the rate (3.4) during the time of the closest approach, $\tau \sim 2r_0/v_0 \sim 2/\omega$, therefore one finds

$$w \sim \frac{4}{3}\alpha\left(\frac{v_0}{c}\right)^2. \tag{3.16}$$

Substituting this relation into Eq.(3.15) and making use of Eq. (3.9), one gets finally[3]

$$\sigma_{\rm rec}^{\rm rad} \sim \sigma_T \frac{I_Z}{\alpha k_B T}. \tag{3.17}$$

Here I substituted $m_e v^2 = 3k_B T$ having in mind thermal plasmas. It is the recombination process that contributes mainly to the radiation energy losses of the plasma at $k_B T \leq I_Z$,. Taking into account that any recombination event is accompanied by radiation with the total energy $E + I_Z \sim k_B T + I_Z \sim I_i$, the total recombination radiation rate is estimated as

$$Q = I_Z \sigma_{\rm rec}^{\rm rad} N_e N_i v \sim \sigma_T \frac{I_Z^2}{\alpha\sqrt{m_e k_B T}} N_e N_i. \tag{3.18}$$

3.3 Collisional recombination.

When a free electron passes by an ion, it could recombine if another electron takes the extra energy. Recombination is possible only if the electron approaches the ion close enough such that the potential energy exceeds the initial electron energy, $b \leq b_0 = Ze^2/k_B T$. Therefore the collisional recombination cross section could be written as

$$\sigma_{\rm rec}^{\rm coll} \sim \pi b_0^2 w, \tag{3.19}$$

where w is the probability for the electron to loose a significant fraction of the energy while passing by the ion. The electron could loose a significant fraction of the energy if it approaches another electron at the distance $b \leq b_1 = e^2/k_B T$. Therefore the probability w is in fact the probability to meet and electron within the volume $\pi b_1^2 b_0$ so that $w = Z(E^2/k_B T)N_e$. Practically the same estimate could be obtained in a different way. Namely w is the probability that another electron collides the first electron during the time of the closest approach to the ion, $\tau \sim b_0/v$. This yields $w = N_e v \cdot \pi b_0^2 \tau = \pi b_0^3 N_e$. Now one finds

$$\sigma_{\rm rec}^{\rm coll} \sim \pi^2 Z^3 \left(\frac{e^2}{k_B T}\right)^5 N_e \approx 300 \frac{a_Z^5}{Z^2}\left(\frac{I_Z}{k_B T}\right)^5 N_e, \tag{3.20}$$

where in the last equality, Eq. (3.14) was used.

[3] In this calculation b is just canceled out therefore the condition (3.13) has not been used. In a more careful consideration, one has to write the recombination cross section as (cf. Eq.(3.1)) $\sigma_{\rm rec} = 2\pi \int w b db \propto \int db/b = \log(b_{\rm max}/b_{\rm min})$. The maximal and the minimal impact parameters are found from the conditions that the photon of the frequency (3.10) should have the energy exceeding $k_B T$ on the one hand (the condition (3.13)), and less than $I_Z + k_B T$ on the other. Since in any reasonable case, the ratio $I_Z/k_B T$ is not very large, one can substitute the logarithmic factor in the cross section by unity.

4 Quantum processes II: when the wave properties are crucial.

4.1 Reactions with slow particles.

In the extreme quantum case, the particle wavelength significantly exceeds the interaction radius. As an example, let us consider reactions of slow neutrons with atomic nuclei. By slow I mean neutrons with the wavelength exceeding the radius of the nucleus,

$$\lambdabar \equiv 1/k = \hbar/p > R \approx 1.3 \cdot 10^{-13} A^{1/3}\,\text{cm}. \tag{4.1}$$

This condition is fulfilled for neutron energies less than $\sim 10A^{-2/3}$ MeV.

In the quantum case, the impact parameter could not be defined together with the particle energy. Instead one can conveniently use the angular momentum, $L = \hbar\sqrt{l(l+1)}$. One can define the corresponding impact parameter as $b_l = L/p = \lambdabar\sqrt{l(l+1)}$; the physical meaning of this quantity in the quantum case is that the wave function of particles with the momentum l drops down at $r < b_l$. One can imagine a particle flow divided into narrow rings (in the plane perpendicular to the flow direction) with the radiuses b_l each. If the particle flux is F, the fraction of particles having the momentum l may be estimated as $dF/F = \pi(b_{l+1}^2 - b_{l-1}^2)/2 = (2l+1)\pi\lambdabar^2$. At the condition (4.1), only neutrons with $l = 0$ could interact with the nucleus. Therefore the reaction cross section may be presented as

$$\sigma = \pi\lambdabar^2 w; \tag{4.2}$$

where $w < 1$ is the reaction probability.

Compound nucleus. The reaction probability is presented as

$$w = w_* \eta, \tag{4.3}$$

where w_* is the probability for the neutron to penetrate the nucleus, η the probability of decay of the compound nucleus in a given channel (generally the compound nucleus could decay in a few channels).

The probability w_* may be estimated by considering the scattering of a zero angular momentum particle on a deep potential well so that $E = p^2/2m \ll V_0$. The wave function of the zero angular momentum particles is spherically symmetric and could be presented as $\psi = u/r$, where u satisfies the 1D Shrödinger equation. One has to match the wave functions and derivatives at the boundary of the nucleus. Since the wavelength outside the nucleus is much larger than inside, matching of derivatives generally implies that the amplitude of the wave function inside the nucleus is much smaller than outside so the ratio of amplitudes inside and outside is $t \sim k/K \simeq \sqrt{E/V_0} \ll 1$, where $k = \sqrt{2mE}/\hbar$ and $K = \sqrt{2mV_0}/\hbar$ are the wave numbers outside and inside the well. The probability for the particle to enter the nucleus is the ratio of particle flux inside the well to the flux of particles towards the well. The particle flux is estimated as $v|u|^2$. Taking into account that v is proportional to the wave number, one estimates this ratio as $w_* \sim t^2 K/k \sim k/K$. Substituting this relation into eqs. (4.2) and (4.3), one finds that the reaction cross section grows with decreasing velocity as $1/v$,

$$\sigma \sim \pi\lambdabar^2 \frac{k}{K}\eta = \frac{\pi\hbar^2\eta}{p\sqrt{mV_0}}. \tag{4.4}$$

In the nuclear physics, this statement is called **"1/v law"**. For thermal neutrons, the absorption cross-section thousands times exceeds the geometrical cross-section of the nucleus. That is why moderators like graphite are used in nuclear reactors in order to slow down neutrons.

The cross section (4.4) is still much smaller than the maximal one, $\sim \lambdabar^2$. This is because the incoming particle is generally reflected from the potential step. The internal and external functions could be matched with nearly equal amplitudes at specific energies (resonances) such that the internal wave function reaches extremum near the boundary. The resonant states exist because a particle with a slightly positive energy is strongly reflected from the surface of the well (the transmission coefficient at a potential step is of the order of $k/K = \sqrt{E/V_0} \ll 1$ for particles moving in both directions) therefore it is almost as confined as a particle with a negative energy. Then the external wave function is matched not with the evanescent wave but with the standing wave. Inasmuch as in standing waves, derivatives are close to zero at the surface of the well (because in the quasi-stationary case, a standing internal wave is matched with a continuous function and its derivative to an outgoing low frequency wave), the external and internal wave functions could now be matched such that their amplitudes are equal. Therefore close to the resonance, the probability for the neutron to find itself within the nucleus is large so that the reaction cross-sections exhibit strong, narrow peaks at the resonance energies. We will consider the resonance cross sections in more details below, when applications of the detailed balance principle will be discussed.

4.2 Tunnelling or why do stars shine

The main energy source in stars is hydrogen burning into helium, which is possible because $4m_p - m_{\rm He} - 2m_e = 27$ MeV > 0. Inasmuch as two protons have to be converted to neutrons, the weak interaction should be involved, which results in a very slow reaction rate. In the $p-p$ cycle, the conversion occurs in the reaction

$$p + p \;\rightarrow\; D + e^+ + \nu \quad (+1.44\,{\rm MeV}), \tag{4.5}$$

which is then followed by the chain:

$$p + D \;\rightarrow\; {}^3{\rm He} + \gamma \quad (+5.49\,{\rm MeV}); \tag{4.6}$$
$${}^3{\rm He} +^3 {\rm He} \;\rightarrow\; {}^4{\rm He} + 2p \quad (+12.85{\rm MeV}). \tag{4.7}$$

The overall reaction rate is determined by the first reaction. It becomes possible if protons approach the nuclear distance, $\sim 10^{-13}$ cm. At this distance, the Coulomb barrier reaches $e^2/r \sim 1$ MeV. Within the stars, the temperature is only $\sim 10^7$ K ~ 1 keV therefore the proton fusion occurs via quantum tunnelling through the barrier.

In the course of the reaction (4.16), one of the protons is converted into a neutron. Inasmuch as the mass of the free neutron exceeds the proton mass, this is possible only within the nucleus. Therefore the reaction rate per pp pair could be roughly presented as

$$W_{pp} \sim PW_{p\to n}. \tag{4.8}$$

Here P is the probability for two protons to find themselves within the distance about the radius of the deuterium nucleus, $r_D \approx 2\cdot 10^{-13}$ cm, $W_{p\to n}$ the proton-to-neutron conversion rate. The last will be discussed in the next section; now let as estimate P. Introducing the wave function of the pair, one can write

$$P \sim \int_{r<r_D} |\psi|^2 dV \tag{4.9}$$

Let us estimate this quantity for a single pair within a normalization volume V. We have to solve the Shrödinger equation for a particle with the reduced mass $m = m_p/2$.

At distances much larger than the classical turning radius, $r \gg r_{\rm cl} = e^2/E$, the wave function of the pp pair is presented as

$$\psi_{\rm ext} = \frac{1}{\sqrt{V}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} = \frac{1}{\sqrt{V}} \left(\frac{\hbar \sin \frac{pr}{\hbar}}{pr} + \sum_{l\geq 1} \dots \right), \tag{4.10}$$

where $p = \sqrt{2mE} = \sqrt{m_p E}$ and the last equality presents the expansion in angular momenta. The distance $r \sim r_D$ could be achieved only by $l = 0$ particle therefore it is the first term in the rhs that should be matched with the wave function within the Coulomb barrier. The $l = 0$ wave function is spherically symmetric and is conveniently presented as $\psi(r) = u(r)/r$, where the function u satisfies the 1D Shrödinger equation

$$\frac{\hbar^2}{m_p} u'' - \left(\frac{e^2}{r} - E \right) u = 0, \tag{4.11}$$

where E is the particle energy. The solution inside the barrier, $r < r_{\rm cl}$, is presented in the WKB approximation

$$u_{\rm int} \sim C \exp\left[-\frac{\sqrt{m_p E}}{\hbar} \int_r^{r_{\rm cl}} \sqrt{\frac{r_{\rm cl}}{r} - 1} dr \right]. \tag{4.12}$$

The rough matching of (4.21) and (4.23) at $r \sim r_{\rm cl}$ yields

$$C \sim \frac{\hbar}{\sqrt{V} p}. \tag{4.13}$$

Now the wave function within the nucleus could be estimated as

$$\psi \sim \psi_{\rm int}(r_D) \sim \frac{\hbar}{r_D (V m_p E)^{1/2}} \exp\left[-\frac{\sqrt{m_p E}}{\hbar} \int_{r_D}^{0} \sqrt{\frac{r_{\rm cl}}{r} - 1} dr \right] \tag{4.14}$$

$$= \frac{\hbar}{r_D (V m_p E)^{1/2}} \exp\left[-\frac{\pi}{2} \frac{e^2}{\hbar} \sqrt{\frac{m_p}{E}} \right]. \tag{4.15}$$

Substituting the above result to (4.20) and then to (4.19) yields the reaction rate per pair

$$W_{pp} \sim W_{p\to n} \frac{\hbar^2 r_D}{V m_p E} \exp\left[-\pi\alpha \sqrt{\frac{m_p c^2}{E}} \right]. \tag{4.16}$$

If there are N protons in the volume V, they form $N(N-1)/2 \approx N^2/2$ pairs therefore the total reaction rate increases $N^2/2$ times. Then the reaction rate per unit volume is presented as

$$q_{pp} \sim W_{p\to n} \frac{\hbar^2 r_D}{m_p E} n^2 \exp\left[-\pi\alpha \sqrt{\frac{m_p c^2}{E}} \right], \tag{4.17}$$

where n is the density of protons.