8.2 Applications of the golden formula

We have seen how the formula for the transition rate Γ, in the process of its construction, gets "healed" from the maladies of the sudden switching-on of a time independent interaction. This procedure which is simple and convincing in the first order becomes more cumbersome when we get to the next order. Let us therefore present some formal operation which leads to unique (and correct!) results in all orders. This operation is an "adiabatic switching-on" of the interaction. We replace

$$V(x,t) = V(x)\, e^{\eta t}\,, \quad \eta > 0 \qquad (V(x,t) \to 0 \quad \text{for} \quad t \to -\infty)\,, \tag{8.39}$$

and then with the result we go to the limit $\eta \to 0$. In other words in the remote past the interaction disappears, and we shall set $t_1 = -\infty$ in (8.22) and (8.23).

Let us apply it to the first approximation (8.22):

$$\begin{aligned} \lambda^{(1)}_{mn}(t_2, -\infty)\, e^{\frac{i}{\hbar}(E_m t_2 - E_n(-\infty))} &= -\frac{i}{\hbar}\int_{-\infty}^{t_2} dt_3\, V_{mn}\, e^{\eta t_3 + \frac{i}{\hbar}(E_m - E_n)t_3} \\ &= -\frac{V_{mn}}{E_m - E_n - i\hbar\eta}\, e^{\eta t_2 + \frac{i}{\hbar}(E_m - E_n)t_2}\,. \end{aligned} \tag{8.40}$$

Thus the probability of transition is

$$P(n \to m) \;=\; |\lambda^{(1)}_{mn}(t_2)|^2 \;=\; |V_{mn}|^2\, \frac{e^{2\eta t_2}}{(E_m - E_n)^2 + (\eta\hbar)^2}\,, \tag{8.41}$$

and the rate is

$$\frac{dP(n \to m)}{dt_2} \;=\; |V_{mn}|^2\, \frac{e^{2\eta t_2}\, 2\eta}{(E_m - E_n)^2 + (\eta\hbar)^2}\,. \tag{8.42}$$

Now we go to the limit $\eta \to 0$ and, since

$$\lim_{\eta \to 0} \frac{2\eta}{(E_m - E_n)^2 + (\eta\hbar)^2} \;=\; \frac{2\pi}{\hbar}\delta(E_m - E_n)\,,$$

we get again the expression for the differential rate

$$\frac{dP(n \to m)}{dt_2} \;=\; \Gamma(n \to m) \;=\; \frac{2\pi}{\hbar}|V_{mn}|^2\, \delta(E_m - E_n)\,, \tag{8.43}$$

although this time we have dealt only with some nonsingular expressions: a singularity appeared only in the last step of going to the limit $\eta \to 0$.

Problem: the adiabatic switching-on of interaction

Let

$$V(x,t) = V(x)\left[e^{i\omega t} + e^{-i\omega t}\right].$$

Find the conditions under which

$$\frac{dP(n \to m)}{dt_2} = \frac{2\pi}{\hbar}|V_{mn}|^2\big[\delta(E_m - E_n + \hbar\omega) + \delta(E_m - E_n - \hbar\omega)\big]\,.$$

End of Problem

Let us discuss now the second order transition amplitude applying the adiabatic switching-on. To this end we substitute in (8.23)

$$V_{mk}(t_4) = V_{mk}\, e^{\eta t_4}\,, \qquad V_{kn}(t_3) = V_{nk}\, e^{\eta t_3}\,, \tag{8.44}$$

and obtain

$$\lambda^{(2)}_{mn}(t_2, t_1)\, e^{\frac{i}{\hbar}(E_m t_2 - E_n t_1)} =$$

$$= -\frac{1}{\hbar^2}\int_{t_1}^{t_2} dt_4 \int_{t_1}^{t_4} dt_3 \sum_k V_{mk}\, e^{\frac{i}{\hbar}(E_m - E_k)t_4 + \eta t_4}\, V_{kn}\, e^{\frac{i}{\hbar}(E_k - E_n)t_3 + \eta t_3}\,.$$

We integrate over t_3 and t_4, take the limit $t_1 \to -\infty$, and obtain

$$\lim_{\eta \to 0} \frac{d}{dt_2}\, |\lambda^{(2)}_{mn}(t_2, -\infty)|^2 =$$

$$= \Gamma(n \to m) \;=\; \frac{2\pi}{\hbar}\left|\sum_k \frac{V_{mk}V_{kn}}{E_n - E_k + i\hbar\eta}\right|^2 \delta(E_m - E_n)\,. \tag{8.45}$$

This is the contribution to $\Gamma(n \to m)$ of the second order. When the first order contribution, eq. (8.31), is non-zero ($V_{mn} \neq 0$), we just add up the two "matrix elements":

$$\Gamma(n \to m) \;=\; \frac{2\pi}{\hbar}\left|V_{mn} + \sum_k \frac{V_{mk}V_{kn}}{E_n - E_k + i\hbar\eta}\right|^2 \delta(E_m - E_n)\,. \tag{8.46}$$

Note that that in (**??**) the amplitudes of the first and second order are being added. Taking $|...|^2$ of the sum and performing the limit $\eta \to 0$ leads to the same factor $\frac{2\pi}{\hbar}\delta(E_m - E_n)$ as in each case taken separately.

As we can see, e.g. from (**??**), the method of the adiabating switching-on of the interaction gives us expressions which are well defined when the numerators become singular ($E_n - E_k = 0$). We have a well defined prescription how to go around the singularities.

Let us discuss now the first and second order corrections to the unperturbed energy eigenvalues. We start with the differential equations (8.26) for $\lambda_{mn}(t_2, t_1)$ and redefine the amplitudes:

$$\lambda_{mn} = \tilde{\lambda}_{mn}\, e^{\frac{i}{\hbar}(-E_m t_2 + E_n t_1)}\,. \tag{8.47}$$

The new amplitudes $\tilde{\lambda}_{mn}$ have the "free system" dependence on time removed, i.e. when $V = 0$ $\tilde{\lambda}_{mn}$ is constant in time. Note also that $\tilde{\lambda}^{(0)}_{mn} = \delta_{mn}$.

Inserting (**??**) into (8.26) we obtain the following equations for $\tilde{\lambda}_{mn}$:

$$\frac{d\tilde{\lambda}_{mn}}{dt_2} = -\frac{i}{\hbar}\sum_k V_{mk}(t_2)\,\tilde{\lambda}_{kn}\,e^{-\frac{i}{\hbar}(E_k-E_m)t_2}\,. \tag{8.48}$$

From (**??**) we know that the amplitude for the system to remain in the same state is

$$\lambda_{nn} = \tilde{\lambda}_{nn}\,e^{-\frac{i}{\hbar}E_n(t_2-t_1)}\,. \tag{8.49}$$

When $V=0$, $\tilde{\lambda}_{nn}$ is time independent but when $V\neq 0$, $\tilde{\lambda}_{nn}$ acquires some time dependence and, being an eigenstate of energy, its time dependence must be of the form

$$e^{-\frac{i}{\hbar}\Delta E_n(t_2-t_1)} \tag{8.50}$$

where ΔE_n is the correction we are looking for.

Let us work out the amplitude for remaining in the same state, e.g. n. It satisfies the equation

$$\frac{d\tilde{\lambda}_{nn}}{dt_2} = -\frac{i}{\hbar}\sum_k V_{nk}(t_2)\,\tilde{\lambda}_{kn}\,e^{-\frac{i}{\hbar}(E_k-E_n)t_2}\,. \tag{8.51}$$

We expand $\tilde{\lambda}_{nn}$ into the perturbation series

$$\tilde{\lambda}_{nn} \;=\; \tilde{\lambda}^{(0)}_{nn} \;+\; \tilde{\lambda}^{(1)}_{nn} \;+\; \tilde{\lambda}^{(2)}_{nn} \;+\; \ldots\,. \tag{8.52}$$

For the first order amplitude we obtain (remember: $\tilde{\lambda}^{(0)}_{kn} = \delta_{kn}$)

$$\frac{d\tilde{\lambda}^{(1)}_{nn}}{dt_2} \;=\; -\frac{i}{\hbar}\sum_k V_{nk}(t_2)\,\tilde{\lambda}^{(0)}_{kn}\,e^{-\frac{i}{\hbar}(E_k-E_n)t_2} \;=\; -\frac{i}{\hbar}\,V_{nn}(t_2)\,. \tag{8.53}$$

From (**??**) we have

$$\Delta E_n \;=\; i\hbar\,\frac{1}{\tilde{\lambda}_{nn}}\,\frac{d\tilde{\lambda}_{nn}}{dt_2}\,. \tag{8.54}$$

Thus the first order correction to the energy is

$$\Delta E^{(1)} \;=\; \lim_{\eta\to 0} V_{nn}\,e^{\eta t_2} \;=\; V_{nn}\,. \tag{8.55}$$

To include the second order we rewrite (**??**) separating the $k=n$ term from the sum, and get

$$i\hbar\,\frac{1}{\tilde{\lambda}_{nn}}\,\frac{d\tilde{\lambda}_{nn}}{dt_2} \;=\; V_{nn}(t_2) \;+\; \sum_{k\neq n} V_{nk}(t_2)\,\frac{\tilde{\lambda}_{kn}}{\tilde{\lambda}_{nn}}\,e^{-\frac{i}{\hbar}(E_k-E_n)t_2}\,. \tag{8.56}$$

To get ΔE_n up to the second order we have to set in the sum on the r.h.s. of (**??**):

$$\tilde{\lambda}_{nn} = 1 \qquad \text{and} \qquad \tilde{\lambda}_{kn} = \tilde{\lambda}^{(1)}_{kn}\,.$$

(Note that $\tilde{\lambda}_{kn}^{(0)}$ cannot contribute to $\sum_{k\neq n}$). But, from (**??**) we obtain

$$\tilde{\lambda}_{kn}^{(1)} = -\frac{i}{\hbar} V_{kn} \int_{-\infty}^{t_2} e^{\frac{i}{\hbar}(E_k - E_n)t_2' + \eta t_2'} \, dt_2' \, . \tag{8.57}$$

We do the integration over t_2, insert the result into (**??**) and take $\eta \to 0$. The result is

$$\begin{aligned} i\hbar \frac{1}{\tilde{\lambda}_{nn}} \frac{d\tilde{\lambda}_{nn}}{dt_2} &= V_{nn} + \sum_{k\neq n} \frac{V_{nk} V_{kn}}{E_n - E_k + i\hbar\eta} \\ &= V_{nn} + \sum_{k\neq n} \mathcal{P} \frac{|V_{nk}|^2}{E_n - E_k} - i\pi \sum_{k\neq n} \delta(E_n - E_k) |V_{kn}|^2 \end{aligned}$$

where we used the identity

$$\frac{1}{x + i\eta} = \mathcal{P}\frac{1}{x} - i\pi\delta(x) \, .$$

Thus we see tha the shift of the energy becomes a complex number, $\Delta E_n - i\hbar\frac{1}{2}\Gamma$, where

$$\Delta E_n = V_{nn} + \sum_{k\neq n} \mathcal{P} \frac{|V_{nk}|^2}{E_n - E_k} \tag{8.58}$$

and

$$\Gamma = \frac{2\pi}{\hbar} \sum_{k} \delta(E_n - E_k) \, |V_{nk}|^2 \, . \tag{8.59}$$