QM-24 Lecture Notes
Approximation Schemes for Time Dependent Problems*
24.2 Transitions to continuum

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§1 Fermi Golden Rule

In this section we assume that the perturbation is either independent of time, or varies periodically with a single frequency and that the energy of the final states lies in continuum. As mentioned in §**??**, we will derive the Fermi Golden rule for the transition probability per unit time.

We shall start from Eq.(**??**) with $\omega = 0$ and a similar treatment can be for the case $\omega \neq 0$.

When the perturbation term is independent of time the probability amplitude, upto first order,(setting $t_0 = 0$) is given by

$$C_f^{(1)}(t) = \langle f|H'|i\rangle \left(\frac{\exp(i\omega_{fi}t) - 1}{-\hbar\omega_{fi}}\right) \tag{1}$$

and the hence one has

$$|C_f^{(1)}(t)|^2 = \frac{4\sin^2(\omega_{fi}t/2)}{\hbar^2\omega_{fi}^2}\,|\langle f|H'|i\rangle|^2. \tag{2}$$

We plot $|C_f^{(1)}(t)|^2$ in the figure below. Note that $|C_f^{(1)}(t)|^2$ is large for $\omega_{fi} \approx 0$,*i.e.* for $E_i \approx E_f$. Only a small range of energy ΔE values

$$\Delta E \approx 2\pi(\hbar/t) \tag{3}$$

have an appreciable transition probability. As $t \to \infty, \Delta E \to 0$ and one recovers conservation of energy. The Eq.(3) suggests that if a measurement is made after time Δt, the accuracy in E will be of the order of $\Delta E \approx h/\Delta t$ which a form of statement of time energy uncertainty relation.

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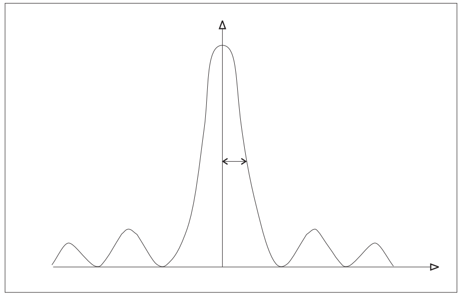

Fig. **1** Golden-Rule

Note that the area under the peak increases as t. Thus if we compute the *transition probability* at time t, given by

$$\int_{E-\Delta E}^{E+\Delta E} |C_f^{(1)}(t)|^2 |dE, \tag{4}$$

to a set of states in the energy range E and $E \pm \Delta E$, the answer will be proportional to *time*. In the case of transitions to a state in continuum, the quantity of interest is the *rate of transitions* to a group of final states having the energy in the range $E \pm \Delta E$, and hence one needs to compute the transition probability per unit time. So we compute

$$\frac{d}{dt}|C_f^{(1)}(t)|^2 = \frac{2}{\hbar}|\langle f|H'|i\rangle|^2 \Big(\frac{\sin \omega_{fi} t}{\omega_{fi}}\Big) \tag{5}$$

and for large t this expression tend to

$$\frac{2\pi}{\hbar^2}|\langle f|H'|i\rangle|^2 \delta(\omega_{fi}) = \frac{2\pi}{\hbar}|\langle f|H'|i\rangle|^2 \delta(E_f - E_i) \tag{6}$$

where use has been made of the standard results

$$\lim_{x\to\infty} \frac{\sin kx}{x} = \pi\delta(x) \tag{7}$$

$$\delta(ax) = \frac{1}{|a|}\delta(x) \tag{8}$$

for the Dirac δ function. Hence the required transition probability per unit time to the group of final states, obtained by differentiating Eq.(4) w.r.t. t and denoted by w_{fi}, is given by

$$w_{fi} = \frac{2\pi}{\hbar} \sum_{\text{final states}} |\langle f|H'|i\rangle|^2 \, \delta(E_f - E_i) \tag{9}$$

Writing

$$\sum_{\text{final states}} (\cdot) = \int dE_f \rho(E_f)(\cdot) \tag{10}$$

where $\rho(E_f)$ is the density of final states. Using Eq.(10) in Eq.(9) give

$$\boxed{w_{fi} = \frac{2\pi}{\hbar}|\langle f|H'|i\rangle|^2 \, \rho(E)} \tag{11}$$

where we have set $E_f = E_i = E$. This result is known as given by Dirac and called Golden Rule by Fermi.

When the perturbation varies harmonically with time, we must analyse Eq.(**??**) and the result is

$$\boxed{w_{fi} = \frac{2\pi}{\hbar}|\langle f|H'|i\rangle|^2 \, \rho(E_f)} \tag{12}$$

The analysis proceeds by keeping only one of the two terms in Eq.(**??**) and showing that the other term is not important. The final energy E_f can have only one of the two values $E_i + \hbar\omega$ or $E_i - \hbar\omega$ only.

§2 Application to Scattering

Use of Fermi golden rule along with the first order first order perturbation theory result leads to the first Born approximation result for the differential cross section.

Let us consider scattering of a beam of particles incident on a target represented by a spherically symmetric potential $V(r)$. The incident beam of particles with momentum $\hbar\vec{k}_i$, and an incident particle will be represented by a plane wave $N\exp(i\vec{k}_\mathrm{i}\cdot\vec{r})$. Let $\hbar\vec{k}_\mathrm{f}$ be the momentum of particles in the outgoing beam. A particle in the outgoing beam be represented by the plane wave $\exp(i\vec{k}_\mathrm{f}\cdot\vec{r})$.

We seek rate of transition into a solid angle $d\Omega$, corresponding to momentum range $\vec{k}_\mathrm{f}$ and $\vec{k}_f+d\vec{k}_\mathrm{f}$.The Fermi golden rule gives the transition probability per unit time w to be

$$dw_{\mathrm{i}\to\mathrm{f}} = \frac{2\pi}{\hbar}\rho(E)|\langle\vec{k}_\mathrm{f}|H'|\vec{k}_\mathrm{i}\rangle|^2 \tag{13}$$

and where the potential energy $V(r)$ is taken to be the perturbation Hamiltonian H'. As it will be seen this rate of transition to group of final states, *i.e.* those corresponding to the momentum in the range $\vec{k}_\mathrm{f}$ and $\vec{k}_f+d\vec{k}_\mathrm{f}$, will be related the differential cross section.

We will work with plane waves with periodic boundary conditions and normalized in a box of size L. The wave functions are

$$u_\mathrm{i}(\vec{r}) = \frac{1}{L^{3/2}}\exp(i\vec{k}_\mathrm{i}\cdot\vec{r}), \qquad u_\mathrm{i}(\vec{r}) = \frac{1}{L^{3/2}}\exp(i\vec{k}_\mathrm{i}\cdot\vec{r}). \tag{14}$$

We only need to compute the density of states $\rho(\vec{E})$ for momentum range $\vec{k}$ and $\vec{k}+d\vec{k}$. The allowed values of $\vec{k}$ in a box are $k_x = 2\pi n_x/L, k_y = 2|pin_y/L, k_z = 2\pi n_z/L$, where n_x, n_y, n_z are positive integers. There will be $(L/2\pi)^3 dk_x dk_y dk_z$ for the propagation vector range $d\vec{k}$ around value $\vec{k}$. The number of states in the small range of momenta around $\vec{k}$ is then given by

$$\frac{L^3}{(2\pi)^3}dk_x dk_y dk_z = \frac{L^3}{(2\pi)^3}\,k^2\,dk\,d\Omega,. \tag{15}$$

Since $E = \hbar^2k^2/(2m)$, the range dE of energy corresponding to a range dk of wave vector is given by

$$E = \frac{\hbar^2k^2}{2\mu} \Longrightarrow dE = \frac{\hbar^2 k}{(2m)}dk \Longrightarrow \frac{dE}{dk} = \frac{\hbar^2k}{\mu},. \tag{16}$$

Therefore the number of states, ((15)) in the small range of momenta around $\vec{k}$ becomes

$$\begin{aligned}\frac{L^3}{(2\pi)^3}\,k^2\,dk\,d\Omega &= \frac{L^3}{(2\pi)^3}\,k^2\left(\frac{\mu}{\hbar^2 k}\right)dE\,d\Omega &(17)\\ &= \frac{L^3}{(2\pi)^3}\left(\frac{\mu k}{\hbar^2}\right)dE\,d\Omega &(18)\end{aligned}$$

Comparing this number of states with the expression $\rho(E)dE$ we get

$$\rho(E) = \frac{L^3}{(2\pi)^3}\left(\frac{\mu k}{\hbar^2}\right)d\Omega \tag{19}$$

Using the expressions for the density of states, wave functions for the initial and final states, the golden rule gives the transition rate to be

$$\begin{aligned} w &= \frac{2\pi}{\hbar}\rho(E)|\langle i|H'|f\rangle|^2\,d\Omega &(20)\\ &= \frac{\mu L^3 k}{(4\pi^2\hbar^3)}|\langle i|H'|f\rangle|^2\,d\Omega. &(21)\end{aligned}$$

Let us now recall the definition of differential cross section. Let a scattering experiment be performed with a total of N particles. The total number of particles scattered into a solid angle $d\Omega$ per unit time is proportional to the solid angle and to the incident flux.

$$\begin{aligned}\mathrm{N}w &= \text{Number of particles scattered per unit time}\\ &= \sigma(\theta)\times d\Omega\times N\times \text{Flux}. &(22)\end{aligned}$$

The incident flux is just the probability current for the initial state and equals

$$\text{incident flux} = \frac{L^3}{(2\pi\hbar)^3}\,\frac{\hbar k}{\mu} \tag{23}$$

'constant of proportionality' is just the differential cross section. And also this number of particles scattered per unit time into solid angle $d\Omega$ is just the total number of incident particles multiplied by the transition probability per unit time, *i.e.* Nw. Therefore substituting Eq.(21) for w, (22) becomes

$$N \times \frac{\mu L^3 k}{(4\pi^2\hbar^3)} |\langle i|H'|f\rangle|^2 \, d\Omega = \sigma(\theta) \times d\Omega \times \left(N\frac{\hbar k}{\mu}\right) \tag{24}$$

Using the expressions for the initial and final state wave functions the differential cross section becomes

$$\boxed{\sigma(\theta) = \left(\frac{\mu}{2\pi\hbar^2}\right)^2} \left|\int e^{i\vec{q}\cdot\vec{r}} V(r) d^3r\right|^2 \tag{25}$$

where $\vec{q} = (\vec{k}_i - \vec{k}_f)$ is the momentum transferred. The above result coincides with the result for the differential cross section in the first Born approximation.

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