Quantum Two

Time Dependent Perturbations

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Fermi's Golden Rule

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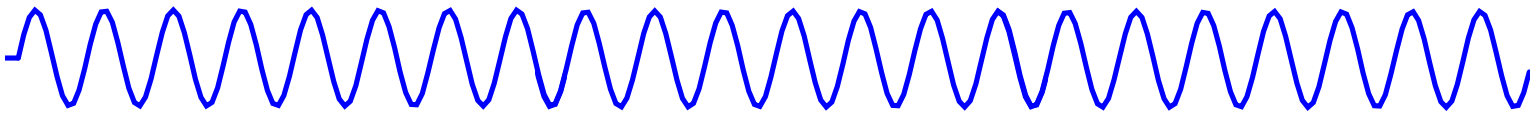

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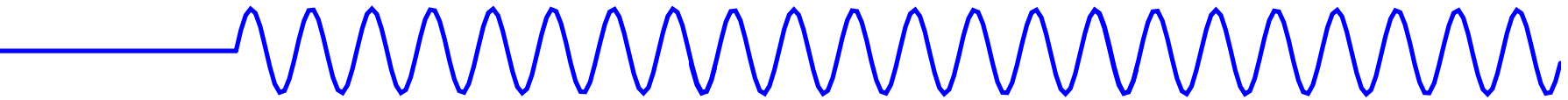

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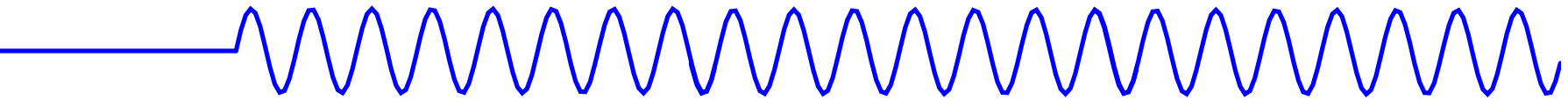

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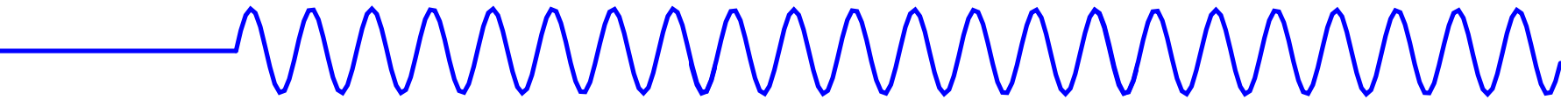

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Such a perturbation could describe, e.g., an electromagnetic wave applied to the system at $t = 0$, with a wavelength much large than the system size.

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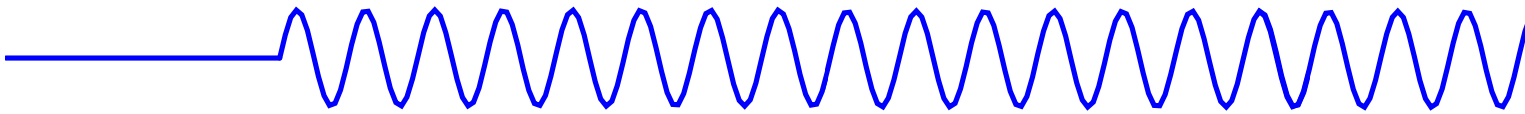
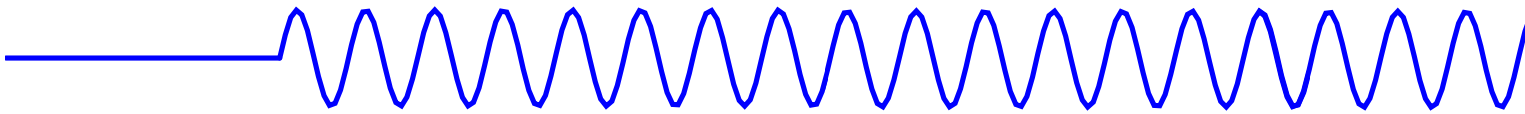


We consider here the situation in which the perturbation is simply left on and calculate, after all the transients of the system have died down, the **steady-state transition rate**

$$\Gamma_{n\to m} = \lim_{t\to\infty} \frac{dW_{n\to m}}{dt}$$



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$$\Gamma_{n\to m} = \lim_{t\to\infty} \frac{dW_{n\to m}}{dt}$$

which gives the **transition probability per unit time** induced by the applied perturbation between an initial state $|n\rangle$ and a final state $|m\rangle$.

Using our basic first order result, the transition probability for this situation can be written in the form

$$W_{n\to m}(t) = \frac{1}{\hbar^2}\left|\int_0^t \left[V_{mn}^{(+)}e^{i\Omega_+ t} + V_{mn}^{(-)}e^{i\Omega_- t}\right] dt\right|^2$$

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$$= \frac{1}{\hbar^2}\left|\frac{V_{mn}^{(+)}\, e^{i\Omega_+ t/2}\sin\left(\Omega_+ t/2\right)}{\Omega_+/2} + \frac{V_{mn}^{(-)}e^{i\Omega_- t/2}\sin\left(\Omega_- t/2\right)}{\Omega_-/2}\right|^2$$

Multiplying the quantity in brackets by its complex conjugate we find

$$W_{n\to m}(t) = \frac{1}{\hbar^2}\left\{\left|V_{mn}^{(+)}\right|^2 \frac{\sin^2(\Omega_+ t/2)}{(\Omega_+/2)^2} + \left|V_{mn}^{(-)}\right|^2 \frac{\sin^2(\Omega_- t/2)}{(\Omega_-/2)^2}\right\}$$
$$+ \frac{2}{\hbar^2}\,\mathrm{Re}\left[e^{-i\omega t} V_{mn}^{(+)} V_{nm}^{(-)*}\right] \frac{\sin(\Omega_+ t/2)}{(\Omega_+/2)} \frac{\sin(\Omega_- t/2)}{(\Omega_-/2)}$$

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To put this in a form useful for exploring the long time limit, we now multiply and divide the first two terms by $2\pi t$ and the last term by π^2 to obtain

$$W_{n\to m}(t) = \frac{2\pi t}{\hbar^2}\left\{\frac{\left|V_{mn}^{(+)}\right|^2}{\pi} \frac{\sin^2(\Omega_+ t/2)}{\Omega_+^2 t/2} + \frac{\left|V_{mn}^{(-)}\right|^2}{\pi} \frac{\sin^2(\Omega_- t/2)}{\Omega_-^2 t/2}\right\} + \frac{2\pi^2}{\hbar^2}\Lambda_{m,n}(t)\left[\frac{1}{\pi}\frac{\sin(\Omega_+ t/2)}{(\Omega_+/2)}\right]\left[\frac{1}{\pi}\frac{\sin(\Omega_- t/2)}{(\Omega_-/2)}\right].$$

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This allows us to write, for times t much greater than typical evolution times of the unperturbed system

$$W_{n\to m}(t) = \frac{2\pi t}{\hbar^2}\left\{\left|V_{mn}^{(+)}\right|^2 \delta(\Omega_+) + \left|V_{mn}^{(-)}\right|^2 \delta(\Omega_-)\right\} + \frac{2\pi^2 \Lambda_{m,n}(t)}{\hbar^2}\delta(\Omega_+)\delta(\Omega_-).$$

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Clearly, the product of delta functions in the last term

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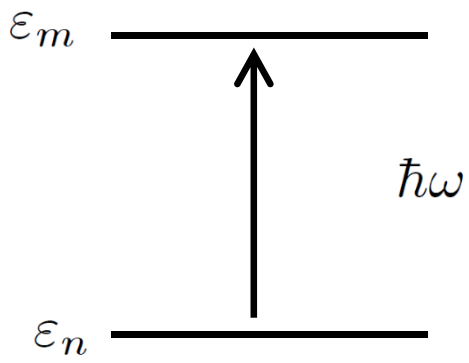
This leaves contributions only from the first two terms, only one of which can be non-zero at a time.

If the final state has an energy **greater** than the initial, so that

$$\omega_m = \omega_n + \omega$$

then the corresponding transition probability



If the final state has an energy **lower** than the initial, so that

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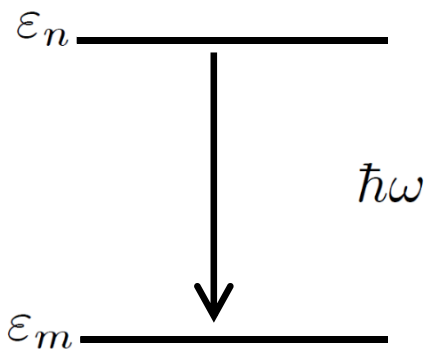
then the transition probability



Thus at long times, the probability of a transition increases linearly with time

$$W^{\pm}_{n\to m}(t) = \frac{2\pi t}{\hbar^2}|V^{(\pm)}_{mn}|^2\ \delta(\omega_m - \omega_n \mp \omega)$$

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This is the simple form of what is referred to as **Fermi's golden rule**.

$$\Gamma^{\pm}_{n\to m} = \frac{2\pi}{\hbar}|V^{(\pm)}_{mn}|^2\delta(\varepsilon_m - \varepsilon_n \mp \hbar\omega)$$

Since the δ-functions makes the transition rate formally infinite or zero, this expression has meaning only when there is a distribution of final states having the right energy that can be integrated over.

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In situations of this sort one typically introduces a density of states function $\rho(\varepsilon)$, which gives the number of states per unit energy in the interval between ε and $\varepsilon + d\varepsilon$, considered a continuous function of the final energy.

When $V_{mn}^{(\pm)}$ is constant over those states in the neighborhood of the energy to which transitions can occur, we can then define the **total probability** for a transition out of the initial state as the integral

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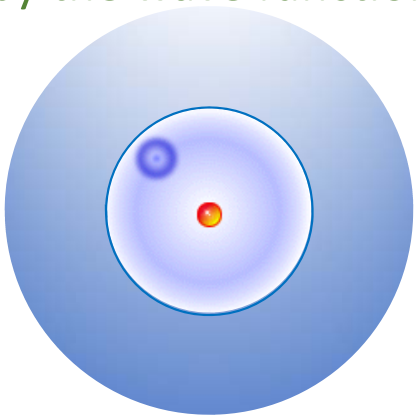
As an example of the application of Fermi's golden rule, and to see how densities of states of the sort typically encountered are constructed, we consider a ground state hydrogen atom, with a single bound electron described by the wave function

$$\psi_0(r) = \left(\pi a_0^3\right)^{-1/2} e^{-r/a_0}$$



to which is applied a harmonic perturbing potential

$$\hat{V}(\vec{r},t) = V_0 \cos(\vec{k}_0 \cdot \vec{r} - \omega t)$$

We are interested in calculating the **differential ionization rate**

$$\frac{d\Gamma_0(\theta,\phi)}{d\Omega}$$

for transitions to free-particle k-states passing through an infinitesimal solid angle $d\Omega$ centered along some particular direction (θ, ϕ).

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To proceed, we note that the perturbation can be written in the form

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where in the position representation

$$V = \frac{1}{2} V_0 e^{i\vec{k}_0 \cdot \vec{r}}$$

is harmonically varying in the electron position coordinate.

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This final energy is assumed to be associated with the final kinetic energy

$$\varepsilon_f = \frac{\hbar^2 k^2}{2m}$$

of the ionized electron,

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Note that this last δ-function involves only the magnitude of the wavevector.

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Working in the spherical coordinate representation in k-space this can be written in the form

$$\sum_{\vec{k}\in d\Omega} \delta(k-k_f) = \int_0^\infty dk\; k^2 d\Omega\; \rho(\vec{k})\delta(k-k_f)$$

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where $\rho(\vec{k}) = \rho(k,\theta,\phi)$ is the density of plane wave states with wavevector $\vec{k}$, i.e., the number of states per unit volume of k-space.

To obtain the density of states, it is convenient to take the entire system to be contained in a large box of edge L, with normalized plane wave states

$$\langle \vec{r} | \vec{k} \rangle = \phi_{\vec{k}}(\vec{r}) = L^{-3/2} e^{i\vec{k}\cdot r}$$

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The allowed wavevectors in this situation are then of the form

$$\vec{k} = \frac{2\pi}{L}(n_x \hat{\imath} + n_y \hat{\jmath} + n_z \hat{k})$$

where $n_x, n_y,$ and n_z are integers.

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The points in k-space thus form a regular cubic lattice with edge length $2\pi/L$ so there is exactly one state in every k-space unit cell volume of $(2\pi/L)^3$.

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Thus, the density of "ionized" electron states along $d\Omega$ takes the form

$$\sum_{k' \in d\Omega} \delta(k' - k) = \int_0^\infty dk\ k^2 d\Omega\ \rho(\vec{k})\delta(k - k_f) = \left(\frac{L}{2\pi}\right)^3 k^2 d\Omega$$

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and dividing through by $d\Omega$, we obtain the following expression for the **differential ionization rate**

$$\frac{d\Gamma_0(\theta, \phi)}{d\Omega} = \frac{2m\pi k}{\hbar^3} \left|V_{\vec{k},0}\right|^2 \rho(\vec{k})$$

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$$= \frac{mL^3 k}{4\pi^2 \hbar^3} \left|V_{\vec{k},0}\right|^2$$

where it is understood at this point that $\left|\vec{k}\right| = k_f$ as given above

$$\frac{d\Gamma_0(\theta,\phi)}{d\Omega} = \frac{mL^3k}{4\pi^2\hbar^3}\left|V_{\vec{k},0}\right|^2$$

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To complete the calculation we need to evaluate the matrix element

$$V_{\vec{k},0} = \langle\vec{k}|V|\psi_0\rangle = \frac{V_0}{2L^{3/2}}\int d^3r\, e^{-i\vec{k}\cdot\vec{r}}e^{i\vec{k}_0\cdot\vec{r}}\psi_0(r)$$

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$$\frac{d\Gamma_0(\theta,\phi)}{d\Omega} = \frac{16mV_0^2a_0^2}{\pi\hbar^3}\frac{ka_0}{(1+a_0^2|\vec{k}-\vec{k}_0|^2)^4}$$

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Note first that it is symmetric about the z -axis (i.e., it is independent of ϕ).

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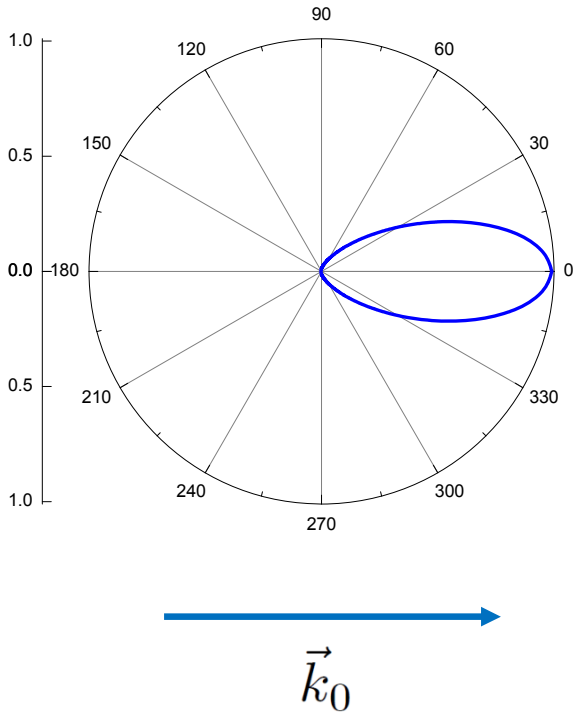
To the left is a polar plot, with the radius of the curve indicating the magnitude of the cross section, as a function of the ejection angle θ of the ionized electron, measured with respect to the wave vector of the incoming plane wave.



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Note the strong maximum along the forward scattering direction relative to the wave vector $\vec{k}_0$ that characterizes the perturbation, suggesting the absorption of both energy and momentum from the perturbing plane wave.