Advanced Quantum Physics

Lecture 15

$$\Gamma_{0\to k} = \frac{2\pi}{\hbar} |H'_{k0}|^2 g(E_k)$$

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Section 4:Transitions

4.2 Time dependent perturbation theory (1)

- We perform a similar analysis to the last lecture - for a more general case.
- This time assume $\hat{H}'(t)$ is small, we turn on the perturbation at $t = 0$
- We use the eigenstates of $\hat{H}_0$: $\hat{H}_0 |\psi_n\rangle = E_n |\psi_n\rangle \equiv \hbar\omega_n |\psi_n\rangle$.
- We must solve the equation: $$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = (\hat{H}_0 + \hat{H}'(t)) |\Psi(t)\rangle$$
- Expand $|\Psi(t)\rangle$ in eigenstates of $\hat{H}_0$: $$|\Psi(t)\rangle = \sum_j c_j(t) e^{-i\omega_j t} |\psi_j\rangle$$

showing the time dependence associated with each $|\psi_j\rangle$.

- Assume initial state: $|\psi_0\rangle$ initial conditions $c_0(0) = 1, c_j(0) = 0$ for $j \neq 0$
- Weak perturbation – transition probability small $c_j(t)$ slowly varying.
- Substituting expansion of $\Psi(t)$ into Schrodinger's equation, cancelling unperturbed terms:

$$i\hbar \sum_j \frac{\partial c_j}{\partial t} e^{-i\omega_j t} |\psi_j\rangle = \sum_j c_j(t) e^{-i\omega_j t} \hat{H}'(t) |\psi_j\rangle$$

Time dependent perturbation theory (2)

•From the last slide:

$$i\hbar\sum_j \frac{\partial c_j}{\partial t} e^{-i\omega_j t}\left|\psi_j\right\rangle = \sum_j c_j(t)e^{-i\omega_j t}\hat{H}'(t)\left|\psi_j\right\rangle$$

•Taking the inner product with $\left\langle\psi_k\right|$, multiply by $e^{i\omega_k t}$ to obtain:

$$\frac{\partial c_k}{\partial t} = \frac{1}{i\hbar}\sum_j c_j(t)e^{i(\omega_k-\omega_j)t}H'_{kj}(t) \quad \text{where} \quad H'_{kj} = \left\langle\psi_k\right|\hat{H}'\left|\psi_j\right\rangle$$

•Exact so far – interesting set of coupled equations…….

•As expected $c_k(t)$ is constant if $\hat{H}'=0$

•If perturbation is small, neglect time dependence of $c_j(t)$

•Approximate $c_0 = 1, c_j = 0$ for $j \neq 0$

•Integrating:

$$c_k(t) = \frac{1}{i\hbar}\int_0^t e^{i(\omega_k-\omega_0)t'}H'_{k0}(t')dt'$$

•$|c_k(t)|^2$ is the probability the system will be in $\left|\psi_k\right\rangle$ at time t - and a transition has occurred from $\left|\psi_0\right\rangle$.

Time dependent perturbation theory (3)

- From the last slide: $$c_k(t) = \frac{1}{i\hbar}\int_0^t e^{i(\omega_k - \omega_0)t'} H'_{k0}(t')dt'$$

- Transitions take place in the presence of the perturbation because the eigenstates of the unperturbed Hamiltonian are no longer stationary states.

- If $H'_{k0} = 0$ for $t < 0$ and $H'_{k0} \to 0$ as $t \to \infty$ then $c_k(\infty)$ is proportional to Fourier Transform of $H'_{k0}(t)$ at:

$$\omega_{k0} = (\omega_k - \omega_0)$$

- So the probability the transition $0 \to k$ will occur at some time $t > 0$ is proportional to intensity (square) of Fourier component of $H'_{k0}(t)$ with appropriate frequency ω_{k0}.

- This is reasonable – a quantum of energy $\hbar\omega_{k0}$ must be absorbed from the source of the perturbation for a transition to take place.

Oscillating perturbation – Fermi's Golden Rule

- Apply these results to a more specific case – a perturbation $\hat{H}'(\mathrm{r})e^{-i\omega t}$ which oscillates at angular frequency ω for $t > 0$.
- We assume that $\hat{H}'(\mathrm{r})$ has no explicit time dependence.
- This could represent interaction of electron with electromagnetic wave.
- In that case $\hat{H}'(\mathrm{r}) \propto \boldsymbol{\varepsilon}_0 \cdot \mathbf{r}$ with $\boldsymbol{\varepsilon}_0$ the amplitude of the electric field oscillation.
- If we want a steady perturbation turned on at $t = 0$ we can set $\omega = 0$.
- The coefficient $c_k(t)$ for a transition $0 \to k$ is given by:

$$c_k(t) = \frac{1}{i\hbar} H'_{k0} \int_0^t e^{i(\omega_k - \omega_0 - \omega)t'} dt' = -\frac{1}{\hbar} H'_{k0} \frac{e^{i(\omega_k - \omega_0 - \omega)t} - 1}{\omega_k - \omega_0 - \omega}$$

- As expected the transition rate is greatest with $\omega \approx \omega_k - \omega_0$ - an absorption process.
- In an absorption process the EM field provides a quantum of the correct energy to allow system to make transition to higher energy level $E_k > E_0$.

Oscillating perturbation – Fermi's Golden Rule (2)

•From the last slide:

$$c_k(t) = -\frac{1}{\hbar} H'_{k0} \frac{e^{i(\omega_k - \omega_0 - \omega)t} - 1}{\omega_k - \omega_0 - \omega}$$

•If $\delta\omega = \omega_k - \omega_0 - \omega$ the transition probability is given by:

$$|c_k(t)|^2 = \frac{|H'_{k0}|^2}{\hbar^2} \left| \frac{e^{i\delta\omega t/2}\left(e^{i\delta\omega t/2} - e^{-i\delta\omega t/2}\right)}{\delta\omega} \right|^2 = \frac{4}{\hbar^2} |H'_{k0}|^2 \left[\frac{\sin \frac{1}{2}\delta\omega t}{\delta\omega} \right]^2$$

•For small t probability of system being in state $|\psi_k\rangle$ is proportional to t^2.

•Hence rate of transition $\propto t$ - surprising since we might expect a constant – e.g radioactive decay.

•Rough explanation: if the perturbation $\hat{H}' e^{-i\omega t}$ is applied for a time t , Fourier spectrum contains a range of frequencies $\sim 1/t$ so energy delivered per unit frequency $\propto t^2$

•In many situations we are not concerned with transitions to a single state but to a range of states close in energy.

•E.g. an atom emitting or absorbing a photon can do so in any direction, as t increases $|c_k(t)|^2$ narrows, narrower range of $\delta\omega$ - less states accessible.

Oscillating perturbation – Fermi's Golden Rule (3)

- We need to calculate the transition probability integrated over final energy states, with density of states: $g(E_k)$ per unit energy around E_k .
- No. of states between E_k and $E_k + dE_k$ is $g(E_k)dE_k$.
- Integrated probability: $$\frac{4}{\hbar^2}\int |H'_{k0}|^2 \left[\frac{\sin\frac{1}{2}\delta\omega t}{\delta\omega}\right]^2 g(E_k)\hbar d(\delta\omega)$$
- Changing variable of integration to $x = \frac{1}{2}\delta\omega t$
- The probability becomes: $$\frac{4}{\hbar}|H'_{k0}|^2 \, g(E_k)\frac{t}{2}\int_{-\infty}^{+\infty}\left[\frac{\sin x}{x}\right]^2 dx$$
- *Tricky* step: $[\sin x/x]^2$ is only significantly different from zero over finite range of $-2\pi < x < 2\pi$ so for sufficiently large t DoS and matrix element are assumed constant – taken out of integral.
- If we approximate the limits of integration as $\pm\infty$, integral equals π .
- Differentiate w.r.t time to get transition rate;

$$\Gamma_{0\to k} = \frac{2\pi}{\hbar}|H'_{k0}|^2 \, g(E_k) \qquad \text{where } E_k = E_0 + \hbar\omega \;.$$

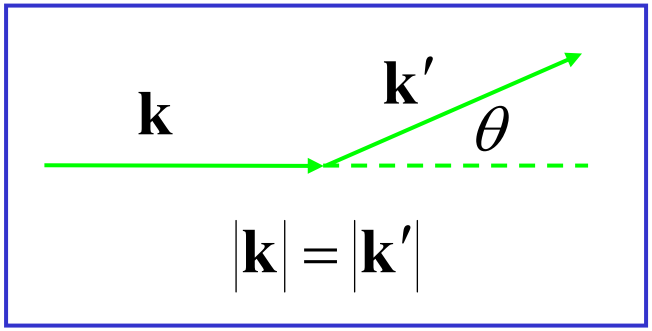
Oscillating perturbation – Fermi's Golden Rule (4)

- From the last slide, transition rate for $0 \to k$:

$$\Gamma_{0\to k} = \frac{2\pi}{\hbar} \,|\, H'_{k0} \,|^2 \, g(E_k)$$

- Known as *Fermi's Golden Rule* – but derived by Dirac!
- So rate of transition proportional to square of perturbation matrix element between states and proportional to density of states.
- Worrying that transition probability increases linearly with time to give a constant transition rate.
- We had to assume t was large so probability might get >1!
- OK - we used first order perturbation theory, valid only for matrix elements small enough so that probability is always small.
- In better calculation we would use higher order effects such as the change in $c_0(t)$ - probability amplitude of initial state as well as emission processes where the system can return to the initial state from the excited state by donating a quantum to the perturbation source.

Scattering



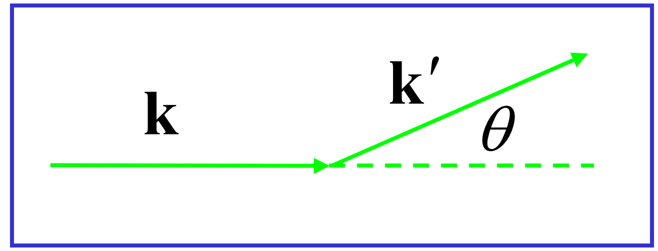
- A important transition occurs in scattering processes.
- Initial state – a free particle approaching the origin from large distance, momentum; $\mathbf{p} = \hbar\mathbf{k}$.
- Particle interacts with potential $V(\mathbf{r})$.
- Final state – particle moving away with deflected momentum $\mathbf{p}' = \hbar\mathbf{k}'$.
- Use Fermi's Golden Rule for the transition rate $\psi \to \psi'$:

$$\Gamma_{i \to f} = \frac{2\pi}{\hbar} |\langle \psi' | V(\mathbf{r}) | \psi \rangle|^2 \; g(E)$$

- Energy of the particle – elastic collision $E = \mathbf{p}^2/2m = \mathbf{p}'^2/2m$.
- Density of final states $g(E)$.
- Initial and final wavefunction: $\psi(\mathbf{r}) = Ae^{i\mathbf{k}\cdot\mathbf{r}}$, $\quad \psi'(\mathbf{r}) = Ae^{i\mathbf{k}'\cdot\mathbf{r}}$
- Assume the wavefunctions are normalised to one particle in a box of volume a^3 so: $|\psi|^2 = A^2 = 1/a^3$

Scattering (2)

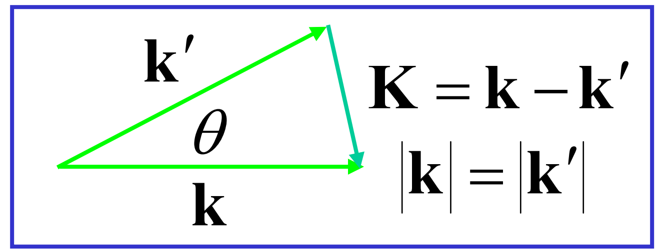
- The matrix element in Fermi's Golden Rule:



$$\langle \psi' | V(\mathbf{r}) | \psi \rangle = \frac{1}{a^3} \int e^{-i\mathbf{k}'\cdot\mathbf{r}} V(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \mathrm{d}^3\mathbf{r}$$

$$= \frac{1}{a^3} \int V(\mathrm{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{d}^3\mathrm{r}$$

where $\mathbf{K} = \mathbf{k} - \mathbf{k}'$



- $\hbar\mathbf{K}$ is the momentum transfer in the collision, and $K \equiv |\mathbf{K}| = 2k \sin\frac{1}{2}\theta$ where θ is the particle scattering angle.

- So…the matrix element is the 3D Fourier transform of the potential.

- Analogous to Fraunhofer diffraction:-

- The integral adds up scattered waves from each point in the potential, taking into account relative phases.

- The weights of components are proportional to $V(\mathbf{r})$.

Scattering (3)

- Density of states calculated as follows:
- For a particle, mass m in a cubical box of side a.
- Wavevector has possible values:

$$\mathbf{k} = \left(\frac{2\pi n_x}{a}, \frac{2\pi n_y}{a}, \frac{2\pi n_z}{a} \right), \qquad n_x, n_y, n_z = 0, 1, 2, 3.....$$

- Each state occupies a volume $(2\pi/a)^3$ of k-space.
- Number of states in solid angle $d\Omega$ and between k and $k + dk$ is: $\dfrac{k^2 dk d\Omega}{(2\pi/a)^3}$
- Density of states in k:

$$g(k) = \frac{dn}{dk} = k^2 d\Omega \left(\frac{a}{2\pi} \right)^3$$

- To convert to density of states in E use $E = \dfrac{\hbar^2 k^2}{2m} \Rightarrow \dfrac{dE}{dk} = \dfrac{\hbar^2 k}{m}$
- Hence

$$g(E) = \frac{dn}{dE} = g(k)\frac{dk}{dE} = \frac{a^3 mkd\Omega}{8\pi^3 \hbar^2}$$

Scattering (4)

- In scattering measure no. of particles scattered per second per unit flux of incident particles.
- Incident flux measured in particles per unit area per second.
- Measured ratio has dimensions of area – called *scattering crossection* (σ)
- *Scattering crossection* can be interpreted as effective area presented by scattering centre to incoming beam.
- To look at no. of particles scattered as a function of angle we use the *differential crossection*:-

$$\frac{d\sigma}{d\Omega} \equiv \frac{\text{Number of particles scattered / unit time into } d\Omega}{\text{Incident flux} \cdot d\Omega}$$

- The incident flux, taking $|\psi\rangle = a^{-3/2} e^{ikz}$ is :

$$-\frac{i\hbar}{2m}\left[\psi^* \nabla \psi - \psi \nabla \psi^*\right] = \frac{\hbar k}{ma^3} = \frac{v}{a^3}$$

where $v = \hbar k / m$ is the incident particle's velocity.

Scattering (5)

- So we have

$$\frac{d\sigma}{d\Omega} \equiv \frac{\text{Number of particles scattered / unit time into } d\Omega}{\text{Incident flux} \cdot d\Omega} = \frac{\Gamma_{i \to f}}{\left(\hbar k / m a^3\right) \cdot d\Omega}$$

and since:

$$\Gamma_{i \to f} = \frac{2\pi}{\hbar} \left| \left\langle \psi' \middle| V(\mathbf{r}) \middle| \psi \right\rangle \right|^2 g(E) = \frac{2\pi}{\hbar} \left| \frac{1}{a^3} \int V(\mathrm{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{d}^3\mathrm{r} \right|^2 \frac{a^3 mk d\Omega}{8\pi^3 \hbar^2}$$

we have:

$$\frac{d\sigma}{d\Omega} \equiv \frac{\frac{2\pi}{\hbar} \left| \frac{1}{a^3} \int V(\mathrm{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{d}^3\mathrm{r} \right|^2 \frac{a^3 mk d\Omega}{8\pi^3 \hbar^2}}{\left(\hbar k / m a^3\right) \cdot d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left| \int V(\mathrm{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{d}^3\mathrm{r} \right|^2$$

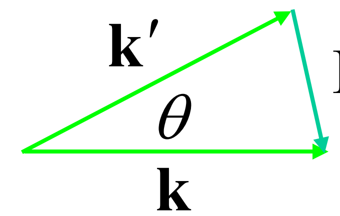
- This is the Born approximation. Based on first order perturbation theory - a good approximation when the scattering potential is a small correction to the Hamiltonian.

- The Born approximation becomes better as energy increases, there will be more about this in TP2 and Particle & Nuclear Physics next term.

Born Approximation – a screened potential

- Applying this to a screened Coulomb potential:

$$V(\mathbf{r}) = \frac{Ze^2}{4\pi\varepsilon_0 r} e^{-\lambda r}$$



- This is a decent approximation for an atom, as $\lambda \to 0$ we get a pure Coulomb potential.

- The Born Approximation: $$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left| \int V(\mathrm{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{d}^3\mathrm{r} \right|^2$$

- Now:

Assume $\mathbf{K}$ is along the z-axis and θ' is the deviation from the z-axis

$$\int V(\mathrm{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{d}^3\mathrm{r} = \frac{Ze^2}{4\pi\varepsilon_0} \iiint \frac{e^{-\lambda r}}{r} e^{i\mathbf{K}\cdot\mathbf{r}} r^2 \sin\theta' dr d\theta' d\phi$$

$u = \cos\theta'$

$$= \frac{Ze^2}{4\pi\varepsilon_0} \int_0^\infty r e^{-\lambda r} dr \int_0^\pi \sin\theta' e^{iKr\cos\theta'} d\theta' \int_0^{2\pi} d\phi = \frac{Ze^2}{2\varepsilon_0} \int_0^\infty r e^{-\lambda r} dr \int_{-1}^{1} e^{iKru} du$$

$$= \frac{Ze^2}{2\varepsilon_0} \int_0^\infty r e^{-\lambda r} dr \left[\frac{e^{iKru}}{iKr} \right]_{-1}^{1} = \frac{Ze^2}{2i\varepsilon_0 K} \int_0^\infty e^{-\lambda r} \left[e^{iKr} - e^{-iKr} \right] dr$$

Born Approximation – a screened potential (2)

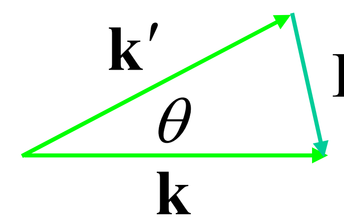
- From the last slide:

$$\int V(\mathrm{r})e^{i\mathbf{K}\cdot\mathbf{r}}\mathrm{d}^3\mathrm{r} = \frac{Ze^2}{2i\varepsilon_0 K}\int_0^\infty e^{-\lambda r}\left[e^{iKr} - e^{-iKr}\right]dr$$

$$= \frac{Ze^2}{2i\varepsilon_0 K}\int_0^\infty e^{(iK-\lambda)r} - e^{-(iK+\lambda)r}dr = \frac{Ze^2}{2i\varepsilon_0 K}\left[\frac{e^{(iK-\lambda)r}}{iK-\lambda} + \frac{e^{-(iK+\lambda)r}}{iK+\lambda}\right]_0^\infty$$

$$= -\frac{Ze^2}{2i\varepsilon_0 K}\left[\frac{1}{iK-\lambda} + \frac{1}{iK+\lambda}\right] = \frac{Ze^2}{2i\varepsilon_0 K}\cdot\frac{2iK}{K^2+\lambda^2}$$

- And since: $K = 2k\sin\tfrac{1}{2}\theta$



$$\mathbf{K} = \mathbf{k} - \mathbf{k}'$$

$$\int V(\mathrm{r})e^{i\mathbf{K}\cdot\mathbf{r}}\mathrm{d}^3\mathrm{r} = \frac{Ze^2}{\varepsilon_0}\cdot\frac{1}{K^2+\lambda^2}$$

$$= \frac{Ze^2}{\varepsilon_0}\cdot\frac{1}{4k^2\sin^2(\theta/2)+\lambda^2}$$

Born Approximation – a screened potential (3)

•From the last slide:

$$\int V(\mathrm{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{d}^3\mathrm{r} = \frac{Ze^2}{\varepsilon_0} \cdot \frac{1}{4k^2 \sin^2(\theta/2) + \lambda^2}$$

•Hence:

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left| \int V(\mathrm{r}) e^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{d}^3\mathrm{r} \right|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left| \frac{Ze^2}{\varepsilon_0} \cdot \frac{1}{4k^2 \sin^2(\theta/2) + \lambda^2} \right|^2$$

$$= \left(\frac{Zme^2}{8\pi\varepsilon_0\hbar^2}\right)^2 \left(\frac{1}{k^2 \sin^2(\theta/2) + \lambda^2/4}\right)^2$$

And if $\lambda \to 0$ - unscreened Coulomb

$$\frac{d\sigma}{d\Omega} = \left(\frac{Zme^2}{8\pi\varepsilon_0\hbar^2 k^2 \sin^2(\theta/2)}\right)^2 = \left(\frac{Zme^2}{8\pi\varepsilon_0 p^2 \sin^2(\theta/2)}\right)^2$$

where $p = \hbar k$

•This is identical to the Rutherford scattering formula – as derived from classical orbits.

•Here we have derived it from Quantum Mechanics using the Born Approximation.

Lecture 15 - Summary

- Time dependent perturbation theory – for a transition , $\psi_0 \rightarrow \psi_k$, the transition probability is $|c_k(t)|^2$, where:

$$c_k(t) = \frac{1}{i\hbar}\int_0^t e^{i(\omega_k-\omega_0)t'} H'_{k0}(t')dt'$$

- Application of an oscillating perturbation, calculation of the transition probability and transition rate - given by *Fermi's golden rule*.

$$\Gamma_{0\rightarrow k} = \frac{2\pi}{\hbar}|H'_{k0}|^2\, g(E_k)$$

- Particle scattering, the Born approximation and calculation of the differential scattering crossection.

$$\frac{d\sigma}{d\Omega} \equiv \left(\frac{m}{2\pi\hbar^2}\right)^2 |\int V(\mathrm{r})e^{i\mathbf{K}\cdot\mathbf{r}}\mathrm{d}^3\mathrm{r}|^2$$

- Example: Scattering from a screened potential using the Born approximation.

Lecture 15

$$\Gamma_{0\to k} = \frac{2\pi}{\hbar} | H'_{k0} |^2 \, g(E_k)$$

The End!!

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