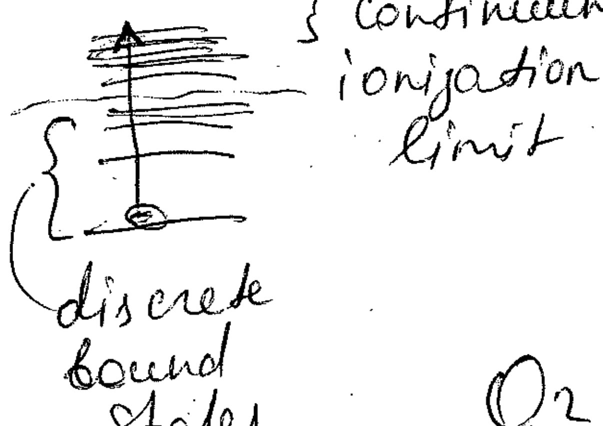
Lecture #5

Transitions between continuum states

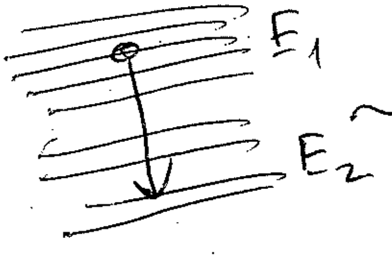
So far we've considered an unperturbed operator that has only a <u>discrete</u> spectrum $\Rightarrow$

$H_0 |\varphi_n\rangle = E_n |\varphi_n\rangle$

What if we deal with ionization of atoms as a consequence of the perturbation field of a charged particle which is passing by



<u>Or</u> bremsstrahlung of charged particles as a result of acceleration or deceleration in the field of other particles



$\rightsquigarrow \hbar\omega = E_1 - E_2$

Consider general case $\Rightarrow$ H_0 has both discrete and continuous spectrum $\Rightarrow$

$H_0 \psi_n(\vec{r}) = E_n \psi_n(\vec{r})$ and $H_0 \psi_\alpha(\vec{r}) = E_\alpha \psi_\alpha(\vec{r})$

discrete index — continuous index

Stationary solutions of the Schrödinger equation: $\psi_{n,\alpha}(\vec{r},t) = \psi_{n,\alpha}(\vec{r}) e^{-\frac{i}{\hbar}E_{n,\alpha} t}$

Normalization: $\int \psi_{n'}^*(\vec{r},t)\, \psi_n(\vec{r},t)\, dV = \delta_{n'n}$

$$\int \psi_\alpha^*(\vec{r},t)\, \psi_{\alpha'}(\vec{r},t)\, dV = \delta(\alpha - \alpha')$$

$$\int \psi_\alpha^*(\vec{r},t)\, \psi_n(\vec{r},t)\, dV = 0$$

Closure: $\sum_n |\psi_n\rangle\langle\psi_n| + \int d\alpha\, |\psi_\alpha\rangle\langle\psi_\alpha| = 1$

At $t = 0 \Rightarrow$ introduce perturbation $V(t)$ $\Rightarrow$

$$i\hbar \frac{\partial \psi}{\partial t} = (H_0 + V(\vec{r},t))\, \psi$$

From Lecture # 3 $\Rightarrow$

$$\psi(\vec{r},t) = \sum_n C_n(t) e^{-\frac{i}{\hbar}E_n t} \psi_n(\vec{r}) + \int d\alpha\, C_\alpha(t)\, e^{-\frac{i}{\hbar}E_\alpha t} \psi_\alpha(\vec{r}), \qquad (6.1)$$

$$\sum_n |C_n(t)|^2 + \int d\alpha\, |C_\alpha(t)|^2 = 1$$

Substitute Eq. (6.1) into Shrödinger equation ③
equation $\Rightarrow$

$$i\hbar\left(\sum_n \frac{dc_n(t)}{dt} e^{-\frac{i}{\hbar}E_n t}\psi_n(\vec{r}) + \int d\alpha \frac{dc_\alpha(t)}{dt} e^{-\frac{i}{\hbar}E_\alpha t}\cdot \psi_\alpha(\vec{r})\right) = \sum_n c_n(t) e^{-\frac{i}{\hbar}E_n t} V(\vec{r},t)\psi_n(\vec{r}) +$$

$$+\int d\alpha\, c_\alpha(t) e^{-\frac{i}{\hbar}E_\alpha t} V(\vec{r},t)\psi_\alpha(\vec{r}); \qquad (6.2)$$

Multiply (6.2) by $e^{\frac{i}{\hbar}E_{n'}t}\psi^*_{n'}(\vec{r})$ and integrate over $\vec{r}$ $\Rightarrow$

$$\underline{i\hbar\frac{dc_{n'}(t)}{dt}} = \sum_n c_n(t) e^{-\frac{i}{\hbar}(E_n - E_{n'})t} V_{n'n} +$$

$$+\int d\alpha\, c_\alpha(t) e^{\frac{i}{\hbar}(E_{n'} - E_\alpha)t} V_{n'\alpha} \underset{\uparrow}{=} \quad \omega_{n'n} = \frac{E_{n'} - E_n}{\hbar} \quad \omega_{n'\alpha} = \frac{E_{n'} - E_\alpha}{\hbar}$$

$$= \sum_n c_n(t) e^{i\omega_{n'n}t} V_{n'n}(t) + \int d\alpha\, c_\alpha(t) e^{i\omega_{n'\alpha}t} V_{n'\alpha}(t) \qquad (6.3)$$

Similarly, if (6.2) is multiplied by $e^{\frac{i}{\hbar}E_{\alpha'}t}\psi^*_{\alpha'}(\vec{r})$ and integrated over $\vec{r}$ $\Rightarrow$

get $$i\hbar \frac{dC_{\alpha'}(t)}{dt} = \underbrace{\sum_n C_n(t) e^{i\omega_{\alpha' n} t} V_{\alpha' n}(t)} +$$

$$+ \underbrace{\int C_\alpha(t) e^{i\omega_{\alpha'\alpha} t} V_{\alpha'\alpha}(t)\, d\alpha} \qquad (6.3)$$

Recall Lecture #3 $\Rightarrow$ $C_n(t) = C_n^{(0)} + \lambda C_n^{(1)} + \ldots$

$C_\alpha(t) = C_\alpha^{(0)} + \lambda C_\alpha^{(1)} + \ldots$

From Eqs. (6.3) $\Rightarrow$

<u>0th order</u>: $i\hbar \frac{dC_{n'}^{(0)}}{dt} = 0$; $i\hbar \frac{dC_{\alpha'}^{(0)}}{dt} = 0$ $\Rightarrow$

$C_{n'}^{(0)}$, $C_{\alpha'}^{(0)}$ are constants

<u>1st order</u>: $$i\hbar \frac{dC_{n'}^{(1)}}{dt} = \sum_n C_n^{(0)} e^{i\omega_{n'n} t} V_{n'n}(t) +$$

$$+ \int d\alpha\, C_\alpha^{(0)} e^{i\omega_{n'\alpha} t} V_{n'\alpha}(t) ;$$

$$i\hbar \frac{dC_{\alpha'}^{(1)}}{dt} = \sum_n C_n^{(0)} e^{i\omega_{\alpha' n} t} V_{\alpha' n}(t) +$$

$$+ \int d\alpha\, C_\alpha^{(0)} e^{i\omega_{\alpha'\alpha} t} V_{\alpha'\alpha}(t) ;$$

- - - -

Let's specify that at $t=0$ our system is in a state k of the discrete spectrum ⇒ (5)

$$C_{n'}^{(0)} = \delta_{n'k} \; ; \quad C_{\alpha'}^{(0)} = 0$$

Then, $i\hbar \frac{dC_{n'}^{(1)}}{dt} = e^{i\omega_{n'k}t} V_{n'k}(t)$

transitions between bound states ⇒ Lecture #3

$$i\hbar \frac{dC_{\alpha'}^{(1)}}{dt} = e^{i\omega_{\alpha'k}t} V_{\alpha'k}(t)$$

transitions between bound and unbound states

⇓

$$C_{\alpha}^{(1)}(t) = \frac{1}{i\hbar}\int_0^t V_{\alpha k}(t')\, e^{i\omega_{\alpha k}t'}\,dt'$$

very similar to what we had for the case of discrete spectrum!

What's different? ⇒ the probability of transition is now $\mathcal{P}_{k\to\alpha} = \int d\alpha\, |C_\alpha(t)|^2$,

$k \neq \alpha$, 1st order

not just $|C_{\underset{n}{\alpha}}(t)|^2$!

What is $d\alpha$? ⇒

$\}\ B(E) \Rightarrow d\alpha = \underbrace{\rho_\alpha(E)}_{\substack{\uparrow \\ \text{density of} \\ \text{states}}} dE$ ← energy

↑ domain in which the electron ends up after the transition

So, $\mathcal{P}_{i \to f} = \int_{B(E)} |C_\alpha^{(1)}(t)|^2 \rho_\alpha(E)\, dE =$

i ↑ discrete state K

f ↑ continuum state α

$$= \int_{B(E)} \frac{1}{\hbar^2} \left| \int_0^t V_{\alpha K}(t')\, e^{i\omega_{\alpha K} t'}\, dt' \right|^2 \rho_\alpha(E)\, dE$$

↑ probability of transition from state K to an "energy region" $B(E)$ in the continuum

If the initial state is in continuum too $\Rightarrow$

$C_K(0) = 0, \quad C_{\alpha'}(0) = \delta(\beta - \alpha') \Rightarrow$

$$\mathcal{P}_{\beta \to \alpha} = \frac{1}{\hbar^2} \int_{B(E)} \left| \int_0^t V_{\alpha\beta}(t')\, e^{i\omega_{\alpha\beta} t'}\, dt' \right|^2 \rho_\alpha(E)\, dE$$

Notes on "sudden" change versus "adiabatic" change in the Hamiltonian

(a) consider a system whose H changes abruptly over a small time interval $\mathcal{E}$. What is the change in the state vector as $\mathcal{E} \to 0$?

Say, $t \in [-\frac{\mathcal{E}}{2}, \frac{\mathcal{E}}{2}]$
↑ change at $t=0$

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = H(t)\,|\Psi(t)\rangle \, ;$$

$$\underbrace{|\Psi(\tfrac{\mathcal{E}}{2})\rangle}_{|\Psi_{\text{after change}}\rangle} - \underbrace{|\Psi(-\tfrac{\mathcal{E}}{2})\rangle}_{|\Psi_{\text{before change}}\rangle} = -\frac{i}{\hbar}\int_{-\frac{\mathcal{E}}{2}}^{\frac{\mathcal{E}}{2}} H(t)\,|\Psi(t)\rangle\, dt$$

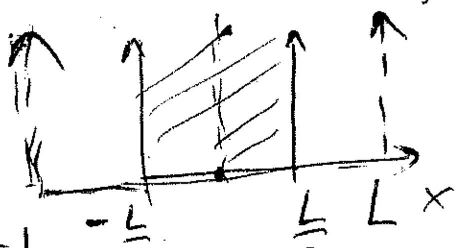
If $H(t)$ is not a δ-function $\Rightarrow \mathcal{E} \to 0 \Rightarrow$
$|\Psi_{\text{after}}\rangle = |\Psi_{\text{before}}\rangle$

(b) now let's say that $H(t)$ changes very slowly from $H(0)$ to $H(\tau)$ in a time τ. If the system starts out at $t=0$ in an eigenstate $|n(0)\rangle$ of $H(0)$, where will it end up at time τ?

<u>adiabatic theorem</u>: if the rate of change of H

is "slow enough", the system will end up (8)
in the corresponding eigenket $|n(\tau)\rangle$ of $H(\tau)$

Recall one of the HW problems from Phys.651.



Particle in the box of length L
Then, the box expands to $2L$.
If the particle is initially in its ground state, where is it going to end up after the change?

"sudden" $\Downarrow$

$$\mathcal{P}(n=1,\text{old} \to n=1,\text{new}) = \left(\frac{8}{3\pi}\right)^2 \sim 81\%$$

(the rest is $\to n=2, \ldots$ new)

"adiabatic" $\Rightarrow \mathcal{P}(n=1,\text{old} \to n=1,\text{new}) \overset{\text{after time } \tau}{=} 1$

But: how slow is slow?! $\Rightarrow$ introduce "natural time scale" for a system $T \sim \frac{1}{\omega_{fi}} \sim \frac{1}{\omega_i}$ ← if $\omega_{fi} \neq 0$ (non-degen.)

Particle-in-the-box $\Rightarrow E_n^0 = \frac{\hbar^2\pi^2}{2mL^2} n^2$

$T \sim \frac{mL^2}{\hbar} \Rightarrow$ so $\tau \gg T$ is <u>slow</u>

<u>Note</u>: the adiabatic theorem suggests that at $\tau \gg T$ time-dependent perturb. theory $\Rightarrow$ time-indep. one!