例 10.1

一在基態上的氫原子，於時間 $t=0$ 時，開始受到一個沿 z 軸方向的均勻電場作用，且其大小 $E=E_0\,e^{-t/\tau}$，求當 $t>>\tau$ 時，此原子被激發至 $n=2$ 狀態的機率為何？

解 氫原子與外加電場之交互作用位能為

$$V=-\vec{p}\cdot\vec{E}=qE\vec{r}\cdot\vec{e}_z=qE_0e^{-t/\tau}Z$$

其對應之運算子則為

$$\hat{H}'=qE_0\,e^{-t/\tau}\hat{Z}=\hat{\mathbf{H}}'f(t)$$

自基態 $n=1$ 躍遷至 $n=2$ 狀態之躍遷矩陣元為

$$\hat{\mathbf{H}}'_{fi}=\langle\varphi_{n=2}|\hat{\mathbf{H}}'|\varphi_{n=1}\rangle=qE_0\langle\varphi_{n=2}|\hat{Z}|\varphi_{n=1}\rangle$$

其中 $\varphi_{n=2}=\varphi_{n\ell m}=\varphi_{200,\,210,\,21\pm1}$、$\varphi_{n=1}=\varphi_{n\ell m}=\varphi_{100}$。當末態 $n=2$ 為 φ_{200} 時，由內積定義，及球面調和函數之正交性，故

$$\begin{aligned}\langle\varphi_{200}|\hat{Z}|\varphi_{100}\rangle&=\iint\langle\varphi_{200}|\vec{r}'\rangle\langle\vec{r}'|\hat{Z}|\vec{r}\rangle\langle\vec{r}|\varphi_{100}\rangle d^3r'd^3r\\&=\iint\varphi^*_{200}(\vec{r}')Z\delta(\vec{r}-\vec{r}')\varphi_{100}(\vec{r})d^3r'd^3r=\int\varphi^*_{200}(r)Z\varphi_{100}(r)d^3r\\&=\sqrt{\frac{4\pi}{3}}\int_0^\infty R_{20}(r)R_{10}(t)r^3dr\int_\Omega Y_2^0Y_1^0Y_0^0d\Omega=0\end{aligned}$$

同理，當末態為 $\varphi_{21\pm1}$ 時，因 $m_1+m_2+m_3=\mp1+0+0=\mp1\neq0$

$$\langle\varphi_{21\pm1}|\hat{Z}|\varphi_{100}\rangle=0$$

但當末態為 φ_{210} 時，

$$\langle\varphi_{210}|\hat{Z}|\varphi_{100}\rangle=\frac{1}{4\sqrt{2}\pi a^4}\int_0^\infty re^{-r/2a}re^{-r/a}r^2dr\int_\Omega\cos\theta\cos\theta\sin\theta d\theta d\varphi$$

因 $\int_0^\infty r^4e^{-3r/2a}dr=\dfrac{4!}{(3/2a)^5}=\left(\dfrac{4}{3}\right)^4a^5$，故

$$\langle \varphi_{210} | \hat{Z} | \varphi_{100} \rangle = \frac{1}{4\sqrt{2}\pi a^4} = \left(\frac{4}{3}\right)^4 a^5 \cdot \frac{4\pi}{3} = \frac{1}{\sqrt{2}}\left(\frac{4}{3}\right)^4 a \cdot \frac{1}{3}$$

另外，含時間部分之積分項為

$$\int_0^t e^{i\omega_{21}t'} f(t')dt' = \int_0^t e^{i\omega_{21}t'} e^{-t'/\tau} dt' = \int_0^t e^{\left(-\frac{1}{\tau}+i\omega_{21}\right)t'} dt' = \int_0^t e^{ct'} dt' = \frac{1}{c}\int_0^t e^{ct'} d(ct')$$

$$= \frac{1}{c}\int_0^{Z=ct} e^{Z'} dZ' = \frac{1}{c}\ [e^{Z'}]_0^{Z=ct} = \frac{1}{c}\ [e^{ct} - e^0] = \frac{1}{c}(e^{ct} - 1)$$

其中 $c = -1/\tau + i\omega_{21}$，且

$$\omega_{21} = 1/\hbar(E_2 - E_1) = -13.6/\hbar(1/4 - 1) = 10.2/\hbar \quad \text{(eV)}$$

因此

$$\left|\int_0^t e^{i\omega_{21}t'} e^{-t'/\tau} dt'\right|^2 = \frac{1}{|c|^2} | e^{-t/\tau} e^{i\omega_{21}t} - 1 |^2 = \frac{1}{|c|^2} | e^{-t/\tau} \cos\omega_{21}t + ie^{-t/\tau} \sin\omega_{21} - 1|^2$$

$$= \frac{1}{(1/\tau)^2 + \omega_{21}^2}[(e^{-t/\tau}\cos\omega_{21}t - 1)^2 + (e^{-t/\tau}\sin\omega_{21})^2]$$

$$= \frac{\tau^2(e^{-2t/\tau} - 2e^{-t/\tau}\cos\omega_{21}t + 1)}{1 + \tau^2\omega_{21}^2} \to \frac{\tau^2}{1 + \tau^2\omega_{21}^2} \quad (\text{當 } t >> \tau)$$

最後，躍遷機率為

$$P_{if}(t) = P_{100\to 210}(t)\left|\frac{\hat{\mathbf{H}}'_{fi}}{\hbar}\right|^2 \left|\int_0^t e^{i\omega_{21}t'} f(t')dt'\right|^2$$

$$= \frac{2^{15}}{3^{10}}\frac{q^2 E_0^2}{\hbar^2} a^2 \left|\int_0^t e^{i\omega_{21}t'} e^{-t'/\tau} dt'\right|^2 = \frac{2^{15}}{3^{10}}\frac{q^2 E_0^2 a^2}{\hbar^2}\frac{\tau^2}{1 + \tau^2\omega_{21}^2}$$

問題 10.5

在 $x=0$ 至 $x=a$ 之無限位能井中，有一粒子於 $t>0$ 時，處於基態，當時間 $t=0$ ，開始受到微擾 $\hat{V}(t)=\varepsilon\, e^{-t^2}$ 之作用，其中 $\varepsilon<<1$ 。計算在時間 $t=+\infty$ 時，粒子被發現處於第一激發態的機率是多少？

解 由基態 $n=1$ 到第一激發態的躍遷機率為

$$P_{1\to 2}=\frac{1}{\hbar^2}\left|\int_0^\infty \langle\psi_2|\hat{V}(t)|\psi_1\rangle e^{i\omega_{21}t}dt\right|^2$$

其中
$$\omega_{21}=\frac{E_2-E_1}{\hbar}=\frac{4\pi^2\hbar}{2ma^2}-\frac{\pi^2\hbar}{2ma^2}=\frac{3\pi^2\hbar}{2ma^2}$$

$$\langle\psi_2|\hat{V}(t)|\psi_1\rangle=\frac{2\varepsilon}{a}e^{-t^2}\int_0^a \sin(\frac{2\pi x}{a})\sin(\frac{\pi x}{a})dx=\frac{16\varepsilon a}{9\pi^2}e^{-t^2}$$

此處我們用到 $E_n=\dfrac{n^2\pi^2\hbar^2}{2ma^2}$ 以及 $\psi_n=\sqrt{\dfrac{2}{a}}\sin(\dfrac{n\pi x}{a})$

故
$$P_{1\to 2}=(\frac{16\varepsilon a}{9\pi^2\hbar^2})^2\left|\int_0^\infty e^{i\omega_{21}t-t^2}\,dt\right|^2$$

利用變數變換 $y=t-\dfrac{i}{2}\omega_{21}$ ，使得 $i\omega_{21}t-t^2=-\dfrac{\omega_{21}^2}{4}-y^2$ 且 $dt=dy$ 。

$$P_{1\to 2}=(\frac{16\varepsilon a}{9\pi^2\hbar^2})^2\left|e^{-\omega_{21}^2/4}\int_0^\infty e^{-y^2}dy\right|^2=(\frac{8\varepsilon a}{9\pi\hbar})^2\frac{1}{\pi}e^{-\omega_{21}^2/2}$$

上式使用了 $\displaystyle\int_0^\infty e^{-y^2}dy=\frac{\sqrt{\pi}}{2}$ 以及 $\omega_{21}=\dfrac{3\pi^2\hbar^2}{2ma^2}$