Lecture 13-QM_II (10/08/00)

Monday, November 1, 2021 2:55 PM

اختلال غیر وابسته به زمان

$$H = H_0 + \lambda H_1 \qquad \lambda \ll 1$$

• تبهگنی نداریم

$$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$$

$$H|n\rangle = E_n |n\rangle$$

تبهگنی داریم

$$H_0 |n_i^{(0)}\rangle = E_n^{(0)} |n_i^{(0)}\rangle \qquad i = 1, \dots l$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

$$|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \dots$$

Key idea : بدون تبهگنی

$$|n\rangle = |n^{(0)}\rangle + \sum_{n \neq k} C_{nk}(\lambda) |k^{(0)}\rangle$$

$E_n^{(0)}$

$$C_{nk}(\lambda) = \sum_{i=1}^{\infty} \lambda^i C_{nk}^{(i)}$$

با تبهگنی

$$|n\rangle = \sum_{i=1}^{l} \alpha_i |n_i^{(0)}\rangle + \sum_{n\neq k} C_{nk}(\lambda) \sum_{j=1}^{l} \beta_j |k_j^{(0)}\rangle$$

بدون تبهگنی

$$E_n^{(1)} = \langle n^{(0)} | H_1 | n^{(0)} \rangle$$

با تبهگنی

$$E_n^{(1)} \vec{\alpha} = \underset{\sim}{H_1} \vec{\alpha}$$

$$E_n^{(1)} \alpha_i = \sum_{j=1}^{l} \langle n_i^{(0)} | H_1 | n_j^{(0)} \rangle \alpha_j$$

اثر Stark (Johannes)

$$E_n^{(0)} = \frac{-1Ry}{n^2}$$

$$H = H_0 + H_1$$

$$H_0 = \frac{P^2}{2m_e} - \frac{Ze^2}{r}$$

هملیتونی اتم هیدروژن $Z = 1$

$$H_1 = e\vec{\mathcal{E}} \cdot \vec{x} = e\mathcal{E} z$$

$$(e\mathcal{E})^n$$

$$\vec{\mathcal{E}} = \mathcal{E}\hat{e}_z$$

غیر تبهگن ? $E_{n=1}^{(1)}$, $E_{n=1}^{(2)}$; $n=1$ $l=0$ $m_l = 0$

$$E_{n=1}^{(0)} = -1Ry$$

$$Ry = \frac{1}{2} m_e c^2 \alpha^2$$

$$\alpha = \frac{e^2}{\hbar c}$$

با تبهگنی ? $E_{n=2}^{(1)}$; $n=2$ $l = 0,1$

$l=0$ $m_l = 0$

$l=1$ $m_l = 0, \pm 1$

$$E_{n=2}^{(0)} = \frac{-1Ry}{2^2}$$

در چه صورتی این عنصر ماتریس غیر صفر می‌شود

$$\langle n\, l\, m_l | z | n' l' m_l' \rangle = ?$$

• قواعد گزینش

b) $\Delta l = l' - l = \pm 1$

a) $\Delta m_l = 0$ ✓

اثبات (a)

$$[L_z, z] = 0$$

$$0 = \langle n\, l\, m_l | [L_z, z] | n' l' m_l' \rangle$$

$$= \langle n l m_l | L_z z | n' l' m_l' \rangle - \langle n l m_l | z L_z | n' l' m_l' \rangle$$

$$= \hbar m_l \langle n l m_l | z | n' l' m_l' \rangle - \hbar m_l' \langle n l m_l | z | n' l' m_l' \rangle$$

$$= \langle n l m_l | L_z z | n' l' m_l' \rangle - \langle n l m_l | z L_z | n' l' m_l' \rangle$$

$$= \hbar m_l \langle n l m_l | z | n' l' m_l' \rangle - \hbar m_l' \langle n l m_l | z | n' l' m_l' \rangle$$

$$0 = \hbar (m_l - m_l') \langle n l m_l | z | n' l' m_l' \rangle$$

اگر $m_l = m_l' \rightarrow \langle n l m_l | z | n' l' m_l' \rangle \neq 0$

در کلی ترین حالت

b) اثبات $\Delta l = l' - l = \pm 1$

$$[\vec{L}^2, [\vec{L}^2, z]] = \underline{2\hbar^2 \{z, \vec{L}^2\}}$$

طرف چپ $$[\vec{L}^2, \vec{L}^2 z] - [\vec{L}^2, z\vec{L}^2] = (\vec{L}^2)^2 z - 2\vec{L}^2 z L^2 + z(\vec{L}^2)^2$$

$$\langle n l m_l | (\vec{L}^2)^2 z - 2\vec{L}^2 z \vec{L}^2 + z(\vec{L}^2)^2 | n' l' m_l' \rangle$$

$$= \{\hbar^4 l^2 (l+1)^2 - 2\hbar^4 l(l+1) l'(l'+1) + \hbar^4 l'^2 (l'+1)^2\}$$

$\vec{L}^2 |nlm\rangle = \hbar^2 l(l+1) |nlm\rangle$ $$\times \langle n l m_l | z | n' l' m_l' \rangle$$

طرف راست $$\langle n l m_l | 2\hbar^2 (z\vec{L}^2 + \vec{L}^2 z) | n' l' m_l' \rangle$$

$$= \{2\hbar^4 l'(l'+1) + 2\hbar^4 l(l+1)\} \langle n l m_l | z | n' l' m_l' \rangle$$

$$\underbrace{\left(\{\ \} - \{\ \}\right)}_{=0} \langle n l m_l | z | n' l' m_l' \rangle = 0$$

$$\begin{cases} l' = l+1 \\ l' = l-1 \\ \cancel{l' = -l} \\ \cancel{l' = -l-2} \end{cases} \qquad l, l' \geq 0$$

اختلال غیرواگن (تعیین تغییر انرژی حالت پایه اتم هیدروژن در حضور میدان الکتریکی) در مرتبه اول اختلال

$$E_{n=1}^{(1)} = \langle 1 0 0 | H_1 | 100 \rangle$$

$$= e\mathcal{E} \langle 100 | z | 100 \rangle = 0$$

$\Delta m_l = 0$
$\Delta l = \pm 1$

n, l, m_l ; n', l', m_l'

$$m_l - m_l' = 0$$
$$l' - l = 0 \neq \pm 1$$

$$\int |\psi_{100}|^2 z \, d^3 r = 0$$

در مرتبه دوم اختلال

$$E_n^{(2)} = \sum_{\substack{k \\ k \neq n}} \frac{|\langle k^{(0)} | H_1 | n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} \qquad H_1 = e\mathcal{E} z$$

$$E_{n=1}^{(2)} = \sum_{\substack{k, l', m_l' \\ k \neq n}} e^2 \mathcal{E}^2 \frac{|\langle k\, l' m_l' | z | 100 \rangle|^2}{E_1^{(0)} - E_k^{(0)}}$$

$m_l' = m_l = 0$
$l' - l = \pm 1$
$l' = l + 1$

$$e^2\mathcal{E}^2 \sum \ |\langle k\, 1\, 0 | z | 100 \rangle|^2$$

$m_\ell = m_{\ell'} = 0$
$\ell' - \ell = \pm 1$
$\ell' = \ell + 1$
$\ell' = 0 + 1$

$$\star = e^2 \mathcal{E}^2 \sum_{\substack{k \neq 1 \\ n=1}} \frac{|\langle k\,1\,0 | z | 100 \rangle|^2}{E_1^{(0)} - E_k^{(0)}}$$

$$|k\,1\,0\rangle = |\varphi_E\rangle \quad ; \quad \sum_{k\neq 1} \to \sum_E \; ; \; E_k^{(0)} \to E$$

$$\langle 100 | z | \varphi_E \rangle \langle \varphi_E | z | 100 \rangle =$$

$$E_{n=1}^{(2)} = e^2 \mathcal{E}^2 \sum_E \frac{\langle 100 | z | \varphi_E \rangle \langle \varphi_E | z | 100 \rangle}{E_1^{(0)} - E}$$

$$\sum_E |\varphi_E\rangle\langle\varphi_E| \cong 1$$

$$E = E_{2=n}^{(0)} > E_1^{(0)} \qquad \frac{1}{E_1^{(0)} - E} < \frac{1}{E_1^{(0)} - E_2^{(0)}}$$

$$E_{n=1}^{(2)} = e^2 \mathcal{E}^2 \sum_E \frac{\text{صورت}}{E_1^{(0)} - E} < \frac{e^2 \mathcal{E}^2}{E_1^{(0)} - E_2^{(0)}} \underbrace{\sum_E \langle 100 | z | \varphi_E \rangle \langle \varphi_E | z | 100 \rangle}_{= \langle 100 | z^2 | 100 \rangle}$$

$$E_{n=1}^{(2)} < \frac{e^2 \mathcal{E}^2}{E_1^{(0)} - E_2^{(0)}} \langle 100 | z^2 | 100 \rangle \stackrel{!}{=} -\frac{8}{3} a_0^3 \mathcal{E}^2$$

$$E_{n=1}^{(2)} = -\frac{9}{4} a_0^3 \mathcal{E}^2$$

$$\langle 100 | z^2 | 100 \rangle = \langle 100 | x^2 | 100 \rangle = \langle 100 | y^2 | 100 \rangle$$

$$\underline{\langle 100 | z^2 | 100 \rangle} = \frac{1}{3} \langle 100 | \vec{r}^{\,2} | 100 \rangle = a_0^2$$

$$\langle n \ell m_\ell | r^2 | n \ell m_\ell \rangle = \frac{a_0^2 n^2}{2} \left(5n^2 + 1 - 3\ell(\ell+1)\right) \Big|_{\substack{n=1 \\ \ell=0 \\ m_\ell=0}}$$

$$= 3a_0^2$$

$$E_1^{(0)} - E_2^{(0)} = \frac{-Ry}{1} + \frac{Ry}{4} = -\frac{3}{4} Ry = -\frac{3}{4}\left(\frac{1}{2} m_e c^2 \alpha^2\right)$$

$$E_{n=1}^{(2)} < \frac{e^2 \mathcal{E}^2}{-\frac{3}{8} m_e c^2 \alpha^2} a_0^2 \underset{\swarrow}{=} -\frac{8}{3} \mathcal{E}^2 a_0^3$$

$$\alpha = \frac{e^2}{\hbar c} \qquad a_0 = \frac{\hbar}{m_e c \alpha}$$