Physics 206, 2004

Final exam

1a). $$f(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int e^{-i\vec{q}\vec{r}} V(\vec{r})\, d^3r\,;$$

$$\vec{q} = \frac{\vec{P}_f - \vec{P}_i}{\hbar} = \vec{k}_f - \vec{k}_i = k\left[\vec{e}_z(\cos\theta - 1) + \vec{e}_x \sin\theta\cos\varphi + \vec{e}_y \sin\theta\sin\varphi\right] = q_z\vec{e}_z + q_x\vec{e}_x + q_y\vec{e}_y$$

$$f(\theta,\varphi) = -\frac{mU}{2\pi\hbar^2}\int_{-a}^{a} dx\, e^{-iq_x x}\int_{-a}^{a} dy\, e^{-iq_y y}\int_{-a}^{a} dz\, e^{-iq_z z} =$$

$$= -\frac{mU}{2\pi\hbar^2}\,\frac{e^{-iq_x a} - e^{iq_x a}}{-iq_x}\,\frac{e^{-iq_y a} - e^{iq_y a}}{-iq_y}\,\frac{e^{-iq_z a} - e^{iq_z a}}{-iq_z} =$$

$$= -\frac{mU}{2\pi\hbar^2}\, 8a^3\, \frac{e^{iq_x a} - e^{-iq_x a}}{2iq_x a}\,\frac{e^{iq_y a} - e^{-iq_y a}}{2iq_y a}\,\frac{e^{iq_z a} - e^{-iq_z a}}{2iq_z a} =$$

$$= -\frac{4mUa^3}{\pi\hbar^2}\,\frac{\sin q_x a}{q_x a}\,\frac{\sin q_y a}{q_y a}\,\frac{\sin q_z a}{q_z a} =$$

$$= -\frac{4mUa^3}{\pi\hbar^2}\,\frac{\sin[ka(1-\cos\theta)]}{ka(1-\cos\theta)}\,\frac{\sin[ka\sin\theta\cos\varphi]}{ka\sin\theta\cos\varphi}\,\frac{\sin[ka\sin\theta\sin\varphi]}{ka\sin\theta\sin\varphi}$$

1b). $$\frac{m}{2\pi\hbar^2}\left|\int \frac{e^{ikr'}}{r'} V(\vec{r}\,') e^{-i\vec{k}\vec{r}\,'} d^3r'\right| \ll 1$$

$$kr' \underset{\sim}{<} ka \ll 1 \Rightarrow$$

$$\frac{m}{\hbar^2}\int^{a} \frac{V(r')}{r'} d^3r' \ll 1 \Rightarrow$$

$$\frac{m}{\hbar^2}\frac{U}{a}a^3 \ll 1 \Rightarrow \underline{\underline{U \ll \frac{\hbar^2}{ma^2}}}.$$

1c). $$f(\theta,\varphi)_{k\to 0} = -\frac{4mUa^3}{\pi\hbar^2}\left(\lim_{x\to 0}\frac{\sin x}{x}\right)^3 = -\frac{4mUa^3}{\pi\hbar^2}$$

$$\sigma = 4\pi|f|^2 = 4\pi\,\frac{16m^2U^2a^6}{\pi^2\hbar^4} = \underline{\underline{\frac{64m^2U^2a^6}{\pi\hbar^4}}}.$$

Dimensions: $$[\sigma] = \frac{[m]^2[E]^2[a]^6}{[E]^4[t]^4} = \frac{[m]^2[a]^6}{[E]^2[t]^4} =$$

$$= \frac{[m]^2[a]^4}{[t]^4}\,\frac{[a]^2}{[E]^2} = \frac{[E]^2}{[E]^2}[a]^2 = \underline{\underline{[a]^2}}$$

1d). Optical theorem:

$$\sigma = \frac{4\pi}{k_0} \operatorname{Im} f(0).$$

$$\sigma = \int d\Omega \frac{\sin^2\theta}{k_0^2} \sim \frac{1}{k_0^2},\ \sigma > 0.$$

$$|f(0)| = \sqrt{\frac{d\sigma}{d\Omega}\Big|_{\theta=0}} = 0.$$

$$0 < \frac{k_0 \sigma}{4\pi} = \operatorname{Im} f(0) \leq |f(0)| = 0.$$

Thus, the results of the experiment contradict the optical theorem.

2a). $\langle\psi|\vec{d}|\psi\rangle = e\int|\psi|^2\vec{r}\,d^3r$. $|\psi|^2$ depends on $|\vec{r}|$ only but $\vec{r}$ changes its sign $\Rightarrow \langle\psi|\vec{d}|\psi\rangle = e\int_{x>0}|\psi(r)|^2(\vec{r}+(-\vec{r}))d^3r = 0$.

2b). $E_1 = \langle\psi|\hat{H}_{dd}|\psi\rangle = \frac{1}{R^3}\Big[\langle\psi_{1atom}|\hat{\vec{d}}_1|\psi_{1atom}\rangle\langle\psi_{2atom}|\hat{\vec{d}}_2|\psi_{2atom}\rangle$

$- 3(\vec{n}\langle\psi_{1atom}|\hat{\vec{d}}_1|\psi_{1atom}\rangle)(\vec{n}\langle\psi_{2atom}|\hat{\vec{d}}_2|\psi_{2atom}\rangle)\Big] =$

$= 0.$

2c). $E = \langle\psi|\hat{H}_w|\psi\rangle = -\frac{e^2}{16R^3}\int\frac{e^{-2r/a_B}}{\pi a_B^3}(r^2+z^2)d^3r$

$$\langle z^2\rangle = \frac{1}{e^2}\langle(\vec{n}\vec{d})^2\rangle = \frac{1}{3}\langle z^2+x^2+y^2\rangle = \frac{1}{3}\langle r^2\rangle$$

$$E = -\frac{e^2}{16R^3}\frac{4}{3}\int\frac{e^{-2r/a_B}}{\pi a_B^3}r^2d^3r = -\frac{e^2}{12R^3\pi a_B^3}4\pi\int e^{-2r/a_B}r^4dr =$$

$$= -\frac{e^2}{3R^3a_B^3}\int_0^\infty e^{-2r/a_B}r^4dr = -\frac{e^2}{3R^3a_B^3}\frac{a_B^5}{32}\int_0^\infty e^{-2r/a_B}\left(\frac{2r}{a_B}\right)^4 d\left(\frac{2r}{a_B}\right)$$

$$= -\frac{e^2a_B^2}{96R^3}\int_0^\infty e^{-x}x^4dx = -\frac{e^2a_B^2}{96R^3}\Gamma(5) = -\frac{e^2a_B^2}{96R^3}24 =$$

$$= -\frac{e^2a_B^2}{4R^3}.$$

2d). $E_{dd} = \sum_n\frac{|\langle 0|H_{dd}|n\rangle|^2}{E_0-E_n}$. $\langle 0|H_{dd}|n\rangle \sim \frac{1}{R^3} \Rightarrow$

$$\Rightarrow E_{dd} \sim \frac{1}{R^6}.$$

2e). $F_{dd} = -\nabla E_{dd} \sim \frac{1}{R^7}.$

2б). $\langle 0 | H_{dd} | n \rangle \sim (e a_B)^2 \frac{1}{R^3}$

$E_0 - E_n \sim Ry.$

$$E_{dd} \sim \frac{1}{R^6} \frac{(e a_B)^4}{Ry} . \qquad Ry \sim \frac{e^2}{a_B}$$

$$E_{dd} \sim \frac{1}{R^6} \frac{e^4 a_B^4}{\frac{e^2}{a_B}} = \frac{a_B^5}{R^6} e^2 \sim \frac{e^2}{a_B}\left(\frac{a_B^6}{R^6}\right) \sim Ry \left(\frac{0.5\,\mathring{A}}{5\,\mathring{A}}\right)^6 =$$

$$= 10^{-6}\, Ry \sim 10^{-6} \cdot 10\,eV \sim 10^{-6} \cdot 10^5\,K = 0.1 \cdot K \sim 10^{-17}\,erg.$$

3a). $$\hat{H} = \frac{1}{2m} \sum_a \left(\hat{p}_a - \frac{e}{c} \bar{A}(\bar{r}_a)\right)^2 + \sum_{a \neq b} \frac{e^2}{|\bar{r}_a - \bar{r}_b|} - Z e^2 \sum \frac{1}{|\bar{r}_a|} -$$

$$- \frac{e\hbar}{mc} \bar{B} \hat{S},$$ where $e = -|e|$, $\bar{r}_a, \hat{p}_a$ are coordinates and momenta of Z electrons.

3б). $$\hat{H}_1 = -\frac{1}{2m} \sum_a \frac{e}{c} \left(\hat{p}_a \bar{A}(\bar{r}_a) + \bar{A}(\bar{r}_a) \hat{p}_a\right) + \frac{|e|\hbar}{mc} \vec{B} \vec{S}$$

$$\hat{p} \bar{A} | \psi \rangle = -i\hbar \frac{\partial}{\partial r_\alpha} \frac{1}{2} \varepsilon^{\alpha\beta\gamma} B_\beta r_\gamma | \psi \rangle =$$

$$= -i\hbar \frac{1}{2} \varepsilon^{\alpha\beta\alpha} B_\beta + \frac{1}{2} \varepsilon^{\alpha\beta\gamma} B_\beta r_\gamma \left(-i\hbar \frac{\partial}{\partial r_\alpha}\right) | \psi \rangle =$$

$$= \bar{A} \hat{p} | \psi \rangle \Rightarrow$$

$$\hat{H}_1 = \frac{|e|}{mc} \sum \bar{A}(\bar{r}_a) \hat{p}_a + \frac{|e|\hbar}{mc} \vec{B} \vec{\hat{S}} =$$

$$= \frac{|e|}{2mc} \sum_a [\vec{B} \times \bar{r}_a] \vec{\hat{p}}_a + \frac{|e|\hbar}{mc} \bar{B} \hat{S} =$$

$$= \frac{|e|}{2mc} \sum \bar{B} [\bar{r}_a \times \hat{p}_a] = \frac{|e|\bar{B}}{2mc} \sum_a [\bar{r}_a \times \hat{p}_a] + \frac{|e|\hbar}{mc} \bar{B} \hat{S} =$$

$$= \frac{|e|\bar{B}\hbar}{2mc} (\hat{L} + 2\hat{S}).$$

3c). $E(M_J) = \langle M_J | \hat{H}_1 | M_J \rangle$ + constant.

$\hat{H}_1$ is a vector operator times $\bar{B}$.

Hence $\langle M_J | \hat{H}_1 | M_J \rangle = \vec{B} \langle M_J | \vec{\hat{V}} | M_J \rangle$,

where $\vec{\hat{V}}$ is a vector operator.

Matrix elements of a vector operator are proportional to matrix elements of $\vec{J}$

$E(M_J) = $ const $+ W \vec{B} \langle M_J | \vec{J} | M_J \rangle$.

$\langle M_J|\hat{J}_z|M_J\rangle \vec{e}_z = \vec{e}_z M_J$

$\langle M_J|\hat{J}_x|M_J\rangle = \langle M_J|\hat{J}_y|M_J\rangle = 0.$

Hence,

$$E(M_J) = \text{const} + W B M_J.$$

3d). $\langle M_J|\hat{\vec{L}} + 2\hat{\vec{S}}|M_J'\rangle = \alpha\langle M_J|\hat{\vec{J}}|M_J'\rangle$

$$\langle M_J|\hat{\vec{J}}(\hat{\vec{L}}+2\hat{\vec{S}})|M_J\rangle = \sum_{N_J}\langle M_J|\hat{\vec{J}}|N_J\rangle\langle N_J|\hat{\vec{L}}+2\hat{\vec{S}}|M_J\rangle =$$

$$= \sum_{N_J}\langle M_J|\hat{\vec{J}}|N_J\rangle\alpha\langle N_J|\hat{\vec{J}}|M_J\rangle = \alpha\langle M_J|\hat{\vec{J}}^2|M_J\rangle =$$

$$= \alpha J(J+1).$$

$$\langle M_J|\hat{\vec{J}}(\hat{\vec{L}}+2\hat{\vec{S}})|M_J\rangle = \langle M_J|\hat{\vec{J}}(\hat{\vec{J}}+\hat{\vec{S}})|M_J\rangle =$$

$$= \langle\hat{\vec{J}}^2\rangle + \langle\hat{\vec{J}}\hat{\vec{S}}\rangle = \langle\hat{\vec{J}}^2\rangle + \frac{1}{2}\langle\hat{\vec{J}}^2 + \hat{\vec{S}}^2 - (\hat{\vec{J}}-\hat{\vec{S}})^2\rangle$$

$$\left([\vec{J},\vec{S}] = [\vec{S},\vec{S}] + [\vec{L},\vec{S}] = 0\,!\right)$$

$$\langle M_J|\hat{\vec{J}}(\hat{\vec{L}}+2\hat{\vec{S}})|M_J\rangle = \langle\hat{\vec{J}}^2\rangle + \frac{1}{2}\langle\hat{\vec{J}}^2 + \hat{\vec{S}}^2 - \hat{\vec{L}}^2\rangle =$$

$$= J(J+1) + \frac{1}{2}\left(J(J+1) + S(S+1) - L(L+1)\right)$$

$$\alpha = 1 + \frac{1}{2}\,\frac{J(J+1) + S(S+1) - L(L+1)}{J(J+1)}$$

$$W = \frac{|e|\hbar}{2mc}\alpha = \left(1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}\right)\frac{|e|\hbar}{2mc}.$$

3e). For a photon $J_{photon} = 1$. Hence M_J changes by 1. (For a photon $|J_z| \le 1$).

$$\hbar\omega_{photon} = \Delta E_{atom}.$$

$$\Delta E_{atom} = W B \Delta M_J = W B \Rightarrow \omega_{photon} = \frac{WB}{\hbar}.$$

Note: this is a magnetic transition with very low probability!

3f). $(3s)^2(3p)^4 \Rightarrow (3p)^4$. $S_{max} \to \uparrow\uparrow\uparrow\downarrow \Rightarrow S = 1$.

L must be maximal for $S = 1$. $\uparrow\uparrow\uparrow$ is a half-filled shell. It makes zero contributi[on] to L. Hence, L is determined by just one p-electro[n]. $L = 1$. There is only one unfilled shell. It is more than half filled. Hence, $J = L + S = 2$.

3g). $$\omega = \frac{|e|\hbar}{2mc}\frac{B}{\hbar}\left(1 + \frac{2\cdot3 - \cancel{2} + \cancel{2}}{2\cdot2\cdot3}\right) = \frac{3}{4}\frac{|e|B}{mc} = \frac{3}{4}\frac{4.8\cdot10^{-10}\cdot10^4}{0.9\cdot10^{-27}\cdot3\cdot10^{10}} =$$

$$= 1.3\cdot10^{11}\ \text{Hz}.$$

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