Department of Physics
IIT-Madras

PCD_STiAP_Self_Assesment_1
15 marks

Q1. Write down the operators $U_R(\delta\phi_x)$ and $U_R(\delta\phi_y)$ for infinitesimal rotations about the Cartesian axes X and Y through infinitesimal rotation angles and find their commutator.

→2 marks

A1: $U_R(\delta\phi_x) = 1 - \frac{i}{\hbar}\delta\phi_x J_x$

$U_R(\delta\phi_y) = 1 - \frac{i}{\hbar}\delta\phi_y J_y$

The operators do not commute since for this operator, rotation through X axis and then through Y axis is not the same when reversed.

Q2. In the Pauli-Lenz quantum vector for the hydrogen atom given by $\vec{A}_{QM} = \frac{1}{2\mu}\left[\vec{p}\times\vec{L} - \vec{L}\times\vec{p}\right] - \kappa\hat{r}$, express κ in terms of the physical properties of the electron and state the dimensions of κ.

→2 marks

A2. κ is the parameter which gives the strength of the centre field potential. The dimensions of κ is $[\vec{v}\times\vec{H}] = LT^{-1}\times L^2T^{-1} = L^3T^{-2}$

Q3. Recall that $[J_+, J_-]_- = 2\hbar J_z$ and $J_+|jm\rangle = \lambda_m\hbar|j,m+1\rangle$ using these relations find $|\lambda_{m-1}|^2 - |\lambda_m|^2$ in terms of the eigenvalue $\hbar m$ of the operator J_z.

→3 marks

A3.

$$[J_+, J_-]_- = 2\hbar J_z$$

$$\langle jm|J_+J_- - J_-J_+|jm\rangle = 2\hbar\langle jm|J_z|jm\rangle$$

$$\langle jm|J_+J_-|jm\rangle - \langle jm|J_-J_+|jm\rangle = 2\hbar\langle jm|J_z|jm\rangle$$

$$\lambda^*_{m-1}\hbar\langle jm|J_+|jm-1\rangle - \lambda_m\hbar\langle jm|J_-|jm+1\rangle = 2\hbar\langle jm|J_z|jm\rangle$$

$$\lambda^*_{m-1}\hbar\lambda_{m-1}\hbar\langle jm||jm\rangle - \lambda_m\hbar\lambda^*_m\hbar\langle jm||jm\rangle = 2\hbar m\hbar\langle jm||jm\rangle$$

$$|\lambda_{m-1}|^2 - |\lambda_m|^2 = 2m$$

Q4. When can a vector $\vec{A}$ be a vector operator $\vec{A}_{op}$? Explain how the condition for $\vec{A}$ to be the vector operator $\vec{A}_{op}$ determines how the angular momentum of a system can be defined.

→2 marks

A4. A vector $\vec{A}$ can be a vector operator $\vec{A}_{op}$ if it transforms under rotation as per $U_R^+ A_i U_R = \sum_{j=1}^{3} R_{ij} A_j$ or equivalently it should follow the commutation relations $\left[A_i, J_j\right] = i\hbar\varepsilon_{ijk} A_k$.

where $\vec{J} = \sum_{j=1}^{3} J_i \hat{e}_i$ is the generator of rotations. It is called as angular momentum.

The transformation of vector A to be an $\vec{A}_{op}$ determines the definition of angular momentum to be the generator of rotations such that the above relations hold good. (If not either the vector A cannot be a vector operator or the angular momentum operator must be defined differently)

Q5. What are the principal objectives of the Foldy-Wouthuysen transformations of the Dirac Hamiltonian? → 1 mark

---

A5. The Principle objective is to decouple the Dirac equation into *two* two-component equations: one reduces to the Pauli description in the non-relativistic limit; the other describes the negative energy states.

Q6. Prove that: $\dfrac{\left(c\vec{\alpha}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\right)^2}{2mc^2} = \dfrac{1}{2m}\left\{\vec{\pi}^2 + i\vec{\sigma}\cdot\vec{\pi}\times\vec{\pi}\right\}1_{4\times4}$ →3 marks

---

A6. $$\frac{\left(c\vec{\alpha}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\right)^2}{2mc^2} = \frac{1}{2m}\left\{\vec{\alpha}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\right\}\left\{\vec{\alpha}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)\right\}$$

$$\frac{\theta^2}{2mc^2} = \frac{1}{2m}\left\{\begin{pmatrix}\vec{0} & \vec{\sigma}\\ \vec{\sigma} & \vec{0}\end{pmatrix}\cdot\vec{\pi}\right\}\left\{\begin{pmatrix}\vec{0} & \vec{\sigma}\\ \vec{\sigma} & \vec{0}\end{pmatrix}\cdot\vec{\pi}\right\}$$
$$= \frac{1}{2m}\begin{pmatrix}\vec{0} & \vec{\sigma}\cdot\vec{\pi}\\ \vec{\sigma}\cdot\vec{\pi} & \vec{0}\end{pmatrix}\begin{pmatrix}\vec{0} & \vec{\sigma}\cdot\vec{\pi}\\ \vec{\sigma}\cdot\vec{\pi} & \vec{0}\end{pmatrix}$$

Where $\theta = c\vec{\alpha}\cdot\left(\vec{p}-\frac{e}{c}\vec{A}\right)$ and $\pi = \left(\vec{p}-\frac{e}{c}\vec{A}\right)$

$$\frac{\theta^2}{2mc^2} = \frac{1}{2m}\begin{pmatrix}\vec{\sigma}\cdot\vec{\pi}\,\vec{\sigma}\cdot\vec{\pi} & 0\\ 0 & \vec{\sigma}\cdot\vec{\pi}\,\vec{\sigma}\cdot\vec{\pi}\end{pmatrix}$$; Using Pauli's identity
$$= \frac{1}{2m}\vec{\sigma}\cdot\vec{\pi}\,\vec{\sigma}\cdot\vec{\pi}\;1_{4\times4}$$

$$\frac{\theta^2}{2mc^2} = \frac{1}{2m}\left\{\vec{\pi}^2 + i\vec{\sigma}\cdot\vec{\pi}\times\vec{\pi}\right\}1_{4\times 4}$$

Q7. Determine if the exchange integral for a pair of electrons can be non-zero if their spins are anti-parallel. →2 marks

The Exchange integral,

$$K = \iint dq_1 dq_2 u^*_{\alpha_i}(q_2) u^*_{\alpha_j}(q_1) \frac{1}{r_{12}} u_{\alpha_i}(q_1) u_{\alpha_j}(q_2)$$

Now, $\int dq \_\_\_\_\_\_ \equiv \iiint dV \_\_\_\_\_\_ \quad \sum_{\zeta} \_\_$

$$K = \iint dV_1 dV_2 u^*_{\alpha_i}(\vec{r}_2) u^*_{\alpha_j}(\vec{r}_1) \frac{1}{r_{12}} u_{\alpha_i}(\vec{r}_1) u_{\alpha_j}(\vec{r}_2) \times \sum_{\zeta_1}\sum_{\zeta_2} \langle \zeta_2 | m_{s_i} \rangle^* \langle \zeta_1 | m_{s_j} \rangle^* \langle \zeta_1 | m_{s_i} \rangle \langle \zeta_2 | m_{s_j} \rangle$$

$$K = \iint \_\_\_\_\_\_ \times \sum_{\zeta_1}\sum_{\zeta_2} \langle m_{s_i} | \zeta_2 \rangle \langle m_{s_j} | \zeta_1 \rangle \langle \zeta_1 | m_{s_i} \rangle \langle \zeta_2 | m_{s_j} \rangle$$

$$K = \iint \_\_\_\_\_\_ \times \langle m_{s_i} | m_{s_i} \rangle \times \langle m_{s_j} | m_{s_j} \rangle$$

$$K = \iint \_\_\_\_\_\_ \times \delta_{m_{s_j} m_{s_i}}$$

$\Rightarrow$ Exchange integral exists only if spins are antiparallel.