(vi) Results: beam splits into two clearly resolved components for large $\partial B_z/\partial z$.

(vii) Conclusions: Magnetic moment is quantized. Hence, angular momentum is quantized. Actually, the experiment with Cs and Ag demonstrates quantization of spin angular momentum.

Q.3–2 *A good answer would include the following points:*

(i) Representation of states: spinors of functions

$$\psi = [\psi_1 \quad \psi_2]^T = \psi_1[1 \quad 0]^T + \psi_2[0 \quad 1]^T.$$

Inner product: $(\mathbf{\Psi}, \mathbf{\Phi}) = \int(\psi_1^*\phi_1 + \psi_2^*\phi_2)\, dV$.

(ii) Representation of angular momentum observables: orbital angular momentum operators $\widehat{\mathrm{L}}^2$, $\widehat{\mathrm{L}}_z$, etc. act on both functions in a spinor of functions, and spin matrices $\mathbf{S}$, $\mathbf{S}_z$, etc. act on spinors of functions as if they were spinors.

Total angular momentum defined $\widehat{\mathbf{J}} = \widehat{\mathbf{L}} + \widehat{\mathbf{S}}$, where $\widehat{\mathbf{L}} = (\widehat{\mathrm{L}}_x, \widehat{\mathrm{L}}_y, \widehat{\mathrm{L}}_z)$, $\widehat{\mathbf{S}} = (\widehat{\mathrm{S}}_x, \widehat{\mathrm{S}}_y, \widehat{\mathrm{S}}_z)$ where $\widehat{\mathrm{S}}_x \equiv \mathbf{S}_x$, etc.

(iii) Example of action of operators on spinors of functions:

$$\begin{aligned}
\widehat{\mathrm{J}}_z\mathbf{\Psi} = \widehat{\mathrm{J}}_z\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} &= \widehat{\mathrm{L}}_z\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} + \widehat{\mathrm{S}}_z\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}\\
&= \frac{\hbar}{\mathrm{i}}\begin{bmatrix}\partial\psi_1/\partial\phi\\ \partial\psi_2/\partial\phi\end{bmatrix} + \frac{\hbar}{2}\begin{bmatrix}\psi_1\\ -\psi_2\end{bmatrix}\\
&= \frac{\hbar}{\mathrm{i}}\begin{bmatrix}\partial\psi_1/\partial\phi + (\mathrm{i}/2)\psi_1\\ \partial\psi_2/\partial\phi - (\mathrm{i}/2)\psi_2\end{bmatrix}
\end{aligned}$$

(iv) Application: *Zeeman effect* – some energy levels and spectral lines of atoms are split by external magnetic field. Or
Spin-orbit perturbation. In chosen case, indicate how perturbation is calculated.

Q.3–3 *A good answer would include the following points:*

(i) Classical hamiltonian

$$\frac{1}{2M}(p_1^2 + p_2^2) + \frac{1}{2m}p_e^2 + \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|^2} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_e|^2} - \frac{1}{|\mathbf{r}_2 - \mathbf{r}_e|^2}\right).$$

(ii) Replace p_1 by $\dfrac{\hbar}{\mathrm{i}}\dfrac{\partial}{\partial x_1}$ etc. to give $\widehat{\mathrm{H}}$ and thence Schrödinger's equation

$$\widehat{\mathrm{H}}\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_e) = E\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_e)$$

9 coordinates!

(iii) Approximations: (a) Remove centre of mass motion and introduce reduced mass of electron; (b) Assume protons are fixed thus eliminating proton kinetic energy terms from $\widehat{\mathrm{H}}$. Proton coordinates are then parameters in V.

(iv) Method of solution: Determine total energy as a function of proton–proton separation, where total energy = proton–proton repulsion plus ground state energy of electron in double potential well. Assume equilibrium configuration of H_2^+ is found by minimizing the total energy, as a function of proton–proton separation.

(v) Ground state energy of electron in double well found by using a variational wave function constructed as a linear combination of hydrogen 1s orbitals.

The combination $\psi_+ = (1/\sqrt{2})[\psi_{1s}(1) + \psi_{1s}(2)]$ leads to binding because of large charge density, $(e|\psi_+|^2)$, between the protons.

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