Quantum Mechanics 3 2001/2002

Solution set 7

(1) The vector $\boldsymbol{\sigma}$ is defined as a vector whose components are matrices: $\boldsymbol{\sigma} = \sigma_1 \hat{\mathbf{x}} + \sigma_2 \hat{\mathbf{y}} + \sigma_3 \hat{\mathbf{z}}$. Taking the dot product with the vector e gives

$$S/(\hbar/2) = (\sin\theta)\sigma_1 + (\cos\theta)\sigma_3 = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}.$$

There is no contribution from σ_2 as $\mathbf{e}$ does not contain $\hat{y}$.

The matrix S represents angular momentum along the vector $\mathbf{e}$, so we expect that the eigenvalues must be $\pm\hbar/2$. It will therefore be easier to work with the matrix $M = S/(\hbar/2)$, whose eigenvalues should be ± 1. To prove this, solve $M\psi = \lambda\psi$ As usual, this requires the zero determinant $|M - \lambda I| = 0$:

$$\begin{vmatrix} \cos\theta - \lambda & \sin\theta \\ \sin\theta & -\cos\theta - \lambda \end{vmatrix} = \lambda^2 - \cos^2\theta - \sin^2\theta = \lambda^2 - 1 = 0.$$

Hence the eigenvalues are as expected.

For the eigenvectors, we therefore need $M\psi = \pm\psi$. Writing ψ as a two-component vector,

$$\psi = \begin{pmatrix} A \\ B \end{pmatrix},$$

we get the two equations

$$A\cos\theta + B\sin\theta = \pm A$$
$$A\sin\theta - B\cos\theta = \pm B.$$

These give

$$A/B = \sin\theta(\pm 1 - \cos\theta)$$
$$A/B = (\cos\theta \pm 1)/\sin\theta$$

but these are the same equation (divide the rhs), so we only get the ratio (reasonably - haven't yet used normalization). Therefore

$$\psi = N \begin{pmatrix} \sin\theta \\ \pm 1 - \cos\theta \end{pmatrix},$$

where N is the normalization factor. We require the vector dot product with its conjugate to be unity, so $|N|^2 = (2 - \pm 2\cos\theta)^{-1}$

Finally, write $|\uparrow\rangle = \alpha\psi_+ + \beta\psi_-$. The coefficients α and β come from the dot product of $|\uparrow\rangle$ with ψ_+ and ψ_-:

$$\alpha = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot N \begin{pmatrix} \sin\theta \\ 1 - \cos\theta \end{pmatrix} = N \sin\theta.$$

The ratio of the two beam intensities is just $|\alpha|^2/|\beta|^2 = |N_+|^2/|N_-|^2$ (the $\sin\theta$ factors cancel), which is $(1+\cos\theta)/(1-\cos\theta)$, or $\cot^2(\theta/2)$.

(2) For a given n, ℓ takes integer values, with a minimum value of 0 and a maximum value of $n-1$. This makes n different values of ℓ in all.

For a given ℓ, m takes integer values, with a minimum value of $-\ell$ and a maximum value of $+\ell$. This makes $2\ell+1$ different values of m for a given value of ℓ. The total degeneracy is therefore

$$\begin{aligned} \sum_{\ell=0}^{\ell=n-1} 2\ell + 1 &= n + 2 \sum_{\ell=0}^{\ell=n-1} \ell \\ &= n + 2\left(\sum_{\ell=1}^{\ell=n} \ell - n \right) \\ &= 2\,\frac{n(n+1)}{2} - n \quad \text{(using given formula)} \\ &= n^2. \end{aligned}$$

The effect of spin is just to double this (each level can take one electron spin up and one spin down).

(3) Normalization requires

$$\int |\psi|^2 dV = 1 = \int |R|^2\, r^2\, dr \int |Y|^2 \sin\theta\, d\theta\, d\phi.$$

If $R \propto r^{-\alpha}$, the radial integral is $\propto \int r^{2-2\alpha}\, dr$. This diverges at $r=0$ if $2-2\alpha < -1$, or $\alpha > 3/2$. Thus, there is no objection to divergent wavefunctions from the point of view of normalization, provided the divergence is not too extreme.

Now consider the energy eigenvalue, which is $\langle H \rangle = \int \psi^* H \psi\, dV$:

$$H\psi = \frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\left(r^2 \psi'\right)' - \frac{\ell(\ell+1)}{r^2}\psi \right] + V\psi.$$

If $\psi \propto r^{-\alpha}$, the term in square brackets is $[\alpha(\alpha-1) - \ell(\ell+1)]\psi/r^2$. This vanishes if $\alpha = -\ell$, but otherwise causes a divergent energy if $\alpha > 1/2$.

Whatever happens with the first term, $\int \psi^* V \psi \, dV$ causes divergence at $r = 0$ if $2 - \alpha - (\alpha + \beta) < -1$ (we assumed $V \propto r^{-\beta}$). Therefore, again the energy diverges if $\alpha > (3 - \beta)/2$.

Recall that we had a choice of $\psi \propto r^\ell$ or $\psi \propto r^{-(\ell+1)}$ in the Hydrogen atom. The reason we reject the second one is not that it can't be normalized (it can, at least for $\ell = 0$), but because it gives divergent energies, which are unphysical. Many books say that the fact that ψ diverges at $r = 0$ is enough reason to reject it, but the above shows that divergent wavefunctions are OK – it's just that $\psi \propto r^{-(\ell+1)}$ is too divergent.