Quantum Theory Solutions

1. (a) [8 marks] [B,S]

(i) [2 marks] The stationary state Schrödinger equation (SSSE) for the wave-function $\psi(x)$ of a particle of mass m moving in one dimension in a potential $V(x)$ is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi.$$

(ii) [4 marks] Set $\phi(x) = \psi(-x)$ then $\phi'(x) = -\psi'(-x)$ and so $\phi''(x) = \psi''(-x)$. Therefore

$$-\frac{\hbar^2}{2m}\phi''(x) + V(x)\phi(x) = -\frac{\hbar^2}{2m}\psi''(-x) + V(-x)\psi(-x) = E\psi(-x) = E\phi(x),$$

QED

Check normalisation:

$$\int_{-\infty}^{\infty} |\phi(x)|^2 dx = \int_{-\infty}^{\infty} |\psi(-x)|^2 dx = \int_{-\infty}^{\infty} |\psi(y)|^2 dy,$$

where $y = -x$, so ϕ is normalised if ψ is.

(iii) [2 marks] Introduce $\psi_{\pm}(x) = \psi(x) \pm \phi(x)$ then linearity of SSSE implies that $\psi_{\pm}$ are both solutions of SSSE with the same E but $\psi_{\pm}$ are respectively even and odd. One or other may be zero but still QED.

(b) [17 marks] [B,S, (iii),(iv) N]

(i) [8 marks] In $-a < x < a$ SSSE becomes

$$\psi'' = -\frac{2m}{\hbar^2}(E + V_0)\psi = -\kappa^2\psi$$

and solution is as indicated, while elsewhere

$$\psi'' = -\frac{2m}{\hbar^2}E\psi = k^2\psi$$

when normalisability leads to solution as indicated in problem.

(ii) [2 marks] For even ψ you need $A = D$ and $C = 0$, so that

$$\psi = B\cos\kappa x \text{ for } -a < x < a$$
$$= A\mathrm{e}^{-kx} \text{ for } x \geqslant a.$$

(iii) [5 marks] We want ψ continuous with continuous derivative at a (when the same will hold at $-a$ by even-ness). Thus

$$A\mathrm{e}^{-ka} = B\cos\kappa a, \quad -kA\mathrm{e}^{-ka} = -B\kappa\sin\kappa a,$$

and take the ratio to obtain

$$\alpha = ka = \kappa a\tan\kappa a = \beta\tan\beta,$$

while

$$\alpha^2 + \beta^2 = a^2(k^2 + \kappa^2) = \frac{2mV_0a^2}{\hbar^2} \qquad (*).$$

QED

(iv) [2 marks] The graph of $\alpha = f(\beta) := \beta\tan\beta$ has a minimum at the origin and tends to infinity as β tends to $\pi/2$ so necessarily it escapes from the circle defined by (*). Any intersection of the two curves (and there is at least one) gives a solution of the desired form.

2. (i) [6 marks] [B] By inspection and self-adjointness of P, X

$$a_+ = P + im\omega X.$$

Then

$$a_+a_- = (P + im\omega X)(P - im\omega X) = P^2 + m^2\omega^2 X^2 + im\omega(XP - PX) = 2mH - m\hbar\omega,$$

QED, while

$$a_-a_+ = (P - im\omega X)(P + im\omega X) = P^2 + m^2\omega^2 X^2 - im\omega(XP - PX) = 2mH + m\hbar\omega,$$

QED and at once

$$[a_-, a_+] = a_-a_+ - a_+a_- = 2m\hbar\omega,$$

QED.

(ii) [5 marks] [B] Various routes, for example first calculate

$$[2mH, a_-] = [a_-a_+ - m\hbar\omega] = [a_-a_+, a_-] = a_-[a_+, a_-] = -2m\hbar\omega a_-$$

and similarly

$$[2mH, a_+] = [a_-a_+, a_+] = [a_-, a_+]a_+ = 2m\hbar\omega a_+$$

so that

$$Ha_-\psi = (Ha_- - a_-H + a_-H)\psi = (E - \hbar\omega)a_-\psi$$

and

$$Ha_+\psi = (Ha_+ - a_+H + a_+H)\psi = (E + \hbar\omega)a_+\psi.$$

Thus $a_\pm\psi$ are eigenstates with eigenvalues $E \pm \hbar\omega$.

(iii) [2 marks] [B] Calculate

$$||a_-\psi||^2 = \langle a_-\psi|a_-\psi\rangle = \langle\psi|a_+a_-\psi\rangle = 2m(E - \frac{1}{2}\hbar\omega)\langle\psi|\psi\rangle = 2m(E - \frac{1}{2}\hbar\omega)||\psi||^2,$$

QED

(iv) [4 marks] [B] So by repeatedly lowering with a_- from an initial ψ with $H\psi = E\psi$ we obtain a sequence $(a_-)^k\psi$ with energy eigenvalues $E - k\hbar\omega$. Since we need $||a_-\psi||^2 \geqslant 0$ for any state this process must stop at some stage, by previous subpart, and can only stop at a state with $E = \hbar\omega/2$. Call this a ground state ψ_0 (not yet *the* ground state), then raising n times gives a state $(a_+)^n\psi_0$ with $E = E_n := (n + 1/2)\hbar\omega$ so these are the only possible energy eigenvalues.

(v) [1 mark] [B] If the ground-state is nondegenerate then there is only one linearly independent ψ_0 (now it is *the* ground state) and the higher states are obtained by raising it (if there were two linearly independent states at level k say then they would lower to independent ground states).

(vi) [4 marks] [S,N]
First remark that eigen-states with different E-values are orthogonal (proof not required but it could be

$$\text{“}E_1\langle\psi_1|\psi_2\rangle = \langle H\psi_1|\psi_2\rangle = \langle\psi_1|H\psi_2\rangle = E_2\langle\psi_1|\psi_2\rangle$$

but $E_1 \neq E_2$ so $\langle\psi_1|\psi_2\rangle = 0$”).

Now if ψ is a state at level k then $\psi \propto (a_+)^k \psi_0$ so

$$\langle \psi | a_- \psi \rangle = \langle a_+ \psi | \psi \rangle \propto \langle (a_+)^{k+1} \psi_0 | (a_+)^k \psi_0 \rangle,$$

which vanishes by previous remark.
So

$$\langle \psi | a_- \psi \rangle = 0 = \langle \psi | P \psi \rangle - im\omega \langle \psi | X \psi \rangle = \mathbb{E}_\psi(P) - im\omega \mathbb{E}_\psi(X),$$

provided ψ is normalised, but both expectations are real so that

$$\mathbb{E}_\psi(P) = 0 = \mathbb{E}_\psi(X).$$

(vii) [3 marks] [S, N] Arguing as in (vi) deduce

$$\langle \psi | (a_-)^2 \psi \rangle = 0 = \langle \psi | (P - im\omega X)^2 \psi \rangle = \langle \psi | P^2 - m^2 \omega^2 X^2 - 2im\omega(PX + XP) \psi \rangle.$$

Real part implies

$$\langle \psi | P^2 \psi \rangle = m^2 \omega^2 \langle \psi | X^2 \psi \rangle,$$

which says

$$\mathbb{E}_\psi(T) = \mathbb{E}_\psi(\frac{P^2}{2m}) = \mathbb{E}_\psi(\frac{m\omega^2 X^2}{2}) = \mathbb{E}_\psi(V),$$

but

$$\mathbb{E}_\psi(T + V) = E$$

so

$$\mathbb{E}_\psi(T) = \mathbb{E}_\psi(V) = E/2.$$

Now

$$\Delta_\psi(X) = \sqrt{\mathbb{E}_\psi(X^2) - (\mathbb{E}_\psi(X))^2} = \sqrt{\mathbb{E}_\psi(X^2)} = \sqrt{\frac{2}{m\omega^2} \mathbb{E}_\psi(V)}$$

which gives answer; similar for P.

3. (i) [2 marks] [B] We have $r\psi = fe^{-\alpha r}$ so that

$$(r\psi)'' = (f'' - 2\alpha f' + \alpha^2 f)e^{-\alpha r}.$$

SE multiplied by $-2mr/\hbar^2$ is

$$(r\psi)'' - \frac{\ell(\ell+1)}{r^2}(r\psi) + \frac{2mKZ}{\hbar^2 r}(r\psi) - \alpha^2(r\psi) = 0,$$

which is precisely

$$e^{-\alpha r}(f'' - 2\alpha f' - \frac{\ell(\ell+1)}{r^2}f + \frac{2mKZ}{\hbar^2 r}f) = 0,$$

QED

(ii) [6 marks] [B] Make the substitution to obtain

$$\sum_k((k+c)(k+c-1) - \ell(\ell+1))a_k r^{k+c-2} - \sum_k(2\alpha(k+c) - 2mKZ/\hbar^2)a_k r^{k+c-1} = 0,$$

and coefficients of all powers must vanish. Lowest power is r^{c-2} with coefficient

$$a_0(c(c-1) - \ell(\ell+1))$$

which must vanish, but $a_0 \neq 0$, whence indicial equation.
Indicial equation factorises as

$$(c+\ell)(c-\ell-1) = 0,$$

but the choice $c = -\ell$ means f begins $a_0 r^{-\ell}$ so ψ begins $r^{-\ell-1}$ and is unbounded at the origin which we forbid on physical grounds. Thus we need the other root: $c = \ell + 1$.

(iii) [8 marks] [B]
The coefficient of r^{k+c-1} is

$$a_{k+1}((k+c+1)(k+c) - \ell(\ell+1)) - 2a_k(\alpha(k+c) - mKZ/\hbar^2)$$

and vanishing of this with value of c plugged in gives answer.
If the series continues forever then asymptotically

$$a_{k+1}/a_k \sim 2\alpha/k$$

so that $f \sim e^{2\alpha r}$ but then $r\psi \sim e^{\alpha r}$ which does not give normalisable ψ. Thus normalisability requires the series to terminate: there must be an n with $a_{n+1} = 0$ and then $a_N = 0$ for $N > n$. This happens provided

$$\alpha(n + \ell + 1) - mKZ/\hbar^2 = 0,$$

QED and then f is a polynomial of degree $n + c = n + \ell + 1$.

(iv) [5 marks] [B,S] For the ground state α has its maximum value (so that E has its minimum value) which requires $n = \ell = 0$, $\alpha = mKZ/\hbar^2$ and $f = a_0 r$. Note $\ell = 0$ means independent of angles. Then

$$\psi(r,\theta,\phi) = \psi(r) = r^{-1}f(r)e^{-\alpha_0 r} = a_0 e^{-\alpha_0 r}.$$

For normalisation, remember that the integral is over $\mathbb{R}^3$ so that

$$1 = \int\int\int |\psi(r)|^2 r^2 \sin\theta dr d\theta d\phi = 4\pi |a_0|^2 \int r^2 e^{-2\alpha_0 r} dr.$$

To do the integral put $R = 2\alpha_0 r$ when

$$\int r^2 e^{-2\alpha_0 r} dr = \frac{1}{8\alpha_0^3} \int R^2 e^{-R} dR = \frac{1}{4\alpha_0^3},$$

whence w.l.o.g. the given a_0.

(v) [4 marks] [B,N] Claim

$$\mathbb{E}_{\psi_0}(r) = \int\int\int r|\psi_0|^2 r^2 \sin\theta dr d\theta d\phi,$$

then

$$= 4\alpha_0^3 \int r^3 e^{-2\alpha_0 r} dr = \frac{1}{4\alpha_0} \int R^3 e^{-R} dR = \frac{3}{2\alpha_0} = \frac{3\hbar^2}{2mKZ}.$$

Take this as a measure of the 'size' of the atom then it is inversely proportional to Z so a helium atom is half the size of a hydrogen atom.