Quantum Mechanics: Practice Exam

Course: FUF040
Responsible: Tom Blackburn
Time allowed: 4 hours
Permitted materials: Physics Handbook (beta), formula sheet
You may answer in either Swedish or English.

1. (2 points) What does a quantum state $|\psi\rangle$ represent?

> **Solution:** A quantum state is a complete set of probability amplitudes for a system, from which we can obtain the probability of each and every possible outcome of each and every possible measurement that can be made of the system.

2. (4 points) What are Hermitian operators and why are they used to represent physical observables?

> **Solution:** A Hermitian operator is equal to its own adjoint, i.e. $\langle a|\hat{Q}|b\rangle^\star = \langle b|\hat{Q}|a\rangle$. They are used to represent because their eigenvalues are real and their eigenvectors, which are mutually orthogonal, form a complete basis.

3. (4 points) If you measure a physical observable Q and get the result q, the state of the system after the measurement is $|q\rangle$. Does that mean the system state was $|q\rangle$ *before* you did the measurement?

> **Solution:** It is an axiom of QM that, on measurement, a quantum state $|\psi\rangle$ 'collapses' to an eigenstate of the operator that is associated with the physical observable being measured: $|\psi\rangle \to |q\rangle$. In this case, the system state before the measurement is *not* $|q\rangle$. However, if a subsequent measurement is made immediately after the first, no collapse takes place. In this case, the system state is indeed $|q\rangle$ before the measurement.

4. (a) (4 points) Prove Ehrenfest's theorem,

$$\frac{d\langle p_x\rangle}{dt} = -\left\langle \frac{\partial V(x)}{\partial x} \right\rangle, \qquad \frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}, \tag{1}$$

where x and p_x are position and momentum respectively, $V(x)$ is the potential energy, and m is the particle mass.

Solution: You could either go general or specific. In the first case, the starting point is the time evolution of an expectation value $\langle Q\rangle = \langle\psi|\,\hat{Q}\,|\psi\rangle$. Differentiate this w.r.t. to time and then substitute the TDSE: $\hat{H}\,|\psi\rangle = i\hbar\frac{\partial}{\partial t}\,|\psi\rangle$. Rearrange, identify the commutator $[\hat{H},\hat{Q}]$ and then specialise to $\hat{x}$ and $\hat{p}$. The tricky bit is the commutator of $[\hat{p},\hat{V}]$: handle this in the position basis, i.e. $\langle\psi|\,[\hat{p},\hat{V}]\,|\psi\rangle = \int_{-\infty}^{\infty} dx\psi^\star(x)[-i\hbar\frac{\partial}{\partial x}, V(x)]\psi(x)$.

(b) (2 points) Ehrenfest's theorem is usually stated as "expectation values obey classical equations of motion." Your colleague, Dr Knowitall, says that this isn't true. Discuss whether he is correct or not.

Solution: A truly classical equation of motion would be $\frac{d\langle p_x\rangle}{dt} = -\frac{\partial V(\langle x\rangle)}{\partial\langle x\rangle}$, which Ehrenfest's theorem is not. So the good doctor is strictly correct. However, if the uncertainty in x is small, these two are very close to being equal. And for simple potentials, such as the harmonic oscillator, they are identical.

5. The state of an electron is given by

$$|\psi\rangle = \frac{2}{3}\,|\uparrow\rangle + \frac{\sqrt{5}}{3}\,|\downarrow\rangle \tag{2}$$

at $t = 0$, where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of the spin operator $\hat{S}_z$, with eigenvalues $S_z = \pm 1$ respectively.

(a) (4 points) At $t = 0$, what is the probability that a measurement of the spin along the z-axis gives $S_z = +1$? What is the probability that a measurement of the spin along the x-axis gives $S_x = +1$?

Solution: $P(S_z = +1) = |\,\langle\uparrow|\psi\rangle\,|^2 = 4/9$. To get the second, you need to express eigenstates of $\hat{S}_x$ in terms of $|\uparrow\rangle$ and $|\downarrow\rangle$. Remembering that the matrix representation of $\hat{S}_x$ is given by the Pauli matrix σ_x, we get $|S_x = +1\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$. So $P(S_x = +1) = 1/2 + 2\sqrt{5}/9 \simeq 0.997$.

(b) (4 points) The Hamiltonian for this system is given by $\hat{H} = \mu\mathcal{B}\hat{S}_z$, where μ and $\mathcal{B}$ are real constants. What is the probability that a measurement of the spin along the z-axis, at time t, gives $S_z = +1$? What is the probability that a measurement of the spin along the x-axis, at time t, gives $S_x = +1$?

> **Solution:** The time-dependent state follows as $|\psi;t\rangle = \frac{2}{3}e^{-i\omega t}|\uparrow\rangle + \frac{\sqrt{5}}{3}e^{i\omega t}|\downarrow\rangle$ where $\omega = \mu B/\hbar$. So $P(S_z = +1) = 4/9$ (stationary states!) and $P(S_z = +1) = 1/2 + 2\sqrt{5}\cos(2\omega t)/9$.

6. A large number N of hydrogen atoms are prepared such that the wavefunction of the electron in each atom, at time $t = 0$, is given by:

$$\psi(\mathbf{r}) = \frac{1}{2\sqrt{\pi}a_0^{3/2}}\left[e^{-r/a_0} + \frac{\sqrt{3}}{4\sqrt{2}}\frac{z}{a_0}e^{-r/(2a_0)}\right] \tag{3}$$

where $a_0 = 4\pi\varepsilon_0\hbar^2/(me^2)$ is the Bohr radius.

(a) (4 points) If we measure the magnitude of the orbital angular momentum of all the electrons, L_i^2, at $t = 0$, what do you predict will be the mean of the results $\langle L^2\rangle = \sum_i L_i^2/N$?

> **Solution:** We need to apply $\hat{L}^2$ to this wavefunction. Only the term with $z = r\cos\theta$ contributes, so we get
>
> $$\hat{L}^2\psi = \underbrace{2\hbar^2}_{\ell(\ell+1)\hbar^2}\frac{1}{2\sqrt{\pi}a_0^{3/2}}\frac{\sqrt{3}}{4\sqrt{2}}\frac{z}{a_0}e^{-r/(2a_0)}, \tag{4}$$
>
> i.e. the same wavefunction back. As such, we recognise the first and second terms as angular momentum eigenstates with $\ell = 0$ and $\ell = 1$ respectively. Now multiply by ψ and integrate, remembering that $d^3\mathbf{r} = r^2\sin\theta dr d\theta d\phi$. There will be two terms, one $\propto\cos\theta$, which vanishes on integration over $0 < \theta < \pi$, and one $\propto\cos^2\theta$, which does not:
>
> $$\langle L^2\rangle = 2\hbar^2\frac{3}{32\times 4\pi a_0^5}\underbrace{\int_0^{2\pi}d\phi}_{2\pi}\underbrace{\int_0^{\pi}d\theta\,\sin\theta\cos^2\theta}_{2/3}\underbrace{\int_0^{\infty}dr\,r^4e^{-r/a_0}}_{24a_0^5} = \frac{3}{2}\hbar^2 \tag{5}$$

(b) (4 points) If we measure the energies of all the electrons, E_i, at $t = 0$, what do you predict will be the mean of the results $\langle E\rangle = \sum_i E_i/N$?

> **Solution:** We need to apply $\hat{H} = \hat{p}_r^2/(2m) + \hat{L}^2/(2m\hat{r}^2) - e^2/(4\pi\epsilon_0\hat{r})$ to this wave-

function. Going term by term,

$$\frac{\hat{p}_r^2}{2m}\psi = -\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) \tag{6}$$

$$= \frac{\hbar^2}{2m}\frac{1}{2\sqrt{\pi}a_0^{3/2}}\left[\left(\frac{2}{a_0 r} - \frac{1}{a_0^2}\right)e^{-r/a_0} + \left(\frac{2}{a_0 r} - \frac{2}{r^2} - \frac{1}{4a_0^2}\right)\frac{\sqrt{3}}{4\sqrt{2}}\frac{z}{a_0}e^{-r/(2a_0)}\right] \tag{7}$$

$$\frac{\hat{L}^2}{2mr^2}\psi = \frac{2\hbar^2}{2mr^2}\frac{1}{2\sqrt{\pi}a_0^{3/2}}\frac{\sqrt{3}}{4\sqrt{2}}\frac{z}{a_0}e^{-r/(2a_0)} \tag{8}$$

$$V\psi = -\frac{\hbar^2}{ma_0 r}\frac{1}{2\sqrt{\pi}a_0^{3/2}}\left[e^{-r/a_0} + \frac{\sqrt{3}}{4\sqrt{2}}\frac{z}{a_0}e^{-r/(2a_0)}\right] \tag{9}$$

and then adding everything together:

$$\hat{H}\psi = \frac{1}{2\sqrt{\pi}a_0^{3/2}}\left[\underbrace{-\frac{\hbar^2}{2ma_0^2}}_{-\mathcal{R}}e^{-r/a_0} + \underbrace{-\frac{\hbar^2}{8ma_0^2}}_{-\mathcal{R}/4}\frac{\sqrt{3}}{4\sqrt{2}}\frac{z}{a_0}e^{-r/(2a_0)}\right] \tag{10}$$

so we can identify a superposition of $n = 1$ and $n = 2$. Now multiply through by ψ. The cross terms vanish on integration because they are proportional to $\cos\theta$. We are left with:

$$\langle E\rangle = \frac{1}{4\pi a_0^3}\int_0^\pi d\theta\,\sin\theta\int_0^{2\pi}d\phi\int_0^\infty r^2 dr\left[-\mathcal{R}e^{-2r/a_0} - \frac{\mathcal{R}}{4}\frac{3}{32}\frac{r^2\cos^2\theta}{a_0^2}e^{-r/a_0}\right] \tag{11}$$

$$= \frac{1}{4}(-\mathcal{R}) + \frac{3}{4}(-\mathcal{R}/4) \tag{12}$$

$$= -\frac{7\mathcal{R}}{16} \tag{13}$$

(c) (4 points) What is the wavefunction as a function of time, $\psi(\mathbf{r}, t)$?

Solution: This part depends on results from the previous two parts. We have a superposition of $\ell = 0$ and $\ell = 1$ from part (a) and a superposition of $n = 0$ and $n = 1$ from part (b), so the state is $|\psi\rangle = \alpha\,|0, 0\rangle + \beta\,|1, 1\rangle$. The constants can be obtained from part (b), so $\alpha = 1/2$ and $\beta = \sqrt{3}/2$, though we don't need them - we just need to put the phase factors into the wavefunction:

$$\psi(\mathbf{r},t) = \frac{1}{2\sqrt{\pi}a_0^{3/2}}\left[e^{-r/a_0}e^{i\mathcal{R}t/\hbar} + \frac{\sqrt{3}}{4\sqrt{2}}\frac{z}{a_0}e^{-r/(2a_0)}e^{i\mathcal{R}t/(4\hbar)}\right] \tag{14}$$

END

Formulas

- The Dirac delta function:

$$f(a) = \int_{-\infty}^{\infty} \delta(x-a) f(x)\, dx, \qquad \delta(x) = \int_{-\infty}^{\infty} e^{ikx} dx \tag{15}$$

- Creation and annihilation operators for the harmonic oscillator, $V(\hat{x}) = \frac{1}{2} m\omega^2 \hat{x}^2$:

$$\hat{a}^\dagger = \frac{\hat{x}}{2L} - \frac{iL\hat{p}}{\hbar}, \qquad \hat{a} = \frac{\hat{x}}{2L} + \frac{iL\hat{p}}{\hbar} \tag{16}$$

where $L = \sqrt{\hbar/(2m\omega)}$.

- Pauli matrices for spin-1/2 particles:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{17}$$

- Pauli matrices for spin-1 particles:

$$\sigma_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \sigma_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{18}$$

- The Hamiltonian in spherical polar coordinates:

$$\hat{H} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V(r), \tag{19}$$

where

$$\hat{p}_r^2 = -\frac{\hbar^2}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \tag{20}$$

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right] \tag{21}$$