FUF040 Quantum Mechanics: Dugga/Exam

Course: FUF040
Time: 2021/10/22, 1400 – 1800
Responsible: Tom Blackburn
Permitted materials: Physics Handbook, attached formula sheet
Questions: 7
Total points: 40
You may answer in either Swedish or English.

1. (4 points) Write down the time-independent and time-dependent Schrödinger equations and define the symbols that you use.

> **Solution:** Time-independent: $\hat{H}\,|E\rangle = E\,|E\rangle$ (or equivalent in position representation). Time-dependent: $\hat{H}\,|\psi\rangle = i\hbar\frac{\partial}{\partial t}\,|\psi\rangle$ (or equivalent in position representation).
>
> 1. $\hat{H}$ is the Hamiltonian/energy operator (or equivalent in terms of kinetic and potential energy).
> 2. E is the energy (total energy/energy eigenvalue).
> 3. $|E\rangle$ is an energy eigenstate (or $\psi(x)$ is the wavefunction of a state of definite energy).
> 4. $|\psi\rangle$ is a general quantum state (or $\psi(x)$ is the wavefunction of a general quantum state).

2. An experiment on a quantum mechanical system has two possible, different, outcomes: A and B. The probability amplitude for outcome A is given by $\alpha(A)$. Outcome B can occur by one of two, mutually exclusive, indistinguishable, routes, X and Y, with probability amplitude $\beta(X)$ and $\beta(Y)$, respectively.

   (a) (1 point) What is the probability for outcome B to occur?

   > **Solution:** $P(B) = |\beta(X) + \beta(Y)|^2$.

(b) (1 point) What is the probability for outcome A or B to occur?

Solution: $P(A|B) = |\alpha(A)|^2 + P(B) = 1$.

3. An operator $\hat{Q}$ is Hermitian if it satisfies $\langle\phi|\,\hat{Q}\,|\psi\rangle = \langle\psi|\,\hat{Q}\,|\phi\rangle^\star$.

(a) (1 point) What is the momentum operator $\hat{p}_x$ in the position representation?

Solution: $\langle x|\,\hat{p}\,|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|\psi\rangle$ or equivalent.

(b) (2 points) Prove that $\hat{p}_x$ is Hermitian and explain any assumptions that you make.

Solution: In the position representation, the trick is to integrate by parts:

$$\begin{aligned}
\langle\phi|\,\hat{p}\,|\psi\rangle &= -i\hbar\int_{-\infty}^{\infty}\phi^\star(x)\frac{\partial\psi(x)}{\partial x}dx && (1)\\
&= -i\hbar\left[\phi^\star(x)\psi(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\frac{\partial\phi^\star(x)}{\partial x}\psi(x)dx\right] && (2)\\
&= i\hbar\int_{-\infty}^{\infty}\psi(x)\frac{\partial\phi^\star(x)}{\partial x}dx && (3)\\
&= \langle\psi|\,\hat{p}\,|\phi\rangle^\star && (4)
\end{aligned}$$

Assumption is that the wavefunction vanishes at $x = \pm\infty$. Equivalent with $|\psi\rangle = |\phi\rangle$ also OK. Alternatively, the Hermiticity of momentum can be proved by requiring the translation operator be unitary.

(c) (3 points) Why are Hermitian operators used to represent physical observables?

Solution:

1. The eigenvalues of Hermitian operator, which give the possible outcomes of a measurement, are real.
2. Eigenstates corresponding to different eigenvalues are orthogonal to each other, thus different physical outcomes do not overlap.
3. The eigenstates form a complete basis, so any quantum state in the relevant Hilbert space can be written as a linear combination of these eigenvectors.

4. (6 points) A particle of mass m is trapped in a 1D harmonic oscillator of natural frequency ω. Show that the product of the uncertainties in position and momentum, $\sigma_x\sigma_p$, for the nth energy level satisfies the uncertainty principle. (The standard deviation of an observable Q is defined by $\sigma_Q = \sqrt{\langle Q^2\rangle - \langle Q\rangle^2}$.)

Solution: The ladder operators for the harmonic oscillator are $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$. Using the formula sheet, we have $\hat{x} = L(\hat{a} + \hat{a}^\dagger)$ and $\hat{p} = \hbar/(2iL)(\hat{a} - \hat{a}^\dagger)$. We have the following expectation values:

- $\langle x\rangle = \langle n|\hat{x}|n\rangle = 0$ as a single application of the ladder operators creates $|n-1\rangle$ or $|n+1\rangle$ which is orthogonal to $|n\rangle$.
- $\langle p\rangle = \langle n|\hat{p}|n\rangle = 0$, by the same reasoning.
- $\langle x^2\rangle = L^2\langle n|\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}|n\rangle$, expanding out the square and discarding terms which have unequal numbers of $\hat{a}$ and $\hat{a}^\dagger$. Thus $\langle x\rangle = L^2(2n+1)$.
- $\langle p^2\rangle = -\frac{\hbar^2}{(2iL)^2}\langle n|\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}|n\rangle = \frac{\hbar^2}{4L^2}(2n+1)$.

As such, $\sigma_x\sigma_p = \frac{\hbar}{2}(2n+1) \geq \hbar/2$ for all $n \geq 0$.

5. A hydrogen atom is prepared such that its state is given by

$$|\psi\rangle = \frac{|n=2,\ell=1,m=1\rangle - |n=2,\ell=1,m=-1\rangle}{\sqrt{2}}, \tag{5}$$

where n is the principal quantum number, ℓ is the orbital angular momentum quantum number, and m is the quantum number associated with the projection of the orbital angular momentum along the z-axis.

(a) (2 points) If the energy is measured, what are the possible outcomes, and the probabilities for those outcomes?

Solution: The state is a superposition of two eigenstates with the same principal quantum number $n = 2$. The only possible outcome is $-\mathcal{R}/4 = -3.4$ eV.

(b) (2 points) If the orbital angular momentum in the z-direction is measured, what are the possible outcomes, and the probabilities for those outcomes?

Solution: The state is a superposition of two eigenstates with $m = +\hbar$ and $m = -\hbar$. A measurement of L_z yields $\pm\hbar$ with equal probability.

(c) (3 points) If the orbital angular momentum in the x-direction is measured, what are the possible outcomes, and the probabilities for those outcomes?

Solution: Here we need to express the state as a linear combination of eigenstates of L_x rather than L_z. Call these eigenstates $|m_x = \pm 1, 0\rangle = \alpha|m_z = +1\rangle + \beta|m_z = 0\rangle + \gamma|m_z = -1\rangle$ and represent them as three-component spinors $(\alpha, \beta, \gamma)^T$. L_x is given by the 3×3 matrix σ_x, which has eigenvalues $\pm 1, 0$. Solving the eigenvalue equation, we get:

- $|m_x = -1\rangle = (1, -\sqrt{2}, 1)^T/2$
- $|m_x = +1\rangle = (1, \sqrt{2}, 1)^T/2$
- $|m_x = 0\rangle = (-1, 0, 1)^T/\sqrt{2}$

The state we have is $|\psi\rangle = (1, 0, -1)^T/\sqrt{2} = -|m_x = 0\rangle$. Therefore a measurement of L_x yields 0 with 100% probability.

6. (6 points) Dr. Knowitall has purchased some overpriced electrons from *Blackburn's Discount Quantum Devices* and is keen to ensure they do not escape the lab. He attempts to confine them to the region $x < 0$ with a very strong, but very narrow, potential barrier: $V(x) = V_\delta \delta(x)$, where V_δ is a real, positive constant. Electrons, with energy E, travel from $x = -\infty$ towards the barrier. Show that the probability that an electron passes through the barrier is

$$P = \left(1 + \frac{m_e V_\delta^2}{2\hbar^2 E}\right)^{-1} \tag{6}$$

You may treat the problem as one-dimensional.

Solution: On the LHS of the barrier, we have $\psi(x) = e^{ikx} + Re^{-ikx}$ where $k = \sqrt{2mE}/\hbar$. On the RHS, we have $\psi(x) = Te^{ikx}$. R and T are the reflection and transmission amplitudes. The wavefunction must be continuous at $x = 0$, so

$$1 + R = T. \tag{7}$$

The boundary condition on the derivative follows by integrating the TISE over a region around $x = 0$:

$$-\frac{\hbar^2}{2m} \left.\frac{\partial \psi(x)}{\partial x}\right|_{-\epsilon}^{+\epsilon} + V_\delta \psi(0) = 0 \tag{8}$$

where ϵ is vanishingly small:

$$-\frac{\hbar^2}{2m}[ikT - (ik - ikR)] + V_\delta T = 0 \tag{9}$$

Eliminating R, we get

$$T = \left(1 + \frac{i m_e V_\delta}{\hbar^2 k}\right)^{-1}. \tag{10}$$

Mod-squaring yields the desired result.

7. A quantum-mechanical system is translated through space, by a 3D displacement $\mathbf{a}$. Its state is transformed as $|\psi'\rangle = \hat{U}|\psi\rangle$, where $\hat{U} = \exp(-i\mathbf{a}\cdot\hat{\mathbf{p}}/\hbar)$.

   (a) (3 points) By considering how $\langle\mathbf{p}\rangle$, the expectation value of momentum, changes under a small translation, show that all components of the momentum operator commute with each other: $[\hat{p}_i, \hat{p}_j] = 0$.

Solution: $\langle\mathbf{p}\rangle$ does not change under translation, so $\langle\psi'|\hat{\mathbf{p}}|\psi'\rangle = \langle\psi|\hat{U}^\dagger\hat{\mathbf{p}}\hat{U}|\psi\rangle = \langle\psi|\hat{\mathbf{p}}|\psi\rangle$. Now consider a small translation, so $\hat{U} = 1 - ia_k\hat{p}_k/\hbar$. Looking at the operators on either side, we need:

$$\left(1 + \frac{ia_k\hat{p}_k}{\hbar}\right)\hat{p}_i\left(1 - \frac{ia_k\hat{p}_k}{\hbar}\right) = \hat{p}_i \tag{11}$$

$$\hat{p}_i + \frac{i}{\hbar}a_k[\hat{p}_k, \hat{p}_i] + O(a^2) = \hat{p}_i \tag{12}$$

Hence the commutator must vanish: $[\hat{p}_i, \hat{p}_k] = 0$.

   (b) (3 points) By considering how $\langle\mathbf{r}\rangle$, the expectation value of position, changes under a small translation, show that the position and momentum operators satisfy: $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$.

Solution: $\langle\mathbf{r}\rangle \to \langle\mathbf{r}\rangle + \mathbf{a}$ under translation by $\mathbf{a}$. so $\langle\psi'|\hat{\mathbf{r}}|\psi'\rangle = \langle\psi|\hat{U}^\dagger\hat{\mathbf{r}}\hat{U}|\psi\rangle = \langle\psi|\hat{\mathbf{r}}|\psi\rangle + \mathbf{a}$. Now consider a small translation, so $\hat{U} = 1 - ia_k\hat{p}_k/\hbar$. Looking at the operators on either side, we need:

$$\left(1 + \frac{ia_k\hat{p}_k}{\hbar}\right)\hat{x}_i\left(1 - \frac{ia_k\hat{p}_k}{\hbar}\right) = \hat{x}_i + a_i \tag{13}$$

$$\hat{x}_i + \frac{i}{\hbar}a_k[\hat{p}_k, \hat{x}_i] + O(a^2) = \hat{x}_i + a_i \tag{14}$$

To get the second term on the LHS equal to a_i, we need the commutator to be $[\hat{p}_k, \hat{x}_i] = -i\hbar\delta_{ik}$, or $[\hat{x}_i, \hat{p}_k] = i\hbar\delta_{ik}$.

   (c) (3 points) Suppose we wished to describe a particle in terms of its position $\mathbf{r}$ and momentum $\mathbf{p}$. Given these commutation relations, how well can we do that? How does this compare to the situation in classical physics?

Solution: In classical physics, it is possible to know all six position and momentum components exactly and simultaneously. In quantum physics, we can only have exact knowledge of two observables simultaneously if their operators commute. Thus we can know only three components exactly at any one time: e.g., p_x, p_y and p_z, or x, y and p_z, etc. The better we know the position in any one direction, the worse our knowledge of the momentum in that direction.

Formulas

- The Dirac delta function:

$$f(a) = \int_{-\infty}^{\infty} \delta(x-a) f(x)\, dx, \qquad\qquad \delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx} dx \tag{15}$$

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

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

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

- Pauli matrices for j or $s = 1/2$ ($\hat{J}_i|\hat{S}_i = \frac{\hbar}{2}\sigma_i$):

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

- Pauli matrices for j, ℓ or $s = 1$ ($\hat{J}_i|\hat{L}_i|\hat{S}_i = \hbar\sigma_i$):

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

- 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

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

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