FUF040 Quantum Mechanics: Omdugga/Re-exam

Course: FUF040
Time: 2022/01/05, 0830 – 1230
Responsible: Tom Blackburn
Permitted materials: Physics Handbook, attached formula sheet
Questions: 6
Total points: 50
You may answer in either Swedish or English.

1. The quantum state of a particle moving in one dimension can be described by its wavefunction in the position representation, $\psi(x)$, or equivalently by its wavefunction in the momentum representation, $\tilde{\psi}(p)$.

   (a) (4 points) Give the wavefunction in the position representation, $\psi(x)$, for a particle with definite momentum p_0. Is this wavefunction properly normalised? Can it represent a physical particle?

   > **Solution:** $\psi(x) = \exp(ip_0x/\hbar)/\sqrt{2\pi\hbar}$. This wavefunction is not normalised properly, $\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx \neq 1$, so it is not physical. Instead, we have $\langle p'|p\rangle = \delta(p - p')$. A real particle would be described by a wavepacket, i.e. a linear combination of these states.

   (b) (2 points) What is the wavefunction in the momentum representation, $\tilde{\psi}(p)$, for the case in part (a)?

   > **Solution:** $\tilde{\psi}(p) = \delta(p - p_0)$.

   (c) (1 point) What is the momentum operator in the momentum representation?

   > **Solution:** $\hat{p}\tilde{\psi}(p) = p\tilde{\psi}(p)$.

   (d) (2 points) What is the position operator in the momentum representation?

   Hint: Transform the wavefunction $\psi(x)$ of a particle with definite position x_0 to the momentum representation.

Solution: The wavefunction of a particle with definite position x_0 is $\psi(x) = \delta(x - x_0)$. Transforming, we obtain $\tilde{\psi}(p) = \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar}/\sqrt{2\pi\hbar}\, dx = \exp(-ipx_0/\hbar)/\sqrt{2\pi\hbar}$. Applying $\hat{p}$ to this $\tilde{\psi}(p)$ must yield $x_0\tilde{\psi}(p)$, so $\hat{p} = i\hbar\frac{\partial}{\partial p}$.

(e) (4 points) Show that the position and momentum operators do not commute. What does this imply?

Solution:

$$[\hat{x}, \hat{p}]\psi(x) = \left[x, -i\hbar\frac{\partial}{\partial x}\right]\psi(x) \tag{1}$$

$$= i\hbar\left[-x\frac{\partial\psi}{\partial x} + \frac{\partial}{\partial x}(x\psi)\right] \tag{2}$$

$$= i\hbar\psi(x) \tag{3}$$

As $[\hat{x}, \hat{p}] \neq 0$, we cannot simultaneously know both the position and momentum of the particle.

2. Suppose you have an infinitely deep, square potential well of width a, such that the potential $V(x) = 0$ for $|x| < a/2$ and infinity otherwise. An electron, of mass m, is trapped inside this well.

(a) (4 points) Derive expressions for the allowed energies E_n and the wavefunctions $\langle x|E_n\rangle$ of the energy eigenstates. How many energy levels are there?

Solution: Solve $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$ with the boundary conditions $\psi(\pm a/2) = 0$. The general solution is $\psi(x) = A\sin(kx) + B\cos(kx)$ where $k = \sqrt{2mE}/\hbar$. The boundary conditions require that $B = 0$ and $ka/2 = n\pi$, or $A = 0$ and $ka/2 = (2n+1)\pi/2$, where n is an integer. The values of A and B are fixed by normalisation: $\int_{-a/2}^{a/2} |\psi(x)|^2\, dx = 1$.

So we have $E_n = \hbar^2\pi^2 n^2/(2ma^2)$ and $\psi_n(x) = \langle x|E_n\rangle = \sqrt{2/a}\cos(n\pi x/a)$ for odd $n \geq 1$ or $\sqrt{2/a}\sin(n\pi x/a)$ for even $n \geq 2$.

There are an infinite number of energy levels.

(b) (5 points) This potential is perturbed by a static electric field, such that $\hat{H}' = e\mathcal{E}\hat{x}$, where $e < 0$ and $\mathcal{E} > 0$. What is the first-order correction to the energy levels ΔE_n? Explain your result physically.

Solution:

$$\Delta E_n = \langle E|\, \hat{H}'\, |E\rangle = e\mathcal{E} \int_{-a/2}^{a/2} \psi_n^{\star}(x)\, x\, \psi_n(x)\, dx \tag{4}$$

$$= \frac{2}{a} \int_{-a/2}^{a/2} x \cos^2(n\pi x/a)\, dx \tag{5}$$

$$= 0 \tag{6}$$

because x is an odd function and $\cos^2$ (or $\sin^2$) are even functions.

The first-order change is zero because the electron is equally likely to be found at $x > 0$ (where the energy is lower) as at $x < 0$ (where the energy is higher).

3. The adjoint $\hat{Q}^\dagger$ of an operator $\hat{Q}$ is defined by

$$\langle f|\, \hat{Q}\, |g\rangle = \langle g|\, \hat{Q}^\dagger\, |f\rangle^\star \tag{7}$$

for all $|f\rangle$ and $|g\rangle$.

(a) (4 points) Prove that the eigenvalues of Hermitian operators are real, and that the eigenstates corresponding to different eigenvalues are orthogonal to each other.

Solution: Let $|f\rangle = |g\rangle = |q_n\rangle$ be an eigenstate of $\hat{Q}$ with eigenvalue q_n. Then the LHS becomes q_n. The RHS can be written as $\langle g|\, \hat{Q}\, |f\rangle^\star = q_n^\star$. So q_n must be real.

Now consider $|f\rangle = |q_m\rangle$ and $|g\rangle = |q_n\rangle$. Then the LHS becomes $q_n \langle q_m|q_n\rangle$. The RHS is $\langle g|\, \hat{Q}\, |f\rangle^\star = q_m^\star \langle q_m|q_n\rangle = q_m \langle q_m|q_n\rangle$. But $q_n \neq q_m$, so this can only be satisfied if $\langle q_m|q_n\rangle = 0$.

(b) (2 points) Why are these two properties necessary for these operators to represent physical observables?

Solution: The allowed results of a measurement are the eigenvalues of the associated operator, which must therefore be real. The eigenstates corresponding to different results must be orthogonal, because if Q is measured, with the result q_n, the probability that an immediate, subsequent measurement yields q_m must be zero: $P = |\langle q_m|\psi\rangle|^2 = |\langle q_m|q_n\rangle|^2 = 0$.

4. A particle of mass m, trapped in a 1D harmonic oscillator with natural frequency ω, is prepared such that its state at $t = 0$ is:

$$|\psi; t = 0\rangle = \frac{|n = 0\rangle - \sqrt{2}\, |n = 1\rangle + |n = 2\rangle}{2}, \tag{8}$$

where $|n\rangle$ is an energy eigenstate with energy E_n.

(a) (3 points) What is the expectation value of a measurement of the energy, $\langle E\rangle$, at time t?

> **Solution:** The expectation value of energy is independent of time, because the Hamiltonian is independent of time. $E_n = (n+1/2)\hbar\omega$. $\langle E\rangle = \sum_n P_n E_n = \frac{1}{4}E_0 + \frac{1}{2}E_1 + \frac{1}{4}E_2 = 3\hbar\omega/2$.

(b) (5 points) What is the expectation value of a measurement of the position, $\langle x\rangle$, at time t?

> **Solution:** The time-dependent state is
>
> $$|\psi;t\rangle = \frac{e^{-i\omega t/2}}{2}\left(|0\rangle - \sqrt{2}e^{-i\omega t}|1\rangle + e^{-i2\omega t}|2\rangle\right). \tag{9}$$
>
> Applying $\hat{x} = L(\hat{a} + \hat{a}^\dagger)$, we get
>
> $$\hat{x}|\psi;t\rangle = L\frac{e^{-i\omega t/2}}{2}\left[|1\rangle - \sqrt{2}e^{-i\omega t}(|0\rangle + \sqrt{2}|2\rangle) + e^{-i2\omega t}(\sqrt{2}|1\rangle + \sqrt{3}|3\rangle)\right]. \tag{10}$$
>
> Bra through by $\langle\psi;t|$ to get:
>
> $$\langle x\rangle = \frac{L}{4}\left[-\sqrt{2}e^{-i\omega t} - \sqrt{2}e^{i\omega t} - 2e^{-i\omega t} - 2e^{i\omega t}\right] \tag{11}$$
>
> $$= -L\left(1 + \frac{1}{\sqrt{2}}\right)\cos\omega t \tag{12}$$

(c) (2 points) Compare your answer to part (c) with the amplitude and frequency of oscillation of a *classical* harmonic oscillator.

> **Solution:** This should read "answer to part (b)". Due to this error, any attempt at question 4 received full marks for this part.
>
> Intended solution: any reasonable response accepted, including: The position oscillates with natural frequency ω for both. The amplitude of oscillation for a classical oscillator with energy $3\hbar\omega/2$ would be $\sqrt{6}L$, which does not agree.

5. The state of a spin-1 particle is given by

$$|\psi\rangle = \frac{|m=-1\rangle - i\sqrt{2}|m=0\rangle - |m=1\rangle}{2}, \tag{13}$$

(a) (3 points) If the component of the spin parallel to z, $\hat{S}_z$, is measured, what are the possible outcomes and the probabilities of those outcomes?

> **Solution:** Possible outcomes are $-\hbar$, 0 and $\hbar$, with probabilities $1/4$, $1/2$ and $1/4$ respectively.

(b) (3 points) If the component of the spin parallel to y, $\hat{S}_y$, is measured, what are the possible outcomes and the probabilities of those outcomes?

> **Solution:** We need to find the eigenstates of $\hat{S}_y$. Use the Pauli matrix representation and solve the eigenvalue equation
>
> $$\frac{1}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\\ \gamma\end{pmatrix} = \lambda\begin{pmatrix}\alpha\\ \beta\\ \gamma\end{pmatrix} \tag{14}$$
>
> for $\lambda = -1$, 0 and 1. We obtain $(-1, i\sqrt{2}, 1)^T/2$, $(1,0,1)^T/\sqrt{2}$, $(-1,-i\sqrt{2},1)^T/2$, respectively. Observe that $|\psi\rangle = -|S_y = -1\rangle$. Therefore in a measurement of the spin component along y, we obtain $-\hbar$ with 100% probability.

6. The energy of the electron in a hydrogen atom is measured. Immediately afterwards, its wavefunction is given by:

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{32\pi a_0^3}}\frac{z}{a_0}\exp\left(-\frac{r}{2a_0}\right) \tag{15}$$

where $a_0 = 4\pi\varepsilon_0\hbar^2/(me^2)$ and m is the reduced mass of the electron-proton system.

(a) (2 points) If the energy is measured again, what is the result?

> **Solution:** The first measurement collapsed the state to an energy eigenstate, so a second measurement must yield the same result again. Hence the given wavefunction satisfies $\hat{H}\psi = E\psi$. We can apply the radial Hamiltonian directly:
>
> $$\hat{H} = -\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hbar^2}{2mr^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] - \frac{e^2}{4\pi\varepsilon_0 r} \tag{16}$$
>
> or look up the wavefunction in the handbook. We obtain $n = 2, \ell = 1, m = 0$ so $E = -R/4$ (−0.85 eV).

(b) (4 points) How much of this energy do we expect to come from the potential energy? And therefore how much do we expect to come from the kinetic energy?
Hint: $\int_0^\infty x^n \exp(-x)dx = n!$

Solution: We need to calculate the expectation value of $\hat{V} = -e^2/(4\pi\varepsilon_0\hat{r})$.

$$\langle V\rangle = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{32\pi a_0^3}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta\ \sin\theta \int_0^{\infty} dr\, r^2\, \frac{r\cos^2\theta}{a_0^2}\exp\left(-\frac{r}{a_0}\right) \tag{17}$$

$$= -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{32\pi a_0^3}\ \underbrace{2\pi}_{\phi\text{ integral}}\ \underbrace{\frac{2}{3}}_{\theta\text{ integral}}\ \underbrace{6a_0^2}_{\text{radial integral}} \tag{18}$$

$$= -\frac{e^2}{16\pi\varepsilon_0 a_0} = -\frac{R}{2} \tag{19}$$

The expectation value of the kinetic energy $\langle T\rangle = R/4$.

END

Formulas

- The Dirac delta function:

$$f(a) = \int_{-\infty}^{\infty} \delta(x-a) f(x)\, dx, \qquad \delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx} dx \tag{20}$$

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

$$\hat{a}^\dagger = \frac{\hat{x}}{2L} - \frac{iL\hat{p}}{\hbar}, \qquad \hat{a} = \frac{\hat{x}}{2L} + \frac{iL\hat{p}}{\hbar} \tag{21}$$

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

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

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{22}$$

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

$$\sigma_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \sigma_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{23}$$

- The Hamiltonian in spherical polar coordinates:

$$\hat{H} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V(r), \tag{24}$$

where

$$\hat{p}_r^2 = -\frac{\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \tag{25}$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{26}$$