FUF040 Quantum Mechanics: Omdugga/Re-exam

Course: FUF040
Time: 2022/08/22, 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. (10 points) Your colleague, Dr. Knowitall, has some quick-fire questions for you.

   (a) (1 point) What wavefunctions satisfy the *time-independent* Schrödinger equation?

   Solution: Only the wavefunctions of energy eigenstates (stationary states).

   (b) (1 point) What wavefunctions satisfy the *time-dependent* Schrödinger equation?

   Solution: All wavefunctions must satisfy the TDSE.

   (c) (1 point) If the quantum state of a system is given by an energy eigenstate at $t = 0$, how does it evolve in time?

   Solution: Via the "wiggle factor": $\psi(t) = \psi(t = 0) \exp(-iEt/\hbar)$ where E is the energy eigenvalue.

   (d) (2 points) What are the wavefunctions in the position and momentum representations, $\psi(x)$ and $\tilde{\psi}(p)$, of a free particle with definite momentum p_0?

   Solution: $\psi(x) = \exp(ip_0 x/\hbar)/\sqrt{2\pi\hbar}$ and $\tilde{\psi}(p) = \delta(p - p_0)$.

   (e) (2 points) Give two important properties of Hermitian operators.

   Solution: They have real eigenvalues, eigenstates (kets/vectors) corresponding to different eigenvalues are orthogonal to each other, the set of eigenstates forms a complete basis.

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

> **Solution:** The eigenvalues represent the possible outcomes of a measurement (which must therefore be real). Eigenstates with different eigenvalues are orthogonal to each other, so different physical outcomes do not overlap. A complete set means that any physical state within the Hilbert space of the system can be represented by a linear combination of the basis states.

(g) (1 point) The three position operators, $\hat{x}$, $\hat{y}$ and $\hat{z}$, and the three momentum operators $\hat{p}_x$, $\hat{p}_y$ and $\hat{p}_z$, can be used to form 15 distinct commutators. How many are zero?

> **Solution:** The only non-zero ones are $[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$, so 12.

2. (6 points) The quantum state of a spin-1 particle is given by

$$|\psi\rangle = -\frac{i}{\sqrt{3}}|m = 0\rangle + \sqrt{\frac{2}{3}}|m = 1\rangle, \tag{1}$$

(a) (2 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 0 and $\hbar$, with probabilities $1/3$ and $2/3$ respectively.

(b) (4 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
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> $$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \lambda \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \tag{2}$$
>
> 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. Now solve $|\psi\rangle = a\,|m_y = -1\rangle + b\,|m_y = 0\rangle + c\,|m_y = 1\rangle$ to obtain $a = 0$, $b = \sqrt{1/3}$ and $c = \sqrt{2/3}$. Therefore in a measurement of the spin component along y, we obtain 0 with $1/3$ probability and $+\hbar$ with $2/3$ probability.

3. (12 points) A particle of mass m is trapped in a narrow, but very deep, potential well at $x = 0$. We will model this potential well as a Dirac δ function $V(x) = V_\delta \delta(x)$.

   (a) (3 points) The energy of the bound state is $E = -mV_\delta^2/(2\hbar^2)$. Show that the wavefunction in the position representation $\psi(x) = N\exp(-\alpha x)$ for $x > 0$ and $N\exp(\alpha x)$ for $x < 0$, where α and N are constants to be determined.

   Solution: Plug the wavefunction into the TISE (working point): $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$ to obtain $\alpha = mV_\delta/\hbar^2$. The wavefunction must be normalised, $\int_{-\infty}^{\infty}\psi(x)^2 dx = 1$, so $N = \sqrt{\alpha} = \sqrt{mV_\delta/\hbar^2}$.

   (b) (5 points) Find the wavefunction in the momentum representation $\tilde{\psi}(p)$.

   Solution: Fourier-transform the wavefunction in the position representation ($k = p/\hbar$):

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int_{-\infty}^{\infty} \langle x|p\rangle^\star \langle x|\psi\rangle \, dx \tag{3}$$

$$= \sqrt{\frac{\alpha}{2\pi\hbar}}\left[\int_{-\infty}^{0} e^{-ikx}e^{\alpha x}dx + \int_{0}^{\infty} e^{-ikx}e^{-\alpha x}dx\right] \tag{4}$$

$$= \sqrt{\frac{\alpha}{2\pi\hbar}}\left[\frac{1}{\alpha - ik} + \frac{1}{\alpha + ik}\right] \tag{5}$$

$$= \sqrt{\frac{2}{\pi\hbar}}\frac{\alpha^{3/2}}{\alpha^2 + k^2} \tag{6}$$

   (c) (2 points) Using your answer to part (b), find the expectation value of the squared momentum $\langle p^2\rangle$. (You may use your answer to part (a) instead – but be *very* careful in your working.)
   Hint: $\int_{-\infty}^{\infty} p^2/[p^2 + b^2]^2 dp = \pi/(2b)$.

   Solution: Working in momentum space, we have $\langle p^2\rangle = \int_{-\infty}^{\infty} p^2\tilde{\psi}(p)^2 \, dp$:

$$\langle p^2\rangle = \frac{2\alpha^3\hbar^2}{\pi}\int_{-\infty}^{\infty}\frac{k^2}{(\alpha^2 + k^2)^2}\, dk = \alpha^2\hbar^2 = \frac{m^2V_\delta^2}{\hbar^2}. \tag{7}$$

(d) (2 points) Show that the bound state satisfies the uncertainty relation.
Hint: $\int_{-\infty}^{\infty} x^2 \exp(-\kappa x) dx = 2/\kappa^3$.

Solution: The position uncertainty is $\langle x^2 \rangle = 2\alpha \int_0^{\infty} x^2 e^{-2\alpha x} dx = 1/(2\alpha^2)$, using the symmetry $\psi(-x) = \psi(x)$. We have therefore that $\sigma_x^2 \sigma_p^2 = \langle x^2 \rangle \langle p^2 \rangle = \hbar^2/2 > \hbar^2/4$.

4. (6 points) The wavefunction of the electron in a hydrogen atom, at $t = 0$, is given by

$$\psi(r, \theta, \varphi) = \sqrt{\frac{15}{16\pi}} R(r) \sin^2\theta \cos(2\varphi) \tag{8}$$

where $R(r)$ is a function of radius r.

(a) (3 points) If the squared magnitude of the orbital angular momentum (L^2) is measured at $t = 0$, what are the possible results and the probabilities to obtain those results?

Solution: $|\psi\rangle = \frac{1}{\sqrt{2}}(|\ell = 2, m = +2\rangle + |\ell = 2, m = -2\rangle)$ so there is 100% probability to obtain $L^2 = 2(2+1)\hbar^2 = 6\hbar^2$.

(b) (3 points) If the z-component of the orbital angular momentum (L_z) is measured at $t = 0$, what are the possible results and the probabilities to obtain those results?

Solution: Using the above representation, we find there is a 50% probability to obtain $L_z = -2\hbar$ or $+2\hbar$.

5. (8 points) A particle of mass m is trapped in a 1D harmonic oscillator of natural frequency ω, which is perturbed by a weak potential $V(x) = (m\omega/\hbar)V_0 x^2$.

(a) (2 points) What is the exact change to the energy of the nth level?

Solution: $V(x) = \frac{1}{2}m\omega^2 x^2 \to \frac{1}{2}m\omega^2 x^2[1 + 2V_0/(\hbar\omega)]$. Thus the natural frequency shifts by $\omega \to \omega\sqrt{1 + 2V_0/(\hbar\omega)}$ and the the exact change in the energy level is

$$\Delta E_n = \hbar\omega\left(n + \frac{1}{2}\right)\left[\sqrt{1 + \frac{2V_0}{\hbar\omega}} - 1\right]. \tag{9}$$

(b) (4 points) Use first-order perturbation theory to determine the change in the energy of the nth level. Show that your result is consistent with your answer to part (a).

Solution: The first-order correction is $\Delta E_n = \langle n|\hat{H}'|n\rangle$, where $\hat{H}' = \frac{1}{2}V_0(\hat{a} + \hat{a}^\dagger)^2$. Thus we obtain $\Delta E_n = V_0(n + 1/2)$. This is consistent with expanding $\sqrt{1 + 2V_0/(\hbar\omega)} \simeq V_0/(\hbar\omega)$.

(c) (2 points) What condition must V_0 satisfy for perturbation theory to be accurate? Explain your reasoning.

> **Solution:** Either: PT works while the energy shift is small compared to the energy itself, i.e. $\Delta E_n/E_n \simeq V_0/(\hbar\omega) \ll 1$. Or: expanding to second order, $\Delta E_n = V_0(n+1/2) - (n+1/2)V_0^2/(2\hbar\omega)$, the next-order correction is small if $V_0/(2\hbar\omega) \ll 1$.

6. (a) (2 points) What physical transformation is associated with the parity operator $\hat{\Pi}$? What does this operator do, when applied to the state (or wavefunction) describing a quantum-mechanical system?

> **Solution:** The parity operator inverts the spatial axes $x \to -x$, etc. In terms of position eigenstates, $\hat{\Pi}\,|x\rangle = |-x\rangle$, or in the position representation, $\langle x|\,\hat{\Pi}\,|\psi\rangle = \hat{\Pi}\psi(x) = \psi(-x)$.

(b) (3 points) By considering how the expectation value of position, $\langle x\rangle$, changes under parity transformation (or otherwise), show that $[\hat{\Pi}, \hat{x}] = 2\hat{\Pi}\hat{x}$.

> **Solution:** The expectation value of the position changes as $\langle\psi'|\,x\,|\psi'\rangle = -\langle\psi|\,x\,|\psi\rangle$ if $|\psi'\rangle = \Pi\,|\psi\rangle$. Therefore $\hat{\Pi}^\dagger\hat{x}\hat{\Pi} = -\hat{x}$. The parity operator is unitary, so apply $\hat{\Pi}$ to both sides, obtaining $\hat{x}\hat{\Pi} = -\hat{x}\hat{\Pi}$. QED. Alternatively, in the position representation, $\langle x|\,[\hat{\Pi}, \hat{x}]\,|\psi\rangle = \hat{\Pi}[x\psi(x)] - \hat{x}[\psi(-x)] = -2x\psi(-x) = \langle x|\,2\hat{\Pi}\hat{x}\,|\psi\rangle$.

(c) (3 points) Under what conditions does the parity operator commute with the kinetic and potential energy operators $\hat{T}$ and $V(\hat{x})$? What does this mean for the wavefunctions $\psi(x) = \langle x|E\rangle$ of the energy eigenstates $|E\rangle$?

> **Solution:** The parity operator always commutes with the kinetic energy operator. The parity operator commutes with the potential energy operator iff the potential $V(x)$ even, i.e. $V(x) = V(-x)$. If $[\hat{\Pi}, \hat{H}] = 0$, it is possible to construct eigenstates that are simultaneously eigenstates of parity and the Hamiltonian; the wavefunctions of these eigenstates would be either even or odd.

END

Formulas

- The Dirac delta function:

$$f(a) = \int_{-\infty}^{\infty} \delta(x-a) f(x)\, dx, \qquad \delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx} dx \tag{10}$$

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

$$\hat{a}^\dagger = \frac{\hat{x}}{2L} - \frac{iL\hat{p}}{\hbar}, \qquad \hat{a} = \frac{\hat{x}}{2L} + \frac{iL\hat{p}}{\hbar} \tag{11}$$

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

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

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{12}$$

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

$$\sigma_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \sigma_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{13}$$

- The Hamiltonian in spherical polar coordinates:

$$\hat{H} = \frac{\hat{p}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + V(r), \tag{14}$$

where

$$\hat{p}_r^2 = -\frac{\hbar^2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \tag{15}$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{16}$$