Part IB Physics A : Lent 2022

QUANTUM PHYSICS EXAMPLES III

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1. For a particle of mass m moving freely in one dimension, show that

$$\frac{\mathrm{d}\langle x^2\rangle}{\mathrm{d}t} = \frac{1}{m}\left\langle \widehat{x}\widehat{p} + \widehat{p}\widehat{x}\right\rangle \qquad \text{and} \qquad \frac{\mathrm{d}^2\langle x^2\rangle}{\mathrm{d}t^2} = \frac{2}{m^2}\left\langle \widehat{p}^2\right\rangle .$$

Show that, if $\mathrm{d}\left\langle x^2\right\rangle/\mathrm{d}t = 0$ at $t = 0$, then at later times t:

$$\left\langle x^2\right\rangle_t = \left\langle x^2\right\rangle_0 + \left\langle p^2\right\rangle_0 \frac{t^2}{m^2} .$$

2. For a certain system, A has eigenvalues a_1 and a_2 corresponding to eigenfunctions:

$$\psi_1 = (u_1 + u_2)/\sqrt{2} \qquad\qquad \psi_2 = (u_1 - u_2)/\sqrt{2}$$

where u_1 and u_2 are stationary states with energies E_1 and E_2. A is measured and found to have value a_1. Find how $\langle A\rangle$ subsequently varies with time.

3. Suppose that $\hat{H}$ is the Hamiltonian of a time-independent system. Using Dirac's bra-ket notation, and bearing in mind the definition of the function of an operator, show that $\hat{H}$ and $\exp\left[i\hat{H}t\right]$ commute.

4. Explain why, when using state vectors, the shift operator introduced in question 6 can be written $\exp\left[-i\hat{p}x_0/\hbar\right]$. Show that the operators corresponding to two different shifts x_{01} and x_{02} commute.

5. Obtain the following commutation relations for the angular momentum operators $\widehat{L} = \widehat{r} \times \widehat{p}$, and comment on the results:

$$\left[\widehat{L}_x, \widehat{x}\right] = 0 \qquad \left[\widehat{L}_x, \widehat{y}\right] = i\hbar\widehat{z}$$

$$\left[\widehat{L}_x, \widehat{p}_x\right] = 0 \qquad \left[\widehat{L}_x, \widehat{p}_y\right] = i\hbar\widehat{p}_z$$

$$\left[\widehat{L}_x, \widehat{L}^2\right] = \left[\widehat{L}_x, \widehat{r}^2\right] = \left[\widehat{L}_x, \widehat{p}^2\right] = 0$$

(All other commutation relations follow by the cyclic permutations $x \to y \to z \to x$.)

6. Use the commutation relations for the angular momentum operators,

$$\left[\widehat{L}_x, \widehat{L}_y\right] = i\hbar\widehat{L}_z \qquad \left[\widehat{L}_y, \widehat{L}_z\right] = i\hbar\widehat{L}_x \qquad \left[\widehat{L}_z, \widehat{L}_x\right] = i\hbar\widehat{L}_y ,$$

and the definitions of angular momentum raising and lowering operators,

$$\widehat{L}_{\pm} = \widehat{L}_x \pm i\widehat{L}_y = \hbar\, e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right),$$

to show that

$$\widehat{L}^2 = \widehat{L}_+\widehat{L}_- + \widehat{L}_z^2 - \hbar\widehat{L}_z$$

and that

$$\left[\widehat{L}_+, \widehat{L}_-\right] = 2\hbar\widehat{L}_z\,.$$

Hence show that

$$\widehat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

and that

$$\widehat{L}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right).$$

Finally, obtain the angular momentum quantum numbers for an electron in the hydrogen atom for the following eigenfunctions:

$$\psi(r,\theta,\phi) = R_1(r) \qquad \psi(r,\theta,\phi) = R_2(r)\sin\theta\, e^{i\phi} \qquad \psi(r,\theta,\phi) = R_3(r)(3\cos^2\theta - 1)\,.$$

7. The orthogonal wave functions $\psi_x = xf(r)$, $\psi_y = yf(r)$ and $\psi_z = zf(r)$ represent three of the electronic bound state solutions for a hydrogen atom. Prove the relations shown in the first row of the table below:

$$\begin{array}{lll} \widehat{L}_x\psi_x = 0 & \widehat{L}_x\psi_y = i\hbar\psi_z & \widehat{L}_x\psi_z = -i\hbar\psi_y \\ \widehat{L}_y\psi_x = -i\hbar\psi_z & \widehat{L}_y\psi_y = 0 & \widehat{L}_y\psi_z = i\hbar\psi_x \\ \widehat{L}_z\psi_x = i\hbar\psi_y & \widehat{L}_z\psi_y = -i\hbar\psi_x & \widehat{L}_z\psi_z = 0 \end{array}$$

Use the results in the table to prove that the expectation value of each component of the angular momentum of any one of ψ_x, ψ_y and ψ_z is zero. Show, however, that each is an eigenfunction of the operator $\widehat{L}^2 = \widehat{L}_x^2 + \widehat{L}_y^2 + \widehat{L}_z^2$ and determine the eigenvalue.
Show that the linear combinations $\psi_\pm = \psi_x \pm i\psi_y$ are eigenfunctions of $\widehat{L}_z$ and determine their orbital angular momentum quantum numbers m and ℓ.

For Questions 8 and 9 you can use the following information about a hydrogen-like atom

The normalised wavefunctions $Y_{\ell m_\ell}(\theta,\phi)$ for $\ell = 0, 1$ and 2 are:

$$\begin{array}{lll} Y_{00} = \sqrt{\frac{1}{4\pi}} & & \\ Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta & Y_{1\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi} & \\ Y_{20} = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) & Y_{2\pm1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi} & Y_{2\pm2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi} \end{array}$$

and the normalised hydrogen-like radial wavefunctions $R_{n\ell}$ for $n = 1, 2$ are:

$$
\begin{aligned}
R_{10} &= (Z/a_0)^{3/2} 2 \exp(-Zr/a_0) \\
R_{20} &= (Z/2a_0)^{3/2} (2 - Zr/a_0) \exp(-Zr/2a_0) \\
R_{21} &= (Z/2a_0)^{3/2} (1/\sqrt{3})(Zr/a_0) \exp(-Zr/2a_0)
\end{aligned}
$$

where a_0 is the Bohr radius and Z is the atomic number.

Note also that $\int_0^\infty x^n e^{-x} dx = n!$.

8. Confirm, for the cases $\ell = 1$ and $\ell = 2$, that

$$
\sum_{m_\ell=-\ell}^{m_\ell=\ell} |Y_{\ell m_\ell}|^2 = \text{constant}\,.
$$

Discuss the significance of this result for the electron probability distributions in the hydrogen atom. (The theorem for general ℓ follows from an addition formula for Legendre polynomials, see Whittaker and Watson, p. 327.)

9. An electron is in the ground state of a hydrogen-like atom with nuclear charge $+Ze$.

(a) What is its average distance from the nucleus?
(b) At what distance from the nucleus is it most likely to be found?
(c) Show that the expectation value of the potential energy operator of the electron is $-Z^2e^2/4\pi\epsilon_0 a_0$.
(d) Show that the expectation value of the kinetic energy operator is $Z^2e^2/8\pi\epsilon_0 a_0$.
(e) Verify that the expectation value of the Hamiltonian is the energy of the ground state.

10. The potential energy for a three-dimensional harmonic oscillator of mass m and frequency ω is $V(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$.

What are the energies and degeneracies of the three lowest levels?
Show that the degeneracy of the n^{th} excited level is $\frac{1}{2}(n + 1)(n + 2)$.

11. In a one-dimensional system two particles each of mass m interact through the potential $\frac{1}{2}m\omega^2(x_1 - x_2)^2$, where x_1 and x_1 are their position coordinates. Find the energy levels of the system when its centre of mass is at rest.

12. The Hamiltonian $\widehat{H}$ of two interacting particles a and b is given by

$$
\widehat{H} = \frac{\widehat{p}_a^2}{2m_a} + \frac{\widehat{p}_b^2}{2m_b} + \widehat{V}(|\boldsymbol{r}|)
$$

where $\boldsymbol{r} = \boldsymbol{r}_a - \boldsymbol{r}_b$ is the relative position of the particles.
Derive the commutation relations of the centre-of-mass and relative position and momentum operators $\widehat{R}$, $\widehat{r}$, $\widehat{P}$ and $\widehat{p}$, where:

$$
\widehat{\boldsymbol{R}} = \frac{m_a\widehat{\boldsymbol{r}}_a + m_b\widehat{\boldsymbol{r}}_b}{m_a + m_b} \qquad \widehat{\boldsymbol{p}} = \frac{m_a m_b}{m_a + m_b}\left(\frac{\widehat{\boldsymbol{p}}_a}{m_a} - \frac{\widehat{\boldsymbol{p}}_b}{m_b}\right)
$$

Comment on your results.

ANSWERS:

2. $\langle A\rangle = a_1 \cos^2 \omega t + a_2 \sin^2 \omega t$, where $\omega = (E_1 - E_2)/2\hbar$.

6. $\ell = 0, m_\ell = 0;\ \ell = 1, m_\ell = 1;\ \ell = 2, m_\ell = 0$.

7. Eigenvalue of $\widehat{L}^2$ is $2\hbar^2$; $\ell = 1, m_\ell = \pm 1$.

8. $\ell = 1$: $3/(4\pi)$; $\ell = 2$: $5/(4\pi)$.

9. (a) $3a_0/2Z$; (b) a_0/Z.

10. $\frac{3}{2}\hbar\omega,\ \frac{5}{2}\hbar\omega,\ \frac{7}{2}\hbar\omega;\ 1, 3, 6$.

11. $E_n = \sqrt{2}(n + \frac{1}{2})\hbar\omega$.

12. $\left[\widehat{R}_j, \widehat{P}_k\right] = [\widehat{r}_j, \widehat{p}_k] = i\hbar\delta_{jk}$, where $j, k = x, y, z$. All other commutators are zero.