QUALIFYING EXAMINATION, Part 3

Solutions

Problem 1: Quantum Mechanics I

(a) The probability $P_{ab}(t)$ is given by

$$P_{ab}(t) = \int_a^b dx\, |\psi(x,t)|^2 \ ,$$

so that

$$dP_{ab}/dt = \int_a^b dx\ (\psi^* \partial_t \psi + c.c.) \ .$$

Using the Schrödinger equation for $\psi(x,t)$

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \partial_x^2 \psi(x,t) + V(x)\psi(x,t) \ ,$$

and its complex conjugate, we find

$$dP_{ab}/dt = i\frac{\hbar}{2m} \int_a^b dx\ \left(\psi^* \partial_x^2 \psi - \psi \partial_x^2 \psi^*\right) \ .$$

Integrating both terms by parts

$$dP_{ab}/dt = i\frac{\hbar}{2m} \left(\psi^* \partial_x \psi|_a^b - \psi \partial_x \psi^*|_a^b + \int_a^b dx\ [-\partial_x \psi^* \partial_x \psi + \partial_x \psi \partial_x \psi^*] \right) \ .$$

The integrand on the r.h.s. vanishes, and we find

$$dP_{ab}/dt = J(a,t) - J(b,t) \ ,$$

where

$$J(x,t) = \frac{i\hbar}{2m} \left(\psi \partial_x \psi^* - \psi^* \partial_x \psi \right)$$

is the probability current.

(b) We determine A from the normalization of the wave function

$$\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2 = \int_{-\infty}^{\infty} dx\, A^2 \exp(-2c|x|) = 2A^2 \int_0^{\infty} dx\ \exp(-2cx) = A^2/c = 1 \ .$$

Therefore

$$A = \sqrt{c} \ .$$

$\langle\hat{x}\rangle(t) = \int dx x|\psi(x,t)|^2 = 0$ since $|\psi(x,t)|^2$ is an even function. For $\langle\hat{x}^2\rangle(t)$ we find

$$\langle\hat{x}^2\rangle(t) = \int_{-\infty}^{\infty} dx\, x^2|\psi(x,t)|^2 = 2c\int_0^{\infty} dx\, x^2\exp(-2cx) = \frac{1}{2c^2} .$$

(c) The time dependence of $\psi(x,t)$ in part (b) is of the form $e^{-iEt/\hbar}$. Substituting this form in the Schrödinger equation, we find that the spatial part of $psi(x,t)$ obeys the time-indepedent Schrödinger equation. Therefore ψ is a stationary state sand all expectation values are time independent

$$\langle\hat{O}\rangle(t) = \langle\hat{O}\rangle(t=0) .$$

(d) Substituting the form of the wave function in (b) into the Schrödinger equation, we find for $x > 0$ or $x < 0$

$$i\hbar\partial_t\psi = E\psi = -\hbar^2c^2/(2m)\psi + V(x)\psi = -\hbar^2/(2m)\partial_x^2\psi + V(x)\psi ,$$

or

$$\left(E + \frac{\hbar^2c^2}{2m}\right)\psi = V(x)\psi .$$

Thus $V(x)$ must be constant for $x \neq 0$. Since $V(x) \to 0$ at large $|x|$, we conclude that $V(x) = 0$ for $x \neq 0$ and also that its energy $E = -\hbar^2c^2/(2m) < 0$, i.e., ψ is a bound state of $V(x)$.

Note that $V(x)$ cannot be zero at $x = 0$ because then it would be zero everywhere, and a free particle does not have bound states.

Next, we integrate the Schrödinger equation around $x = 0$ over a narrow interval $-\epsilon < x < \epsilon$ for $\epsilon > 0$ and then take the limit $\epsilon \to 0$. We find

$$E\int_{-\epsilon}^{\epsilon} dx\,\psi = -\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon} dx\,\partial_x^2\psi + \int_{-\epsilon}^{\epsilon} dx\,\psi V(x) = -\frac{\hbar^2}{2m}\partial_x\psi|_{-\epsilon}^{\epsilon} + \psi(0,t)\int_{-\epsilon}^{\epsilon} dx\,V(x) .$$

Since the wave function ψ is continuous, The expression on the l.h.s. vanishes in the limit $\epsilon \to 0$. Using the actual form of $\psi(x,t)$ from part (b) in the r.h.s. of the above equation, we find

$$0 = A\frac{\hbar^2c}{m} + A\int_{-\epsilon}^{\epsilon} dx\,V(x) ,$$

or

$$\int_{-\epsilon}^{\epsilon} dx\,V(x) = -\frac{\hbar^2c}{m} .$$

Since $V(x) = 0$ for $x \neq 0$ and its integral around $x = 0$ is a constant, it must be proportional to the Dirac δ function. Therefore

$$V(x) = -\frac{\hbar^2c}{m}\delta(x) .$$

Problem 2: Quantum Mechanics II

(a) There are fours states, one $2s$ state, $|2s, m_l = 0\rangle$, and three $2p$ states, $|2p, m_l = +1\rangle$, $|2p, m_l = 0\rangle$, and $|2p, m_l = -1\rangle$

(b) The potential has odd parity, and therefore the matrix elements between $2s$ states or $2p$ states must vanish. As the zero component of a spherical tensor of rank one, V can only connect states with the same m_l. Thus the only non-vanishing matrix elements are between $|2s, m_l = 0\rangle$ and $|2p, m_l = 0\rangle$. The matrix element $\Delta E_\pm = \pm 3e\epsilon a_0$. In first-order degenerate perturbation theory, we diagonalize the corresponding 2×2 matrix of V

$$\begin{pmatrix} 0 & 3e\epsilon a_0 \\ 3e\epsilon a_0 & 0 \end{pmatrix} .$$

The energy shifts are given by the eigenvalues of this matrix

$$\Delta E_\pm = \pm 3e\epsilon a_0 .$$

The energies of the $|2p, m_l = +1\rangle$ and $|2p, m_l = -1\rangle$ states are not shifted.

(c) These are the eigenvectors of the matrix in (b)

$$|\pm\rangle = \frac{1}{\sqrt{2}} \left(|2s, m_l = 0\rangle \pm |2p, m_l = 0\rangle \right) .$$

(d) In the limit $e\epsilon a_0 \ll \delta$, we can ignore the splitting δ between the $2s_{1/2}$ states and the $2p_{1/2}$ states, and solve the problem in first-order degenerate perturbation theory. Since V conserves m_j, the only non-vanishing matrix elements of V are between $|2s_{1/2}, m_j = +1/2\rangle$ and $|2p_{1/2}, m_j = +1/2\rangle$, and also between $|2s_{1/2}, m_j = -1/2\rangle$ and $|2p_{1/2}, m_j = -1/2\rangle$. The Stark shift in each case is linear in ϵ, as determined by degenerate perturbation theory.

(e) In the limit $e\epsilon a_0 \ll \delta$, we can consider the Stark shift separately for the $2s_{1/2}$ states and the $2p_{1/2}$ states. For each such set of degenerate states (with $m_j = \pm 1/2$) there are no off-diagonal matrix elements, and the diagonal matrix elements also vanish (since V has odd parity). Therefore there is no contribution in first-order perturbation theory, and one must proceed to second-order perturbation theory. The Stark shift of each level is thus quadratic in ϵ. Non-degenerate perturbation theory *can* be used.