PHYS3701 Introduction to Quantum Mechanics I (Spring 2021)

Final Exam Thursday 29 April 2021

There are **four questions** and you are to work all of them. You are welcome to use your textbook, notes, computer, or any other resources, other than consulting with another human. If you have questions, please ask the person proctoring the exam. **Good luck!**

(1) The Hamiltonian for a certain spin-1/2 particle is $\hat{H} = (A/\hbar)\hat{S}_z + (B/\hbar)\hat{S}_x$ where $\hat{S}_x$ and $\hat{S}_z$ are the usual spin operators, and A and B are real constants, with $B \ll A$.
(a) Find the exact energy eigenvalues in terms of A and B.
(b) Treating the term $(B/\hbar)\hat{S}_x$ as a perturbation, find the approximate energy eigenvalues to first order and compare to the exact expressions.
(c) Calculate the second order correction, and again compare to the exact expressions.

(2) A particle of mass m scatters from the localized central potential energy function

$$V(r) = \begin{cases} -V_0 & r \le a \\ 0 & r \ge a \end{cases}$$

(a) Find the differential scattering cross section in the Born approximation as a function of momentum transfer $q = |\mathbf{q}|$. It will be useful to know that $\int x \sin x \, dx = -x\cos x + \sin x + C$.
(b) If a measurement of the cross section goes to zero at $q = q_0$, how would you use this information to find the well radius a?

(3) Labeling the states of the simple harmonic oscillator with frequency ω in one dimension as $|n\rangle$, where $n = 0, 1, 2, \ldots$, a particle of mass m is in the state

$$|\psi\rangle = N\left[|0\rangle + 2i|1\rangle + \sqrt{3}|2\rangle\right]$$

where N is a normalization constant.
(a) What is the probability that a measurement of the energy gives (i) zero or (ii) $3\hbar\omega/2$?
(b) What is the average value of a large number of identical measurements of the energy?
(c) Obtain an expression for the normalized time-evolved wave function $|\psi(t)\rangle$.

(4) An electron in a hydrogen atom is in the state

$$|\psi\rangle = \frac{1}{2}|1s\rangle + \frac{1}{2}|2p, m=0\rangle + \sqrt{\frac{1}{2}}|2p, m=1\rangle$$

(a) Find the expectation value of the position component $\hat{z}$.
(b) Find the expectation value for the total orbital angular momentum $\hat{\mathbf{L}}^2$.
(c) Find the expectation value for the z-component of orbital angular momentum $\hat{L}_z$.

Solutions

(1) This is very similar to Problem #11 on Homework #14. In the $|\pm\mathbf{z}\rangle$ basis, we have

$$\hat{H}|E\rangle = E|E\rangle \qquad \Longrightarrow \frac{1}{2}\begin{pmatrix} A & B \\ B & -A \end{pmatrix}\begin{pmatrix} \langle +\mathbf{z}|E\rangle \\ \langle -\mathbf{z}|E\rangle \end{pmatrix} = E\begin{pmatrix} \langle +\mathbf{z}|E\rangle \\ \langle -\mathbf{z}|E\rangle \end{pmatrix}$$

leading to the characteristic equation

$$(A/2-E)(-A/2-E)-(B/2)^2 = E^2-(A^2+B^2)/4 = 0 \;\text{ so }\; E = \pm\frac{1}{2}\left(A^2+B^2\right)^{1/2} \equiv E_\pm$$

For comparison to perturbation theory, it will be useful to expand in powers of B/A, that is

$$E_\pm = \pm\frac{1}{2}A^2\left(1+\frac{B^2}{A^2}\right)^{1/2} = \pm\frac{1}{2}A\left(1+\frac{1}{2}\frac{B^2}{A^2}+\cdots\right) = \pm\frac{A}{2}\pm\frac{B^2}{4A}+\cdots$$

In perturbation theory terminology, $B=0$, gives $\hat{H}_0 = (A/\hbar)\hat{S}_z$ and therefore $E_\pm^{(0)} = \pm A/2$ and $|\phi_\pm^{(0)}\rangle = |\pm\mathbf{z}\rangle$. Since $\hat{S}_x = (\hat{S}_+ + \hat{S}_-)/2$, we determine the first order corrections to be

$$E_\pm^{(1)} = \langle\phi_\pm^{(0)}|\hat{H}_1|\phi_\pm^{(0)}\rangle = \frac{B}{\hbar}\frac{1}{2}\langle\pm\mathbf{z}|(\hat{S}_+ + \hat{S}_-)|\pm\mathbf{z}\rangle = 0$$

which is consistent with the expansion of the exact eigenvalues.

Since there are only two eigenstates, the "sum over all the other eigenstates" needed for the second order correction just includes the one other eigenstate. Therefore

$$\begin{aligned} E_+^{(2)} &= \frac{|\langle\phi_-^{(0)}|\hat{H}_1|\phi_+^{(0)}\rangle|^2}{E_+^{(0)}-E_-^{(0)}} = \frac{B^2}{4\hbar^2}\frac{\langle -\mathbf{z}|(\hat{S}_+ + \hat{S}_-)|+\mathbf{z}\rangle|^2}{A/2-(-A/2)} = +\frac{B^2}{4A} \\ E_-^{(2)} &= \frac{|\langle\phi_+^{(0)}|\hat{H}_1|\phi_-^{(0)}\rangle|^2}{E_-^{(0)}-E_+^{(0)}} = \frac{B^2}{4\hbar^2}\frac{\langle +\mathbf{z}|(\hat{S}_+ + \hat{S}_-)|-\mathbf{z}\rangle|^2}{-A/2-(A/2)} = -\frac{B^2}{4A} \end{aligned}$$

which agrees with the first nonzero terms in the expansions of each of the exact eigenvalues.

(2) The cross section $d\sigma/d\Omega = |f(\theta,\phi)|^2$, and in the Born approximation we have

$$\begin{aligned}
f(\theta,\phi) &= -\frac{m}{2\pi\hbar^2}\int d^3r\, V(r) e^{i\mathbf{q}\cdot\mathbf{r}} \\
&= \frac{mV_0}{\hbar^2}\int_0^a r^2 dr \int_0^\pi \sin\theta d\theta\, e^{iqr\cos\theta} \\
&= \frac{mV_0}{\hbar^2}\int_0^a r^2 dr \int_{-1}^1 d\mu\, e^{iqr\mu} = \frac{mV_0}{\hbar^2}\int_0^a r^2 dr \frac{1}{iqr}\left(e^{iqr} - e^{-iqr}\right) \\
&= \frac{mV_0}{\hbar^2}\frac{2}{q}\int_0^a r\sin(qr)\, dr \\
&= \frac{mV_0}{\hbar^2}\frac{2}{q^3}\int_0^{qa} x\sin x\, dx = \frac{mV_0}{\hbar^2}\frac{2}{q^3}(-qa\cos qa + \sin qa) \\
&= \frac{2mV_0 a}{\hbar^2 q^2}\left[\frac{\sin qa}{qa} - \cos qa\right]
\end{aligned}$$

The factor in square brackets will go to zero when $\sin q_0 a = q_0 a \cos q_0 a$, that is, $q_0 a$ equal to some transcendental number (the first of which turns out to be 4.49). Known q_0 from the measurement, we get $a = 4.49/q_0$.

(3) The first step is to determine the normalization constant N. We have

$$\langle\psi|\psi\rangle = 1 = |N|^2(1+4+3) = 8|N|^2 \qquad \text{so} \qquad N = \frac{1}{2\sqrt{2}}$$

(a) We know that $\hat{H}|n\rangle = E_n|n\rangle = (n+1/2)\hbar\omega|n\rangle$, and our postulates tell us that we can only measure eigenvalues E_n. Therefore the probability of measuring (i) zero is zero, and (ii) the probability of measuring $3\hbar\omega/2 = (1+1/2)\hbar\omega$ is the probability of observing the state $|1\rangle$, namely $|2i/2\sqrt{2}|^2 = 1/2$.

(b) Here we are being asked for the expectation value of the energy, so

$$\langle E\rangle = \frac{1}{8}\left[\frac{1}{2}\hbar\omega\times 1 + \frac{3}{2}\hbar\omega\times 4 + \frac{5}{2}\hbar\omega\times 3\right] = \frac{\hbar\omega}{16}\left[1+12+15\right] = \frac{7}{4}\hbar\omega$$

(c) We just apply the time evolution operator $\hat{U}(t) = \exp(-i\hat{H}t/\hbar)$ to the state $|\psi\rangle$, so

$$\begin{aligned}
e^{-i\hat{H}t/\hbar}|\psi\rangle &= \frac{1}{2\sqrt{2}}\left[e^{-i\omega t/2}|0\rangle + 2ie^{-3i\omega t/2}|1\rangle + \sqrt{3}e^{-5i\omega t/2}|2\rangle\right] \\
&= \frac{e^{-i\omega t/2}}{2\sqrt{2}}\left[|0\rangle + 2ie^{-i\omega t}|1\rangle + \sqrt{3}e^{-2i\omega t}|2\rangle\right]
\end{aligned}$$

(4) (a) Although it first appears that $\langle\psi|\hat{z}|\psi\rangle$ has nine terms, each requiring an integration, most of those terms vanish. The first thing to realize is that the expectation value $\langle z\rangle$ vanishes in any eigenstate of the hydrogen atom, from parity symmetry. Second, matrix elements between states with different m also vanish, as shown in Townsend (11.43). (Or, just realize that the integrand for the matrix element between $m=0$ and $m=1$ states will have a factor of $e^{i\phi}$, which integrates to zero.) Therefore the only remaining terms are

$$\langle\psi|\hat{z}|\psi\rangle = \frac{1}{4}\langle 1s|\hat{z}|2p, m=0\rangle + \frac{1}{4}\langle 2p, m=0|\hat{z}|1s\rangle = \frac{1}{2}\langle 1s|\hat{z}|2p, m=0\rangle$$

where we realize that each term is real, so the complex conjugates are equal. (Much of this reasoning just follows the discussion in Section 11.3 of Townsend.) We have

$$\begin{aligned}
\langle\psi|\hat{z}|\psi\rangle &= \frac{1}{2}\int d^3r\,\langle 1s|\hat{z}|\mathbf{r}\rangle\langle\mathbf{r}|2p, m=0\rangle \\
&= \frac{1}{2}\int_0^{2\pi} d\phi \int_0^{\pi}\sin\theta\,d\theta\int_0^{\infty} r^2 dr\,\left[R_{10}(r)\sqrt{\frac{1}{4\pi}}\right] r\cos\theta\left[R_{21}(r)\sqrt{\frac{3}{4\pi}}\cos\theta\right] \\
&= \frac{\sqrt{3}}{4}\int_{-1}^{1} d\mu\,\mu^2\int_0^{\infty} r^3\frac{2}{\sqrt{3}}\frac{1}{2^{3/2}}\frac{1}{a_0^3}\frac{r}{a_0}e^{-3r/a_0}dr = \frac{1}{2}\frac{1}{2^{3/2}}\frac{1}{a_0^4}\int_0^{\infty} r^4 e^{-3r/a_0}dr
\end{aligned}$$

Quizzes #8 and #9 gave the formula here, namely $\int_0^\infty x^n e^{-ax}dx = n!/a^{n+1}$, so

$$\langle\psi|\hat{z}|\psi\rangle = \frac{1}{4\sqrt{2}}\frac{1}{a_0^5}5!\left(\frac{a_0}{3}\right)^6 = \frac{10}{3^5\sqrt{2}}a_0$$

Parts **(b)** and **(c)** are similar to Example 10.2 in Townsend. Writing the eigenstates in $|n,l,m\rangle$ notation, we have

$$|\psi\rangle = \frac{1}{2}|1,0,0\rangle + \frac{1}{2}|2,1,0\rangle + \sqrt{\frac{1}{2}}|2,1,1\rangle$$

The expectation values of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ are simple to read off from this. We have

$$\begin{aligned}
\langle\hat{\mathbf{L}}^2\rangle &= \frac{1}{4}(0)(1)\hbar^2 + \frac{1}{4}(1)(2)\hbar^2 + \frac{1}{2}(1)(2)\hbar^2 = \frac{3}{2}\hbar^2 \\
\langle\hat{L}_z\rangle &= \frac{1}{4}(0)\hbar + \frac{1}{4}(0)\hbar + \frac{1}{2}(1)\hbar = \frac{\hbar}{2}
\end{aligned}$$