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Solution to final exam
FY2045 Quantum Mechanics I
Thursday December 14, 2017

Problem 1

In this problem, you do not have to show your reasoning or calculations.

a) The easiest way to solve this problem is by dimensional analysis and some simple reasoning. We know that k, being a wave number, has units of inverse length. From this, we can immediately see that σ has units of length, since the argument to the exponential in the definition of $\phi(k)$ should be dimensionless. From this information, we can rule out option C, as is has inconsistent units for the momentum, and we can rule out option E, as it has wrong units for the variance of the position.

Furthermore, it is stated in the problem that $\phi(k)$ has a peak at $k = k_0$, which implies that the expectation value for the momentum should be $\hbar k_0$. This rules out option A. Finally, since the width of the distribution of k is finite, the uncertainty in momentum is finite, and hence the uncertainty in position must also be finite (i.e., not 0). This rules out option B.

We are left with the only possible alternative being option **D**.

b) Fermi's golden rule describes transition probabililty per unit time. If you didn't remember, you could guess this from the expression, since $\Gamma_{i\to f}$ has units of inverse time, and since it contains the absolute square of a matrix element it seems likely a probability, not an amplitude.

The answer is option **C**.

c) The triangular inequality for addition of angular momenta says that

$$|l_1 - l_2| \le l \le l_1 + l_2.$$

Hence, the answer is option **E**.

d) The amount of energy required to liberate an electron from a piece of metal, known as the work function of the metal, is the depth of the potential well, minus the Fermi energy, i.e. $V_0 - E_F$. The wavelength of a photon with this energy is $\frac{hc}{V_0 - E_F}$.

The correct answer is option **A**.

e) By calculating the norms and inner products, we find that all of the vectors have unit length, but the vectors in option **B** are not orthogonal to each other.

f) From the time independent Schrödinger equation (given in the Appendix), we find that the energy of a particle in this box is given by

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2mL^2} \left(\frac{n_x^2}{4} + \frac{n_y^2}{1} + \frac{4n_z^2}{9} \right).$$

Since the particles have spin $3/2$, we can have four particles in each spatial state, meaning there will be four particles in the ground state, and one particle in an excited state. The particle in the excited state will have to have $n_x = 2,\ n_y = 1,\ n_z = 1$, as this is the excited state with the lowest energy. The Fermi energy of the system is thus equal to

$$E_{211} = \frac{\hbar^2 \pi^2}{2mL^2} \left(\frac{4}{4} + \frac{1}{1} + \frac{4}{9} \right) = \frac{11}{9} \frac{\hbar^2 \pi^2}{mL^2}.$$

The correct answer is option **D**.

Problem 2

a) Since the energy is proportional to the square of $\Pi_n^{(l)}$, the state with the lowest energy is simply that corresponding to the smallest value of $\Pi_n^{(l)}$. The spatial state with the lowest energy is thus the state with $n = 1,\ l = 0$. In this state, we can place 2 particles, each with $m = 0$, and with opposite spin. The next available state with the lowest energy corresponds to $n = 1,\ l = 1$. In this state, the particles can have $m = -1$, $m = 0$ and $m = 1$, and again opposite spin, for a total of 6 particles. Finally, in the state $n = 1,\ l = 2$, we can have 10 particles, with $m = -2 \ldots 2$, and opposite spin. The energy thus becomes

$$\frac{\hbar^2}{2ma^2} \left[2 \left(\Pi_1^{(0)} \right)^2 + 6 \left(\Pi_1^{(1)} \right)^2 + 10 \left(\Pi_1^{(2)} \right)^2 \right] \approx 473 \frac{\hbar^2}{2ma^2}.$$

b) We have that the work done by the system on the surroundings, if there is an infinitesimal increase in the volume of the box, is

$$\mathrm{d}W = P\mathrm{d}V.$$

Since work done by the box corresponds to a reduction in the internal energy of the box, we have

$$P = -\frac{\mathrm{d}E}{\mathrm{d}V}.$$

Using that for a sphere of radius a, we have

$$\frac{\mathrm{d}V}{\mathrm{d}a} = 4\pi a^2,$$

we find

$$\begin{aligned} P &= -\frac{\mathrm{d}E}{\mathrm{d}V} \\ &= -\frac{1}{4\pi a^2}\frac{\mathrm{d}E}{\mathrm{d}a} \\ &= \left[2\left(\Pi_1^{(0)}\right)^2 + 6\left(\Pi_1^{(1)}\right)^2 + 10\left(\Pi_1^{(2)}\right)^2\right]\frac{\hbar^2}{4\pi m a^5} \\ &\approx 473\frac{\hbar^2}{4\pi m a^5} \end{aligned}$$

c) In this case, the next available state with the lowest energy is $n = 2,\ l = 0$, since $\Pi_2^{(0)} < \Pi_1^{(3)}$. The energy then becomes

$$\frac{\hbar^2}{2ma^2}\left[2\left(\Pi_1^{(0)}\right)^2 + 6\left(\Pi_1^{(1)}\right)^2 + 10\left(\Pi_1^{(2)}\right)^2 + \left(\Pi_2^{(0)}\right)^2\right] \approx 512.5\frac{\hbar^2}{2ma^2}.$$

d) We rewrite the integral

$$\int \psi^*_{nlm}(\boldsymbol{r})\, z\, \psi_{100}(\boldsymbol{r})\ \mathrm{d}^3r = \int R_{nl}(r)Y_{lm}(\phi,\theta)\ r\cos\theta\ R_{10}(r)Y_{00}(\phi,\theta)\ r^2\mathrm{d}\Omega\mathrm{d}r.$$

We then use the second part of the hint, and find that $Y_{10} = \sqrt{3}Y_{00}\cos\theta$, and we get

$$\frac{1}{\sqrt{3}}\int Y_{lm}(\phi,\theta)\ Y_{10}(\phi,\theta)\ \mathrm{d}\Omega \int R_{nl}(r)\ r\ R_{10}(r)r^2\ \mathrm{d}r.$$

From the orthogonality of the spherical harmonics, we can then tell that the integral will be zero, except when $l = 1,\ m = 0$.

Problem 3

a) If we calculate $V'(r) = V_0(r) + \hat{V}(r)$, where $V_0(r)$ is the potential energy of the unperturbed hydrogen atom, we find

$$V'(r) = \begin{cases} -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} & \text{for} \quad r > R \\ \frac{e^2}{4\pi\epsilon_0}\left(\frac{r^2}{2R^3} - \frac{3}{2R}\right) & \text{for} \quad r \leq R \end{cases},$$

which is what we want: The unperturbed potential for $r < R$, and the potential inside a uniformly charged sphere for $r > R$.

b) To solve this problem, it is necessary to remember (or guess from the given expression) that the first order correction to the energy of a state is given by

$$E_1^{(1)} = \langle \psi_n^{(0)} | \hat{V} | \psi_n^{(0)} \rangle,$$

where $\psi_n^{(0)}$ is the unperturbed state. Using this, and the ground state of the hydrogen atom (the relevant radial function and spherical harmonic are given in the appendix), we find

$$E_1^{(1)} = \int R_{10} Y_{00} \; \hat{V} \; R_{10} Y_{00} \; \mathrm{d}^3 r.$$

Since the perturbation depends only on r (and not θ and ϕ), we can separate out the angular part, which gives a factor of 1 since the spherical harmonics are orthonormalised. Since the perturbation is 0 for $r > R$, we integrate only from 0 to R, and we get

$$\begin{aligned} E_1^{(1)} &= \int_0^R R_{10} \; \hat{V} \; R_{10} \; r^2 \mathrm{d}r \\ &= \frac{e^2}{\pi\epsilon_0 a_0^3} \int_0^R \mathrm{e}^{-2r/a_0} \left(\frac{r^2}{2R^3} - \frac{3}{2R} + \frac{1}{r} \right) r^2 \mathrm{d}r. \end{aligned}$$

c)

$$
\begin{aligned}
E_1^{(1)} &= \frac{e^2}{\pi\epsilon_0 a_0^3}\int_0^R \left(\frac{r^2}{2R^3} - \frac{3}{2R} + \frac{1}{r}\right) r^2 \mathrm{d}r \\
&= \frac{e^2}{\pi\epsilon_0 a_0^3}\left[\frac{r^5}{10R^3} - \frac{r^3}{2R} + \frac{r}{2}\right]_0^R \\
&= \frac{1}{10}\frac{R^2 e^2}{\pi\epsilon_0 a_0^3} \\
&= \left(-\frac{4}{5}\frac{R^2}{a_0^2}\right)\left(-\frac{e^2}{8\pi\epsilon_0 a_0}\right).
\end{aligned}
$$

As was stated in the problem, $R/a_0 \approx 10^{-5}$, which means that this perturbation modifies the ground state energy of hydrogen by a factor of about 10^{-10}. In other words, this is a tiny effect.

d) As the perturbation is a function of r, we expect states with different radial probability distribution to be differently affected. Hence, states with the same n, but different l will be affected differently. Thus, the energy of a state in the perturbed system depends not only on n, but also on l.

Problem 4

a)

$$
\begin{aligned}
\hat{S}_z \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix},
\end{aligned}
$$

$$
\begin{aligned}
\hat{S}_z \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\end{aligned}
$$

We see that χ_+ and χ_- are eigenvectors of the operator $\hat{S}_z$, and their eigenvalues are $\hbar/2$ and $-\hbar/2$.

b) To find the eigenvalues, we solve the equation

$$\det\begin{pmatrix} -\lambda & \hbar/2 \\ \hbar/2 & -\lambda \end{pmatrix} = 0$$
$$\Rightarrow \lambda^2 - \frac{\hbar^2}{4} = 0$$
$$\Rightarrow \lambda = \pm\frac{\hbar}{2}.$$

We find that $S_{+x} = \hbar/2$ and $S_{-x} = -\hbar/2$.

To find the eigenvectors, we solve the equation

$$(A - \lambda I)\,\boldsymbol{\xi} = 0$$

for each of the eigenvalues.

For $\lambda = \hbar/2$, we get

$$\frac{\hbar}{2}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 0$$
$$\Rightarrow a = b.$$

Then we use the normalisation condition, $a^2 + b^2 = 1$, to obtain

$$\chi_{+x} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Similarly, for the eigenvalue $-\hbar/2$, we obtain

$$\chi_{-x} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

c) First, we rewrite the Hamiltonian, using the given definition of ω, and the fact that $\mathbf{B}$ only has a non-zero component along the x direction:

$$\hat{H} = -\frac{\omega}{2}\hat{S}_x = -\frac{\hbar\omega}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Then, we insert this into the Schrödinger equation:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = -\frac{\hbar\omega}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix}.$$

This gives us two coupled differential equations:

$$\frac{\partial}{\partial t}a(t) = \mathrm{i}\frac{\omega}{4}b(t), \tag{1a}$$
$$\frac{\partial}{\partial t}b(t) = \mathrm{i}\frac{\omega}{4}a(t). \tag{1b}$$

Differentiating the second equation once with respect to time, and inserting the result into the first equation, and vice versa, we get

$$\frac{\partial^2}{\partial t^2}a(t) = -\frac{\omega^2}{4^2}a(t),$$
$$\frac{\partial^2}{\partial t^2}b(t) = -\frac{\omega^2}{4^2}b(t).$$

Using the general solution from the hint for each of these equations, we get

$$a(t) = A_+\mathrm{e}^{\mathrm{i}\frac{\omega}{4}t} + A_-\mathrm{e}^{-\mathrm{i}\frac{\omega}{4}t}, \tag{2a}$$
$$b(t) = B_+\mathrm{e}^{\mathrm{i}\frac{\omega}{4}t} + B_-\mathrm{e}^{-\mathrm{i}\frac{\omega}{4}t}. \tag{2b}$$

To find the coefficients, we first insert Eqs. (2a) and (2b) into Eq. (1a), which gives the additional conditions

$$A_+ = B_+,$$
$$-A_- = B_-.$$

We then use the given initial condition,

$$\psi(t=0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

to find

$$a(t=0) = A_+ + A_- = 1,$$
$$b(t=0) = A_+ - A_- = 0,$$

which finally gives us

$$A_+ = 1/2, \quad A_- = 1/2.$$

To find the state of the electron at time $t = \frac{\pi}{2\omega}$, where $\omega = g_e \frac{eB_0}{m_e}$, we can then just insert these values into Eqs. (2a) and (2b):

$$\psi(t = \frac{\pi}{2\omega}) = \begin{pmatrix} \frac{1}{2}\mathrm{e}^{\mathrm{i}\frac{\pi}{8}} + \frac{1}{2}\mathrm{e}^{-\mathrm{i}\frac{\pi}{8}} \\ \frac{1}{2}\mathrm{e}^{\mathrm{i}\frac{\pi}{8}} - \frac{1}{2}\mathrm{e}^{-\mathrm{i}\frac{\pi}{8}} \end{pmatrix},$$

$$= \begin{pmatrix} \cos\frac{\pi}{8} \\ \mathrm{i}\sin\frac{\pi}{8} \end{pmatrix}.$$