Solution

PHY 308 Midterm 2, Spring 2018

Stony Brook University

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6 problems and 100 points total. The following information may or may not be useful

Planck's constant: $\hbar = 1.055 \times 10^{-34}$ J-s $= 6.582 \times 10^{-16}$ eV-s
Speed of light: $c = 3 \times 10^8$ m/s
Mass of the electron: $m_e = 9.1 \times 10^{-31}$ kg
The electron volt: 1 eV $= 1.6 \times 10^{-19}$ J
The fine structure constant $\alpha = 1/137$
The gradient in spherical coordinates: $\vec{\nabla} f(r,\theta,\phi) = \hat{e}_r \frac{\partial f}{\partial r} + \hat{e}_\theta \frac{1}{r}\frac{\partial f}{\partial \theta} + \hat{e}_\phi \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}$
The Laplacian in spherical coordinates: $\nabla^2 f(r,\theta,\phi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial f}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}$

Table 4.2: The first few spherical harmonics, $Y_l^m(\theta,\phi)$.

$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$	$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$
$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$	$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$
$Y_1^{\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$	$Y_3^{\pm 1} = \mp\left(\frac{21}{64\pi}\right)^{1/2} \sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$
$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$	$Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta\cos\theta e^{\pm 2i\phi}$
$Y_2^{\pm 1} = \mp\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{\pm i\phi}$	$Y_3^{\pm 3} = \mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta e^{\pm 3i\phi}$

TABLE 4.7: The first few radial wave functions for hydrogen, $R_{nl}(r)$.

$R_{10} = 2a^{-3/2}\exp(-r/a)$
$R_{20} = \frac{1}{\sqrt{2}} a^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$
$R_{21} = \frac{1}{\sqrt{24}} a^{-3/2}\frac{r}{a}\exp(-r/2a)$
$R_{30} = \frac{2}{\sqrt{27}} a^{-3/2}\left(1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$
$R_{31} = \frac{8}{27\sqrt{6}} a^{-3/2}\left(1 - \frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$
$R_{32} = \frac{4}{81\sqrt{30}} a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$
$R_{40} = \frac{1}{4} a^{-3/2}\left(1 - \frac{3}{4}\frac{r}{a} + \frac{1}{8}\left(\frac{r}{a}\right)^2 - \frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$
$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}} a^{-3/2}\left(1 - \frac{1}{4}\frac{r}{a} + \frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$
$R_{42} = \frac{1}{64\sqrt{5}} a^{-3/2}\left(1 - \frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$
$R_{43} = \frac{1}{768\sqrt{35}} a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$

1 True/False (14 points)

Circle **T** if the statement is always true. Otherwise circle **F** for false. 2 points each

T **F** For a single electron bound to a nucleus with charge Z, the spatial extent of the stationary states (i.e. orbitals) decreases as Z is increased.

T **F** For a single electron bound to a nucleus with charge Z, the spacing between the energy levels decreases as Z is increased.

T **F** When the spin angular momenta of two identical particles are added, the z-component of the total angular momentum cannot exceed the z-component of either particle.

T **F** When the spin angular momenta of two identical particles are added, the eigenstates of the total spin angular momentum, $\hat{S}^2$, are either symmetric or antisymmetric under interchange of the two particles.

T **F** Electrons are Fermions.

T **F** The variational principle states that for any quantum system, the expectation value of the Hamiltonian evaluated using any normalized trial wave function will always be greater than or equal to the energy of the system's ground state.

T **F** In spherical coordinates (r, θ, ϕ), any function of the angles $f(\theta, \phi)$ can be written as a linear combination of spherical harmonics.

2 Multiple Choice (16 points)

Circle **one** answer for each question. 4 points each.

Which property applies to identical particles that are labeled "Bosons":
- a) they possess integer spin angular momentum
- b) their angular momentum cannot be added.
- c) they always have $\langle \hat{S}^2 \rangle = 0$
- d) they obey the Pauli principle.
- e) none of the above.

The atomic unit of length is (circle the closest answer):
- a) 0.529 nm
- b) 0.529 Å
- c) 0.529 μm
- d) 13.6 eV
- e) none of the above

Which of the following is *not* a valid set of quantum numbers for the orbitals of the hydrogen atom $\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_\ell^m(\theta, \phi)$:
- a) $n = 1, \ell = 0, m = 0$
- b) $n = 27, \ell = 26, m = -26$
- c) $n = 2, \ell = 1, m = -1$
- d) $n = 2, \ell = 1, m = 2$
- e) none of the above.

The energy-time uncertainty principle
- a) only applies to decaying excited states.
- b) only applies to wave packets.
- c) assures that in atomic spectra the spectral width of an observed transition between two quantum states is always inversely related to the upper state lifetime.
- d) none of the above.

many line broadening mechanisms in expt.
Only true for natural linewidth

3 The Virial Theorem (15 points)

For the hydrogen atom as we have treated it in class (nucleus fixed, neglecting fine and hyperfine structure, etc.)

a) What are the normalized ground state wave function and binding energy (i.e. the energy required to remove the electron from the atom)?

b) Calculate the expectation value of the potential energy $\langle \hat{V} \rangle$ for a hydrogen atom in its ground state?

c) Calculate the expectation value of the kinetic energy $\langle \hat{T} \rangle$ for a hydrogen atom in its ground state?

Express your answers in atomic units ($e = \hbar = m_e = \frac{1}{4\pi\epsilon_0} = 1$).

a) $\psi_{100} = \frac{1}{\sqrt{\pi}} e^{-r}$ $\quad E_1 = -\frac{1}{2}$ $\quad$ Binding energy $= +\frac{1}{2}$

b) $$\langle \hat{V} \rangle = \int_{4\pi} d\Omega \int_0^\infty dr\, r^2 \frac{1}{\sqrt{\pi}} e^{-r} \left(\frac{-1}{r}\right) \frac{1}{\sqrt{\pi}} e^{-r}$$

$$= -\frac{4\pi}{\pi} \int_0^\infty dr\, r\, e^{-2r}$$

$$= -4 \int_0^\infty dr\, r\, e^{-2r}$$

Tabular Method

r	e^{-2r}
1 (+)	$-\frac{1}{2} e^{-2r}$
0 (−)	$+\frac{1}{4} e^{-2r}$

$\cancel{-\frac{1}{2} r e^{-2r}} \Rightarrow$ 0 at both bounds

$$-\frac{1}{4} e^{-2r} \Big|_0^\infty = \left[-\frac{1}{4} e^{-\infty} - \frac{-1}{4} e^{-0}\right] = \frac{1}{4}$$

$$\Rightarrow \boxed{\langle \hat{V} \rangle = -4\left(\frac{1}{4}\right) = -1}$$

c) $\langle \hat{T} \rangle + \langle \hat{V} \rangle = E_1$

$$\Rightarrow \boxed{\langle \hat{T} \rangle = -\frac{1}{2} + 1 = +\frac{1}{2}}$$

4 Angular Momentum Basics (16 points)

A certain state $|\Psi\rangle$ is an eigenstate of the total angular momentum $\hat{L}^2$ and z-component $\hat{L}_z$ such that

$$\hat{L}_z |\Psi\rangle = \hbar\ell |\Psi\rangle \quad \text{and} \quad \hat{L}^2 |\Psi\rangle = \hbar^2\ell(\ell+1) |\Psi\rangle$$

a) Calculate the expectation value $\langle \hat{L}_z \rangle$ for this state.

b) Show that for this state, one must have $\langle \hat{L}_x \rangle = \langle \hat{L}_y \rangle = 0$. *Hint: Consider what the ladder operators would do to this state.*

c) Calculate the expectation value $\langle \hat{L}_x^2 \rangle$ for this state. *Hint: You can assume symmetry with respect to x and y such that $\langle \hat{L}_x^2 \rangle = \langle \hat{L}_y^2 \rangle$.*

d) Calculate the uncertainties in the x and y components of the angular momentum for this state. Are your results consistent with the generalized uncertainty principle?

a) $\langle \Psi | \hat{L}_z | \Psi \rangle = \hbar \ell \langle \Psi | \Psi \rangle = \hbar \ell$

b) $\hat{L}_+ |\Psi\rangle = 0$ since on top rung $(m=\ell)$

so $\langle \hat{L}_x + i\hat{L}_y \rangle = \langle \hat{L}_x \rangle + i \langle \hat{L}_y \rangle = 0$

since $\hat{L}_x$ and $\hat{L}_y$ are Hermitian, expectation values must be real, thus each term above must be zero independently $\Rightarrow \langle \hat{L}_x \rangle = \langle \hat{L}_y \rangle = 0$

c) $\langle \hat{L}_x^2 \rangle + \langle \hat{L}_y^2 \rangle = \langle \hat{L}^2 \rangle - \langle \hat{L}_z^2 \rangle$

$2\langle \hat{L}_x^2 \rangle = \ell(\ell+1)\hbar^2 - \ell^2\hbar^2$

$= \ell \hbar^2$

$\Rightarrow \langle \hat{L}_x^2 \rangle = \langle \hat{L}_y^2 \rangle = \frac{\ell}{2}\hbar^2$

d) $(\Delta L_x)^2 = \langle \hat{L}_x^2 \rangle - \underbrace{\langle \hat{L}_x \rangle^2}_{0} = \frac{\ell}{2}\hbar^2$

$(\Delta L_y)^2 = \langle \hat{L}_y^2 \rangle - \langle \hat{L}_y \rangle^2 = \frac{\ell}{2}\hbar^2$

$\frac{1}{2} |\langle [\hat{L}_x, \hat{L}_y] \rangle| = \frac{1}{2} |\langle i\hbar \hat{L}_z \rangle|$

$= \frac{1}{2}\hbar^2 \ell$

Generalized uncertainty $\longrightarrow$ $\sigma_{L_x}\sigma_{L_y} = \sqrt{\frac{\ell\hbar^2}{2}}\sqrt{\frac{\ell\hbar^2}{2}} = \frac{\ell\hbar^2}{2} \geq \frac{\ell\hbar^2}{2}$ ✓ Yes!

5 Addition of Angular Momenta (20 points)

Consider two particles with spin 1/2. Answer the following questions about what happens when their angular momenta are added. **No partial credit.**

a) What are the possible m values for the z component of the total spin angular momentum $\hat{S}_z$, such that $\hat{S}_z |\psi\rangle = m\hbar |\psi\rangle$? (4 points)

$1, 0, -1$

b) What are the possible s values for the total spin angular momentum $\hat{S}^2$ such that $\hat{S}^2 |\psi\rangle = s(s+1)\hbar^2 |\psi\rangle$? (4 points)

$1, 0$

$s_1 + s_2 = 1$

$|s_1 - s_2| = 0$

and all integer steps in between

c) How many eigenstates of the total spin angular momentum are there? (4 points)

$(2\times\frac{1}{2}+1)(2\times\frac{1}{2}) = (2\times 1+1) + (2\times 0+1) = 4$

d) Write down all the eigenstates of the total angular spin angular momentum and z-component of the total, $|\frac{1}{2}\frac{1}{2}; sm\rangle$ in terms of the eigenstates of the z-components of the individual particles $|\frac{1}{2}\frac{1}{2}; m_1 m_2\rangle$? (8 points)

$s \; m \qquad m_1 \; m_2$

singlet $|\frac{1}{2}\frac{1}{2}; 0\,0\rangle = \frac{1}{\sqrt{2}}|\frac{1}{2}\frac{1}{2}; \frac{1}{2}\,\frac{-1}{2}\rangle - \frac{1}{\sqrt{2}}|\frac{1}{2}\frac{1}{2}; \frac{-1}{2}\,\frac{1}{2}\rangle$

$|\frac{1}{2}\frac{1}{2}; 1\,1\rangle = |\frac{1}{2}\frac{1}{2}; \frac{1}{2}\,\frac{1}{2}\rangle$

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

$|\frac{1}{2}\frac{1}{2}; 1\,-1\rangle = |\frac{1}{2}\frac{1}{2}; \frac{-1}{2}\,\frac{-1}{2}\rangle$

6 Three-dimensional Harmonic Oscillator (19 points)

Consider a particle of mass m moving in three dimensions with the spherically symmetric potential $V(r)$ expressed in spherical coordinates as

$$V(r) = \frac{1}{2}m\omega^2 r^2 \tag{6.1}$$

where ω is a real positive constant with units of angular frequency.

a) Since the potential is spherically symmetric, this problem is separable. Taking the stationary state wave functions of the separable form

$$\psi(r,\theta,\phi) = \frac{u(r)}{r} f(\theta,\phi) \tag{6.2}$$

insert equation (6.2) into the time-independent Schrödinger equation for this system and derive differential equations for $u(r)$ and $f(\theta,\phi)$, i.e. the "radial equation" and the "angular equation" for this system, as we did for the Hydrogen atom.

b) What are the solutions to the angular equation?

c) What is the ground state wave function and ground state energy for this system?

a) $$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m\omega^2 r^2\psi = E\psi$$

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\hat{L}^2\psi$$

w/ $$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$ only depends on angles

Now

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\left(\frac{u}{r}f\right)\right) = \frac{f}{r^2}\frac{d}{dr}\left(r^2\left(\frac{1}{r}\frac{du}{dr} - \frac{u}{r^2}\right)\right)$$

$$= \frac{f}{r^2}\frac{d}{dr}\left(r\frac{du}{dr} - u\right)$$

$$= \frac{f}{r}\frac{d^2u}{dr^2}$$

✓ (1)

So the TISE reads

$$-\frac{\hbar^2}{2mr} f\frac{d^2u}{dr^2} + \frac{1}{2mr^2}\frac{u}{r}\hat{L}^2 f + \frac{1}{2}m\omega^2 r^2\frac{u}{r}f = E\frac{u}{r}f$$

or multiplying (1) by $2m\left(\frac{fu}{r^3}\right)^{-1}$ and rearranging

$$\underbrace{-\hbar^2 \frac{r}{u}\frac{d^2u}{dr} + \left(\frac{1}{2}m\omega^2 r^2 - E\right)2mr^2}_{\text{only depends on } r} + \underbrace{\frac{1}{f}\hat{L}^2 f}_{\text{only depends on } f} = 0$$

$\Rightarrow$ Must both be equal to a constant $\pm C$ so gives two equations

$$\boxed{\begin{gathered}\hat{L}^2 f = cf \\ -\hbar^2 \, r^2\frac{d^2u}{dr^2} + \left(\frac{1}{2}m\omega^2 r^2 - E\right)2mr^2 u = -Cu\end{gathered}} \quad (2)$$

b) Need eigenfcns of $\hat{L}^2$ or Spherical Harmonics Y_ℓ^m

$$\hat{L}^2 Y_\ell^m = \ell(\ell+1)\hbar^2 Y_\ell^m$$

c) Inserting result from b) into (2) gives

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{1}{2}m\omega^2 r^2 + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right]u = Eu$$

For the ground state, take $\ell = 0$

Even More Space! (If you would like to be graded on this work, please indicate which problem corresponds to which work)

$l=0 \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \frac{1}{2}m\omega^2 r^2 u = Eu$

Now this is the standard simple harmonic oscillator differential equation, and the solutions are

Hermite Polynomial

$$U_n = N_n H_n(r)\, e^{-\frac{m\omega}{2\hbar}r^2}$$

Now normally, we would take the ground state to be $n=0$ and u is just a Gaussian, but here this diverges since $\psi_{ground} = \frac{u(r)}{r} Y_0^0$, so we need $u \to 0$ at $r=0$, so take the next state

$$u(r) = N r e^{-\frac{m\omega}{2\hbar}r^2}$$ w/ N a normalization constant

and then

$$\boxed{\psi = \left(\frac{1}{4\pi}\right)^{\frac{1}{2}} N\, e^{-\frac{m\omega}{2\hbar}r^2} \qquad E = \left(1+\frac{1}{2}\right)\hbar\omega = \frac{3}{2}\hbar\omega}$$

Normalization

$$1 = \int_{4\pi} d\Omega \int_0^\infty dr\, r^2 |\psi|^2 = N^2 \int_0^\infty dr\, r^2 e^{-\alpha r^2}$$ w/ $\alpha = \frac{m\omega}{\hbar}$

The integral can be done by parts

$$\int_0^\infty dr\, r^2 e^{-\alpha r^2}$$

$u = r \qquad dv = r e^{-\alpha r^2} dr \qquad v = \int dr\, r e^{-\alpha r^2}$

$du = dr$

$z = \alpha r^2$

$dz = 2 r \alpha dr$

$r dr = \frac{dz}{2\alpha}$

$\Rightarrow v = \int \frac{dz}{2\alpha} e^{-z}$

$= \frac{-e^{-z}}{2\alpha} = \frac{-e^{-\alpha r^2}}{2\alpha}$

so $\int_0^\infty dr\, r^2 e^{-\alpha r^2} = \overset{0}{\cancel{r\, r e^{-\alpha r^2}\Big|_0^\infty}} - \int_0^\infty dr\, \frac{-e^{-\alpha r^2}}{2\alpha}$

$= \frac{1}{2\alpha} \underbrace{\int_0^\infty dr\, e^{-\alpha r^2}}_{\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}} = \frac{\sqrt{\pi}}{4} \alpha^{-3/2}$

standard Gaussian integral

$\Rightarrow N^2 \frac{\sqrt{\pi}}{4} \alpha^{-3/2} = 1$

$N = 2\alpha^{3/4}/\pi^{1/4}$

$$\boxed{N = 2\left(\frac{1}{\pi}\right)^{1/4}\left(\frac{m\omega}{\hbar}\right)^{3/4}}$$

So putting it all together

$$\boxed{\psi = \left(\frac{1}{4\pi}\right)^{1/2} \cancel{2} \left(\frac{1}{\pi}\right)^{1/4} \left(\frac{m\omega}{\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar} r^2}}$$

$$\boxed{\psi = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar} r^2}}$$

$$\boxed{E_{ground} = \frac{3}{2}\hbar\omega}$$

Actually much easier to obtain this result in Cartesian coordinates

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \quad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega^2 y^2$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{1}{2}m\omega^2 z^2$$

$\Rightarrow$ easily separable $\psi_{ground} = \psi_0(x)\,\psi_0(y)\,\psi_0(z)$

$E_{ground} = \frac{1}{2}\hbar\omega + \frac{1}{2}\hbar\omega + \frac{1}{2}\hbar\omega = \frac{3}{2}\hbar\omega$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}y^2} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}z^2}$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar}(x^2+y^2+z^2)}$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-\frac{m\omega}{2\hbar}r^2}$$