

## PH102: Modern Physics Homework 2 (Due: 1/30/2012) with Hints

1. (20 points) Textbook: Harris, Chapter 7 Conceptual Question #7

2. (20 points) Textbook: Harris, Chapter 7 Conceptual Question #9

3. (20 points) Textbook: Harris, Chapter 7 Conceptual Question #14

The translation invariance means that the Hamiltonian is translationally invariant. The rotational invariance means that the Hamiltonian is rotationally invariant.

The formal definition of the (full; see comment below) translational invariance is that  $H(x, y, z) = H(x + a, y + b, z + c)$  for any constants  $a, b, c$ , where  $x, y, z$  are the Cartesian coordinates. The formal definition of the (full; see comment below) rotational invariance is that  $H(r, \theta, \phi) = H(r, \theta + a, \phi + b)$  for any constants  $a, b$ , where  $r, \theta, \phi$  are spherical coordinates. However, the following information, derivable from this formal definition, is sufficient.

First, note that

$$H = T \text{ (kinetic energy)} + U \text{ (potential energy)}.$$

The kinetic energy is both translationally and rotationally invariant.

The potential energy is translationally invariant if it is independent of  $x, y, z$  when it is expressed as a function of the Cartesian coordinates,  $x, y, z$ . (If the potential is independent of a certain Cartesian coordinate only, then the system is partially translationally invariant.)

The potential energy is rotationally invariant if it is independent of  $\theta, \phi$ , when it is expressed as a function of the spherical coordinates,  $r, \theta, \phi$ . (If the potential is independent of one angle only (like  $\phi$ ), then the system is partially rotationally invariant.)

If the system is translationally invariant, then the momentum is conserved. In QM, this means that the Hamiltonian eigenstate can be written as a momentum eigenstate ( $e^{ikx}$  for example).

If the system is rotationally invariant, then the angular momentum is conserved. In QM, this means that the Hamiltonian eigenstate can be written as an angular momentum eigenstate ( $Y_{lm}(\theta, \phi)$  or  $e^{im\phi}$ ).

Remember that  $H$  for the 3d infinite box and  $H$  for the hydrogen atom are different because of what type of potential a particle is in:

Schrodinger Equation:  $\frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{x}) + U(\vec{x})\psi(\vec{x}) = E \psi(\vec{x})$

Hamiltonian:  $H = \frac{-\hbar^2}{2m} \nabla^2 + U(\vec{x})$

For the 3d Infinite box  $U(\vec{x}) = \begin{cases} 0 & 0 < x < L_x, 0 < y < L_y, 0 < z < L_z \\ \infty & \text{otherwise} \end{cases}$

For the hydrogen atom  $U(r) = \frac{1}{4\pi\epsilon_0} \frac{-e^2}{r}$

You can discuss the wave functions for the Hamiltonian eigenstates in view of these invariances or the lack thereof. Note that even the 3d infinite box is not a translationally invariant problem since the potential is dependent on x, y, z coordinates, but the translationally invariant problem (the zero potential case) does shed light on it when we limit the particle behavior within the box.

4. (20 points) Unsöld's theorem states that, for any value of the orbital quantum number  $l$ , the probability densities summed over all possible states from  $m_l = -l$  to  $m_l = +l$  yield a constant independent of angles  $\theta$  or  $\phi$ , that is

$$\sum_{m_l=-l}^l |\Theta_{l,m_l}|^2 |\Phi_{m_l}|^2 = \text{Constant}$$

(a) Verify Unsöld's theorem for  $l = 0, l = 1,$  and  $l = 2.$

Where

$$l = 0, m_l = 0, \quad \Theta_{00} = \frac{1}{\sqrt{2}}, \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$l = 1, m_l = 0, \quad \Theta_{10} = \frac{\sqrt{6}}{2} \cos\theta, \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$l = 1, m_l = \pm 1, \quad \Theta_{1\pm 1} = \frac{\sqrt{3}}{2} \sin\theta, \Phi_{\pm 1} = \frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$$

$$l = 2, m_l = 0, \quad \Theta_{20} = \frac{\sqrt{10}}{4} (3 \cos^2\theta - 1), \Phi_0 = \frac{1}{\sqrt{2\pi}}$$

$$l = 2, m_l = \pm 1, \quad \Theta_{2\pm 1} = \frac{\sqrt{15}}{2} \sin\theta \cos\theta, \Phi_{\pm 1} = \frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$$

$$l = 2, m_l = \pm 2, \quad \Theta_{2\pm 2} = \frac{\sqrt{15}}{4} \sin^2\theta, \quad \Phi_{\pm 2} = \frac{1}{\sqrt{2\pi}} e^{\pm 2i\phi}$$

(b) Explain what this theorem tells about the charge distribution of the closed shell atoms such as Helium and Argon.

5. (20 points) Let us consider the angular wave functions for  $l = 1.$  We leave  $n$  as unspecified and general: it is a fixed, but arbitrary, positive integer. Thus, this problem applies to  $2p$  orbitals,  $3p$  orbitals, or  $4p$  orbitals, etc., regardless of the fixed value of  $n.$

(Note:  $\Theta_{l,m_l} \Phi_{m_l} = Y_l^{m_l}$ , spherical harmonics).

- (a) Show that the angular wave function  $Y_1^0$  has the same angular dependence ( $\theta$  and  $\phi$ ) as the coordinate  $z$  expressed in terms of the spherical coordinates  $(r, \theta, \phi)$ .
- (b) Show that by proper linear combinations of  $Y_1^1$  and  $Y_1^{-1}$ , it is possible to construct two wave functions that have the same angular dependence as the coordinates  $x$  and  $y$  respectively. Let us call these two new wave functions  $Y_x(\theta, \phi)$  and  $Y_y(\theta, \phi)$ .
- (c) Show that  $Y_x, Y_y,$  and  $Y_z$  (where  $Y_z = Y_1^0$ ) are mutually orthogonal to each other.

Note that this new set of vectors,  $Y_x, Y_y,$  and  $Y_z,$  also provide a complete description of  $p$  orbitals, just as the original  $Y_l^{m_l}$ 's. This new set may be familiar to you from chemistry textbooks: they are the so-called  $p_x, p_y,$  and  $p_z$  orbitals. While the two different sets for  $p$  orbitals,  $\{p_x, p_y, p_z\}$  and  $\{Y_1^1, Y_1^{-1}, Y_1^0\}$ , are completely equivalent for describing atomic orbitals, the  $\{p_x, p_y, p_z\}$  set provides a definitely more natural way to describe  $p$  orbitals in chemical bonds.

To test the orthogonality among  $Y_x, Y_y,$  and  $Y_z,$  use the following:

Orthogonality between  $Y_x, Y_y,$  check whether  $\int_0^\pi \int_0^{2\pi} Y_x^* Y_y \sin\theta d\theta d\phi = 0.$

Orthogonality between  $Y_y, Y_z,$  check whether  $\int_0^\pi \int_0^{2\pi} Y_y^* Y_z \sin\theta d\theta d\phi = 0.$

Orthogonality between  $Y_x, Y_z,$  check whether  $\int_0^\pi \int_0^{2\pi} Y_x^* Y_z \sin\theta d\theta d\phi = 0.$

6. Briefly describe your idea for the final course project in a paragraph. If you have multiple ideas, please describe them. The idea(s) you are presenting may not be the final project you end up presenting, which is OK.