Quantum Mechanics Week 5: Class Prep

Please study this worksheet before Wednesday's Week 5 tutorial, and submit your solutions to the Class Prep exercises by the end of Tuesday. The estimated total time requirement is 2 hours.

Overview

This week we'll study how to solve the Schrödinger equation in 3 dimensions. We'll learn about:

- How the 3D Schrödinger equation can be solved for a particle in a cubical box
- Radial and angular solutions for particles moving in central potentials
- The energy eigenvalues and eigenfunctions of the hydrogen atom

This worksheet will help you get the most out of this week's tutorial, by covering some introductory aspects in advance of the class.

Resources for Learning

Please study the Week 5 resources. The estimated time requirement is 1 hour.

Video: The Week 5 video summarises the topics we'll study this week. The running time is 25:31.

Textbook: You can find more information on these topics in Chapter 4.1-4.2.

You are free to search for and use other resources in addition to (or instead of) the above, as long as you can answer the following Class Prep exercises.

Class Prep Exercises

Please answer these short exercises on paper and submit your scanned answers by the end of Tuesday. After studying the above resources, the estimated time requirement for these exercises is 1 hour.

1) Write down the Bohr formula for the energy of a hydrogen atom as a function of the quantum number n. In the following parts, we'll see how these energy values arise.

2) Write down the time-independent Schrödinger equation for the wavefunction $\psi(x, y, z)$ of a particle of mass μ moving in a 3D potential V(x, y, z).

When we solve the time-independent Schrödinger equation in spherical co-ordinates for a central potential V(r), we obtain $\psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$, where $Y(\theta, \phi)$ is an eigenfunction of angular momentum and the radial function R(r) satisfies,

$$-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2}\right]R = ER$$

3) If we define a new function u(r) = r R(r), show that $\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = \frac{1}{r} \frac{d^2 u}{dr^2}$.

Substituting this relation and using the potential of the hydrogen atom is $V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$, the radial equation becomes in this case,

$$-\frac{d^2u}{dr^2} + \left[-\frac{2}{ar} + \frac{l(l+1)}{r^2}\right]u = \frac{2\mu E}{\hbar^2}u$$

where $a = 4\pi\varepsilon_0 \hbar^2/\mu e^2$.

4) Show that $u_{10}(r) = re^{-r/a}$ is a solution of this equation for l = 0. What is the energy of this state? Check it agrees with the Bohr formula for n = 1. [Note: we write the eigenfunctions in the form $u_{nl}(r)$]

5) Show that $u_{21}(r) = r^2 e^{-r/2a}$ is solution for l = 1. What is the energy of this state? Check it agrees with the Bohr formula for n = 2.

6) The full energy eigenfunctions of the hydrogen atom may be written

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r) Y_{lm}(\theta,\phi) = \frac{u_{nl}(r)}{r} Y_{lm}(\theta,\phi)$$

where the energy depends only on the value of *n*. How many distinct eigenfunctions have n = 3?

Grading and getting help

How this is graded: Class Prep assignments are always graded on *completeness & effort*. If you submit a reasonable effort for all parts on time, you will receive full marks regardless of all details being correct. Otherwise, you will not receive a grade. Each Class Prep assignment represents 1% of the unit grade.

After you have studied this week's learning resources, these exercises are not supposed to take more than 1 hour to complete. If you've been working purposefully on these exercises for 30 minutes and you're struggling with the content, please stop and ask for help. You can work with a friend, e-mail the instructor (<u>cblake@swin.edu.au</u>) or ask a question on the Week 5 Discussion Board in Canvas.

The rest of this week's activities

In Wednesday's tutorial class we'll expand on the Class Prep exercises to:

- Normalise wavefunctions in 3 dimensions
- Identify the quantum numbers of a 3D wavefunction of the hydrogen atom
- Determine the expectation value of the radial co-ordinate of the electron in a hydrogen atom

Finally, **please complete the Week 5 Online Quiz** (10 multiple choice questions) by the end of Sunday Week 5. Each Online Quiz represents 1% of the unit grade.