

Homework assignment

Due Date: 02/14 by 11:59 pm

Fill in your solutions in the Pluto notebook provided below. Once completed, execute the notebook and export it as a PDF. Upload the PDF to Gradescope for grading, and assign the pages to the respective exercises. Please ensure that all of your solutions, including the code you wrote, are visible and legible in the exported PDF before submitting it to Gradescope. Keep in mind that adjustments to assignments after the submission deadline will not be accommodated.

Conceptual Problems

Exercise 1:

Prove that the Laplace operator in spherical coordinates is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$

Solution:

Your solution goes here ...

```
1 md" #### Solution:
2
3 Your solution goes here ...
4 "
```

Exercise 2:

Prove that the Laplacian is spherically symmetric.

Solution:

Your solution goes here ...

```
1 md" #### Solution:
2
3 Your solution goes here ...
4 "
```

Exercise 3:

Prove that the spin- $\frac{1}{2}$ operator for a single particle satisfies

$$S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4} I_2$$

Use this result to show that $[S^2, S_\alpha] = 0$ for $\alpha = x, y, z$

Solution:

Your solution goes here ...

Programming Problems

We will follow the exercises outlined in Section 5.5 in Computational Physics (Second Edition) by Jos Thijsen please see the reference for additional information on the programming assignment.

Exercise 4:

'Combine the integration routine and the root-finding routine into a method for finding the $\ell = 0$ states of a radial potential.

Check: Test your program for the hydrogen atom.'

```
1 # Your code goes here ...
```

Exercise 5:

'Add an extra integration to your program which solves Eq. (5.77).

It is useful to check for correctness by using the hydrogen atom as an example. The normalised ground state density (in the sense of (5.76)), found at $E = -0.5$ a.u., is $4e^{-2r}$ and we must solve

$$\frac{d^2}{dr^2}U(r) = -4re - 2r,$$

with the boundary conditions $U(0) = 0, U(\infty) = 1$, so

$$U(r) = -(r + 1)e - 2r + 1$$

Check: Check whether your program produces these results '

```
1 # Your code goes here ...
```