Numerical projects in Quantum mechanics

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Quantum dots in three dimensions, one ad two electrons

We are first interested in the solution of the radial part of Schroedinger's equation for one electron. This equation reads

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{l(l+1)}{r^2}\right)R(r)+V(r)R(r)=ER(r).$$

In our case $V(r)$ is the harmonic oscillator potential $(1/2)kr^2$ with $k=m\omega^2$ and E is the energy of the harmonic oscillator in three dimensions. The oscillator frequency is ω and the energies are

$$E_{nl}=\hbar\omega\left(2n+l+\frac{3}{2}\right),$$

with $n=0,1,2,\dots$ and $l=0,1,2,\dots$.

Spherical coordinates

Since we have made a transformation to spherical coordinates it means that $r \in [0, \infty)$. The quantum number l is the orbital momentum of the electron. Then we substitute $R(r) = (1/r)u(r)$ and obtain

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + \left(V(r) + \frac{l(l+1)}{r^2}\frac{\hbar^2}{2m}\right)u(r) = Eu(r).$$

The boundary conditions are $u(0) = 0$ and $u(\infty) = 0$.

Making the equations dimensionless

We introduce a dimensionless variable $\rho = (1/\alpha)r$ where α is a constant with dimension length and get

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\rho^2}u(\rho) + \left(V(\rho) + \frac{l(l+1)}{\rho^2}\frac{\hbar^2}{2m\alpha^2}\right)u(\rho) = Eu(\rho).$$

In project 2 we choose $l = 0$. Inserting $V(\rho) = (1/2)k\alpha^2\rho^2$ we end up with

$$-\frac{\hbar^2}{2m\alpha^2}\frac{d^2}{d\rho^2}u(\rho) + \frac{k}{2}\alpha^2\rho^2 u(\rho) = Eu(\rho).$$

We multiply thereafter with $2m\alpha^2/\hbar^2$ on both sides and obtain

$$-\frac{d^2}{d\rho^2}u(\rho) + \frac{mk}{\hbar^2}\alpha^4\rho^2 u(\rho) = \frac{2m\alpha^2}{\hbar^2}Eu(\rho).$$

And introducing a natural length scale

We have thus

$$-\frac{d^2}{d\rho^2}u(\rho)+\frac{mk}{\hbar^2}\alpha^4\rho^2u(\rho)=\frac{2m\alpha^2}{\hbar^2}Eu(\rho).$$

The constant α can now be fixed so that

$$\frac{mk}{\hbar^2}\alpha^4=1,$$

or

$$\alpha=\left(\frac{\hbar^2}{mk}\right)^{1/4}.$$

Defining

$$\lambda=\frac{2m\alpha^2}{\hbar^2}E,$$

we can rewrite Schroedinger's equation as

$$-\frac{d^2}{d\rho^2}u(\rho)+\rho^2u(\rho)=\lambda u(\rho).$$

Discretizing I

We use the by now standard expression for the second derivative of a function u

$$u'' = \frac{u(\rho + h) - 2u(\rho) + u(\rho - h)}{h^2} + O(h^2), \tag{1}$$

where h is our step. Next we define minimum and maximum values for the variable ρ, $\rho_{\mathrm{min}} = 0$ and ρ_{max}, respectively. You need to check your results for the energies against different values ρ_{max}, since we cannot set $\rho_{\mathrm{max}} = \infty$.

Discretizing II

With a given number of steps, n_{step}, we then define the step h as

$$h = \frac{\rho_{\mathrm{max}} - \rho_{\mathrm{min}}}{n_{\mathrm{step}}}.$$

Define an arbitrary value of ρ as

$$\rho_i = \rho_{\mathrm{min}} + ih \qquad i = 0, 1, 2, \ldots, n_{\mathrm{step}}$$

we can rewrite the Schrödinger equation for ρ_i as

$$-\frac{u(\rho_i + h) - 2u(\rho_i) + u(\rho_i - h)}{h^2} + \rho_i^2 u(\rho_i) = \lambda u(\rho_i),$$

or in a more compact way

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \rho_i^2 u_i = -\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + V_i u_i = \lambda u_i,$$

where $V_i = \rho_i^2$ is the harmonic oscillator potential.

Discretizing III

Define first the diagonal matrix element

$$d_i = \frac{2}{h^2} + V_i,$$

and the non-diagonal matrix element

$$e_i = -\frac{1}{h^2}.$$

In this case the non-diagonal matrix elements are given by a mere constant. *All non-diagonal matrix elements are equal*.
With these definitions the Schroedinger equation takes the following form

$$d_i u_i + e_{i-1} u_{i-1} + e_{i+1} u_{i+1} = \lambda u_i,$$

where u_i is unknown. We can write the latter equation as a matrix eigenvalue problem

From one to two electrons, studying the role of the repulsive Coulomb force

We are going to study two electrons in a harmonic oscillator well which also interact via a repulsive Coulomb interaction. Let us start with the single-electron equation written as

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r)+\frac{1}{2}kr^2u(r)=E^{(1)}u(r),$$

where $E^{(1)}$ stands for the energy with one electron only. For two electrons with no repulsive Coulomb interaction, we have the following Schroedinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr_1^2}-\frac{\hbar^2}{2m}\frac{d^2}{dr_2^2}+\frac{1}{2}kr_1^2+\frac{1}{2}kr_2^2\right)u(r_1,r_2)=E^{(2)}u(r_1,r_2).$$

Rewriting the equations

Note that we deal with a two-electron wave function $u(r_1, r_2)$ and two-electron energy $E^{(2)}$.
With no interaction this can be written out as the product of two single-electron wave functions, that is we have a solution on closed form.
We introduce the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and the center-of-mass coordinate $\mathbf{R} = 1/2(\mathbf{r}_1 + \mathbf{r}_2)$. With these new coordinates, the radial Schroedinger equation reads

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} - \frac{\hbar^2}{4m}\frac{d^2}{dR^2} + \frac{1}{4}kr^2 + kR^2\right) u(r, R) = E^{(2)} u(r, R).$$

Center of mass and relative coordinates

The equations for r and R can be separated via the ansatz for the wave function $u(r, R) = \psi(r)\phi(R)$ and the energy is given by the sum of the relative energy E_r and the center-of-mass energy E_R, that is

$$E^{(2)} = E_r + E_R.$$

We add then the repulsive Coulomb interaction between two electrons, namely a term

$$V(r_1, r_2) = \frac{\beta e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{\beta e^2}{r},$$

with $\beta e^2 = 1.44$ eVnm.

The equation for the relative motion

Adding this term, the r-dependent Schroedinger equation becomes

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2}+\frac{1}{4}kr^2+\frac{\beta e^2}{r}\right)\psi(r)=E_r\psi(r).$$

This equation is similar to the one we had previously in parts (a) and (b) and we introduce again a dimensionless variable $\rho = r/\alpha$. Repeating the same steps, we arrive at

$$-\frac{d^2}{d\rho^2}\psi(\rho)+\frac{mk}{4\hbar^2}\alpha^4\rho^2\psi(\rho)+\frac{m\alpha\beta e^2}{\rho\hbar^2}\psi(\rho)=\frac{m\alpha^2}{\hbar^2}E_r\psi(\rho).$$

Further manipulations

We want to manipulate this equation further to make it as similar to the one-lectron case as possible. We define a 'frequency'

$$\omega_r^2 = \frac{1}{4}\frac{mk}{\hbar^2}\alpha^4,$$

and fix the constant α by requiring

$$\frac{m\alpha\beta e^2}{\hbar^2} = 1$$

or

$$\alpha = \frac{\hbar^2}{m\beta e^2}.$$

The new equation to solve

Defining

$$\lambda = \frac{m\alpha^2}{\hbar^2}E,$$

we can rewrite Schroedinger's equation as

$$-\frac{d^2}{d\rho^2}\psi(\rho) + \omega_r^2\rho^2\psi(\rho) + \frac{1}{\rho}\psi(\rho) = \lambda\psi(\rho).$$

We treat ω_r as a parameter which reflects the strength of the oscillator potential.
With no repulsive Coulomb interaction you should get a result which corresponds to the relative energy of a non-interacting system. Make sure your results are stable as functions of $\rho_{\max}$ and the number of steps.
We are only interested in the ground state with $l = 0$. We omit the center-of-mass energy.
For specific oscillator frequencies, the above equation has analytic

The Python code

The code sets up the Hamiltonian matrix by defining the the minimun and maximum values of r with a maximum value of integration points. These are set in the initialization function. It plots the eigenfunctions of the three lowest eigenstates.

```
#Program which solves the one-particle Schrodinger equation
#for a potential specified in function
#potential(). This example is for the harmonic oscillator in 3d

from  matplotlib import pyplot as plt
import numpy as np
#Function for initialization of parameters
def initialize():
    RMin = 0.0
    RMax = 10.0
    lOrbital = 0
    Dim = 400
    return RMin, RMax, lOrbital, Dim
# Here we set up the harmonic oscillator potential
def potential(r):
    return r*r

#Get the boundary, orbital momentum and number of integration points
RMin, RMax, lOrbital, Dim = initialize()

#Initialize constants
Step    = RMax/(Dim+1)
```