EXCITONS

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January 8, 2019

1. In this first task you make the first step towards implementing the numerical techniques for solving the radial Schrödinger equation

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}+V(r)\right\}\zeta(r)=E\zeta(r);\quad r\in[0;\infty). \tag{1}$$

Consider $V(r)=\frac{1}{2}\mu\omega^2 r^2$ the potential of a spherical 3D harmonic oscillator. This problem can be solved analytically. The eigenvalues are given by

$$E_n=\left(n+\frac{3}{2}\right)\hbar\omega;\ \text{with } n=2k+l \text{ and } k=0,1,2,...;\ l=0,1,2,.... \tag{2}$$

As usual, l is the angular momentum quantum number,[1] and n is the principal quantum number. The degeneracy of the energy levels (the number of energy levels with the same energy) is given by $(n+1)(n+2)/2$. To be complete, I give you the eigenfunctions as well

$$\zeta_{k,l}(r)=A_{kl}r^{l+1}e^{-\nu r^2}L_k^{(l+\frac{1}{2})}(2\nu r^2);\quad \text{with}\quad \nu=\frac{\mu\omega}{2\hbar}, \tag{3}$$

A_{kl} a normalization constant, and $L_k^{(l+\frac{1}{2})}(x)$ a generalized Laguerre polynomial (where $k=(n-l)/2$ integer, see Eq. 2).
We are going to solve Eq. 1 numerically.

   (a) *Description:* A 1D harmonic oscillator (Griffiths, Sec 2.3) has eigenvalues $E_n=\left(n+\frac{1}{2}\right)\hbar\omega;\ n=0,1,2,....$ Explain the eigenvalues of the isotropic 3D harmonic oscillator, on the basis of of the 1D harmonic oscillator. [Hint: think of cartesian coordinates.]
   Deliverables: A short derivation.

   (b) *Description:* derive the degeneracies of the energy levels.
   Deliverables: A short derivation.

   (c) *Description:* Choose $V_0=\hbar\omega$. Write down the radial Schrödinger equation in dimensionless (energies and distances) form. Write a matlab routine that determines the the outer turning point. Plot the position of the outer turning point as function of energy (all in dimensionless units) for $l=0$. What analytical form does this curve have?
   Deliverables: The radial Schrödinger equation in dimensionless form. What (simple) form does the potential have? A plot of the outer turning point; an explanation of the curve.

[1] As always in spherical problems, one has the additional quantum number $m=-l,-l+1,...,l-1,l$, but the energy levels do not depend on these $2l+1$ different m values.

(d) *Description:* Using the central difference expression for the second derivative, write a matlab routine that solves the radial Schrödinger equation by forward and backward propagation to the outer turning point. Choose $l = 0$, $E/V_0 = \frac{3}{2}$. Find a grid

$$\rho_j = a + jh;\ j = 0, 1, ..., N \tag{4}$$

that covers the whole extend of the wave function, and that gives you the wave function $\zeta(\rho)$ with sufficient accuracy. We aim at obtaining a *minimum* N (and adapt a and h accordingly), such that the accuracy

$$|\zeta_{f,b}(\rho_j) - \zeta_{0,0}(\rho_j)| < \epsilon;\ j = 0, 1, ..., N \tag{5}$$

where $\epsilon = 3 \times 10^{-4}$, and $\zeta_{k=0,l=0}(\rho)$ is the analytical solution of Eq. 3. [Some tricks: rescale your forward and backward solutions, such that you have a continuous function $\zeta_f(\rho_M) = \zeta_b(\rho_M)$ at the matching point. Normalize your functions, $\int_0^\infty \left|\tilde{\zeta}(\rho)\right|^2 d\rho = 1$, to compare numerical and analytical solutions.]
Deliverables: A plot of the numerical (matched) forward $\zeta_f(\rho)$ and backward $\zeta_b(\rho)$ solutions; a plot of of the error compared to the analytical solution $e(\rho) = \zeta(\rho) - \zeta_{0,0}(\rho)$. A short description of those plots, such as the values of a, h, and N used. You have to motivate your choice of a, h, and N. Can/should we choose $a = 0$? What is the mininum N that gives the required accuracy? (N within a factor of two or so is sufficient.) What happens to $e(\rho)$ at the outer turning point?

2. In the second task you improve and complete the numerical techniques applied to the same problem as in 1. In 2(a) you demonstrate that, using the same grid as in 1(d), Numerov's method increases the accuracy. Fixing this grid and using Numerov's method, you then implement the shooting method, first using bisection, and then using the improved method. [Hint: an order of magnitude number of iterations needed to converge the eigenvalue asked in this problem is 10^1.]

   (a) *Description:* Again $l = 0$, $E/V_0 = \frac{3}{2}$. Write down the forward and backward propagation algorithms (LN[2] sec 1.2) using Numerov's method (LN sec 1.5). Modify your matlab routine of 1(d) to implement Numerov's method for solving the radial Schrödinger equation.
   Deliverables: A description of the propagation algorithms using Numerov's method. The same deliverables as for 1(d). How much of an imnprovement is Numerov's method?

   (b) *Description:* Again $l = 0$. Write a matlab routine that implements the shooting method for determining the lowest eigenvalue. Use the bisection method for root searching, starting with the bracket $E_{\min}/V_0 = 0.3$ and $E_{\max}/V_0 = 1.8$. Aim at a numerical eigenvalue E/V_0 to within 10^{-4} of the analytical result.
   Deliverables: A plot of the numerically obtained $\zeta(\rho)$ for $E_{\min}/V_0$ and for $E_{\max}/V_0$, and a plot of $\zeta(\rho)$ for the converged eigenvalue. What are the main qualitative differences in these plots? A list or table with E/V_0 and $F(E/V_0)$ (LN sec. 1.3) for each iteration. A short discussion of these results.

[2] "LN" means "lecture notes".

(c) *Description:* Same conditions as 2(b). Write a matlab routine that implements the improved method of eigenvalue search. Aim at a numerical eigenvalue E/V_0 to within 10^{-7} of the analytical result. Start with a guess $E/V_0 = 0.4$.
Deliverables: A list or table with E/V_0 and $F(E/V_0)$ for each iteration. Comment on the convergence of the eigenvalue.

3. In the third task we consider the more challenging Coulomb potential $V(r) = -e^2/(4\pi\epsilon r)$. Obviously one cannot choose $a = 0$ in Eq. 4, so we have to use displaced grids. Choose $V_0 = R_x = \mu e^4/(32\pi^2\epsilon^2\hbar^2)$, the Rydberg constant, to make the radial Schrödinger equation dimensionless. We aim at an accuracy of a numerical eigenvalue E/V_0 to within 10^{-5} of the analytical result. The grid spacing h, the start point a, and the end point $a + Nh$ all influence this accuracy. For a logarithmic grid (LN sec 1.6), we have an additional parameter τ_1 influencing the accuracy.
We want to achieve the accuracy in E/V_0 with a *minimum* number of points N, and call this the *optimal grid*. The background idea is that the computational cost scales with N, so it pays off to keep this number as small as possible , but not so small that one looses too much accuracy. [3]

   (a) *Description:* Choose $l = 1$. Making use of the matlab routines you have written, find the lowest eigenvalue E/V_0 and the wave function $\zeta(\rho)$ that belongs to that eigenvalue. Find the optimal grid. N within a factor of two or three from the minimum is sufficient here. You have to play with a and h.
   Deliverables: Write down the dimensionless Schrödinger equation for the Coulomb potential. A description of the grid that gives a sufficient accuracy, a plot of the numerically obtained $\zeta(\rho)$ and the converged eigenvalue. Convince us that you have actually found the lowest eigenvalue, and you have sufficient accuracy.

   (b) *Description:* Again $l = 1$. Switch to a logarithmic grid. Modify your matlab routines accordingly. Find the optimal (logarithmic) grid with $\tau_1 = 0$. [Hint: think carefully about the range and spacing of your logarithmic grid.]
   Deliverables: as in (a). Discuss whether it is advantageous to use a logarithmic grid.

   (c) *Description:* Choose $l = 0$. Focus on the lowest eigenvalue. As in (b), find the optimal logarithmic grid with $\tau_1 = 0$.
   Deliverables: A description of the grid that gives a sufficient accuracy. What are the main differences with the grid you found in (b).

   (d) *Description:* As (c), but now find the optimal *shifted* logarithmic grid with $\tau_1 \neq 0$.
   Deliverables: A description of the grid that gives a sufficient accuracy. Does the extra degree of freedom (τ_1) allow you to use a coarser grid for the same accuracy?

[3] In the present application, the computational costs are kept low on purpose anyway, which allows you to do the project quasi-interactively. In a real-life application, one may want to solve the Schrödinger equation many times over, for instance to fit/construct a potential such that it reproduces experimental spectra. To keep the computational costs low, this then requires the use of an efficient numerical routine, i.e., one that uses an optimal grid.

4. Table 1 gives the energies $\hbar\omega$ of selected exciton lines of the semiconductor Cu_2O, extracted from the experimental spectra. Table 2 contains the parameters we will use to calculate those lines. You are going to study how good (or how bad) some potentials are reproducing the experiment.
You set up a single grid that gives you sufficient accuracy for all the requested eigenvalues. From experiment you know what accuracy is required, and for the Coulomb potential you know the analytical results. Make sure you don't miss an eigenvalue; you have the wave functions to check whether you found the correct ones. [Hint: also think about what relative sign the wave function $\zeta(\rho)$ should have for $\rho \to 0$ and for $\rho \to \infty$ to find which eigenvalue.]

   (a) *Description:* Calculate the eigenvalues of the nS; $n = 1, 2, 3, 4, 5$ states using the Coulomb potential, and the routines you have developed above. Calculate the eigenvalues of the 2P and 3D states.
   Deliverables: A description of the grid you used for your calculations. A list/table with the converged eigenvalues of the calculated states in scaled units. Convince us that you are converged; discuss (briefly) how they compare to the analytical values, and what the degeneracies are. Plots of the 1S and of the 5S wave functions (vs. ρ). Comment on the usefulness of having a logarithmic grid.

   (b) *Deliverables:* The reduced mass in m_0, the scale factor r_0 in nm, and the Rydberg constant for this system in eV. What is the extend in nm of the 5S wave function you plotted in (a)? A list/table with the converged eigenvalues of the calculated states in eV. Discuss (briefly) how they compare to the values derived from experiment.

   (c) In order to incorporate size/frequency-dependent screening, Haken modified the Coulomb potential to

$$V(r) = -\frac{e^2}{4\pi\epsilon r}\left\{[1 - f_1(r)] + \frac{\epsilon}{\epsilon_1}[f_1(r) - f_2(r)] + \frac{\epsilon}{\epsilon_2} f_2(r)\right\},$$

   with

$$f_1(r) = \frac{1}{2}\left\{\exp\left[-\frac{r}{r_{+,1}}\right] + \exp\left[-\frac{r}{r_{-,1}}\right]\right\} \text{ and } f_2(r) = \frac{1}{2}\left\{\exp\left[-\frac{r}{r_{+,2}}\right] + \exp\left[-\frac{r}{r_{-,2}}\right]\right\}.$$

   The parameters are given in Table 2.
   Deliverables: Plots of the Haken potential $V(\rho)/V_0$ vs. ρ in comparison with the (scaled) Coulomb potential. Discuss (briefly) the main differences between the two potentials.

   (d) *Description:* Repeat the calculations of (a) with this potential.
   Deliverables: A list/table with the converged eigenvalues of the calculated states in scaled units and in eV. What happens to the degeneracies you observed in (a)? A comparison to the results of (a) and to the experimental values, and a brief discussion thereof. Is the Haken potential an improvement?

state	E_{exp}(eV)	state	E_{exp}(eV)	state	E_{exp}(eV)
1S	2.0212	3D	2.16202	5S	2.16801
2S	2.1378	4S	2.16555	5P	2.16829
2P	2.1484	4P	2.16609	5D	2.16846
3S	2.16027	4D	2.16629	5F	2.16851
3P	2.16135	4F	2.16652		

Table 1: Experimental exciton lines in Cu_2O, collected by *F. Schweiner, J. Main, G. Wunner, and C. Uihlein, Phys. Rev. B 95, 195201 (2017).*

parameter	symbol	value
electron mass	m_-	0.99 m_0
hole mass	m_+	0.57 m_0
band gap	E_g	2.17202 eV
diectric constant	ϵ	7.5 ϵ_0
Haken potential	ϵ_1, ϵ_2	7.11, 6.45 ϵ_0
	$r_{+,1}, r_{-,1}$	3.573, 2.711 nm
	$r_{+,2}, r_{-,2}$	1.656, 1.257 nm

Table 2: Parameters for calculating the excitions in Cu_2O, from *F. Schweiner, J. Main, G. Wunner, and C. Uihlein, Phys. Rev. B 95, 195201 (2017).*