Writing a DFT program for the helium atom in Matlab

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Script 1: Poisson equation

We are looking for a solution on an equidistant mesh and therefore rewriting the equation using finite differences:

$$\frac{y_{i+1} - 2\,y_i + y_{i-1}}{h^2} = -4\,\pi\,x_i\,n(x_i)\,.$$

$y(0)=0$
$y(x_{max})=q$

Rewrite in matrix form **Ay=b**,

$$\boldsymbol{y} = \begin{pmatrix} y_2 \\ y_3 \\ \cdot \\ \cdot \\ \cdot \\ y_{N-1} \end{pmatrix} \qquad \boldsymbol{b} = \begin{pmatrix} -h^2\,4\pi\,x_2\,n(x_2) - 0 \\ -h^2\,4\pi\,x_3\,n(x_3) \\ \cdot \\ \cdot \\ \cdot \\ -h^2\,4\pi\,x_{N-1}\,n(x_{N-1}) - q \end{pmatrix}$$

A is a tridiagonal (N-2)x(N-2) matrix with $A_{i,i}$=-2 and $A_{i,i\pm1}$=1.

Script 2: Schrödinger equation

Radial Schrödinger equation using equidistant finite differences:

$$-\frac{1}{2}y''(x)+V(x)\,y(x)\approx-\frac{1}{2}\frac{y_{i-1}-2y_i+y_{i+1}}{h^2}+V(x_i)\,y_i=\lambda\,y_i$$

Reorganize the terms on the left side:

$$-\frac{1}{2h^2}\left(y_{i-1}+(-2-2h^2V(x_i))\,y_i+y_{i+1}\right)=\lambda\,y_i. \qquad y(0)=y(x_{max})=0$$

Rewrite in matrix form **Ay**=λ**y**, ***A*** is a tridiagonal (N-2)x(N-2) matrix

$$\boldsymbol{y}=\begin{pmatrix} y_2 \\ y_3 \\ \cdot \\ \cdot \\ \cdot \\ y_{N-1} \end{pmatrix}$$

$$A_{i,i}=-\frac{1}{2h^2}\left(-2-2h^2V(x_i)\right)$$

$$A_{i,i\pm1}=-\frac{1}{2h^2}$$

Script 3: Self-consistent cycle

1. Construct suitable starting guess for the charge density (hydrogen times 2)
2. Using this density, calculate potential terms: Hartree, exchange&correlation, external potential
3. Solve differential equation as in script 2
4. Calculate new density from the solution
5. Mix new and old densities (half-half)
6. Repeat steps 2-5 until self consistency