Time-independent Schödinger equation solver

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We are solving the time independent Schrödinger equation:

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\Psi = E\Psi \tag{1}$$

One approach is to use a basis of harmonic oscillators[1] to be able to find a matricial form for the operators. Here, we will use a finite difference method, as described in the paper from Graen and Grubmmüller [2].

We start with the approximation

$$\frac{\partial\Psi(x)}{\partial x} \simeq \frac{\Psi(x+\varepsilon) - 2\psi(x) + \Psi(x-\varepsilon)}{\varepsilon^2} \tag{2}$$

where ε is a small quantity. Ψ will be discretized in a grid of N steps of width ε.

For a 1D case, we can introduce this result in the Schrödinger equation and obtain (with atomic units[3]):

$$\frac{-1}{2m\varepsilon^2}\left(\Psi_+ - 2\Psi + \Psi_-\right) + V\Psi = E\Psi \tag{3}$$

Where we use the alleviated notation $\Psi(x) := \Psi$, $\Psi(x \pm \varepsilon) = \Psi_\pm$. We define the adimensional potential $V' = 2m\varepsilon^2 V$ and the adimensional energy $E' = 2m\varepsilon^2 E$, and rewrite the Schrödinger equaton as

$$-\Psi_+ + 2\Psi - \Psi_- + V'\Psi = E'\Psi \tag{4}$$

If we arrange Ψ as a vector of $N = 3$ elements, we can express the previous equation as an eigenvalue equation:

$$\begin{pmatrix} 2 & -1 & \\ -1 & 2 & -1 \\ & -1 & 2 \end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\\ \Psi_3\end{pmatrix} + \begin{pmatrix} V_1' & & \\ & V_2' & \\ & & V_3' \end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\\ \Psi_3\end{pmatrix} = E'\begin{pmatrix}\Psi_1\\ \Psi_2\\ \Psi_3\end{pmatrix}$$
$$\underbrace{\begin{pmatrix} 2+V_1' & -1 & \\ -1 & 2+V_2' & -1 \\ & -1 & 2+V_3' \end{pmatrix}}_{M+V'}\Psi = E'\Psi \tag{5}$$

Numerically, we only have to build the matrix $M + V'$ for the desired N and find its eigenvalues $\lambda = E'$ and eigenvectors $v \propto \Psi$.

The 2D case is similar, but we wave N^2 elements in the vector $\Psi(x, y) = \Psi_{ij}$. After defining $\Psi^\pm_\pm := \Psi(x \pm \varepsilon, y \pm \varepsilon)$, the resulting Schrödinger equation results

$$-\Psi_+ + 2\Psi - \Psi_- - \Psi_+ + 2\Psi - \Psi_- + V'\Psi = E'\Psi \tag{6}$$

[1] H Korsch and M Glück. Computing quantum eigenvalues made easy. *European Journal of Physics*, 23:413, 07 2002

[2] Timo Graen and Helmut Grubmüller. Nusol — numerical solver for the 3d stationary nuclear schrödinger equation. *Computer Physics Communications*, 198:169 – 178, 2016

[3] In atomic units $\hbar$,e,m_e and $\frac{1}{4\pi\varepsilon_0}$ are set to one. The unit of length is the Bohr radius ($\sim 5 \times 10^{-11}$ m), and the unit of energy is the *Hartree* ($\sim 4 \times 10^{-18}$ J $\simeq 27$ eV).

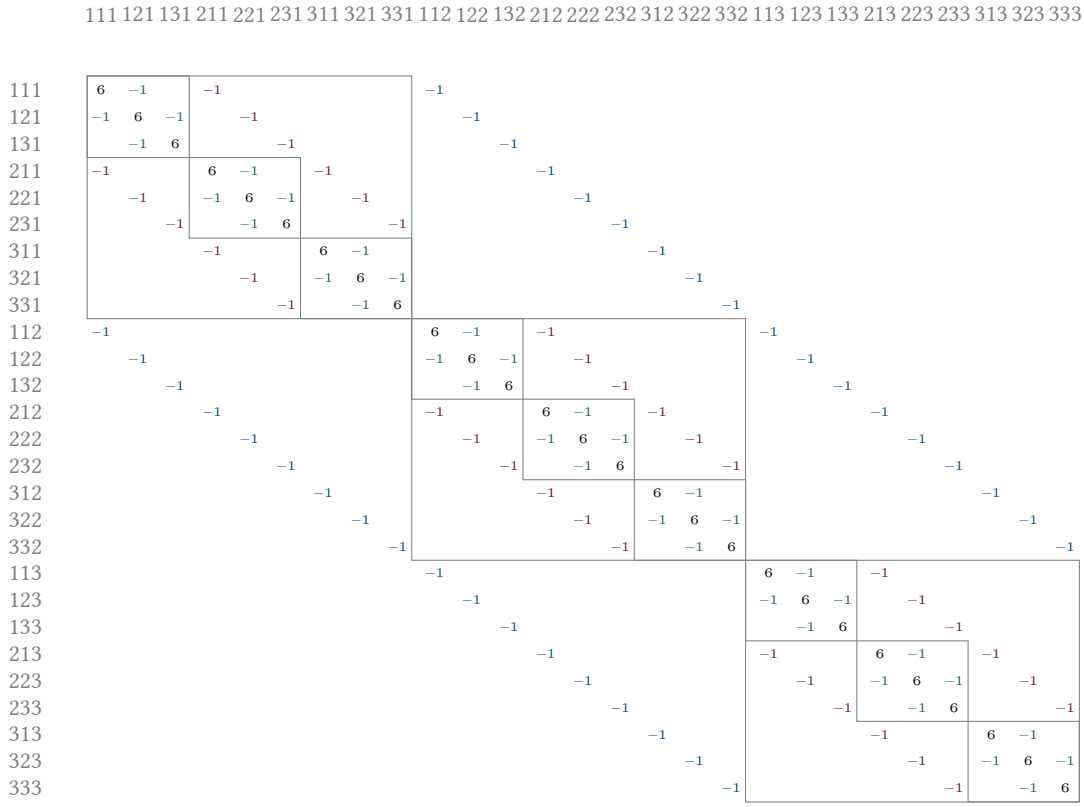
Ordering Ψ as $\Psi = (\Psi_{11}, \Psi_{12}, \Psi_{13}, \dots, \Psi_{1N}, \Psi_{21}, \dots, \Psi_{NN})$, we obtain the following matrix M:

	11	12	13	21	22	23	31	32	33
11	4	−1		−1					
12	−1	4	−1		−1				
13		−1	4			−1			
21	−1			4	−1		−1		
22		−1		−1	4	−1		−1	
23			−1		−1	4			−1
31				−1			4	−1	
32					−1		−1	4	−1
33						−1		−1	4

The diagonal blocks are the same as in the 1D case. The first diagonal of ones connect the elements i, j of Ψ with $i \pm 1, j$ (terms $\Psi_{\pm}$ in the equation) whereas the second one connects i, j with $i, j \pm 1$ (terms $\Psi^{\pm}$).[4]

In the 3D case, we have $\Psi(x, y, z)$; the new dimension amounts only to adding another diagonal of ones:

[4] Remember that $\Psi(x, y)$ is a 1D vector, despite its intrinsic 2D nature.



References

[1] Timo Graen and Helmut Grubmüller. Nusol — numerical solver for the 3d stationary nuclear schrödinger equation. *Computer Physics Communications*, 198:169 – 178, 2016.

[2] H Korsch and M Glück. Computing quantum eigenvalues made easy. *European Journal of Physics*, 23:413, 07 2002.