

Numerical solution of the Schrödinger equation
for the quantum harmonic oscillator

Derek W. Harrison

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Introduction

The nonrelativistic Schrödinger equation for the hydrogen atom is solved numerically using the finite volume method.

Model equations

The one-dimensional time independent Schrödinger equation for the harmonic oscillator is:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi = E \psi \quad (1)$$

Where \hbar is a constant, m the particle mass, ω the frequency, x the coordinate with respect to the origin, ψ the dependent variable and E the associated energy.

Discretization

The domain V of the system is partitioned into n_x nodes. Central differencing is applied to the diffusion term. The resulting eigen value problem is solved using the QR algorithm to obtain the eigen values, corresponding with the associated energies, and eigen vectors.

Normalization

The computed eigen vectors need to be normalized:

$$\psi = \frac{\psi}{\sqrt{\int_V \psi^2 dx}} \quad (2)$$

Note that the statement (2) above is not an equality, but an assignment.

Verification

In order to verify that the computations proceed correctly the results obtained numerically are compared with the analytical solutions for the first few energy levels. The ground state solution is:

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-m\omega x^2 / 2\hbar} \quad (3)$$

The equation for the first excited state is:

$$\psi_1 = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \sqrt{\frac{2m\omega}{\hbar}} x e^{-m\omega x^2 / 2\hbar} \quad (4)$$

And the equation for the second excited state is given by:

$$\psi_2 = C \left(1 - 2 \frac{m\omega x^2}{\hbar} \right) e^{-m\omega x^2/2\hbar} \quad (5)$$

A comparison between numerical and analytical solutions is shown in figures 1, 2 and 3. The comparison shows that the discrepancy between analytical and numerical results is relatively small. Discrepancies increase however at higher energy levels.

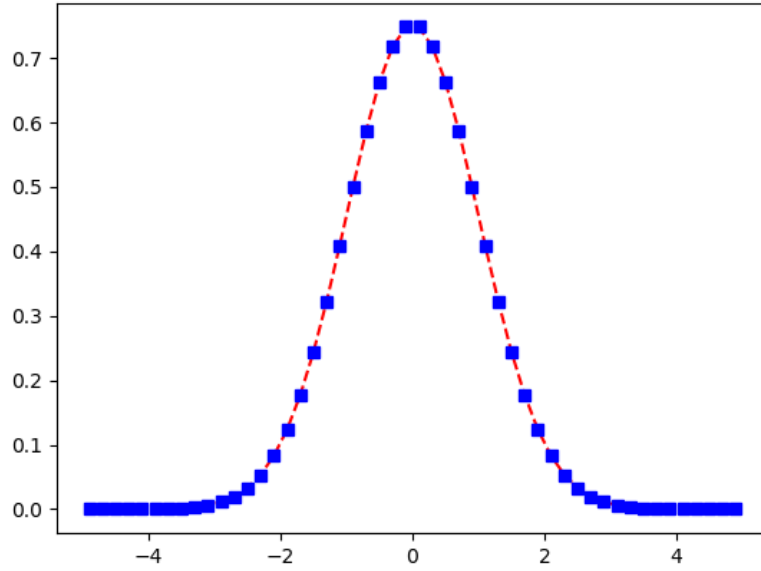


Figure 1: Analytical vs numerical results for the ground state. The dashed red line denotes the analytical solution and the blue squares the numerical solution

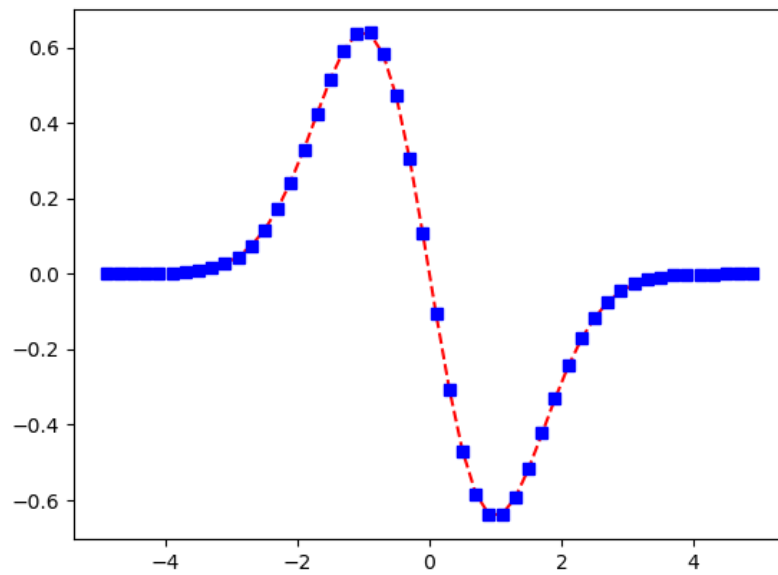


Figure 2: Analytical vs numerical results for the first excited state. The dashed red line denotes the analytical solution and the blue squares the numerical solution

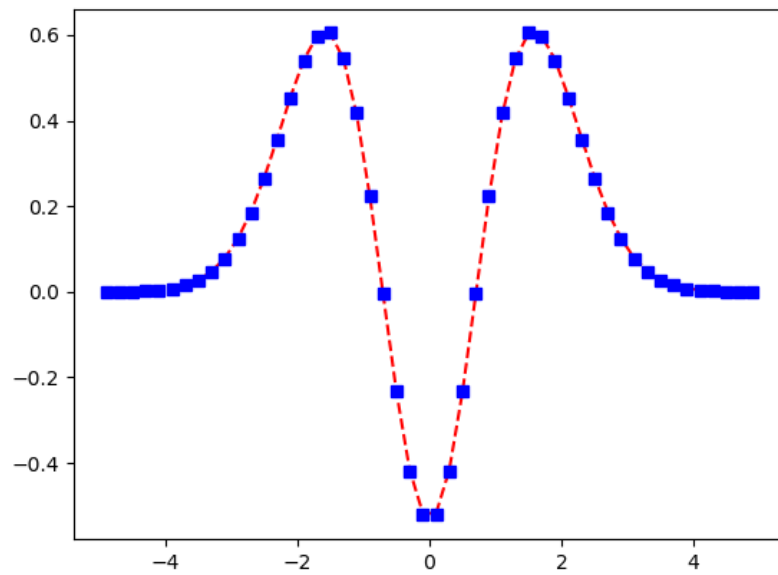


Figure 3: Analytical vs numerical results for the second excited state. The dashed red line denotes the analytical solution and the blue squares the numerical solution