

Simulation of time dependent hamiltonian

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Abstract

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Parametres

The 1D time dependent Schrödinger equation is given by

$$\hat{H}\Psi(x, t) = i\hbar \frac{\partial}{\partial t} \Psi(x, t), \quad \hat{H} = -\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + V(x, t),$$

for some potential $V(x)$. However, it is cumbersome to work with dimensionfull constants, especially numerically, when values for \hbar in the si-system is of order 10^{-34} . This can lead to inaccuracies when doing numerical simulations. But, by choosing some defining, problem-dependent sizes and grouping together the constants, this can be eliminated by the introduction of dimensionless variables. We are going to be working with potentials which are infinite outside some local region, i.e. the boundary conditions $\psi(0 > x > L) = 0$, so it is natural to choose the length of the potential, L , as a defining quantity. Noticing that

$$\left[\frac{\hbar}{2mL^2} \right] = \frac{\text{kg m}^2 \text{s}^{-1}}{\text{kg m}^2} = \text{s}^{-1},$$

we make the variable change

$$\frac{\hbar}{2mL^2} t \rightarrow t, \quad \frac{1}{L} x \rightarrow x.$$

This gives the new, dimensionless Schrödinger equation

$$\hat{H}\Psi(x, t) = -i \frac{\partial}{\partial t} \Psi(x, t), \quad \hat{H} = -\frac{\partial^2}{\partial x^2} + V(x, t), \quad (1)$$

where I have done the change $2mL/\hbar^2 V(x, t) \rightarrow V(x, t)$. All sizes now are in units defined by the problem and the constants of the equation, and the new boundary condition is

$$\Psi(0 > x > 1) = 0.$$

Time independent problems

Assuming, for now, that the potential is independent of time, we can get the time independent Schrödinger equation from (1) by separation of variables. Assuming $\Psi(x, t) = \psi(x)\phi(t)$ yields the time independent Schrödinger equation and the equation for the time dependence:

$$\left[-\frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x) = \hat{H}\psi = E\psi(x), \quad \frac{\partial}{\partial t} \phi(t) = -iE\phi(t). \quad (2)$$

The equation for time is elementary, and gives the solution

$$\phi(t) = \exp(-iEt).$$

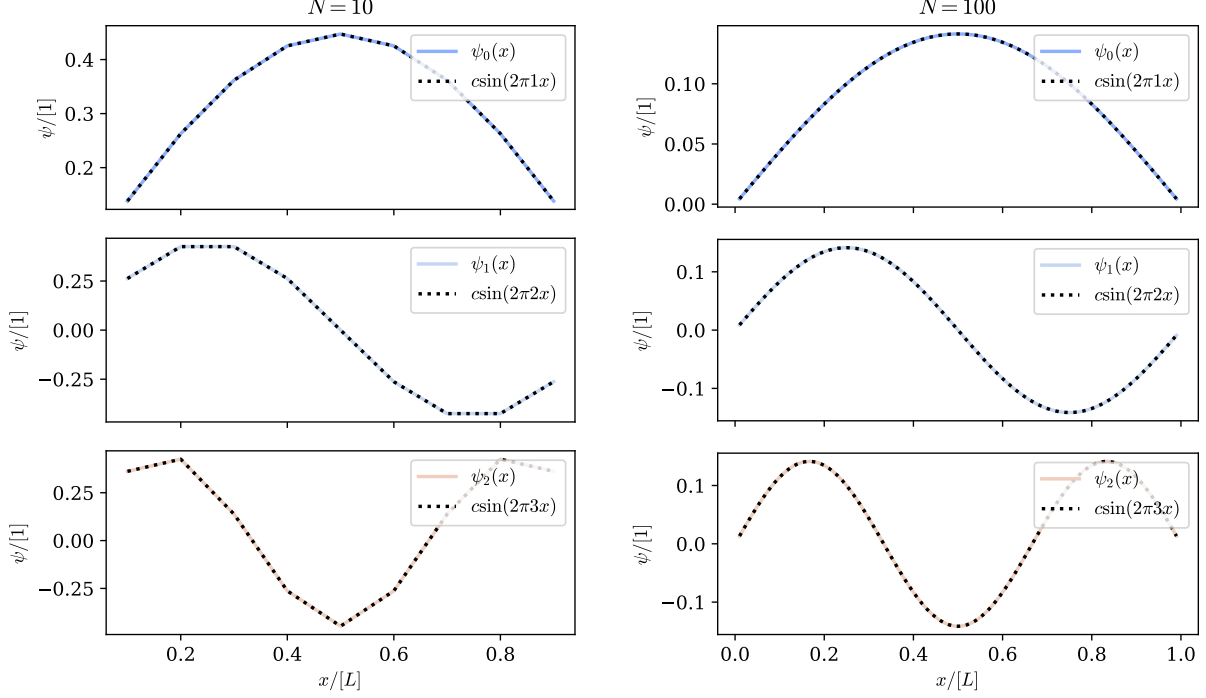


Figure 1: The numerical simulation and analytical solution to a prticle in a box

The time independent schrödinger equation is a eigenvalue problem, and can be solved by discretizing the hamiltonian, and thus also ψ . We are first going to look at a particle in a box, i.e. $V(0 < x < 1) = 0$. The euqaiion to discretize is thus

$$\frac{\partial^2}{\partial x^2} \psi(x) = E\psi(x).$$

Using a finite difference scheme with $N + 1$ nodes, there will be $N - 1$ possibly non-zero nodes. The end node are given by the boundary conditions $\psi(0) = \psi(1) = 0$, and the interior points are given by the matrix equation

$$D\psi_n = E_n\psi_n, \quad D_{ii} = 2N^2, D_{ii\pm 1} = -N^2.$$

Here, ψ_n is a vector such that $\psi_n^{(j)} = \psi_n((j + 1)/N)$. This is shown in the figure bleow.

$$\psi_n^{(0)} = 0 \quad \psi_n^{(1)} \quad \dots \quad \psi_n^{(N)} \quad \psi_n^{(N+1)} = 0$$

The result of the simulation, togheter with the analytical solution, is shown in figure 1. The normalization is such that the sum $\psi_n^{j\dagger} \psi_n^j = 1$ holds. The analytical solution for the eigenvalues are $E_n = (n\pi)^2$. By the finite nature of this simulation, the values are going to be less accurate for the higher energies, as they are waves where the wave length is short, and is aproaching the resolution of the discretization. Figure 2 shows the numerically computed eigenvalues, and compares them to the analytical solution. We see the error always wil increas rapidly for higher values, but we also get rapidly more accurate values by increasing N , i.e. decreasing the steplenght $\Delta x = 1/N$. In figure 3, we can se the trend of the error as the stepsize decrease. It is evident that the error decreases as the square of the steplength, or the inverse of the square of the number of points.

A straight forward way to implement the inner product of this discretizised eigenvectors are the usual inner product,

$$\langle \psi | \phi \rangle = \sum_i \psi_i^\dagger \phi_i.$$

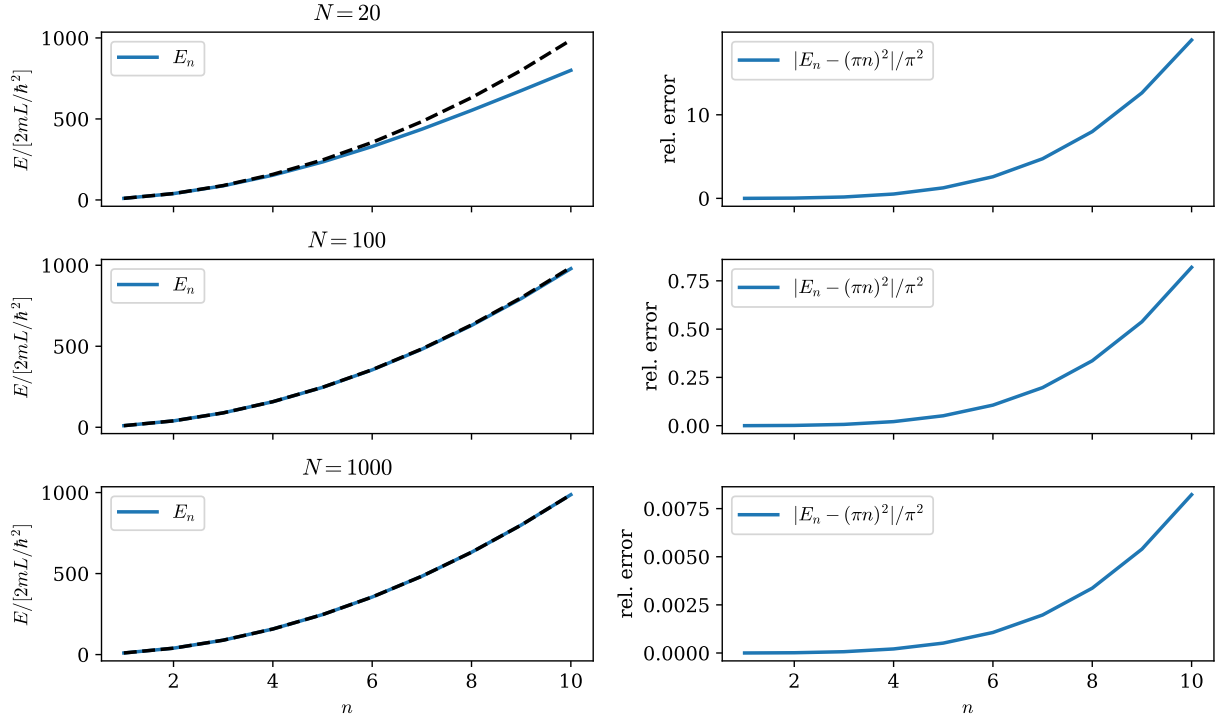


Figure 2: The numerical eigenvalues, compared with the analytical solution.

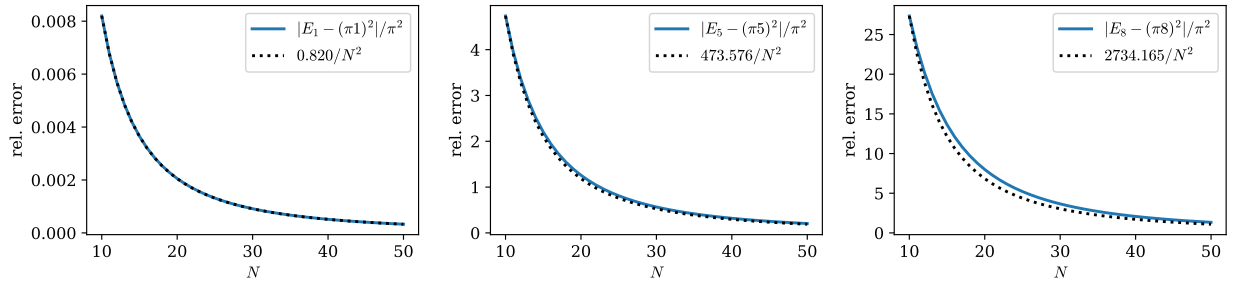


Figure 3: The errors for some of the few first eigenvalues, compared to the square of the steplength

This fits together with the normalization chosen earlier. The eigenvectors should be orthonormal, which they are, up to about a factor 10^{-15} .