

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 $\phi(t) = \exp(-iEt)$. The time independent schrödinger equation is an eigenvalue problem, and can be solved by discretizing the hamiltonian, and thus also ψ .

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

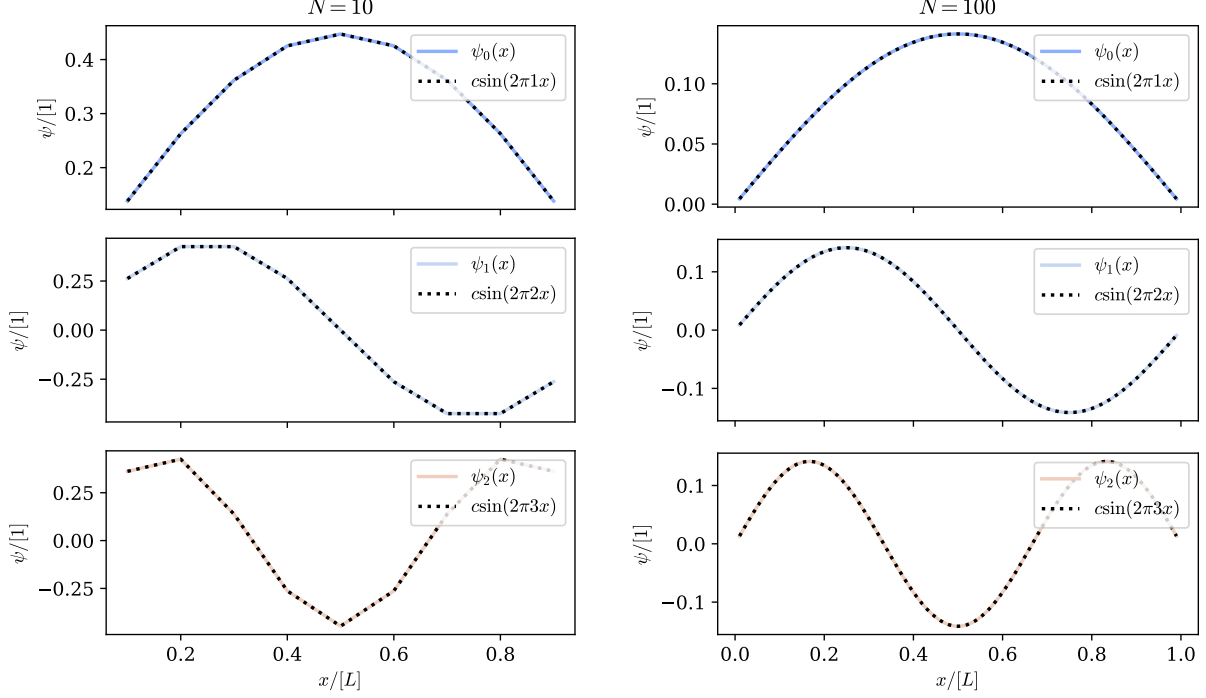


Figure 1: The numerical simulation and analytical solution to a prticle in a box

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

$$H\psi_n = E_n\psi_n, \quad H_{ii} = 2N^2 + V_i, D_{ii\pm 1} = -N^2.$$

Here, ψ_n is a vector such that $\psi_n^{(i)} = \psi_n((i + 1)/N)$, and V_i is the potential evaluated at that node. This is shown in the figure bleow.

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

Particle in a box

The method is first tested at a particle in a box, i.e. $V(0 < x < 1) = 0$. 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 steplenght, or the inverse of the square of the number of points.

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

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

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

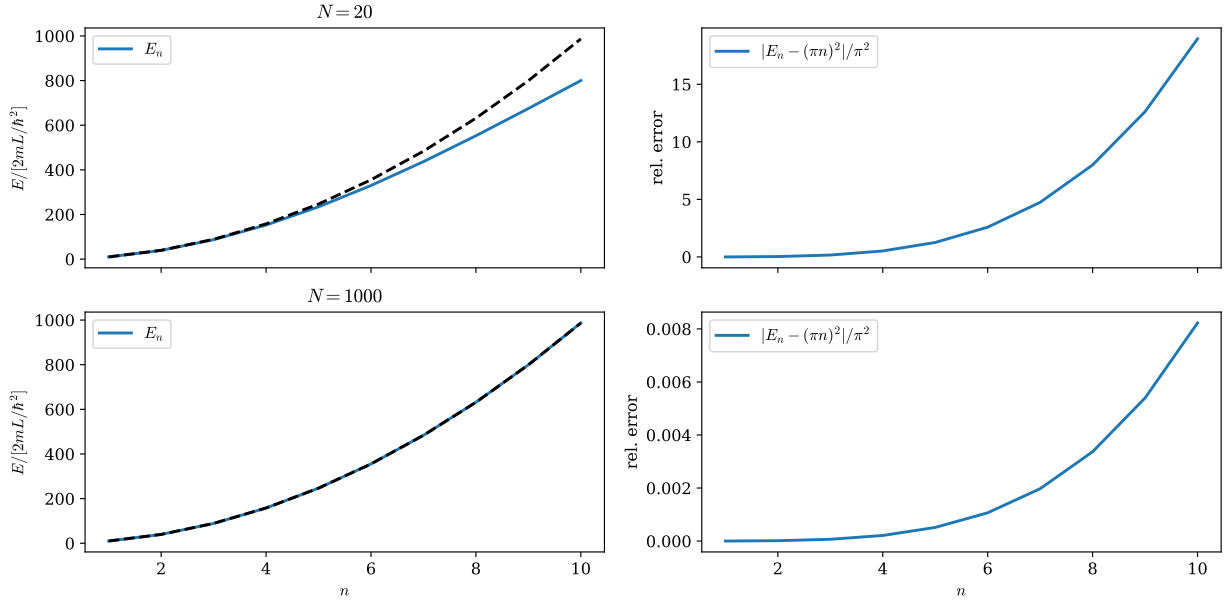


Figure 2: The numerical eigenvalues, compared with the analytical solution.

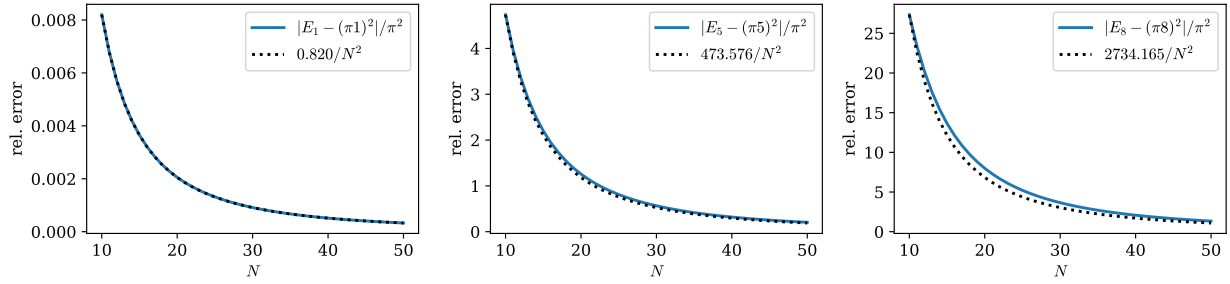


Figure 3: The errors for some of the few first eigenvalues, compared to the square of the steplength

A box with a barrier

Next, we put a barrier in the middle of the potential,

$$V(x) = \begin{cases} 0, & x \in (0, L/3] \cup [2L/3, L) \\ V_0, & x \in (L/3, 2L/3), \end{cases}$$

with the same boundary conditions as before. We will first study the case of $V_0 = 1000$, as shown in 4. We see there are 6 bound, the eigenvectors with positive curvature over the barrier. These have the twin eigenvalues which are almost equal. However they are not exactly equal, as there can be no degeneracy in 1D. These are, however, so close that they can be hard to calculate correctly. The bound values are given by the roots of

$$f(\lambda) = \exp(\kappa/3) \left[\kappa \sin(k/3) + k \cos(k/3) \right]^2 - \exp(-\kappa/3) \left[\kappa \sin(k/3) - k \cos(k/3) \right]^2,$$

where $\kappa = \sqrt{\lambda}$, $k = \sqrt{V_0 - \lambda}$. To find these roots, we use the secant method,

$$x_{n+1} = x_n - f(x_n) \frac{x_{n-1} - x_{n-2}}{f(x_{n-1}) - f(x_{n-2})}.$$

However, as there are several roots, and some of them are very close, it is important to choose good starting values. We can exploit the shape of the graph to do this, as the pseudo code below showcases. This program finds the local minima of the function, and runs the secant method on starting points in the minima and just to the left, and in the minima and just to the right, finding the two almost degenerate roots.

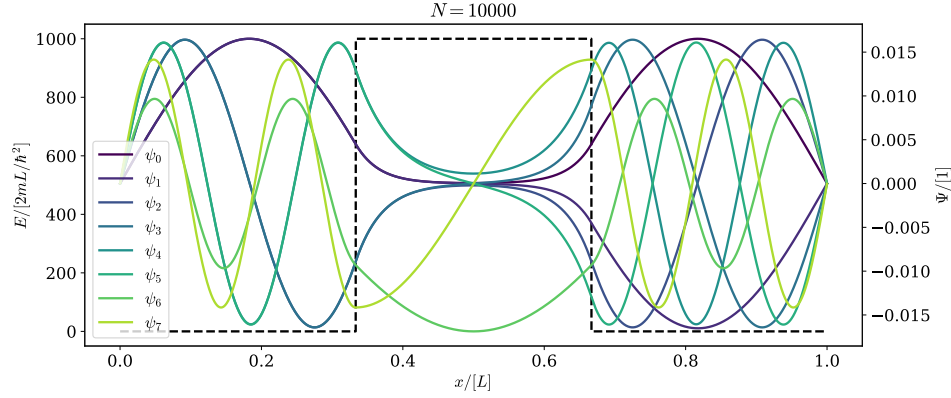


Figure 4: The first eigenstates of the system. The bound states have positive curvature at the barrier.

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x ← [0, dx, 2dx]
while x2 < xmax do
  while f(x0) > f(x1) < f(x2) do
    x ← x + dx
  end while
  roots ← roots ∪ secant(x0, x1)
  roots ← roots ∪ secant(x1, x2)
  x ← [0, dx, 2dx]
end while

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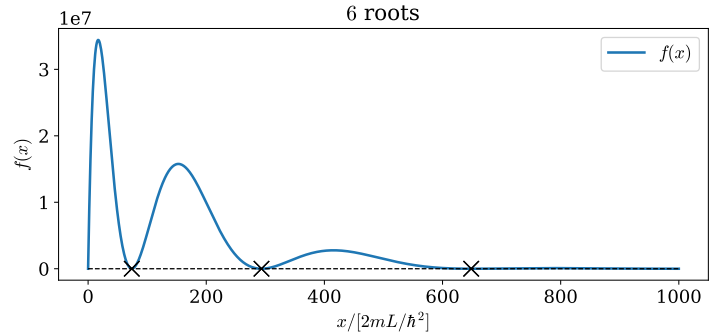


Figure 5: The shape of the function $f(x)$, shown to the right, makes it possible to effectively choose starting points for the secant method.

Time evolution

Given a starting condition of the wave function, $\Psi(x, 0) = f(x)$, it can be evolved in time by combining the solutions we found from separation of variables, 2, by using the fact that the eigenfunctions are a complete set,

$$|\Psi(0)\rangle = \langle \psi_n | f \rangle |\psi_n\rangle \implies |\Psi(t)\rangle = \langle \psi_n | f \rangle |\psi_n\rangle \exp(-itE_n) = \alpha_n |\psi_n\rangle \exp(-itE_n).$$

By taking a superposition of the first two eigenfunctions from the box with a barrier, $f(x) = (\psi_1(x) - \psi_2(x))/\sqrt{2}$, we can see that this starts almost only being on the right side, then it teleports over to the left. However, if the function has parts that are varying quickly, the numerics will be increasingly imprecise, as higher and higher eigenvalues and eigenvectors are needed, which might have larger errors, as we have seen. The computation of the eigenvalues and vectors can be skipped, by using the time evolution operator,

$$\hat{U} = \exp[-it\hat{H}].$$

A first approximation is to Taylor expand this, as $\hat{U} = I - i\Delta t\hat{H}$, and then iteratively taking a lot of small steps. The problem with this, however, is that the time evolution operator is a unitary operator, which this expansion is not. This leads to instabilities, and for probability not to be conserved. However, by using the Padé approximant of the exponential function instead,

$$\hat{U} = \frac{I - i\Delta t/2\hat{H}}{I + i\Delta t/2\hat{H}},$$

the operator is unitary, at the cost of having to find the inverse of the denominator. The stark difference in stability is shown in figure 8.

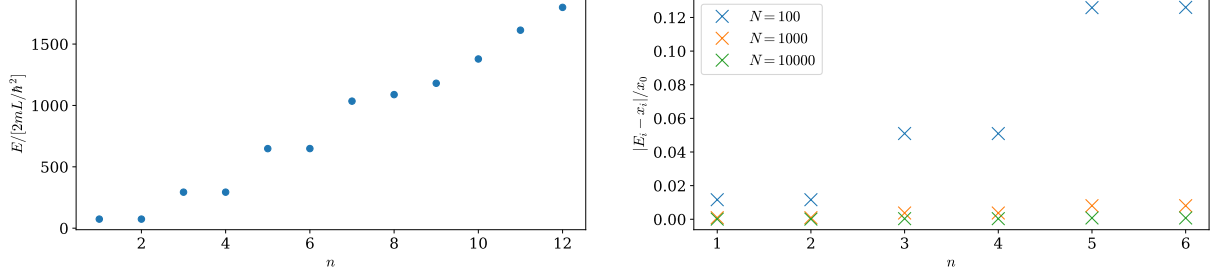


Figure 6: The shape of the function $f(x)$, shown to the left, makes it possible to effectively choose starting points for the secant method. The error from computing eigenvalues is shown to the right

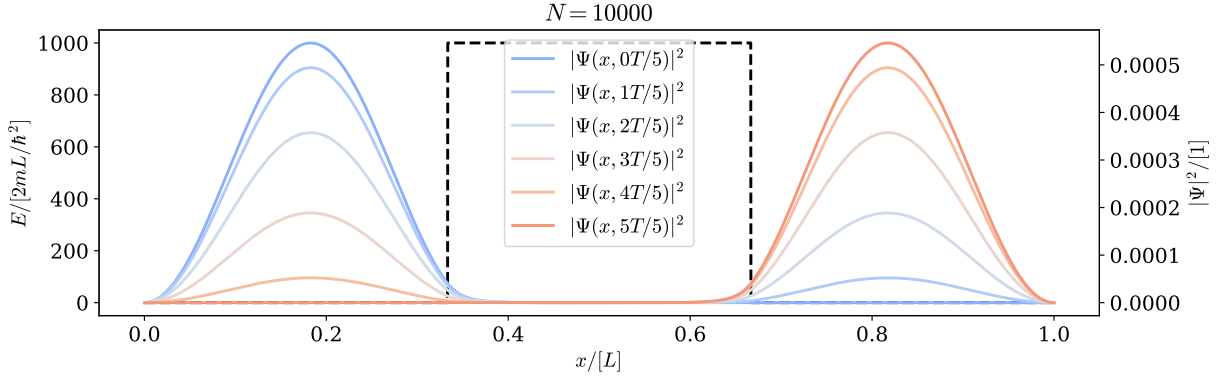


Figure 7: Time evolution of $(\psi_1(x) - \psi_2(x))/\sqrt{2}$. It starts out on the right side, but after a time $T = \pi/(E_2 - E_1)$, it has teleported over to the other side.

Periodic detuning

We now introduce a time dependence to the to the right part of the potential,

$$V(x) = \begin{cases} 0, & x \in (0, L/3] \\ V_0, & x \in (L/3, 2L/3) \\ V_r(t), & [2L/3, L). \end{cases}$$

Lets look at the system with $V_r(t) = \tau \sin(\omega t)$, where $\tau \ll \epsilon_0 = E_2 - E_1$. We therefore assume that, if the particle starts out in a superposition of 2 states, it will stay so. Furthermore, the ground states, and thus also ϵ_0 , are almost constant. We can thus write the full state as a linear combination of the two lowest states,

$$|\Psi(t)\rangle = \sum_k a_k(t) \exp[-itE_k] |k\rangle, \quad \langle x|k\rangle = \psi_k(x)$$

We can then write $\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t)$, and thus

$$\begin{aligned} -i \frac{d}{dt} |\Psi(t)\rangle &= -i \dot{a}_k(t) \exp[-itE_k] |k\rangle + a_k(t) E_k \exp[-itE_k] |k\rangle \\ &= a_k(t) \hat{H}_0 \exp[-itE_k] |k\rangle + a_k(t) \hat{H}_1(t) \exp[-itE_k] |k\rangle \\ / -i \exp[itE_j] \langle j| \cdot &\implies \dot{a}_j(t) = -i H_{jk} a_k(t) \exp[-it(E_j - E_k)], \quad H_{jk} = \langle j| \hat{H}_1(t) |k\rangle. \end{aligned}$$

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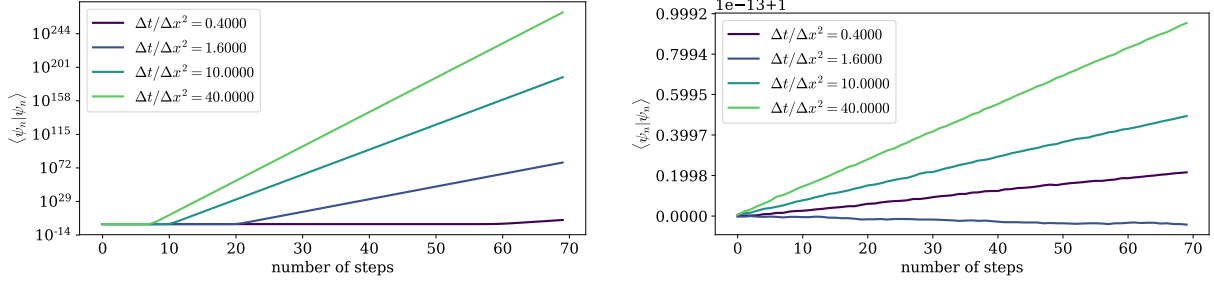


Figure 8: The drift in probability using the naïvé taylor expansion on the left, and the padé aproximat at the right. Be aware of the difference between the y-axis.

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$$|\psi(t)\rangle = |\psi(0)\rangle - i \int_0^t dt' \hat{H}(t') |\psi(t')\rangle.$$

This is discretized as a sum,

$$\psi_i^l = \psi_i^0 - i\Delta t \sum_{k=0}^l \sum_{j=1}^2 H_{ij}^k \psi_j^k, \implies A_{ij}^l \psi_j^l = b_i^l, \quad A_{ij}^l = \delta_{ij} + i\Delta t H_{ij}^l, \quad b_i = \psi_i^0 - i\Delta t \sum_{k=0}^{l-1} \sum_{j=1}^2 H_{ij}^k \psi_j^k.$$