

Numerical simulation of time dependent hamiltonian

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March 30, 2020

Parametres

The 1D time dependent Schrödinger equation is given by

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

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

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

we make the variable change

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

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 . We are first going to look at a particle in a box, i.e. $V(0 < x < 1) = 0$. The equation to discretize is thus

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

Using a finite difference scheme with N , this becomes a matrix equation,

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

This has automatically built in the boundary conditions, as D_{10} and D_{NN+1} does not exist, and is thus not included.