QUANTUM MANY-BODY SIMULATIONS IN HASKELL

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Abstract

Applying numerical methods in quantum mechanics has always been necessary in analyzing complex structures of quantum mechanical systems. The technical progress of computer performance has enabled physicists and mathematicians to simulate complex many-body systems. With these methods tangible progress in quantum physics can be made, to analyze quantum phenomena on the level of many-particle interactions. This article focuses on the implementation of numerical methods for many-body simulation in the functional programming language **Haskell**. Functional programming languages get more and more interesting for physicists through their mathematical way of implementation. In this article simple quantum systems are simulated first and an overview of different numerical methods for solving the Schrödinger equation will be given following an attempt to proceed to many-body systems from simple quantum systems.

CONTENTS

1 SIMPLE QUANTUM SYSTEMS

In this chapter simple quantum systems will be studied. Consider a particle in a three-dimensional potential $V(\vec{x})$. The corresponding wave function $\psi(\vec{x},t)$ is the solution of the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t) = H\psi(\vec{x},t) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{x},t) + V(\vec{x})\psi(\vec{x},t), \tag{1}$$

where Δ is the Laplacian differential operator: $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. For a time-independent potential $V(\vec{x})$ the Schrödinger equation can be formally solved by

$$\psi(\vec{x},t) = U(t,t_0)\psi(\vec{x},t_0) = \exp\left\{-\frac{i(t-t_0)}{\hbar}H\right\}\psi(\vec{x},t_0). \tag{2}$$

For a time-dependent potential like an oscillating laserfield, the time evolution of the wave function becomes

$$\begin{aligned}\psi(\vec{x},t) = U(t,t_0)\psi(\vec{x},t_0) &= \hat{T}_t \exp\left\{\frac{i}{h}\int_{t_0}^{t} H(\tau)d\tau\right\}\psi(\vec{x},t_0) \\ &= \sum_{n=0}^{\infty}\frac{1}{n}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ldots \int_{t_0}^{t} dt_n \hat{T}_t \left\{H(t_1)H(t_2)\ldots H(t_n)\right\},\end{aligned} \tag{3}$$

where $\hat{\mathrm{T}}_t$ is the time ordering operator. A simple approach is to divide the interval $[0 \dots t]$ into a sequence of N steps so that

$$\mathrm{U}(t, t_0) = \mathrm{U}(t, t_{N-1}) \dots \mathrm{U}(t_2, t_1)\mathrm{U}(t_1, t_0) \tag{4}$$

and to neglect small deviations of the Hamiltonian in the small interval $\Delta t = t_n - t_{n-1}$.

1.1 *Discretization of the kinetic Energy*

Dividing the Hamiltonian H into $H = T + V$, the nonlocal kinetic energy operator can be written as

$$T\psi(\vec{x}, t) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{x}, t). \tag{5}$$

1.1.1 *Method of Finite Differences*

Taking a grid (k, l, m) in three dimensions, the kinetic energy operator can be approximated by finite differences

$$T\psi(\vec{x}, t) = -\frac{\hbar^2}{2m}\left(\frac{\psi^n_{(k+1,l,m)} - 2\psi^n_{(k,l,m)} + \psi^n_{(k-1,l,m)}}{\Delta x^2} + \right.$$
$$\left.\frac{\psi^n_{(k,l+1,m)} - 2\psi^n_{(k,l,m)} + \psi^n_{(k,l-1,m)}}{\Delta y^2} + \frac{\psi^n_{(k,l,m+1)} - 2\psi^n_{(k,l,m)} + \psi^n_{(k,l,m-1)}}{\Delta z^2}\right) \tag{6}$$

with higher order terms $\mathcal{O}(\Delta x^2, \Delta y^2, \Delta z^2)$ where n represents the discrete time index of the wave function. Considering the time independent Schrödinger equation we can write the operator in one dimension as a matrix satisfying the eigenvalue equation

$$\left[\begin{pmatrix} 2 & -1 & & \dots & 0 \\ -1 & 2 & -1 & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & \dots & & -1 & 2 \end{pmatrix} + V_{kk}\right]\begin{pmatrix} \psi_1 \\ \vdots \\ \psi_k \\ \vdots \\ \psi_N \end{pmatrix} = E\begin{pmatrix} \psi_1 \\ \vdots \\ \psi_k \\ \vdots \\ \psi_N \end{pmatrix} \tag{7}$$

where $\vec{\psi}$ are the values of the wave function on the evaluation points x_k. V_{kk} represents the potential for each x_k, thus it is a diagonal matrix.

For the example of a particle in a box the potential is

$$V_{kk} = \begin{cases} \infty & \text{for} \quad k = 0,\ k = N \\ 0 & \text{else} \end{cases} . \tag{8}$$

Solving the above eigenvalue equation yields the eigenfunctions ψ_n with eigenenergies E_n. The boundary conditions $V = \infty$ at $k = 0$ and $k = N$ are satisfied even when the boundary conditions are left out. An example of the first four eigenstates is shown in figure 1. To reduce the problem of a particle in three dimensions to a simple matrix equation, the spatial wave function $\vec{\psi}$ can be stacked, to obtain an N^3 dimensional vector

$$\vec{\psi}_{k,l,m} = \begin{pmatrix} \vec{\psi}_{1,1,m} \\ \vdots \\ \vec{\psi}_{1,N,m} \\ \vdots \\ \vec{\psi}_{N,1,m} \\ \vdots \\ \vec{\psi}_{N,N,m} \end{pmatrix}, \text{ through nested vectors.} \tag{9}$$

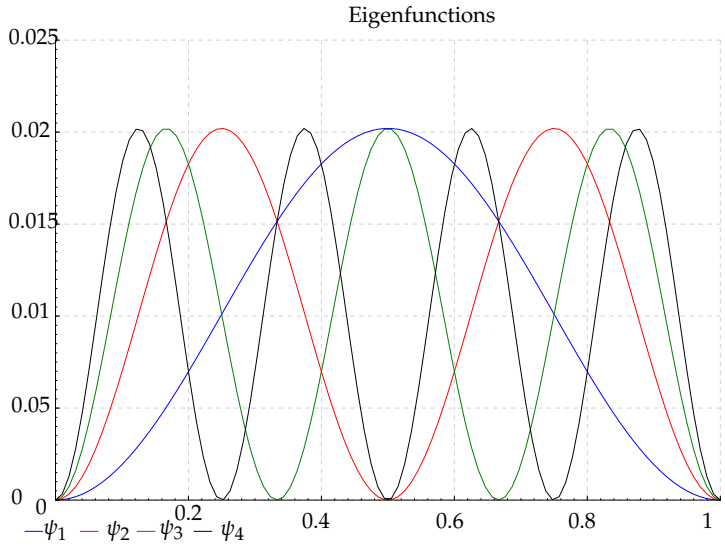

Figure 1: Propability densities for the calculated eigenfunctions ψ_n, with the method of finite differences and a grid of $N = 100$ for $n = 1, 2, 3$ and 4 in one dimension. For simplicity the prefactor $\frac{\hbar^2}{2m}$ was set to one, obtaining non-normalized eigenfunctions.

For two dimensions the approximated kinetic energy operator T thus becomes the tridiagonal block matrix

$$T \approx \begin{pmatrix} 4 & -1 & & -1 & & & 0 \\ & \ddots & & & \ddots & & \\ & -1 & 4 & & & -1 & \\ -1 & & & 4 & -1 & & \ddots \\ & \ddots & & & \ddots & & \\ 0 & & -1 & & & -1 & 4 \end{pmatrix}. \tag{10}$$

In figure 2 an example of an eigenstate for a particla in a two dimensional box is shown.

1.2 *A Subsection*

2 A SECTION

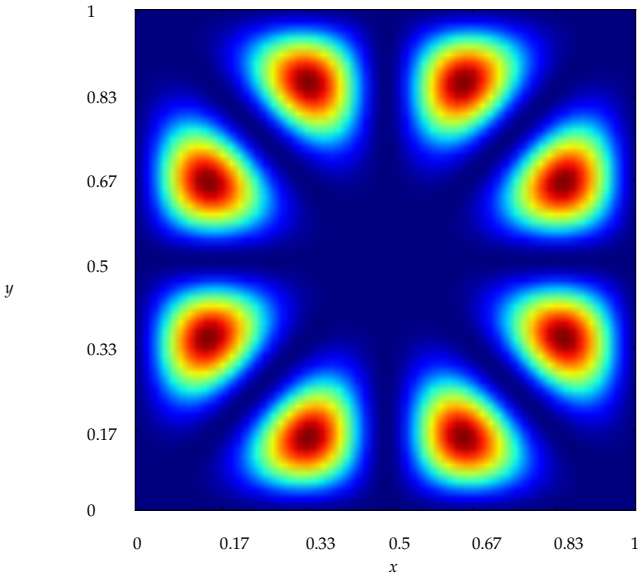

Figure 2: Propability densities for the calculated eigenfunction ψ_{12}, with the method of finite differences and a grid of $N = 60$ in two dimensions. For simplicity the prefactor $\frac{\hbar^2}{2m}$ was set to one, obtaining a non-normalized eigenfunction.