Computational Physics: Exact Diagonalization

Iasonas Andronis - ph4783 (UOC Department of Physics)

Introduction

Exact Diagonalization is a numerical method that is widely used for solving problems in quantum mechanics. In essense a Hamiltonian matrix is constructed and then diagonalized to find the eigenstates and eigenenergies so any observable can be then calculated from those.

Construction of the Hamiltonian

The Hamiltonian used in this problem is known as the Tight Binding Hamiltonian for a single electron in a 1d Lattice. Periodic Boundary conditions are assumed. The Hamiltonian is of the form:

$$H = \lambda \sum_n (|n+1\rangle\langle n| + |n\rangle\langle n+1|) + V_{nn} \sum_n |n\rangle\langle n|$$

where λ is the hopping term between lattice sites and V_{nn} are the diagonal elements of a diagonal potential matrix. The i, j-th element of the hamiltonian is calculated like so:

$$\langle i|H|j\rangle = \langle i| \left(\lambda \sum_n (|n+1\rangle\langle n| + |n\rangle\langle n+1|) + V_{nn} \sum_n |n\rangle\langle n| \right) |j\rangle$$

$$= \langle i| \left(\lambda \sum_n (|n+1\rangle\langle n|j\rangle + |n\rangle\langle n+1|j\rangle) + V_{nn} \sum_n |n\rangle\langle n|j\rangle \right)$$

$$= \lambda\langle i|j+1\rangle + \lambda\langle i|j-1\rangle + V_{nn}\langle i|j\rangle$$

$$= \lambda\delta_{i,j+1} + \lambda\delta_{i,j-1} + V_{nn}\delta_{i,j}$$

where $\delta_{n,m}$ is the Kronecker delta. We used a step potential.

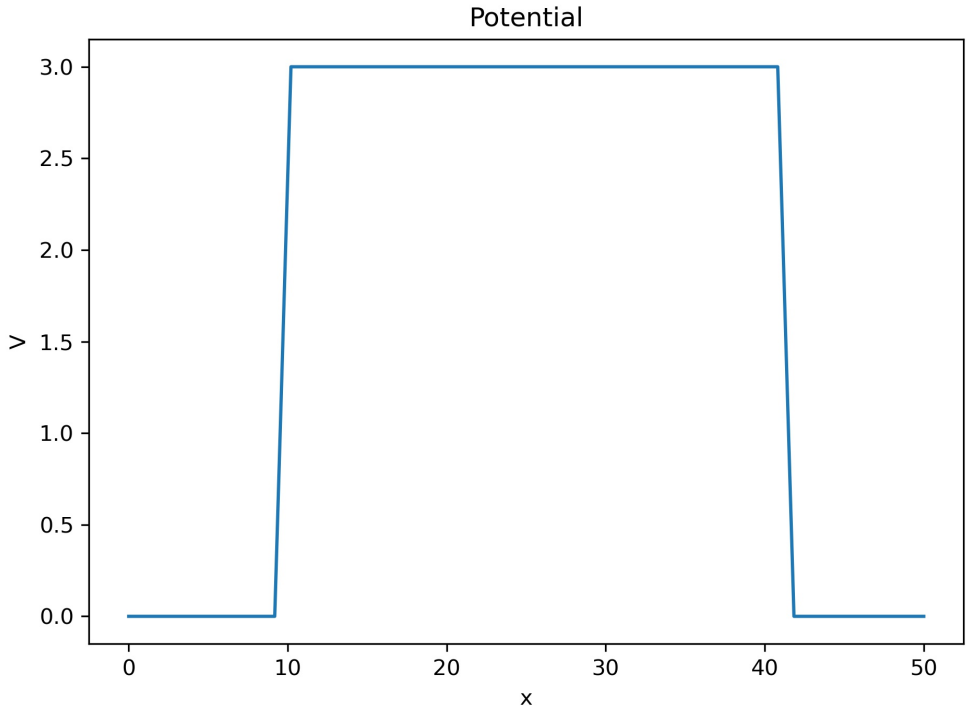

Figure 1 - Plot of the diagonal elements of the potential matrix.

The initial Gaussian distribution of the wave packet is:

$$C(i) = e^{(-0.04(x-25)^2)}$$

Now that we have a matrix (which we already can see that it is tridiagonal) we can compute numerically its eigestates and eigenenergies using functions from the Header Library Eigen or any other way we want. An example observable that we can calculate is the position x.

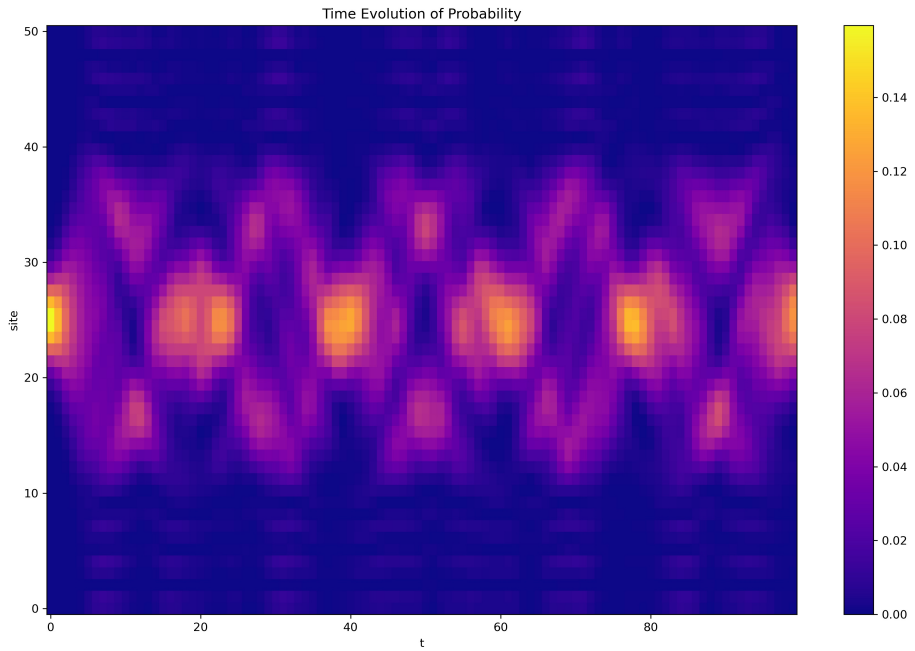

Figure 2 - Time evolution of the probability density of the electron.

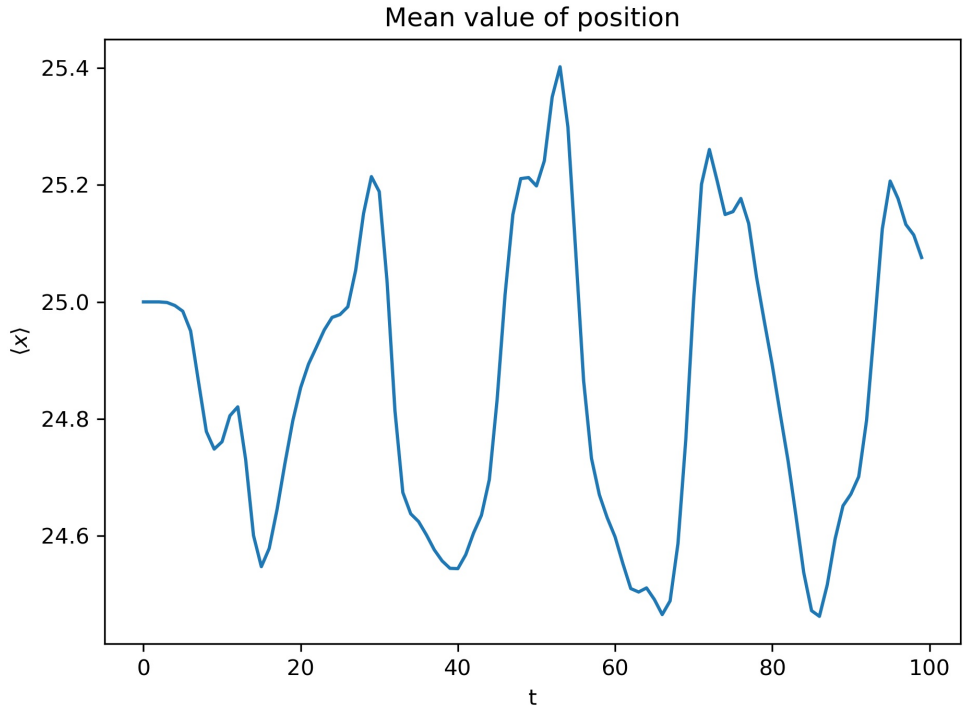

Figure 3 - Mean value of position with respect to time.

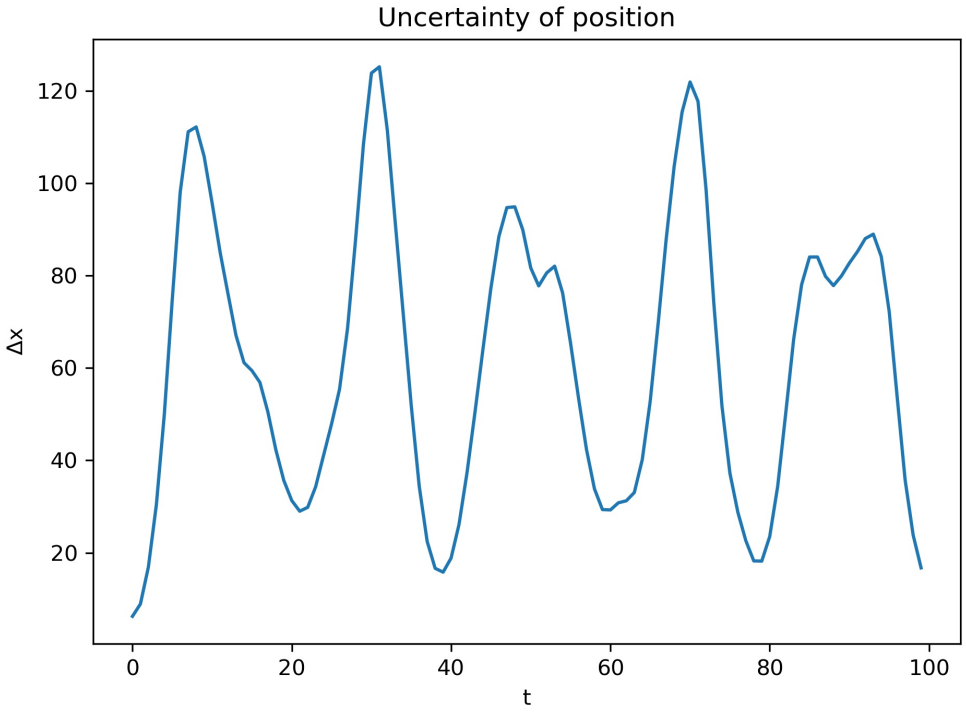

Figure 4 - Position uncertainty with respect to time.