

Information Theory and Computation

Exercise 7

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Theory

Split operator method

Suppose we want to propagate the wavefunction according to some (possibly time dependent) Hamiltonian $H(t)$. For a small time interval the propagator is:

$$U(t + \tau, t) \approx e^{-\frac{i}{\hbar} H(t) \tau} \quad (1)$$

Since the Hamiltonian is $H = \frac{p^2}{2m} + V(x, t)$ we can use the BCH formula and split the evolution operator as:

$$e^{-\frac{i}{\hbar} \hat{H}(t) \tau} = e^{-\frac{i}{\hbar} \frac{\hat{V}(x, t)}{2} \tau} e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m} \tau} e^{-\frac{i}{\hbar} \frac{\hat{V}(x, t)}{2} \tau} + o(\tau^2) \quad (2)$$

Now if we have the wavefunction at time t , $|\psi(x, t)\rangle$ and we want to apply the evolution operator we may proceed in the following way: we apply first, in space representation, the operator $e^{-\frac{i}{\hbar} \frac{\hat{V}(x, t)}{2} \tau}$; then, by means of Fourier Transform, we represent the result in momentum space, which makes $e^{-\frac{i}{\hbar} \frac{\hat{p}^2}{2m} \tau}$ diagonal. After applying it, we go back to space representation and we apply the last operator.

Code Development

Results

Self Evaluation