

Homework 00

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Introduction

This report is a short overview on solving the nonlinear Schrodinger equation. In the Split Operator method, we split the Hamiltonian into momentum space components, $H_p = \frac{\hbar^2}{2m} \nabla_z^2$ and position space components, $H_r = V(x)$. If we assume a some what general solution to our quantum system:

$$\psi(x, t + dt) = e^{-\frac{i\hat{H}dt}{\hbar}} \psi(x, t) = e^{\frac{-i(\hat{H}_p + \hat{H}_r)dt}{\hbar}} \psi(x, t) \quad (1)$$

and assume we are simulating our system by a series of small timesteps (dt), we can perform similar splitting by using the Baker-Campbell-Housdorff formula:

$$\psi(x, t + dt) = e^{\frac{-i(\hat{H}_p)dt}{\hbar}} e^{\frac{-i(\hat{H}_r)dt}{\hbar}} e^{\frac{-i([\hat{H}_p, \hat{H}_r])dt^2}{2\hbar}} \psi(x, t) + \mathcal{O}(dt^2) \quad (2)$$

This accrues a small amount of error (dt^2) related to the commutation of the real and momentum-space components of the Hamiltonian. In order to change the (dt^2) error to (dt^3), we can split the system by performing a half-step in position space before doing a full-step in momentum space, through a process called Strang Splitting:

$$\psi(x, t + dt) = e^{\frac{-i(\hat{H}_r)dt}{2\hbar}} e^{\frac{-i(\hat{H}_p)dt}{\hbar}} e^{\frac{-i(\hat{H}_r)dt}{2\hbar}} \psi(x, t) + \mathcal{O}(dt^3) \quad (3)$$

We can then address each part of this solution in parts, first in position space, then in momentum space, then in position space again by using Fourier Transforms.

$$\psi(x, t + dt) = \left[\hat{U}_r(dt/2) \mathcal{F}^{-1} \left[\hat{U}_p(dt) \mathcal{F} \left[\hat{U}_r(dt/2) \psi(x, t) \right] \right] \right] + \mathcal{O}(dt^3) \quad (4)$$

where $\hat{U}_r(dt) = e^{\frac{-i(\hat{H}_r)dt}{\hbar}}$ and $\hat{U}_p(dt) = e^{\frac{-i(\hat{H}_p)dt}{\hbar}}$.

A code for a simple system is attached [here](#).