Quantum Information and Computing

2022 - 2023

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Exercise #05

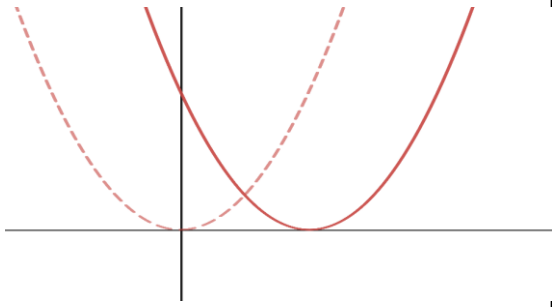
Physics of Data

Continuous time-dependent Schrodinger eq

Theory

We consider the time-dependent one-dimensional quantum harmonic defined by the Hamiltonian: $H = \frac{1}{2m}\hat{p}^2 + \frac{\omega^2}{2m}(\hat{q} - q_0)^2$

K, kinetic — V(t), potential



Given the ground state $|\psi_0> = |\, n = 0>$, we aim to solve the problem of finding the evolved state $|\psi(t)>$ under $\hat{H}$:

$$\hat{H} = \frac{1}{2}\,\hat{p} + \frac{1}{2}\left(\hat{q} - \frac{t}{T}\right)^2$$

$$|\psi(t)\rangle = U(t, t_0)|\psi(0)\rangle = e^{-i\Delta t\left(\hat{T}+\hat{V}\right)}|\psi(0)\rangle$$

Where: $e^{-i\Delta t\left(\hat{T}+\hat{V}\right)} \simeq e^{-i\frac{\Delta t}{2}\hat{V}} e^{-i\Delta t\hat{T}} e^{-i\frac{\Delta t}{2}\hat{V}}$

$$= e^{-i\Delta t\left(\hat{T}+\hat{V}\right)}|\psi(0)\rangle \simeq e^{-i\frac{\Delta t}{2}\hat{V}} e^{-i\Delta t\hat{T}} e^{-i\frac{\Delta t}{2}\hat{V}}|\psi(0)\rangle$$

Continuous time-dependent Schrodinger eq

The space interval [-a, a] and time interval $[t_0, t_f]$, we discretize both into N_x, N_t smaller interval of width Δx, Δt:

$$x_i = -a + i\Delta x$$
$$t_j = -t_0 + j\Delta t$$

The formal solution of Schrodinger equation for the wave function after a time step Δt is given by:

$$|\psi_x(t+\Delta t)\rangle = e^{-i\frac{\Delta t}{2}\hat{V}} F^{-1}\left[e^{-i\Delta t\hat{T}} F\left[e^{-i\frac{\Delta t}{2}\hat{V}}|\psi_x(t)\rangle\right]\right]$$

Algorithms:

1. Evolve $\hat{V}$
2. Apply Fourier transform F: $\psi_x \rightarrow \psi_k$
3. Evolve with $\hat{T}$
4. Apply inverse Fourier transform F^{-1}: $\psi_k \rightarrow \psi_x$
5. Evolve $\hat{V}$

Continuous time-dependent Schrodinger eq

Code Development

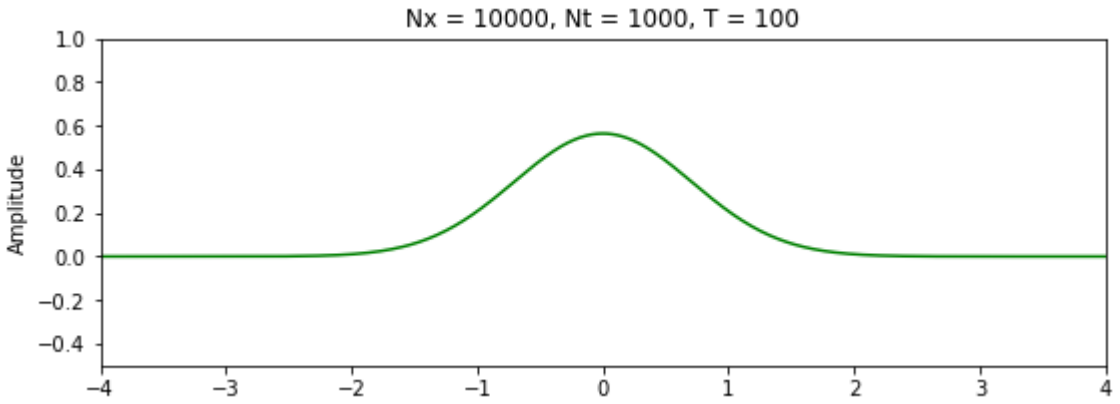
- The parameter are created as user input.
- We exploit the dfftw_plan_dft_1d and dfftw_execute_dft subroutines contained in the fftw3 library.
- To compile it: **gfortran schro.f90 -o schrp -Wall -llapack -lfftw3 –frecursive**

```
program shroedingertimedependent
  use debugmod
  use q_util
  use, intrinsic :: iso_c_binding
  use fftw3

  implicit none


  double precision            :: Lx, Lp, T, dx, dt, dp
  integer                     :: Nx, Nt, xx, tt
  character(20)               :: folder
  integer                     :: iostat  ! Checking types in READ(*,*)

  double precision, dimension(:), allocatable :: xgrid, pgrid, ps
  double complex, dimension(:), allocatable   :: Uv, Ut

  ! Vectors for:
  ! tmp_k1: after Ux, Fourier transformed
  ! tmp_k2: after Uk
  ! tmp_x2: after inverse transforming
  complex(kind=8), dimension(:), allocatable   :: psi_x0, psi_x1, psi_k1, psi_k2,
psi_x2, psi_x3, psi_k3

  ! Constants
  double precision :: pi

  ! For debugging
  logical :: DEBUG, DEBUG2

  ! FFTW Related
  integer*8 :: dfft_plan, idfft_plan, jdfft_plan

  ! General
  DEBUG =  .FALSE.
  ! Too check if first step matches with theory
  DEBUG2 = .FALSE.
```

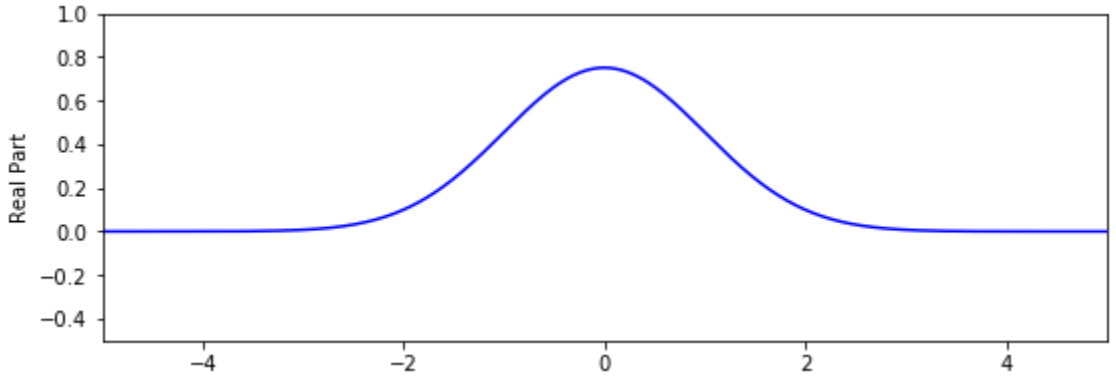
```
qi@qi-VirtualBox:~/Assignment5$ gfortran schro.f90 -o schro -llapack -Wall -lfft
w3 -frecursive
qi@qi-VirtualBox:~/Assignment5$ ./schro
 +   TIME DEPENDENT SCHROEDINGER EQUATION   +
 + Lx:  Lenght of x space                   +
 + Lp:  Lenght of p space                   +
 + Nx:   Number of points                   +
 + Nt:  Number of time-points               +
 + T:   Total time                          +
 +-----------------------------------------+
 + Type: Lx, Lp, Nx, Nt, T and folder:      +
 + 50
50
1000
100
50
c
 + Data will be saved in: ./c
 + Lenght of x space     (Lx):    50.000000000000000
 + Lenght of p space     (Lp):    50.000000000000000
 + Number of points       (N):         1000
 + Number of time-points (Nt):          100
 + Total time            (T):    50.000000000000000
 +-----------------------------------------+
```

Continuous time-dependent Schrodinger eq

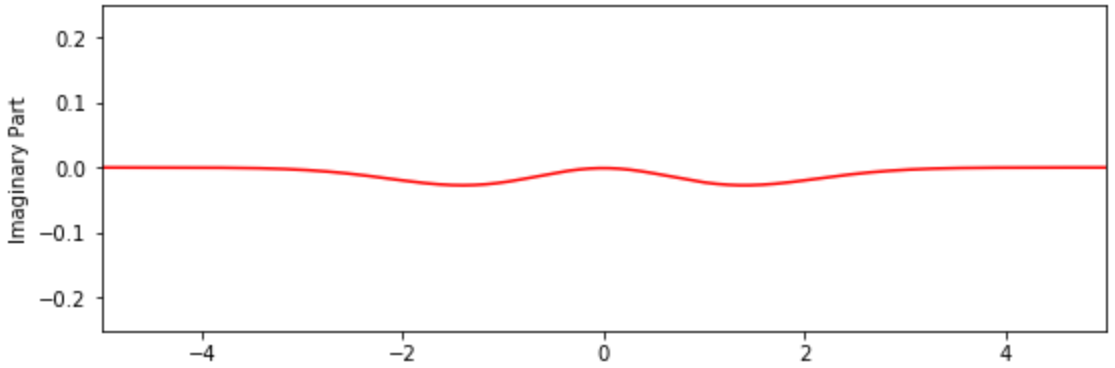
$|\psi_0(x,t)|^2$

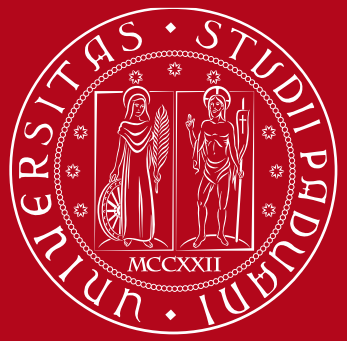


$Re[\psi_0(x,t)]$



$\mathrm{Im}[\psi_0(x,t)]$





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Thanks for the attention