Quantum Information and Computing

2021 - 2022

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06/12/21

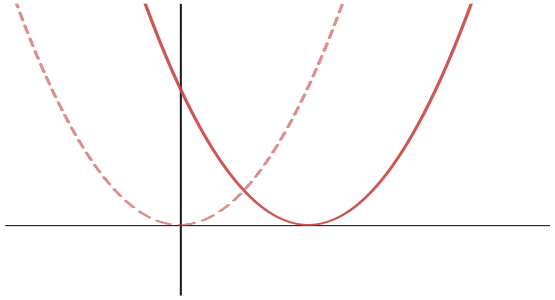
Exercise 5

Split-Operator Application in a Time Dependent Hamiltonian

Physics of Data

Theory

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



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

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

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

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

Algorithm:

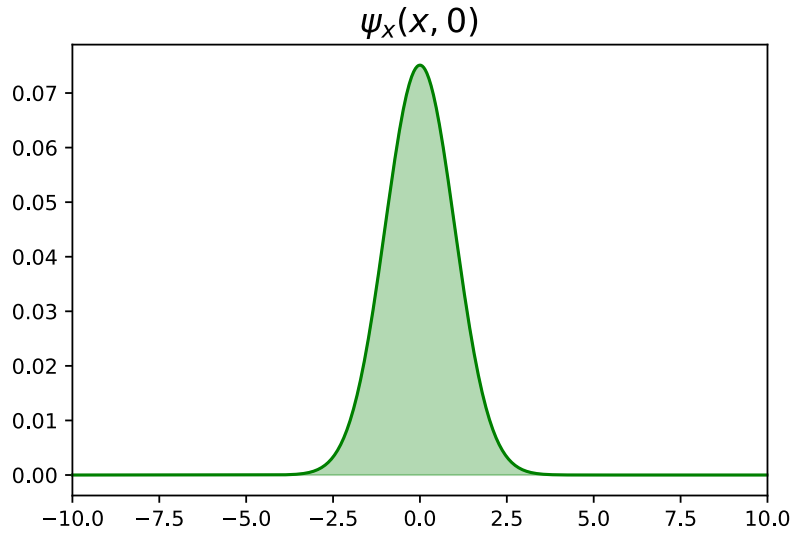
1. Evolve with $\hat{V}$
2. Apply Fourier transform F: $\psi_x \rightarrow \psi_k$
3. Evolve with $\hat{T}$
4. Apply inverse Fourier transform F^{-1}: $\psi_k \rightarrow \psi_x$
5. Evolve with $\hat{V}$

Code Development

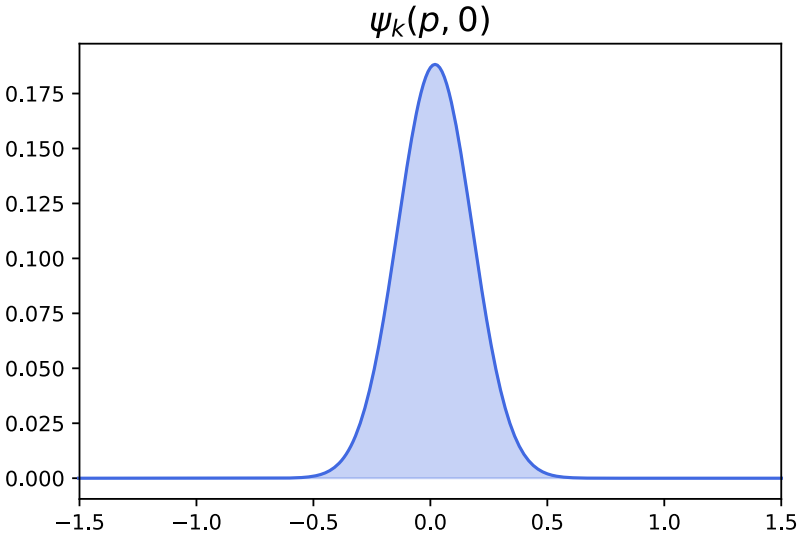
```
include 'fftw3.f03'

integer*8 :: dfft_plan
complex(kind=8), dimension(:), allocatable   :: psi_x1, psi_k1

⋮

! dfft_plan contains all information necessary to compute the transform
! including the pointers to the input and output arrays.

! Creates the plan
call dfftw_plan_dft_1d(dfft_plan,  Nx, psi_x1, psi_k1, FFTW_FORWARD,FFTW_MEASURE)

! Transform x -> k
call dfftw_execute_dft(dfft_plan, psi_x1, psi_k1)

⋮

! Destroy the plan
call dfftw_destroy_plan(dfft_plan)
```

To compile it:
gfortran time_dep_qho.f03 -o tqho -Wall -llapack **-lfftw3** -frecursive

Code Development




```
call dfftw_execute_dft(dfft_plan, psi_x1, psi_k1)
```

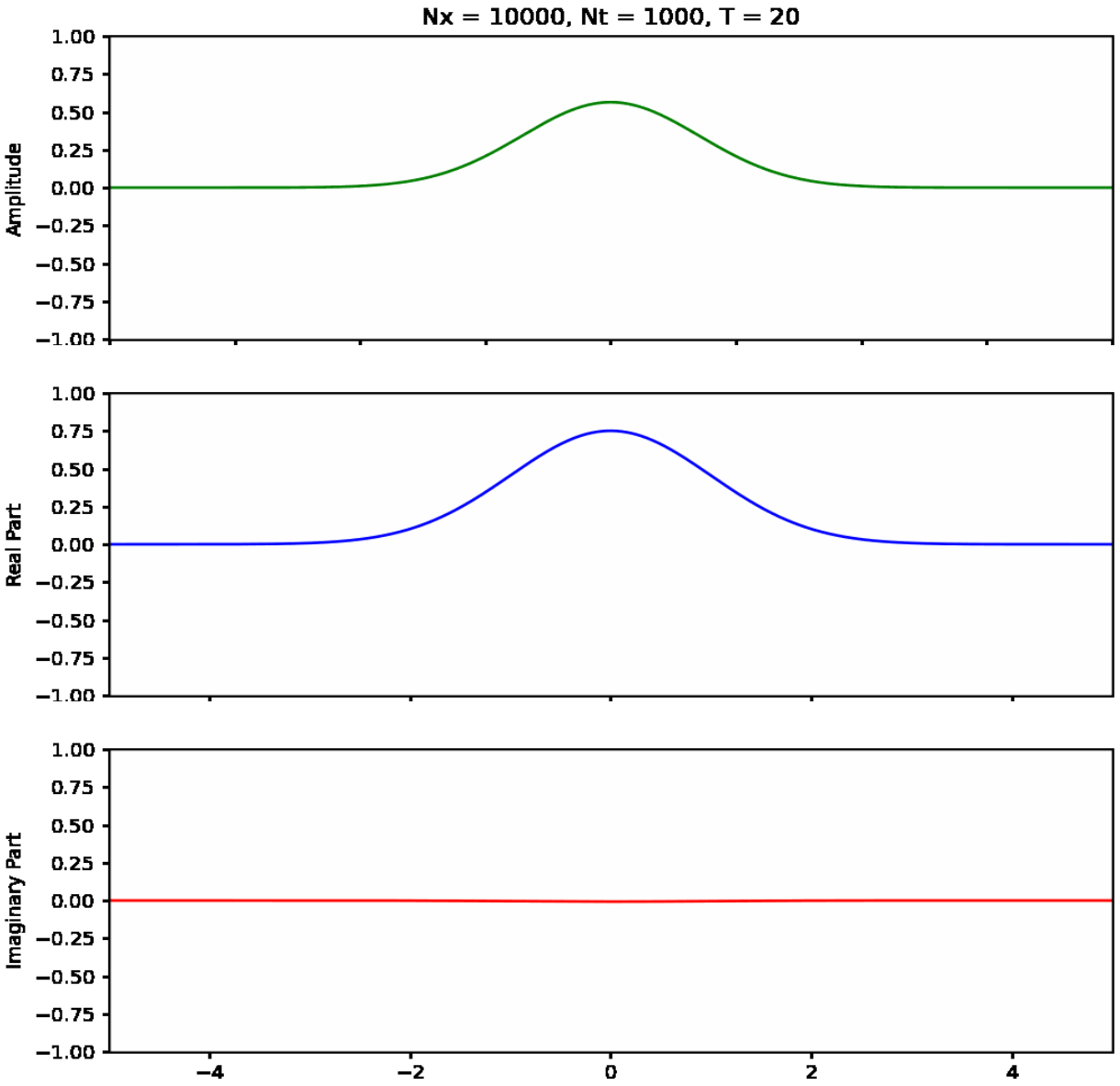


Results

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

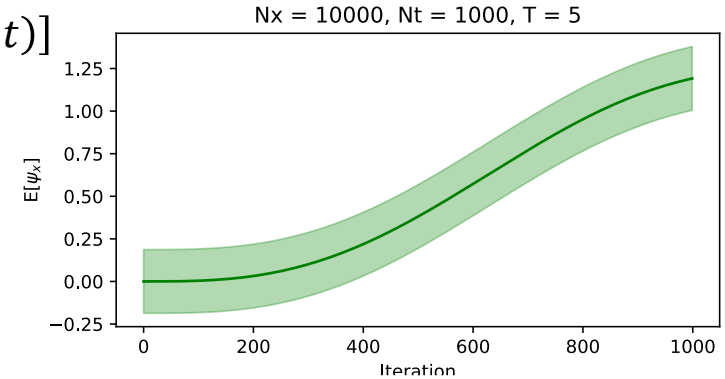
$Re[\psi_0(x,t)]$

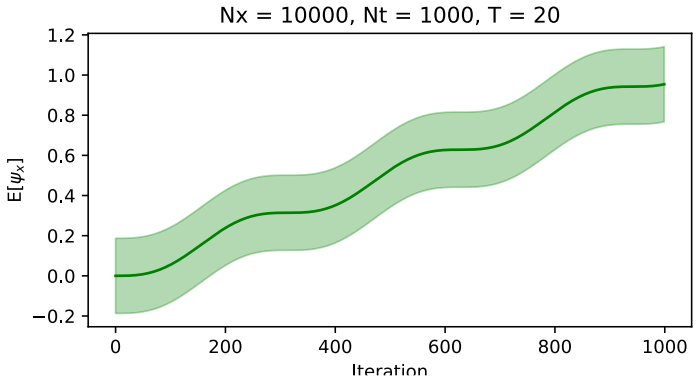
$\mathrm{Im}[\psi_0(x,t)]$

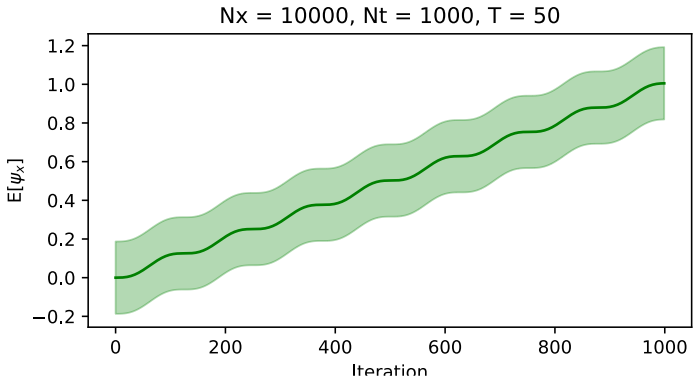


Results

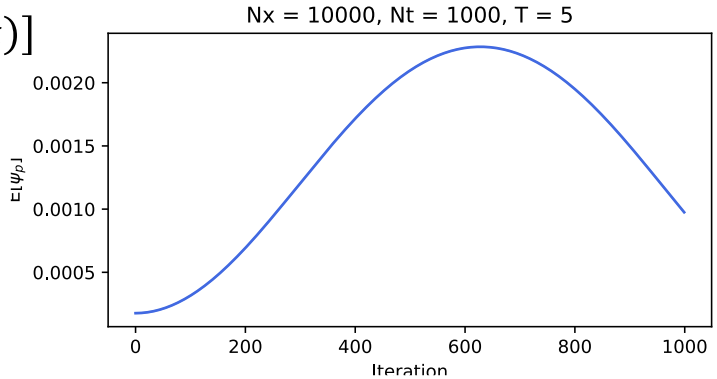
$E[\psi_0(x,t)]$

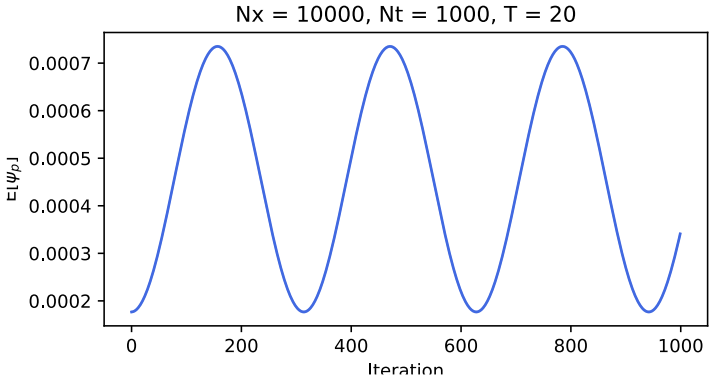


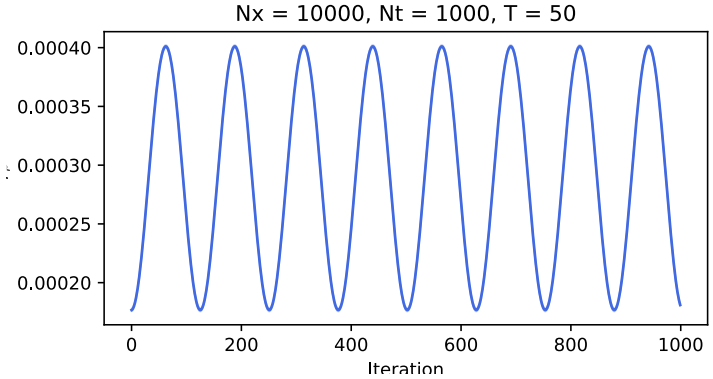




$E[\psi_0(p,t)]$







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Thanks for the attention