Information Theory and Computation
Exercise 7

Vincenzo Maria Schimmenti - 1204565

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Theory

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

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

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

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

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

In our task we had to evolve using the time dependent Hamiltonian:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x - \frac{t}{T}\right)^2 \tag{3}$$

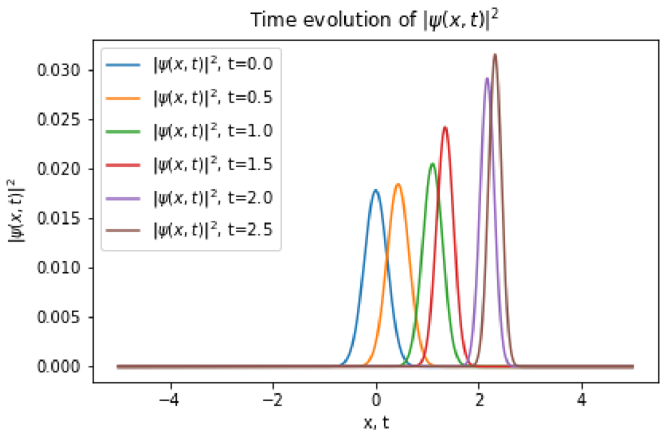
the ground state of the Harmonic Oscillator $|\psi_0\rangle$. First of all we used the subroutine **zheev** from **lapack** in order to diagonalize the Hamiltonian and compute the ground state, for which we used a lattice of spacing $a = 0.01$ going from -5.0 to 5.0 and $\hbar = 1.0$, $m = 1.0$, $\omega = 1.0$. As mentioned in the first section, we used the split operator method to propagate in time the function; the implementation has been done with the following code

```
factor = complex(0, -0.5*tGrd%a*4*acos(-1.0)/(hbar*m*(grd%a*grd%sz)**2))
psi(:,1)=psi0

call dfftw_plan_dft_1d(planf,grd%sz,temp,temp2,FFTW_FORWARD,FFTW_ESTIMATE);
call dfftw_plan_dft_1d(planb,grd%sz,temp2,temp,FFTW_BACKWARD,FFTW_ESTIMATE);

temp = psi0
t = 0.0
do idx=2, tGrd%sz
! potential part, first half
call propagate_hov_shifted(temp,grd,tGrd%a/2,hbar,m,omega,t,Tmax)
! momentum space
call dfftw_execute_dft(planf,temp,temp2)
! multiply by kinetic term
do jdx=1,grd%sz/2
temp2(jdx)=temp2(jdx)*exp(factor*jdx*jdx)
end do

do jdx=1+grd%sz/2, grd%sz
temp2(jdx)=temp2(jdx)*exp(factor*(grd%sz-jdx)**2)
end do
! position space
call dfftw_execute_dft(planb, temp2, temp)
! potential part, second half
call propagate_hov_shifted(temp,grd,tGrd%a/2,hbar,m,omega,t,Tmax)
psi(:,idx)=temp/grd%sz
temp = psi(:,idx)
t = t + tGrd%a
end do
```

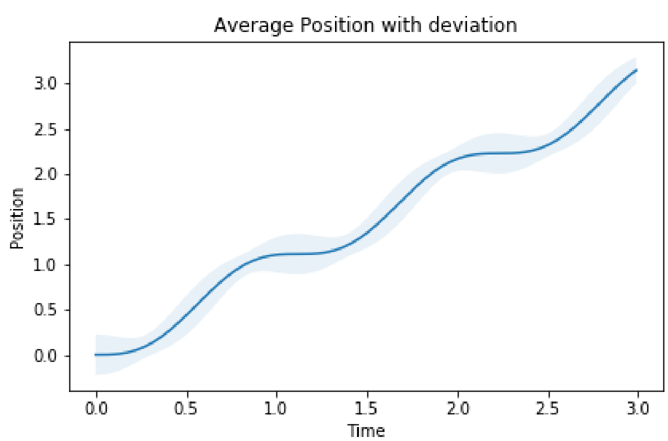
In the code *grd* and *tGrd* are custom types characterizing respectively the space grid and the time grid; the subroutine *propagate_hov_shifted* multiplies the wave-function by the potential part of the evolution operator (i.e. by $e^{-\frac{i\tau}{2}V(x,t)}$). The subroutine *dfftw_plan_dft_1d* is internal of **fftw** and prepares the system for using the Discrete Fourier Transform while *dfftw_execute_dft* computes it: we use it twice, once forward and once backward and, in the middle, we multiply by the kinetic part of the evolution operator, i.e. $e^{-i\tau\frac{p^2}{2m}}$ which, again, is diagonal in momentum space. The library **fftw** stores in the first half of the transformed wave function the positive momentum component while in the second half, reversed, the negative ones; if we denote the momenta as $p_j = \frac{2\pi}{2La\hbar}j$ (with $2L$ the global system size, N the number of points and a the lattice spacing), we will find first the momenta $p_0, \dots, p_{N/2-1}$ and then $p_{-1} \dots p_{-N/2}$.

Results

Below we show three instants of the wavefunction evolution using its squared norm:



We can really appreciate the time evolution if we look at the average position of the particle:



This result recalls the classical case of an harmonic particle in a moving frame with constant velocity: its position fluctuates according to a sinusoidal wave with resting point given by $\frac{t}{T}$.