Time Dependent Schrödinger equation

Abstract

Solution for the time evolution of the ground state of a static harmonic oscillator subjected to a potential of the same shape but that moves with constant velocity.

1 Theory

The goal of this project is to solve the time dependent one dimensional Schrödinger equation in the case of an harmonic potential that at time $t = 0$ starts moving with constant velocity $v = \frac{1}{T}$.

$$i\hbar\frac{d}{dt}|\Psi(x,t)\rangle = \hat{H}|\Psi(x,t)\rangle \tag{1}$$

where $\hat{H}$ is

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

Let at time $t = 0$, $\Psi(x, t = 0)$ be the eigenfunction with the lowest energy of a time independent static harmonic oscillator. This, our initial condition, will evolve under the action of $\hat{H}$ according to equation [1], explicitly:

$$\Psi(x,t) = e^{-\frac{i}{\hbar}\int_0^t \hat{H}(s)ds}\Psi(x,0) \tag{3}$$

Computing numerically the equation [3] generally can be inconvenient since the Hamiltonian is not a diagonal matrix, so it can be useful to approximate it as follows:

$$e^{-\frac{i}{\hbar}\int_0^t \hat{H}(s)ds} = e^{-\frac{i}{2\hbar}\int_0^t \hat{V}(s)ds} \cdot F^{-1} \cdot e^{-\frac{i}{\hbar}\tilde{K}t} \cdot F \cdot e^{-\frac{i}{2\hbar}\int_0^t \hat{V}(s)ds} + O(t^3) \tag{4}$$

Where F and F^{-1} is the Fourier transform, $\tilde{K}$ the kinetic part of the Hamiltonian in Fourier Transform basis, and V the potential term of the Hamiltonian. Now every Matrix at the exponent is diagonal and the computation of the operator is trivial.

1.1 Coherent State

It can be shown that $\Psi(x, 0)$ is a coherent state for the Hamiltonian $\hat{H}$. For this reason the modulus square of the wave function will oscillate harmonically without dispersion with respect to the centre of the potential. And hence:

$$\bar{x} = vt - \frac{v}{\omega} sin(\omega t) \tag{5}$$

where $\bar{x} = \int_{-\infty}^{+\infty} x|\Psi(x, t)|^2 dx$.

2 Code Development

To perform temporal advancement I used the **update** function which evolve the wave function by a step dt (*tdschrodinger.F90*). The only choice not prescribed by the theory regarded the evaluation of the integrals appearing in the potential energy terms. These have been computed analytically since they were just integrals of polinomials, neglecting only the third power of the timestep dt. To compute the Fourier transform I used the **fftw3** library, but since the call of its functions are quite intricate, I coded an interface to perform the task more easily, and more safely thanks to the debug function of the **debugqic** module. The interface for fftw3 appears in *tdschrodinger.F90* and it is called **zfft**.

3 Results

The following results have been computed using a spatial mesh of 1201 units from $x = -5.0$ to 5.0, a temporal step of $dt = 1e - 4$, and velocity $v = \frac{1}{T} = 0.5$. Additionally I set $m = \hbar = 1$. As we can see in Fig.1, the $|\Psi(t, x)|^2$ function evolve as expected.Moreover its standard deviation remains constant. It has been performed a linear fit on the standard deviation reporting an angular coefficient of $m = -5.31872e - 07$. About the harmonic fluctuations of the wave function we can see in Fig.2 that these have an amplitude equal to $\frac{v}{\omega}$. For what regards the frequency of the harmonic oscillations I did not find perfect agreement with the theory. This can be seen also in figure 2 where lines with $\omega = 5$ and 10 do not display a good overlap of the x coordinate among nodes or stationary points. This issue could derive from lack of precision in the computation, but its precise causes remain unknown.

4 Self Development

This project have been more challenging that the others, not because difficulties in programming, but because I did not know what to expect from the results. Fortunately this problem has an analytical solution that I have been able to compute. In the end the code worked properly, but clearly to be sure of its correct functioning more tests are needed.

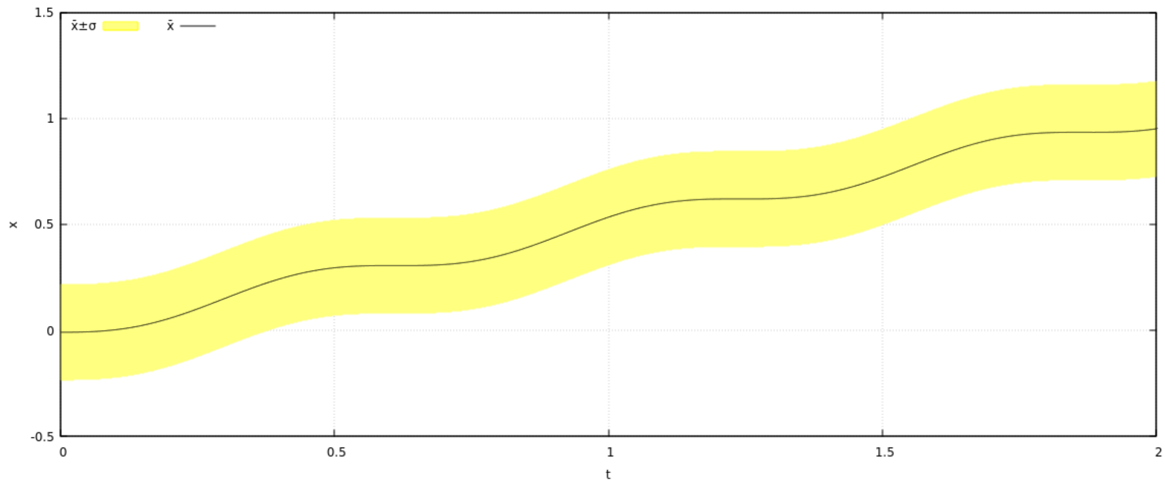

Figure 1: Average position of the wave function with respect to the time. The yellow ribbon represents the x coordinates inside the standard deviation of the PDF associated to the wave function

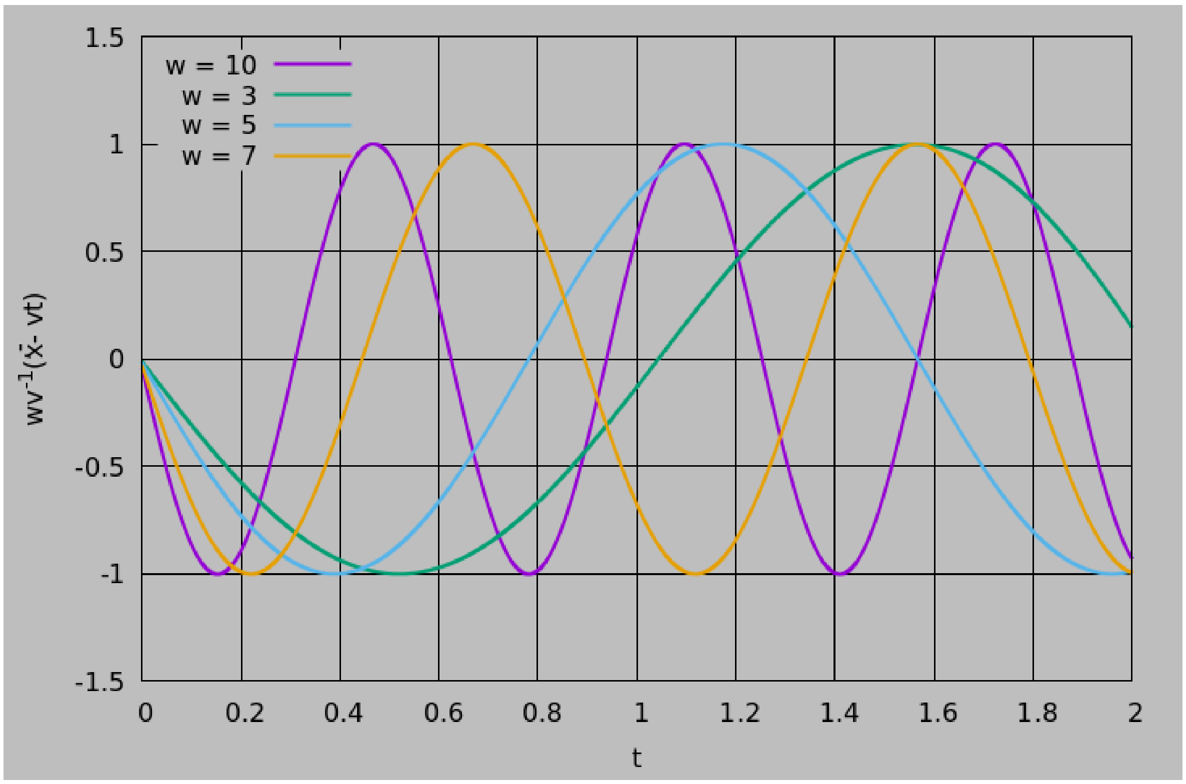

Figure 2: Fluctuation of the average position with respect to the centre of the bin for different ω. The values have been normalized with $v\omega^{-1}$ to show the agreement with the oscillations of coherent states. In fact each curve approaches ± 1.