Quantum Information and Computing (QIaC)

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Theory

We study the solution of a time-dependent Schrödinger 1D equation that obeys the following Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 (\hat{q} - q_0(t))^2 \tag{1}$$

where $q_0(t) = t/T$ is a **time dependent shift** ($t \in (0, T]$). Making use of the work done last week, we solve for the ground state and we let him evolve exploiting the **split operator method**. Starting from the application of the time evolution operator

$$|\psi(x, t + \Delta t)\rangle = e^{-i\Delta t \hat{H}} |\psi(t)\rangle \overset{(a)}{\approx} e^{-\frac{1}{2} i\Delta t \hat{V}} e^{i\Delta t \hat{T}} e^{-\frac{1}{2} i\Delta t \hat{V}} |\psi(x, t)\rangle \tag{2}$$

we use in (a) the Baker-Campbell-Hausdorff formula. Noticing that $\hat{T}$ is diagonal in the **momentum basis** and $\hat{V}$ is diagonal in the **position basis**, we perform proper Fourier transformations of the wave function.

$$|\psi(x, t + \Delta t)\rangle = e^{-i\Delta t \hat{H}} |\psi(t)\rangle \approx e^{-\frac{1}{2} i\Delta t \hat{V}} \mathscr{F}^{-1} e^{i\Delta t \hat{T}} \mathscr{F} e^{-\frac{1}{2} i\Delta t \hat{V}} |\psi(x, t)\rangle \tag{3}$$

After the application of each Fourier transform we normalize the wave functions. The last equation propagates the state for `dt`, so we apply it **iteratively** to reach the T_{max} value.

Code development - Two main functions

- Initialization of the **kinetic part** of the hamiltonian. Given a discretization with width $L = L_{max} - Lmin$, we populate the momentum vector (after reading `FFTW3`'s manual) with **positive frequencies** $\left[0, \frac{2\pi}{L} \cdot aa\right]$ in the first half $aa \in [0, N/2]$, and with **negative frequencies** $\left[-\frac{2\pi}{L} \cdot (aa - N - 1), 0\right]$ in the second half $aa \in [N/2 + 1, N + 1]$:

```
1  FUNCTION H_kinetic_part(N, Lmin, Lmax, m) RESULT(K)
2  ![...]
3  DO aa=1,INT(N/2)
4      K(aa) = (0.5d0/m) * (4.0d0*ASIN(1.0d0)*(aa)/(Lmax-Lmin))**2
5  ENDDO
6  DO aa=INT(N/2)+1,N+1
7      K(aa) = (0.5d0/m) * (4.0d0*ASIN(1.0d0)*(aa-N-1)/(Lmax-Lmin))**2
8  ENDDO
9  ![...]
```

- Initialization of the **potential part** of the hamiltonian.

```
1  FUNCTION H_potential_part(N, Lmin, Lmax, m, omega, time, T) RESULT(V)
2  ![...]
3  dx = (Lmax-Lmin)/N
4  DO aa = 1, N+1
5      V(aa) = 0.5*m*omega**2*(Lmin+(aa-1)*dx-time/T)**2
6  ENDDO
7  ![...]
```

Code development - Two main functions

- The *delicate* `myFFTW(input)` function (`myAFFTW(input)` for the inverse is similar):

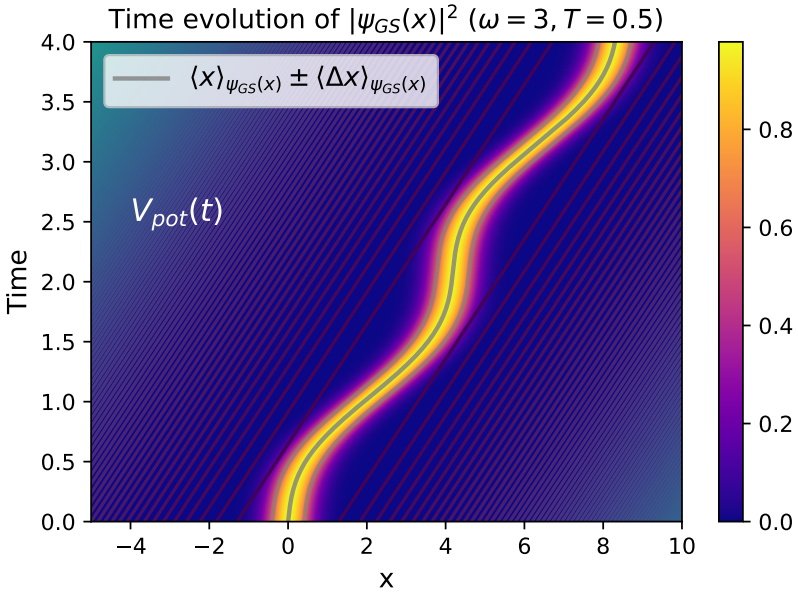
```
1     INTEGER(8)                                          :: plan
2     INTEGER                                             :: FFTW_FORWARD
3     PARAMETER(FFTW_FORWARD=-1)
4     INTEGER                                             :: FFTW_MEASURE
5     PARAMETER(FFTW_MEASURE=64)
6     !initialize the array once the plan is created
7     temp = input
8     CALL dfftw_plan_dft_1d( plan, N, input, output, FFTW_FORWARD, FFTW_MEASURE)
9     CALL dfftw_execute_dft( plan, temp, output)
10    output = output/SQRT(1.0d0*N)
11    CALL dfftw_destroy_plan(plan)
12    ![...]
```

- The function `evolve_dt(wf, dt, Lmin, Lmax, m, omega, time, T)`:

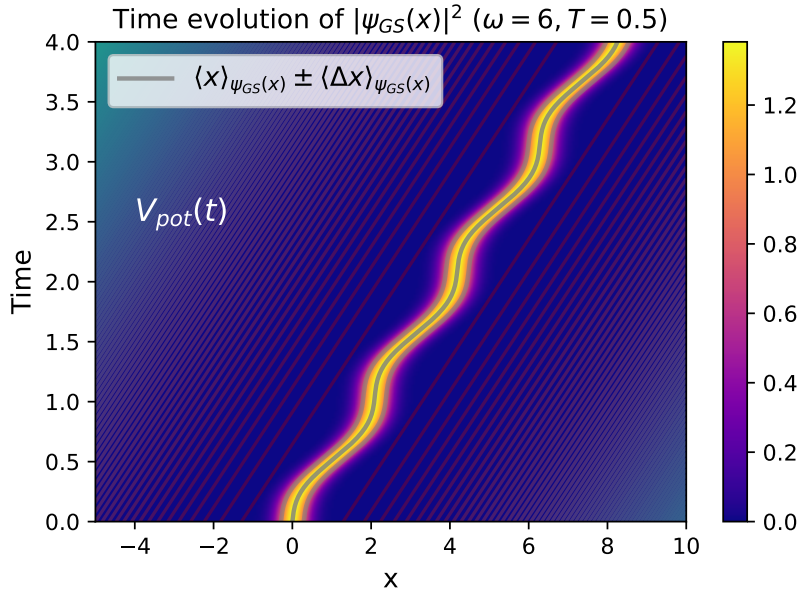
```
1     DO aa = 1, N+1
2         wf(aa) = EXP(COMPLEX(0.0d0, - 1.0d0 / 2.0d0 * dt * V(aa))) * wf(aa)
3     END DO
4     wf = myFFTW(wf)
5     DO aa = 1, N+1
6         wf(aa) = EXP(COMPLEX(0.0d0, -1.0d0 * dt * K(aa))) * wf(aa)
7     END DO
8     wf = myAFFTW(wf)
9     ![...]
```

Time evolution

We report in the following graphs the results obtained by computing the **probability density function** $|\psi(x)|^2$ at each time step and at each point of the discretized space lattice. For this simulations we set the time of the potential equal to $T = 0.5$ and $m = 1$.



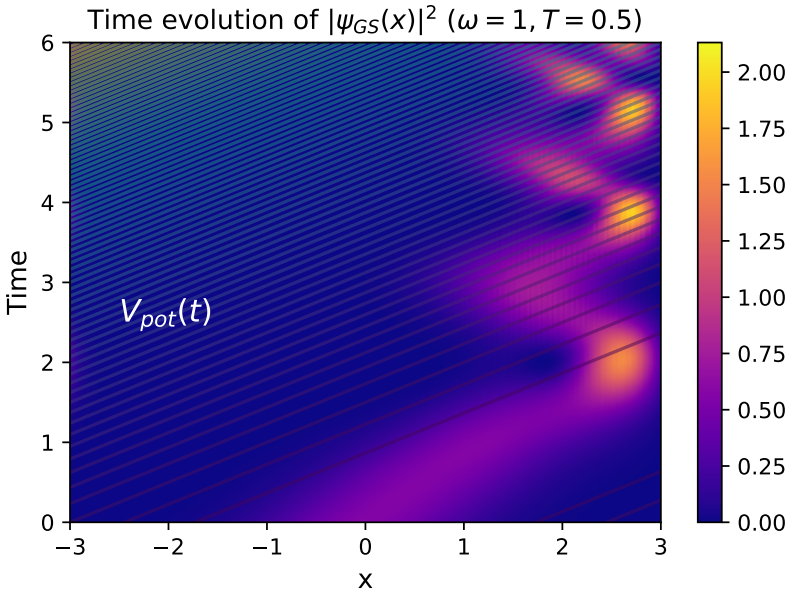
The harmonic potential moves to the right at a **constant speed**, and the position expectation value $\langle x \rangle_{\psi_{GS}(x)}$ does the same but with an **oscillatory component**.

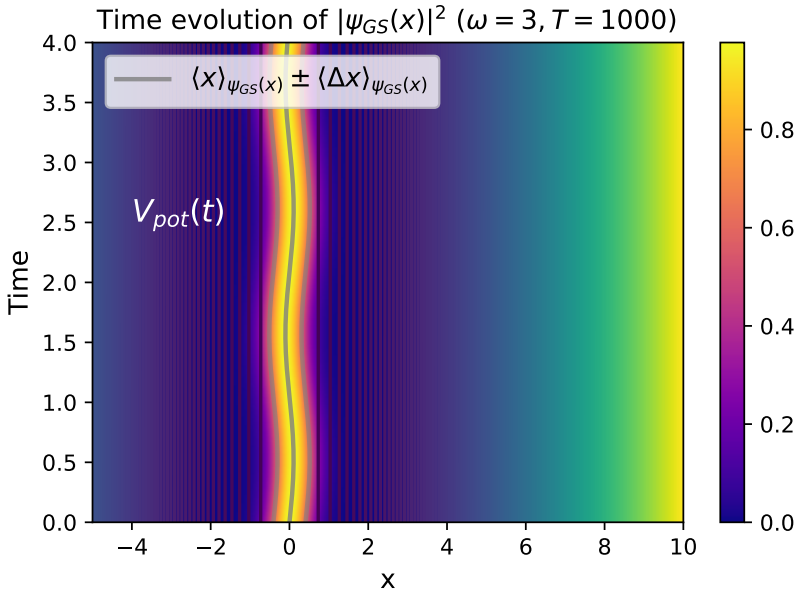


The oscillatory behavior is accentuated as the **angular frequency increases**. We did not investigate further but, at first sight, the fluctuation seems decreased in this case.

Two special cases

We now discuss two special cases achievable with our simulation: where we **extend the time window** (left graph) and where we recover the case in which the harmonic potential is **not practically moving** in a small time window (right graph).





We set $T_{max} = 6$. It is interesting to notice that the wave function hits the right border, goes in the opposite direction and the potential forces it to invert again the direction. The wave function **bounces off the right-hand side** of the interval.

We try to emulate what happens when $T = 1000$. In this case, in a $T_{max} = 4$ time window we are still seeing the ground state **oscillating at the bottom of the potential** (contrary to expectations). This may be due to some errors inserted in the code, we did not investigate further.