Computational Quantum Physics
Exercise 2

PHYS-463
Prof. G. Carleo

Problem 2.1 Exact diagonalization for an Harmonic Well

In this exercise we will approach the general problem of finding bound states of a quantum model. The quantum mechanical description of this problem is based on an eigenvalue problem (the time-independent Schrödinger equation),

$$H|\Psi\rangle = E|\Psi\rangle \tag{1}$$

where

- $|\Psi\rangle \in \mathcal{H}$ is a vector in some Hilbert space $\mathcal{H}$,
- H is the Hamiltonian operator which acts on vectors in $\mathcal{H}$,
- E are the energy eigenvalues.

The goal of this exercise is to find bound-state solutions ($E < 5$) to the 1D time-independent Schrödinger equation for an harmonic well, i.e. for a potential $V(x)$ satisfying

$$V(x) = x^2/2. \tag{2}$$

Construct the main and off-diagonal of the hamiltonian for a the potential choosing a suitable interval $[x_0, x_f]$ and a discretization interval δ, as described in section 3.1.1 of the lecture script. Use a suitable eigenvalue solver for this symmetric tridiagonal matrix.

- Check the convergence of the ground and first excited states as a function of δ.
- What happens if we make the interval $[x_0, x_f]$ smaller or larger?
- Plot the bound-state spectrum and the wavefunctions of the first and excited state and compare it to the exact solutions of the Harmonic oscillator.

Now add an anharmonic term λx^4 to the potential to obtain

$$V_\lambda(x) = x^2/2 + \lambda x^4, \tag{3}$$

- What happens to the energy gap between the ground state and the first excited state when λ is varied?
- Compare the results with those obtained with first order perturbation theory

Problem 2.2 Particles against a wall

Here, we will study the dynamics of a quantum particle in one dimension being reflected off a tilted wall by using the techniques described in the lecture notes. As initial state at $t = 0$, we choose a Gaussian wave packet going in x-direction

$$\Psi(x) = \mathcal{N} e^{ik_0 x} e^{-(x-x_0)^2/a^2},$$

with center $x_0 = -10$, spread $a = 1$ and $k_0 = 5$. The normalization constant $\mathcal{N} = (\pi a^2/2)^{-1/4}$ is chosen such that $\int_{-\infty}^{\infty} dx\, |\Psi(x)|^2 = 1$.

1. Show that the operator $\left(1 + \frac{i\Delta_t}{2\hbar} H\right)^{-1} \left(1 - \frac{i\Delta_t}{2\hbar} H\right)$ is unitary.
2. Numerically compute the free time evolution of the particle in the absence of any potential. Compare the performance of the different methods in the lecture notes.
   (a) Start by implementing the spectral method from section 3.3.1 in the lecture notes.
   (b) Compare it to the implicit integrator from section 3.3.2 in the lecture notes.
   (c) Plot $\mathrm{Re}\,[\Psi(x,t)]$, $\mathrm{Im}\,[\Psi(x,t)]$ and the density $|\Psi(x,t)|^2$ at different times t.

   Hint: Compare your results with the exact solution ($\hbar = 1$, $m = 1$):

$$\Psi(x,t) = \mathcal{N} \left(\frac{a^2}{a^2 + 2it} \right)^{1/2} e^{i(k_0 x - k_0^2 t/2)} e^{-(x-x_0-k_0 t)^2/(a^2+2it)}. \tag{4}$$

3. Modify your code to include an infinite wall at $x = 0$, as described by the following potential:

$$V(x) = \begin{cases} 0 & x < 0 \\ \infty & x \geq 0 \end{cases}$$

4. We now insert a tilted wall at $x = 0$,

$$V(x) = \begin{cases} 0 & x < 0 \\ \tan(\theta)\, x & x \geq 0 \end{cases}$$

   where θ is the tilting angle. In this case, the solution can no longer be found analytically.

   Investigate the behaviour of the wave packet numerically as it hits the wall. In particular, study the time evolution of the velocity of the wave packet

$$v(t) = \int_{-\infty}^{\infty} \mathrm{Im}[\Psi(x,t)^* \frac{d}{dx} \Psi(x,t)]\, dx$$

   for different tilting angles.

   Hint: You can use finite differences for computing the spatial derivative.

Part 1)

The goal of this exercise is to find bound-state solutions ($E < 5$) to the 1D time-independent Schrödinger equation for an harmonic well, i.e. for a potential $V(x)$ satisfying

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- ✓ Check the convergence of the ground and first excited states as a function of δ.
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From finite-difference approximation, we have obtained the tridiagonal $\hat{H}_\delta$ Hamiltonian matrix with

diagonal terms: $V_n + \frac{1}{\delta^2}$

off-diagonal terms: $\frac{-1}{2\delta^2}$

what's it for?

Step 1: Define Hamiltonian (V, xs, dx, return_sparse_matrix = False)

Step 2: Define $V(x)$

Define the interval and the discretization

xs = np.arange (xmin, xmax, dx)

Step 3: Define $\psi(x,n)$, $E(n) \rightarrow n + \frac{1}{2}$

$$\frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \exp\left(-\frac{1}{2}x^2\right) H_n(x)$$

↳ Hermite polynomials

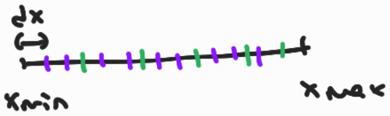
Step4: Get bound states, and E → what's the difference from (l → λ)

$$\psi = \text{eigh\_tridiagonal}(\text{main\_diag}, \text{off\_diag}, \dots)$$

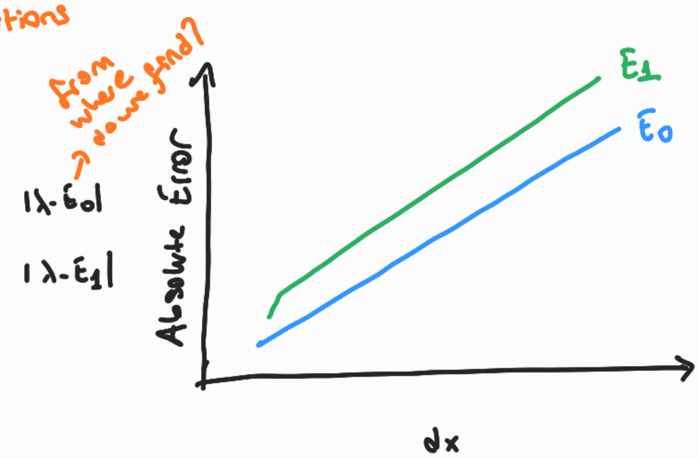
Get bound eigenvalues

$$l = \text{eigvalsh\_tridiagonal}(\dots)$$
(λ)

Step 5: Understand the effect of changing interval:

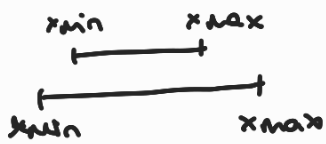


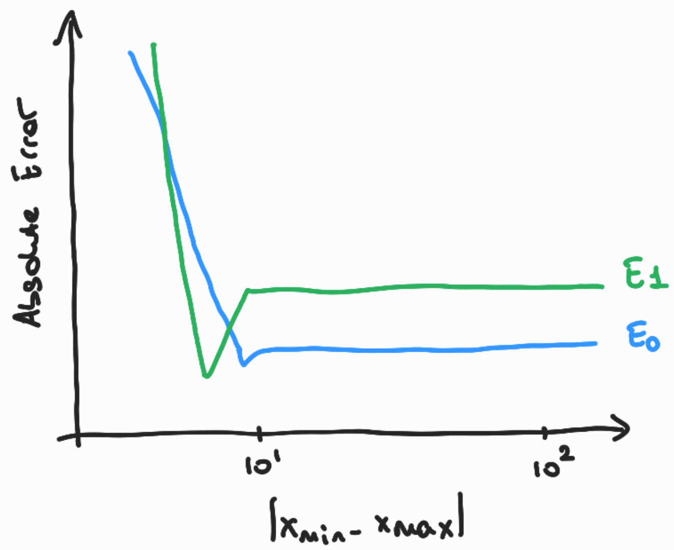
(exact) solutions



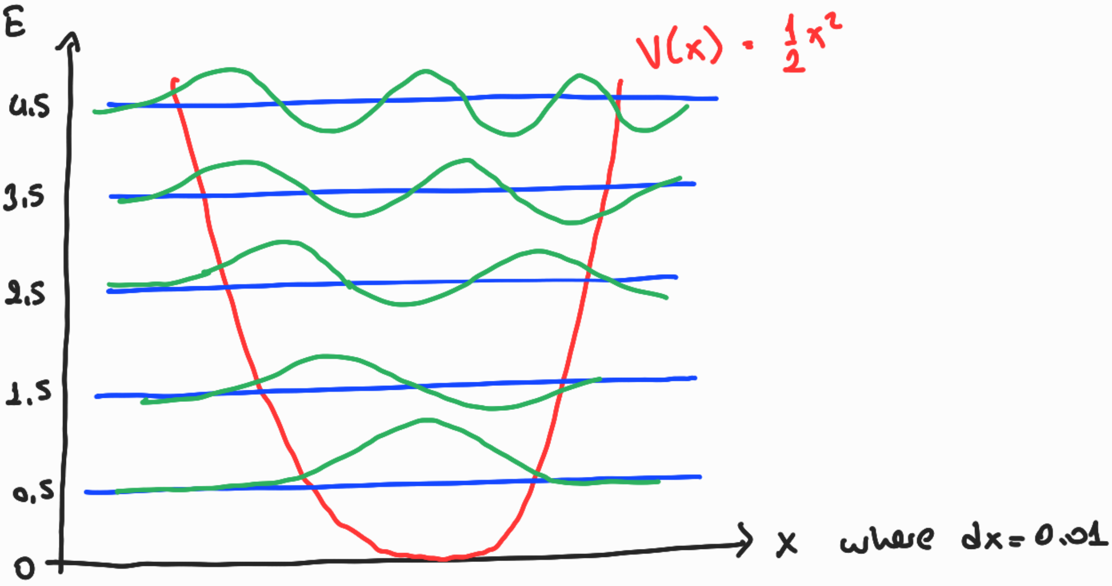
Decreasing dx yields more realistic solutions

Step6: Plot the effect of interval length

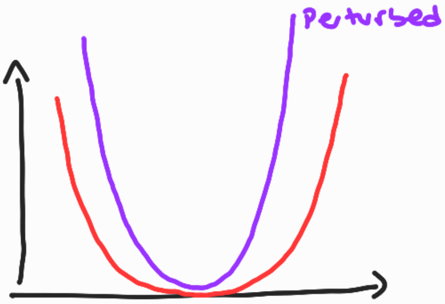




Step 7: Plot the bound states, Energy, $\psi(x, n)$



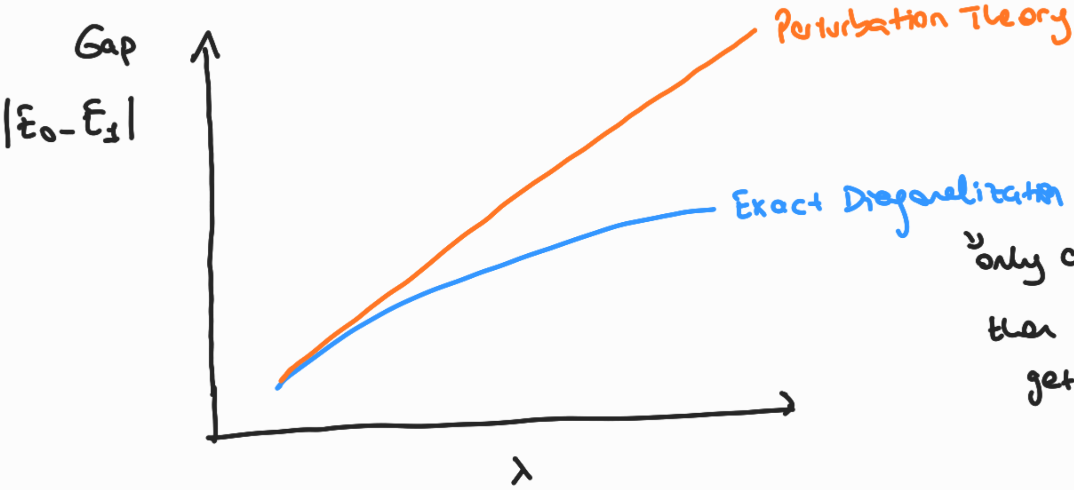
Step 8: Adding anharmonicity $V(x) = \frac{1}{2}x^2 + \lambda x^4$



additional energy in E_0 add. energy in E_1

Step 4: Calculate the 1^{st} order perturbation $\langle \psi_0 | \lambda x^4 | \psi_0 \rangle$ & $\langle \psi_1 | \lambda x^4 | \psi_1 \rangle$

$|(E_0 + E_0') - (E_1 + E_1')|$



↳ only change V
then compute as above
get_bound_eigvals

Problem 2.2 Particles against a wall

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1. Show that the operator $\underbrace{\left(1 + \frac{i\Delta_t}{2\hbar} H\right)^{-1}}_{A} \left(1 - \frac{i\Delta_t}{2\hbar} H\right)$ is unitary.

$A \cdot A^{\dagger} = I$

$A^{\dagger} A = I$

2. Numerically compute the free time evolution of the particle in the absence of any potential. Compare the performance of the different methods in the lecture notes.

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   Hint: Compare your results with the exact solution ($\hbar = 1$, $m = 1$):

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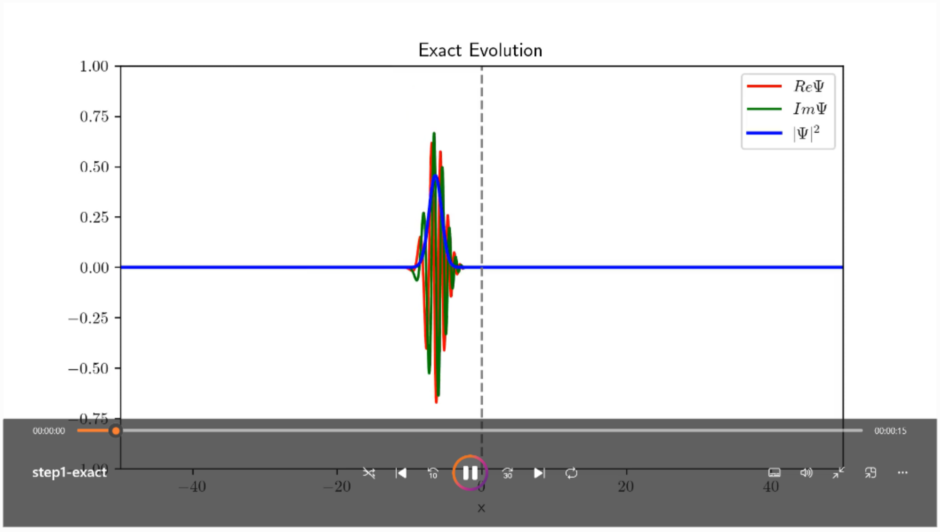
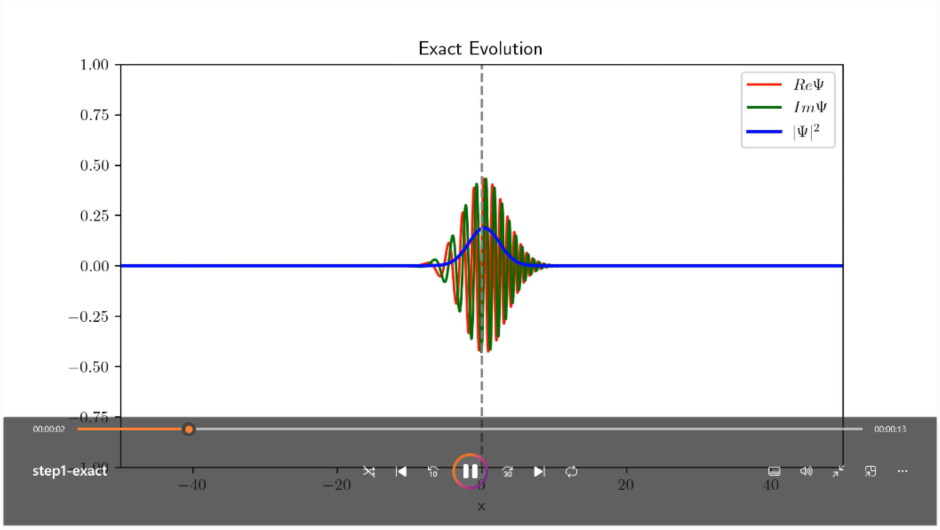
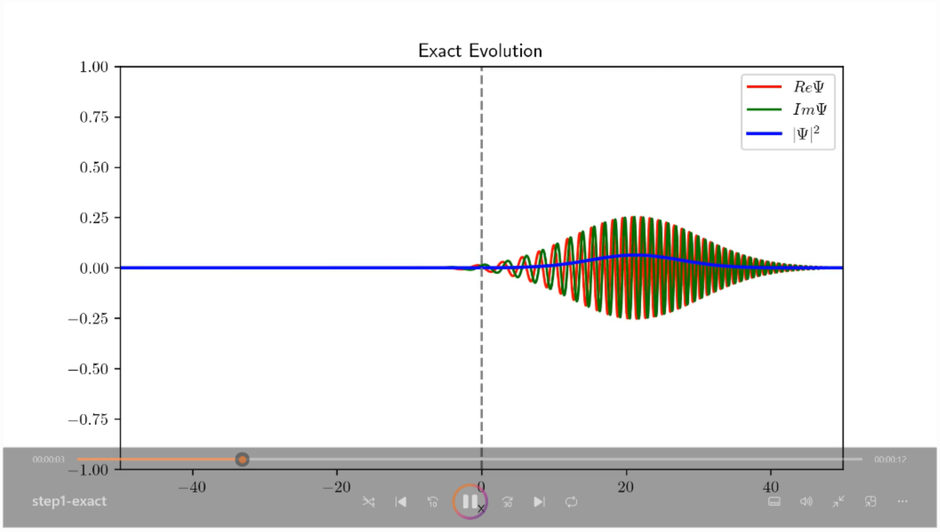
Step 1: Wavepacket Function $\Psi(x,t)$



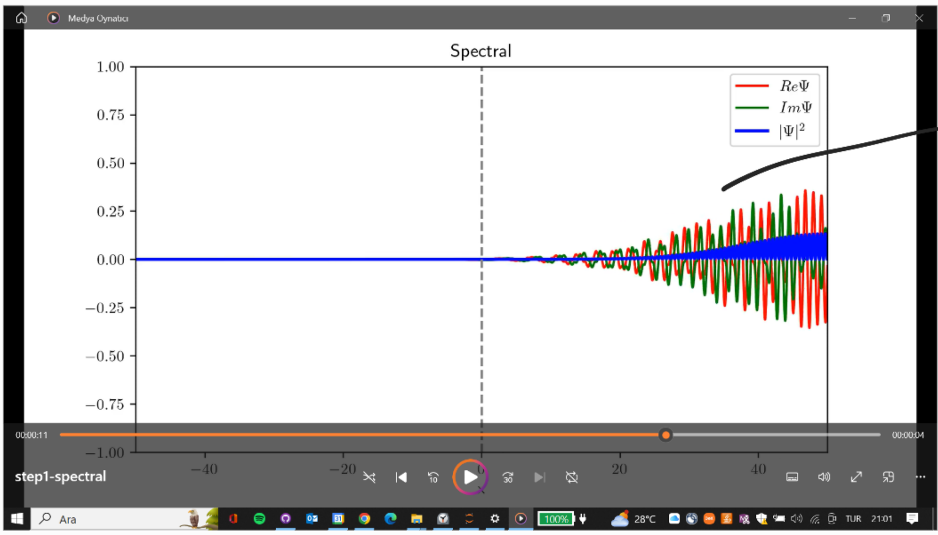




Step 2: Discretize the Hamiltonian with previous methods (tridiagonal)

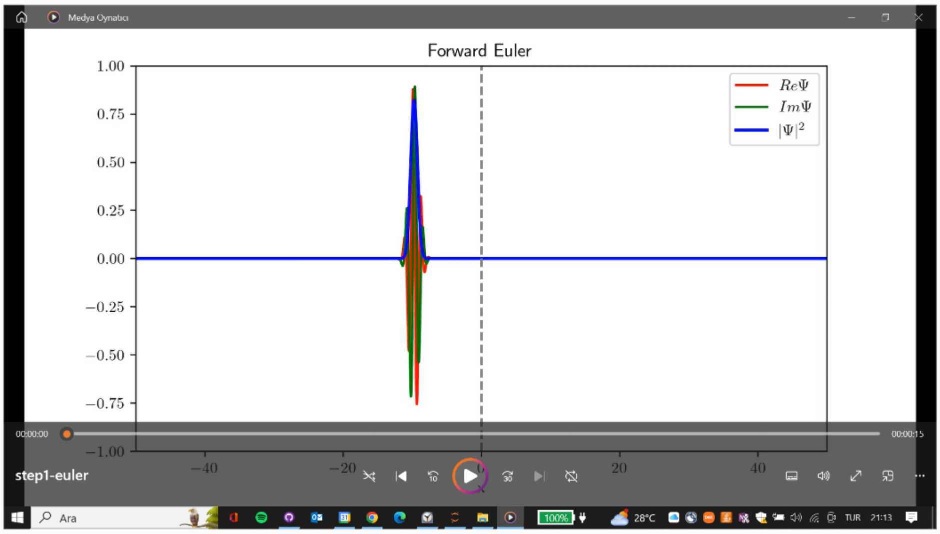
Step 3: 1st Method: Spectral Evolution

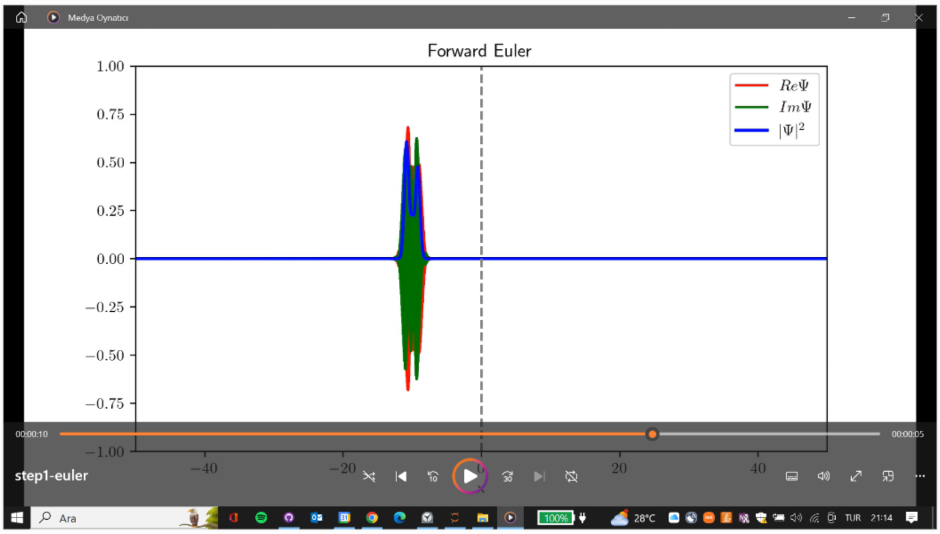
$$|\psi(t_0)\rangle = \sum_n c_n |\phi_n\rangle \qquad |\psi(t)\rangle = \sum_n c_n e^{-iE_n(t-t_0)} |\phi_n\rangle$$



It bounces back cmp. with the exact evolution

Step 4: Forward Euler (unstable)





No time evolution

Step 5: Forward / Backward Unitary Scheme

It's similar to spectral solution (result)

* Due to sparsity of unitary scheme

$\left(I - \frac{i\Delta t}{2}\hat{H}\right) \rightarrow$ is not Hermitian

Thus, (previous tridiagonal) hermitian solver can not employed

↓

Instead banded solver is used (sparse matrix)

Step 6: Split-Operator Method

It uses FFT (fast fourier transform)

position space $\rightleftarrows$ momentum space

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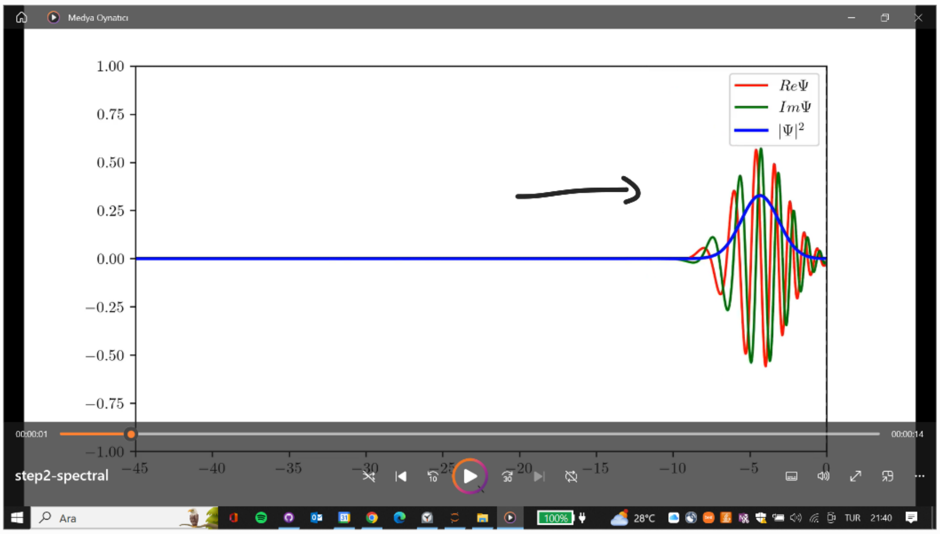
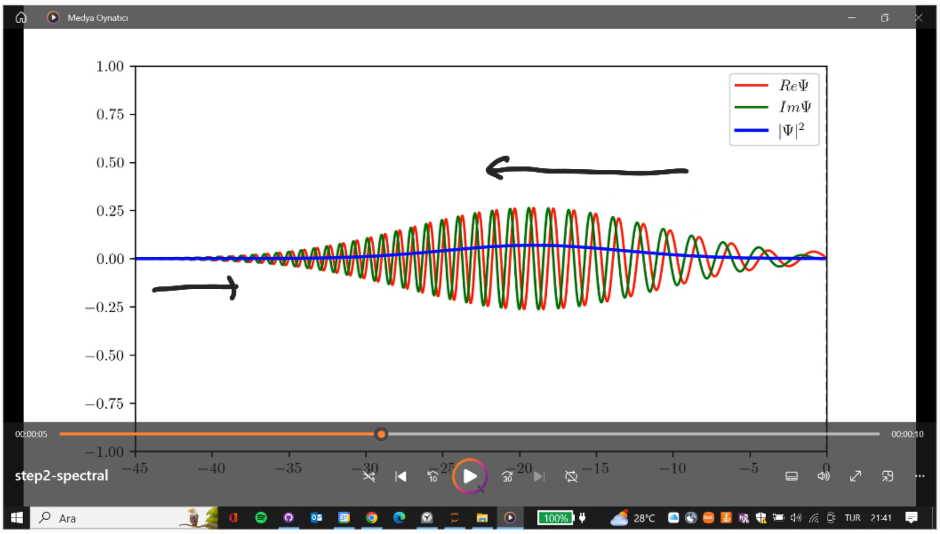




4. We now insert a tilted wall at $x = 0$,

$$V(x) = \begin{cases} 0 & x < 0 \\ \tan(\theta)\, x & x \geq 0 \end{cases}$$

WHY?

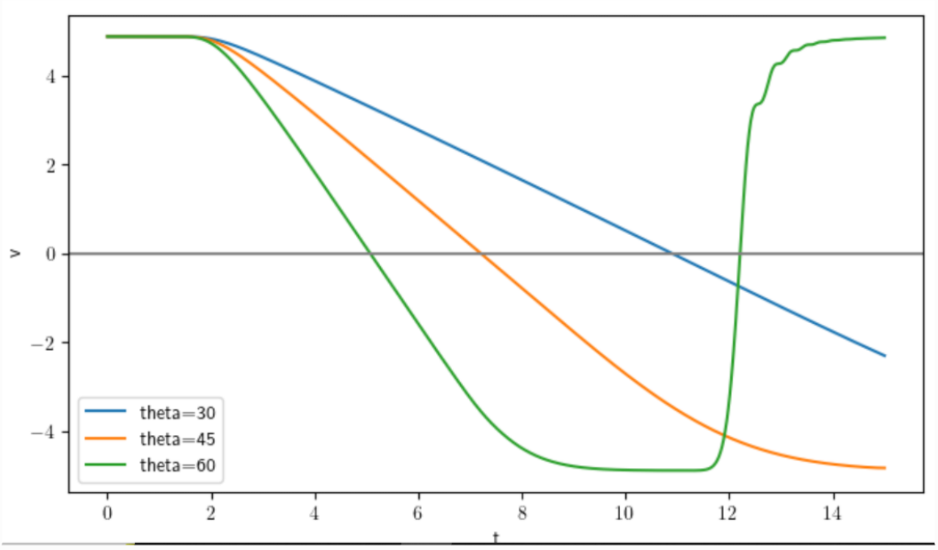
where θ is the tilting angle. In this case, the solution can no longer be found analytically.

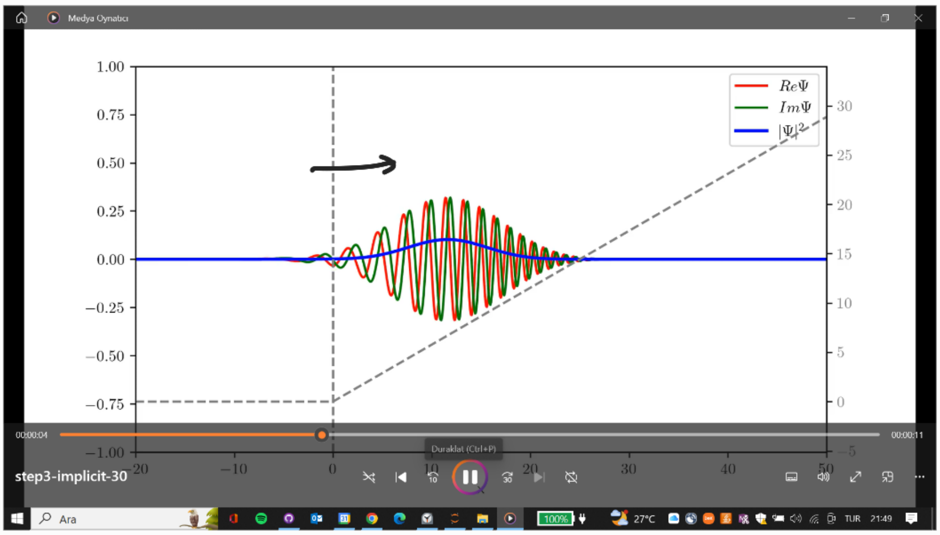
Investigate the behaviour of the wave packet numerically as it hits the wall. In particular, study the time evolution of the velocity of the wave packet

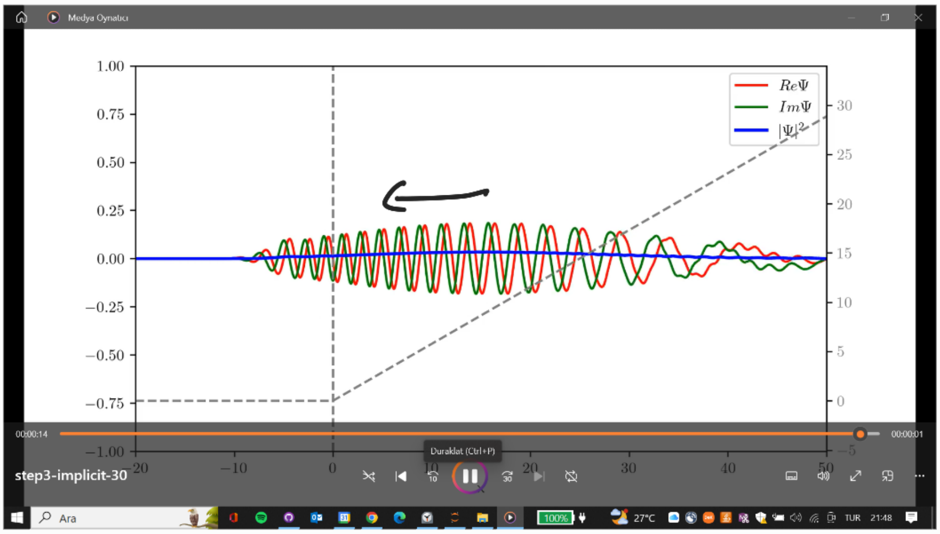
$$v(t) = \int_{-\infty}^{\infty} \mathrm{Im}[\Psi(x,t)^* \frac{d}{dx}\Psi(x,t)]\, dx$$

for different tilting angles.

Hint: You can use finite differences for computing the spatial derivative.



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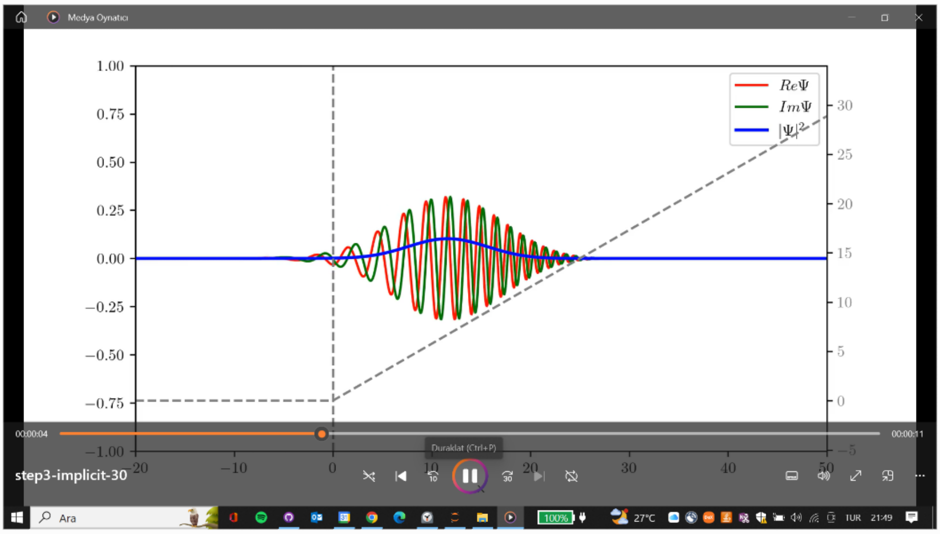
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