Lab9 Report

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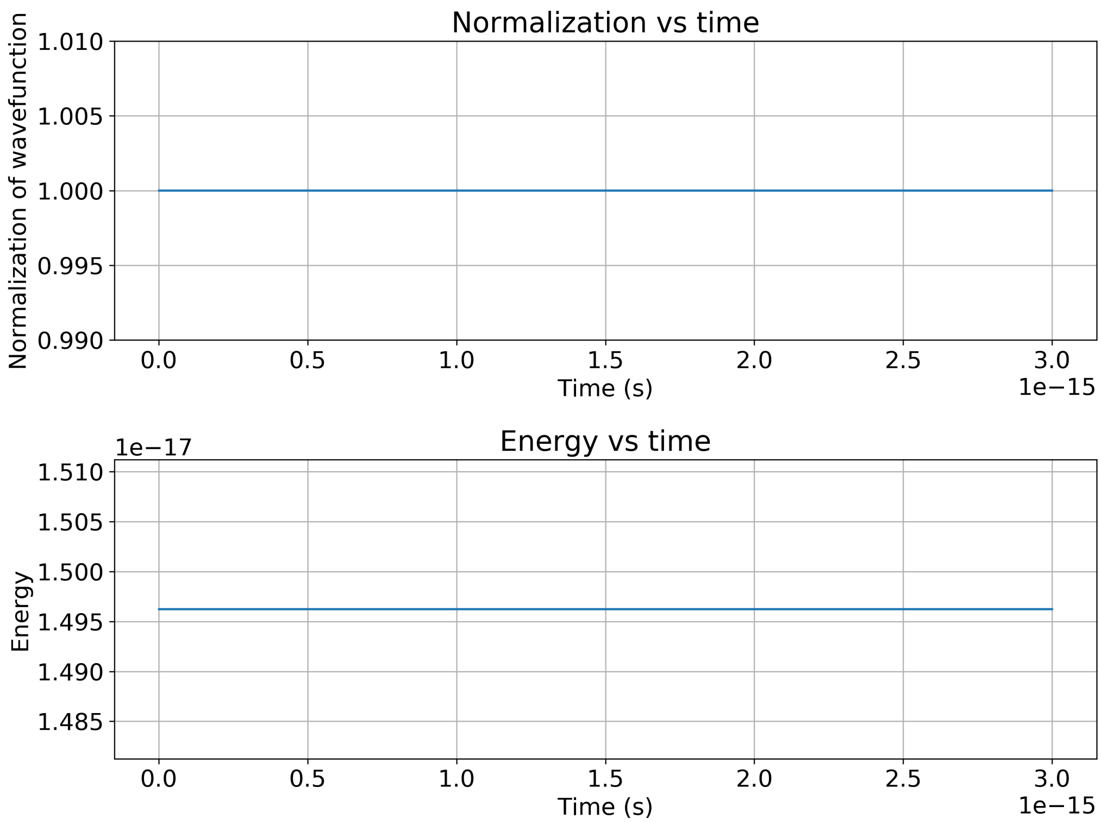
1 Question 1

1.1 Problem restatement and procedure

In this question, we are asked to solve the time-dependent Schrodinger equation within a box defined between [-L/2, L/2], by implementing a Crank-Nicolson (C-N) scheme. The initial condition of wavefunction ψ is given, and the constants on the dimension of the space are also provided. Infinity boundary conditions are set so that ψ is always zero at x=-L/2 and x=L/2. We are going to deal with 3 different potential functions: square well, harmonic oscillator and double well.

Considering the time-consuming nature of this simulation, I wrote up a code to do the simulation part and visualization part separately. Wavefunctions at each time step, and the state variables of the system (energy, expected location and normalization factor) are all outputted and stored in zipped files. To visualize this dynamical process, I plotted wavefunction ψ and probability density function (pdf) of the particle (or $\psi * \psi$) for 4 specific time steps (t=0, t=T/4, t=T/2, t=3T/4). I plotted the 4 steps with different colors, and label the expected position of the particle $< X >$ on the time series using the corresponding color later. The general finding is that the Ehrenfest theorem is held for this scenario, i.e. the wavefunction is moving like a particle and as long as the wave packet remains localized the expected location of the particle is the same as the centre of the wave packet.

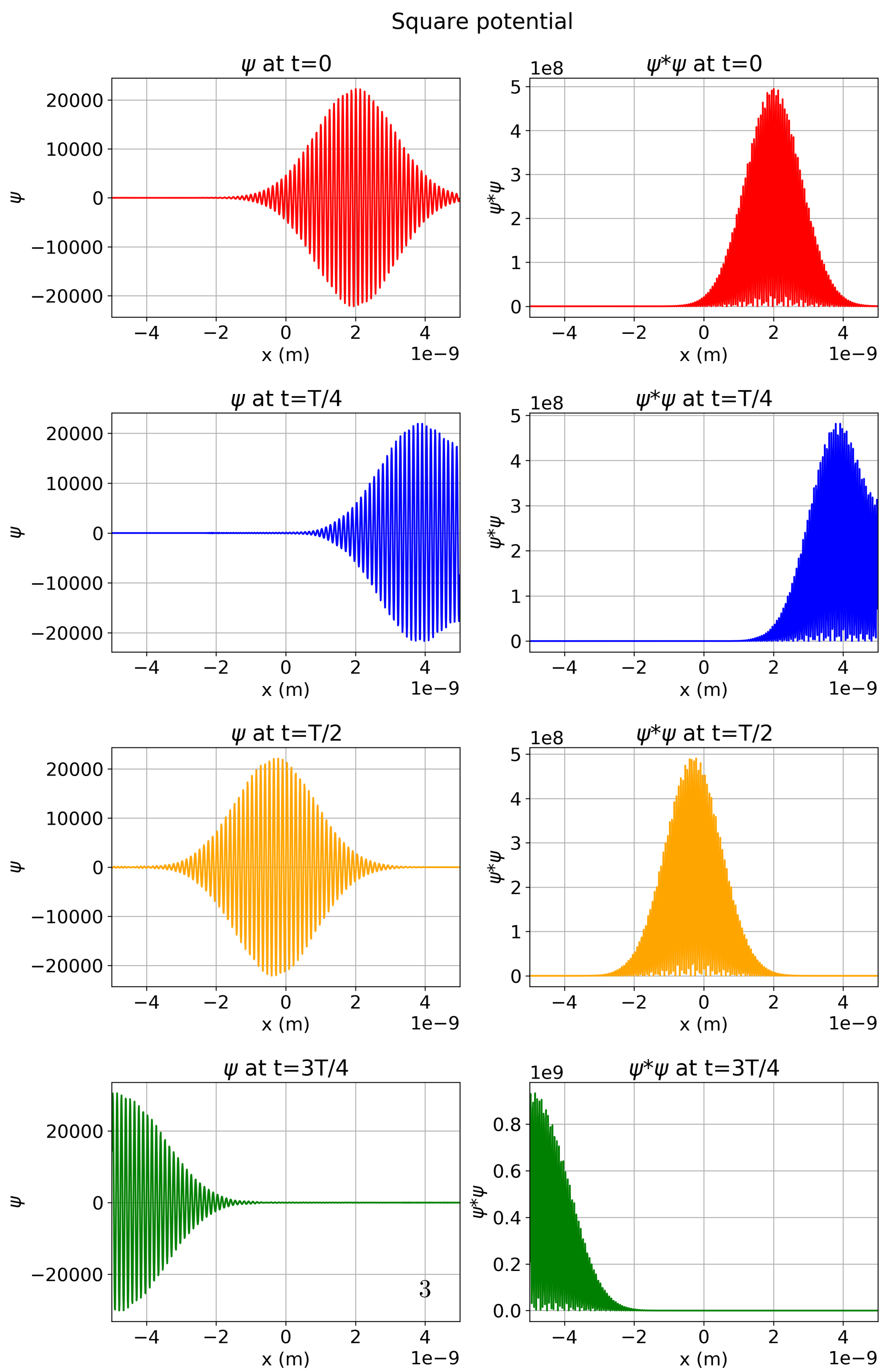
1.2 Q1 (a) Results

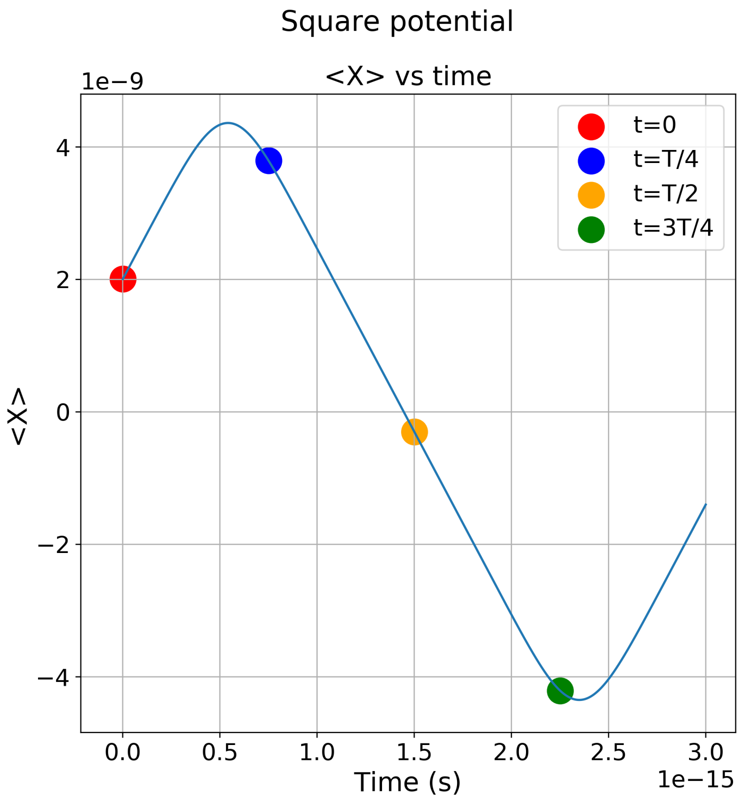


1.3 Q1 (a) Comments

To ensure my C-N scheme works properly, I plotted the time series of normalization factor of the wavefunction and the energy. You can see that both normalization factor and energy of the wave-particle remains constant throughout the simulation time period, which satisfies the low of conservation of energy.

1.4 Q1 (b) Results

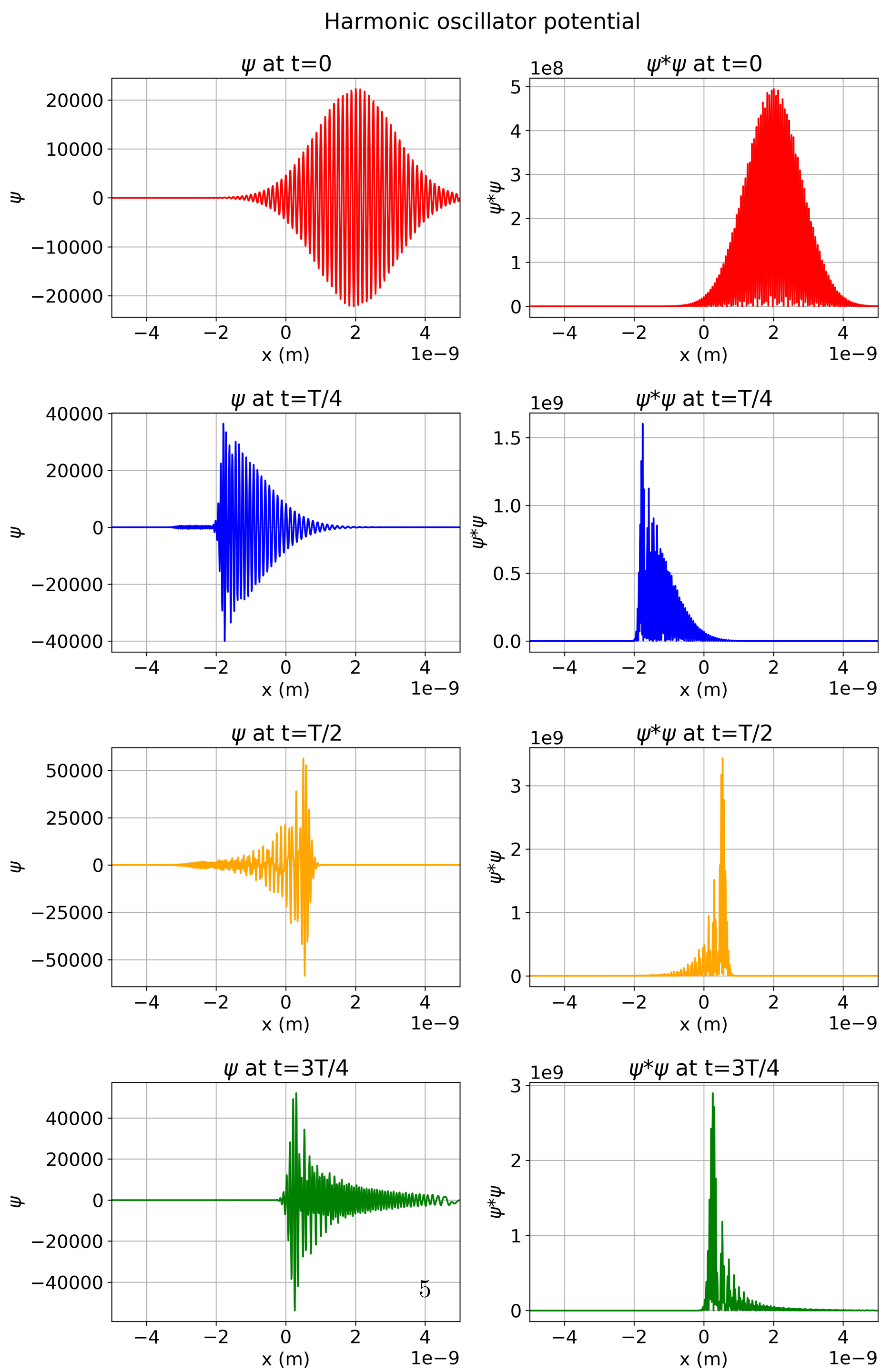


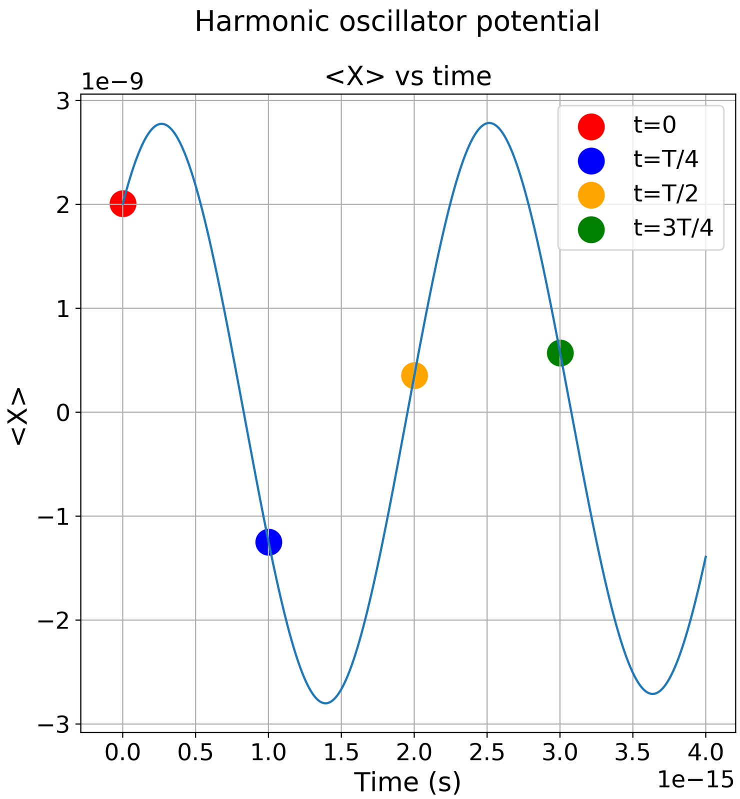


1.5 Q1 (b) Comments

Results for the square well potential are shown above. As mentioned in the problem restatement section, ψ and pdf of centre of the wave packet are plotted for 4 different time steps. You can see that the wave is bouncing between the 2 boundaries, just like a particle. Referring to the time series of expected location of the particle, you can see that the expected location of the particle is moving along with its wave packet. The wavefunction behaves just like the particle, bouncing between the boundaries. This just demonstrates the wave-particle duality and Ehrenfest theorem.

1.6 Q1 (c) Results

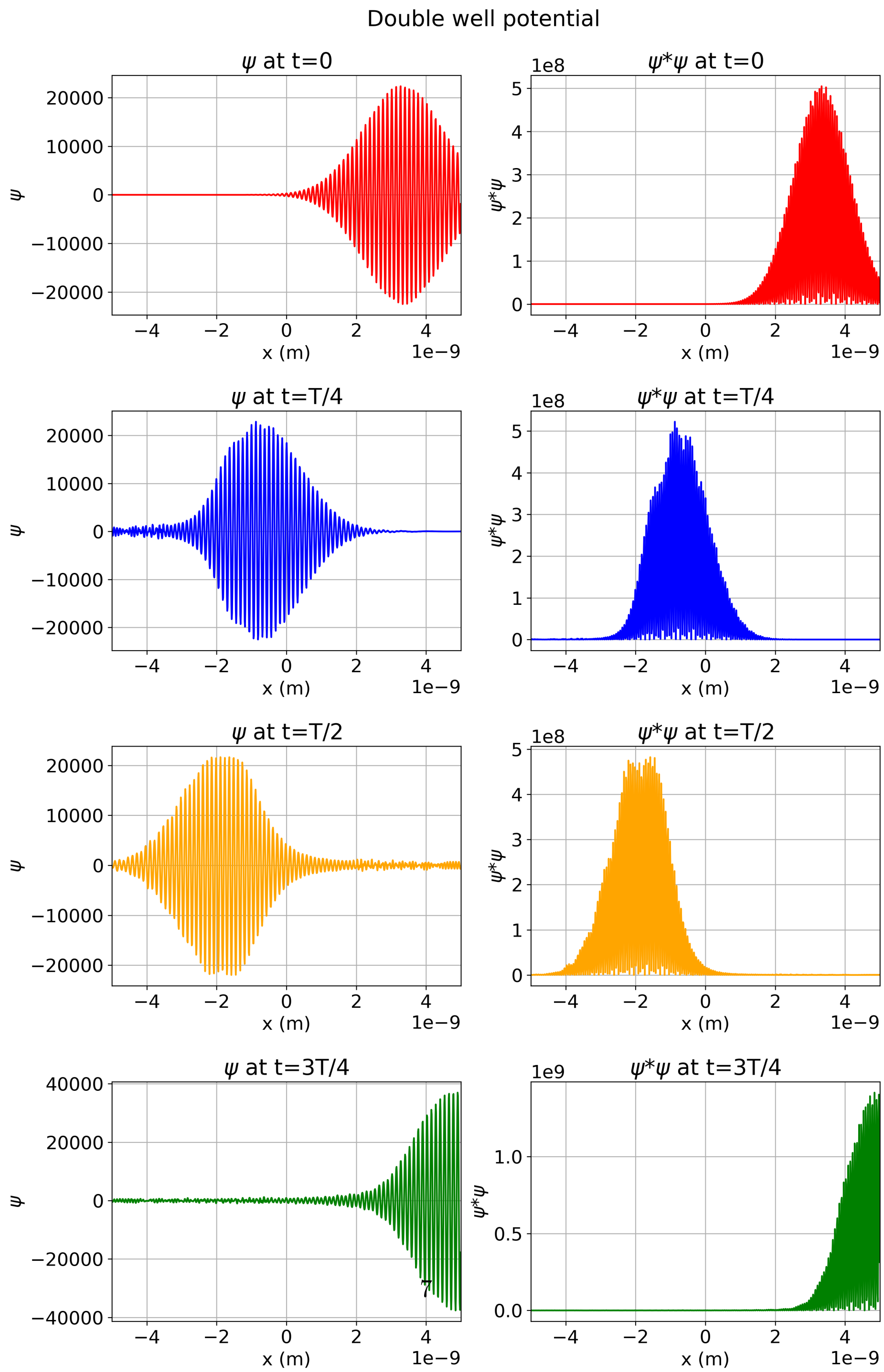


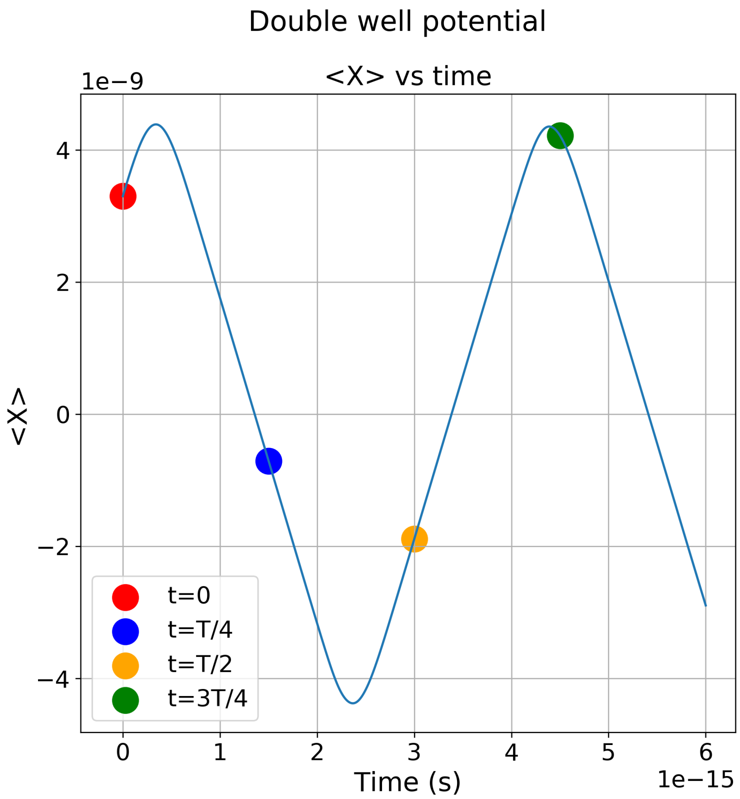


1.7 Q1 (c) Comments

Results for the harmonic oscillator potential are shown above. It is interesting to see that the pdf of the position of the particle is not Gaussian as in a square well, however, now the distribution is slightly skewed. This physically makes sense because the potential is no longer zero inside the box. The particle is now affected by the interaction between itself and the potential. And the expected position of the particle is now undergoing a more sinusoidal motion, just as expected for a harmonic oscillator. This again shows the wave-particle duality and Ehrenfest theorem.

1.8 Q1 (d) Results





1.9 Q1 (d) Comments

Results for the double well potential are shown above. For this double well case, the interaction between the particle and the potential is even more obvious. For example, at t=T/4, the particle is moving to left, so that the potential is "pushing" the particle right. Similarly, at t=T/2, now the particle is leaving away from the boundary (see time series of $< X >$), and now the potential is "accelerating" the motion of the wave packet. As a result, the distribution of pdf of $< X >$ of the wavefunction gets "distorted" to be skewed in the corresponding directions. This again proves the wave-particle duality and Ehrenfest theorem.

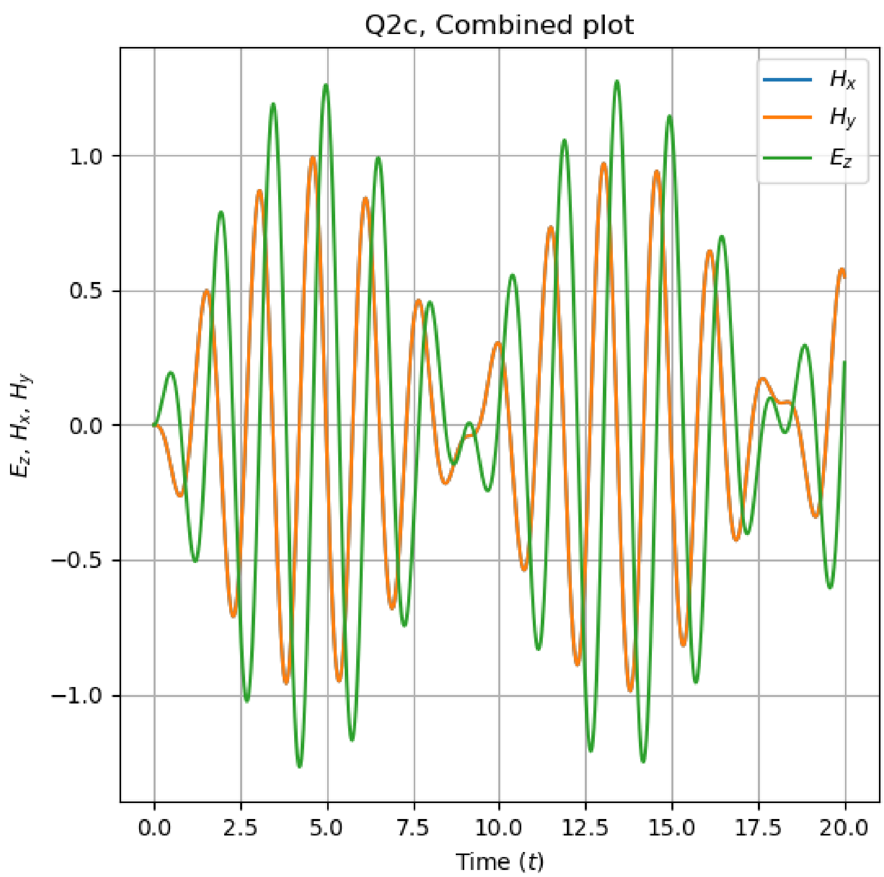
2 Question 2, 2D Resonant cavity

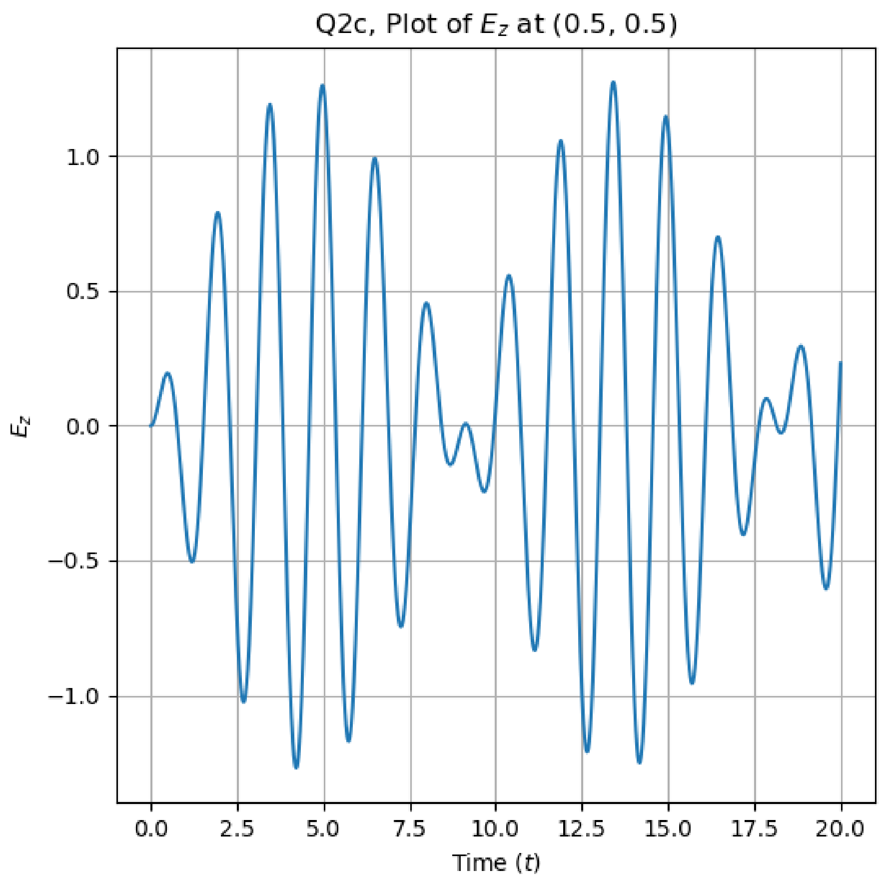
2.1 Q2a, Explanation of why the decomposition in Eqns. (10) satisfy the boundary conditions

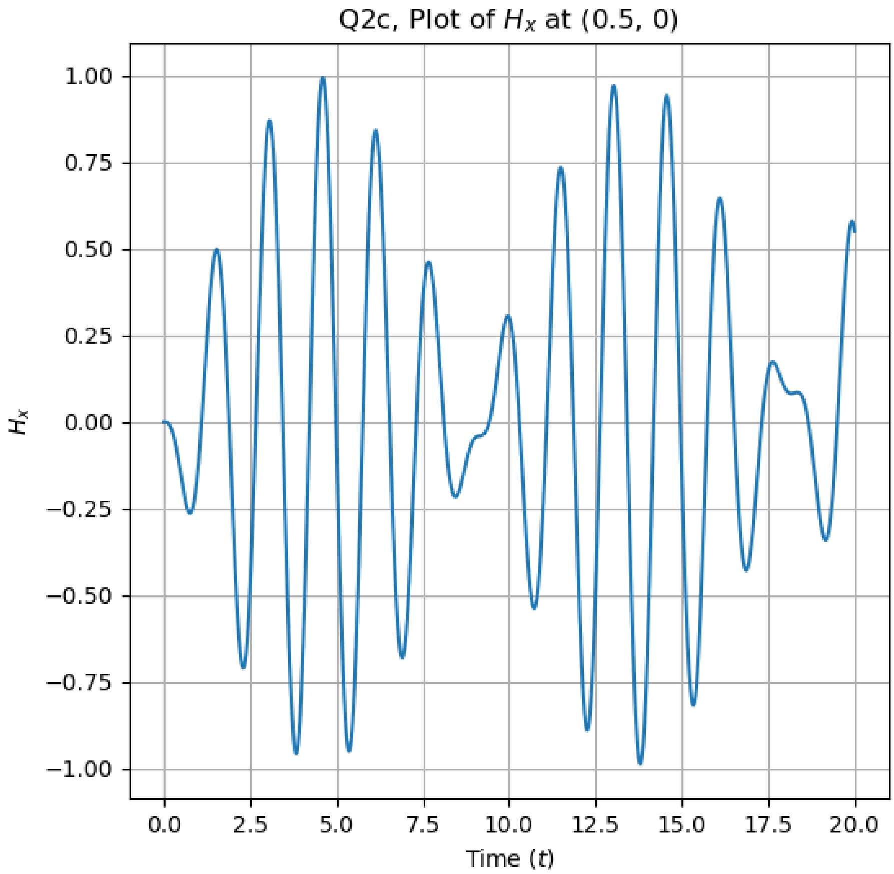
For E_z, we decompose both x and y into sine functions. So at boundary where $x = 0, L_x$ and $y = 0, L_y$, we have $p' = 0, P$ and $q' = 0, P$ respectively. Due to the property of sine functions, we can easily conclude that Eqn. (10a) satisfies $E_z = 0$ ($x = 0, L_x$ and $y = 0, L_y$).
For H_x, we decompose the x-direction into sine functions and y-direction into cosine functions. Due to the property of sine functions, we know they are 0 at x-boundaries. Also we know from the property of cosine functions, the partial derivative along y-axis is 0 at y-boundaries. So the decomposition satisfies the boundary condition: $H_x = 0\,(x = 0, L_x)$ and $\partial_y H_x = 0\,(y = 0, L_y)$.
So similarly, we can conclude for H_y, by just swapping x-axis and y-axis, and say the decomposition satisfies the boundary condition: $H_y = 0\,(y = 0, L_y)$ and $\partial_x H_y = 0\,(x = 0, L_x)$.

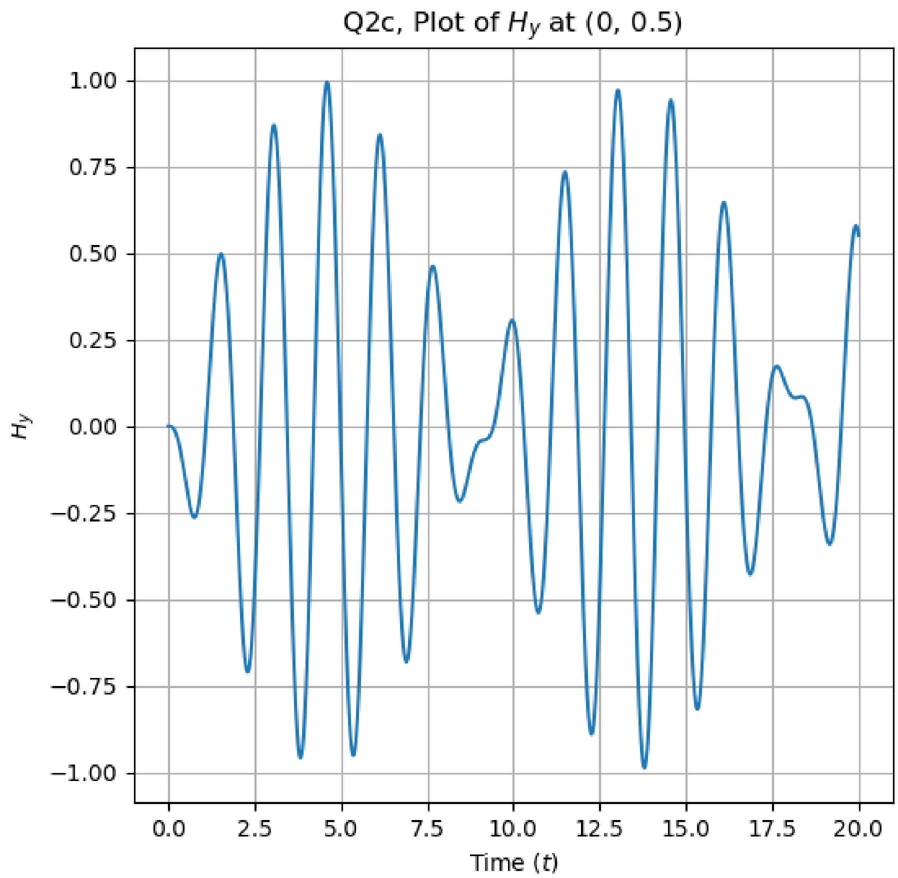
2.2 Q2c, Driving frequency $\omega = 3.75$. Explanatory notes and Plots of the traces $H_x(x = 0.5, y = 0.0)$, $H_y(x = 0.0, y = 0.5)$, and $E_z(x = 0.5, y = 0.5)$

Here I present 4 plots, one plot for each $H_x(x = 0.5, y = 0.0)$, $H_y(x = 0.0, y = 0.5)$, and $E_z(x = 0.5, y = 0.5)$ respectively, and a combined plot.
Please note, I omit all units on axes, since all the constant are scaled to 1. They don't have real physical meanings.



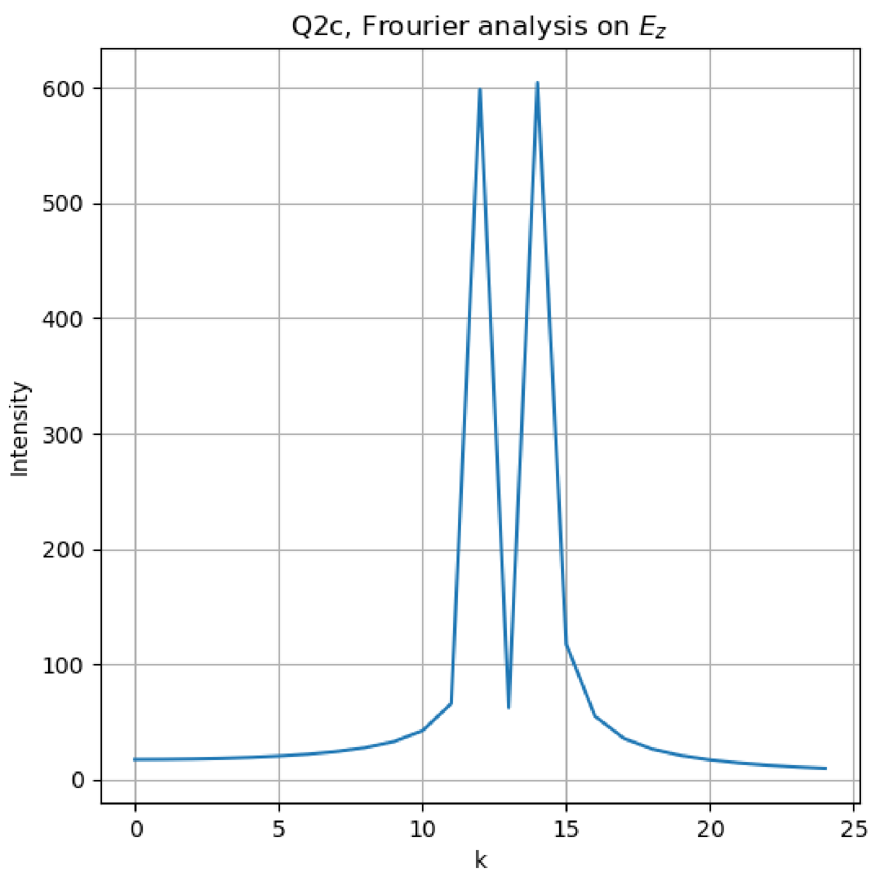

Q2c, Plot of E_z at (0.5, 0.5)
E_z
1.0
0.5
0.0
−0.5
−1.0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
Time (t)


Q2c, Plot of H_x at (0.5, 0)
H_x
Time (t)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0



Q2c, Plot of H_y at (0, 0.5)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
H_y
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
Time (t)

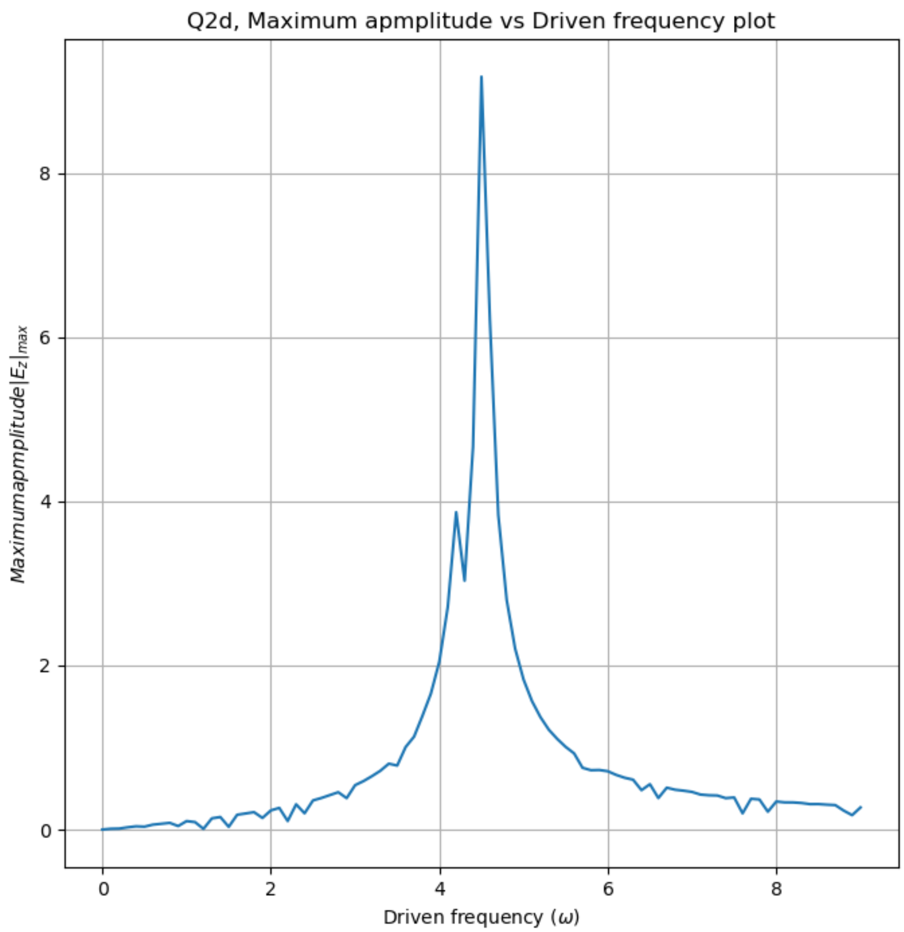
From the plots, we can tell that the amplitudes for $H_x(x = 0.5, y = 0.0)$ and $H_y(x = 0.0, y = 0.5)$ are identical, so they overlap each other in the combined plot. $E_z(x = 0.5, y = 0.5)$ has higher amplitude than $H_x(x = 0.5, y = 0.0)$ and $H_y(x = 0.0, y = 0.5)$. But they all follow a similar pattern.
From the plots, we can tell that they oscillate according to a relatively high frequency within packs with a lower frequency. To find out what is actually happening here, I performed a Fourier transform on the signal of E_z:



I find two k values. For $k = 12$, it corresponds to the driving frequency $\omega = 3.75$, for $k = 14$, it corresponds to $\omega \simeq 4.39$, which is called *normal frequencies* from the latter part.
After some googling, this pattern is caused by the interference between the driving frequency and the normal frequency.

2.3 Maximum amplitude of E_z vs ω plot and explanatory notes

So I plot the maximum amplitude of E_z $(x = 0.5, y = 0.5)$ verses the driving frequency ω:

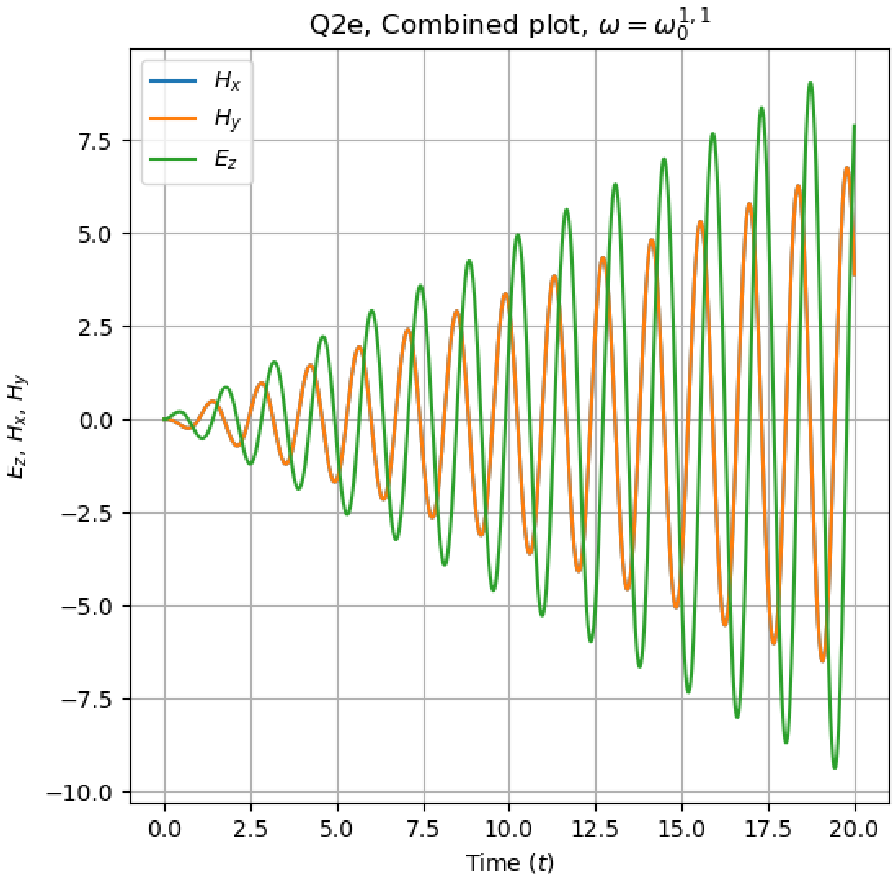


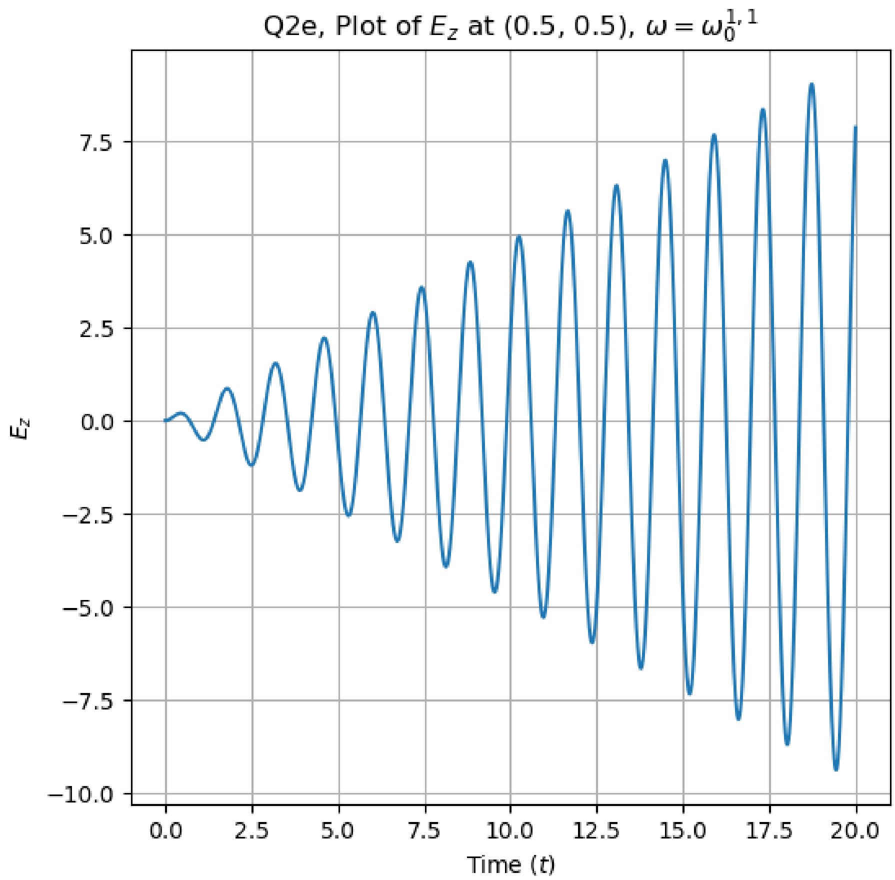
From the plot we can tell that the peak happens around $\omega = 4.4$.
The peaking frequency agree with the value calculated by the formula given in the lab handout:

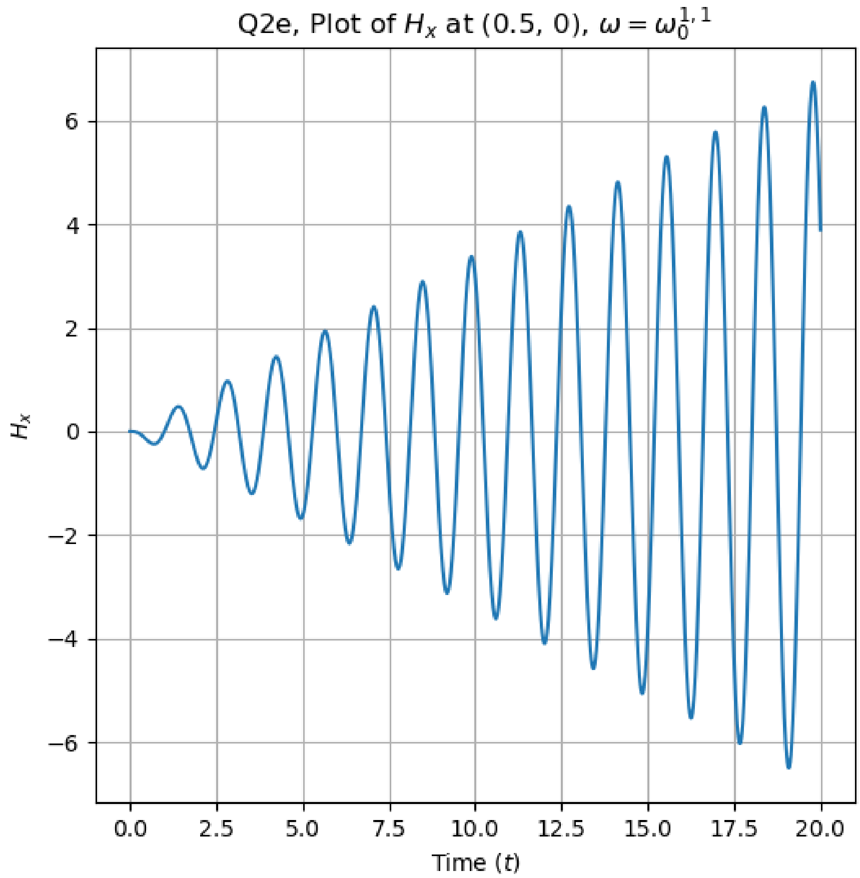
$$\omega_0^{m,n} = \pi c\sqrt{(nL_x)^{-2} + (mL_y)^{-2}} = \pi\sqrt{2} \simeq 4.44$$

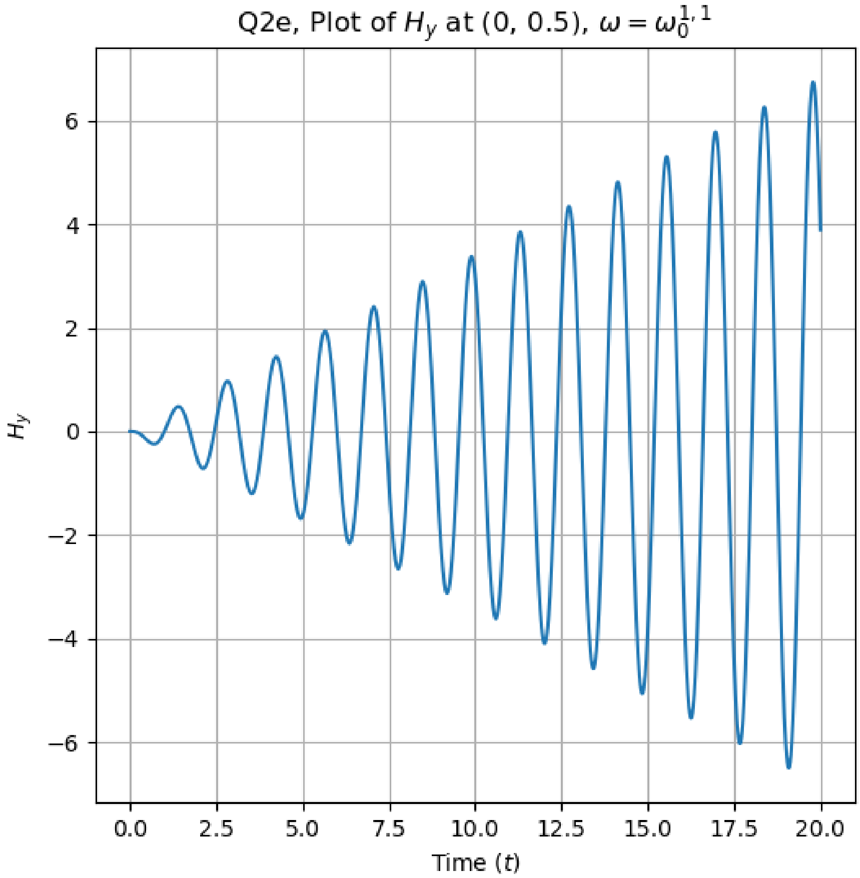
2.4 Plots at driving frequency equals to normal frequency, $\omega = \omega_0^{1,1}$, and Explanatory notes

Here I present 4 plots, one plot for each $H_x(x = 0.5, y = 0.0)$, $H_y(x = 0.0, y = 0.5)$, and $E_z(x = 0.5, y = 0.5)$ respectively, and a combined plot.
Please note, I omit all units on axes, since all the constant are scaled to 1. They don't have real physical meanings.



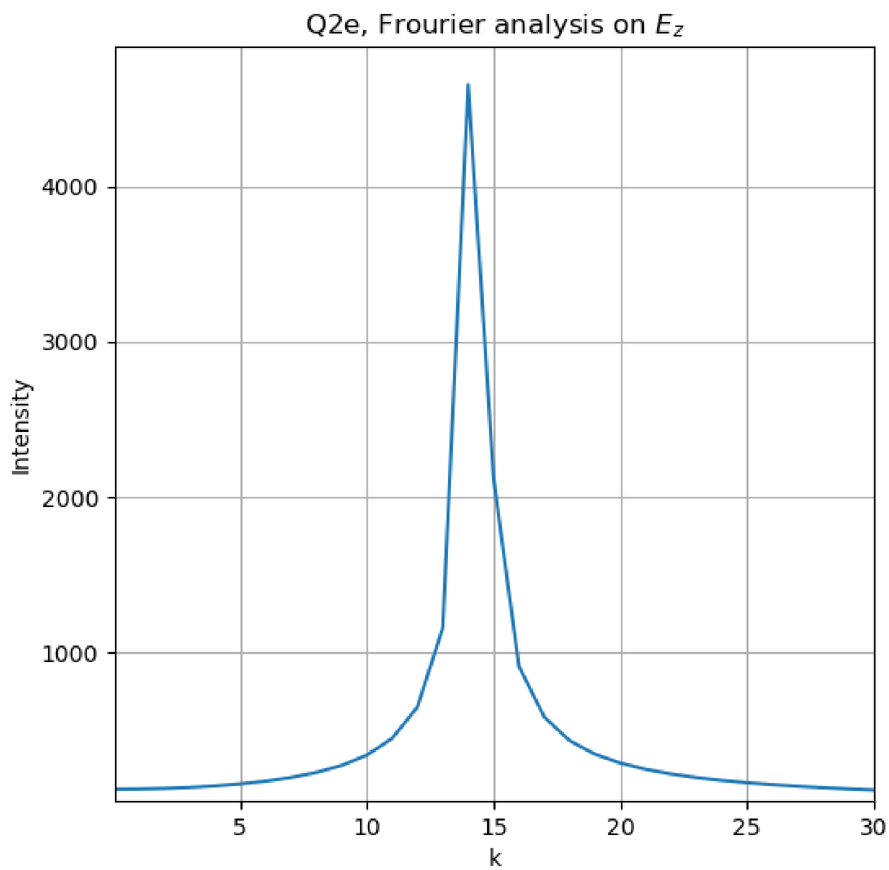

Q2e, Plot of E_z at (0.5, 0.5), $\omega = \omega_0^{1,1}$
E_z
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
Time (t)


Q2e, Plot of H_x at (0.5, 0), $\omega = \omega_0^{1,1}$
H_x
Time (t)
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
6
4
2
0
−2
−4
−6



Q2e, Plot of H_y at (0, 0.5), $\omega = \omega_0^{1,1}$
H_y
Time (t)
6
4
2
0
−2
−4
−6
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0

From the plot, we can tell that there is no longer pack-like behaviour. There is only one sine wave but its amplitude grows linearly over time. This means the energy in the cavity will also grow over time. It is like the energy is being accumulated and never released.
Just for fun, I performed a Fourier transform:



We can see that this time there is only 1 peak at $k = 14$, which is corresponds to the normal frequency or resonant frequency of the cavity.
This phenomenon is called the resonance of rectangular wave guide.