PHY407 Lab09

(Yonatan Eyob Q1), (Kivanc Aykac Q2)
Student Numbers: 1004253309, 1004326222

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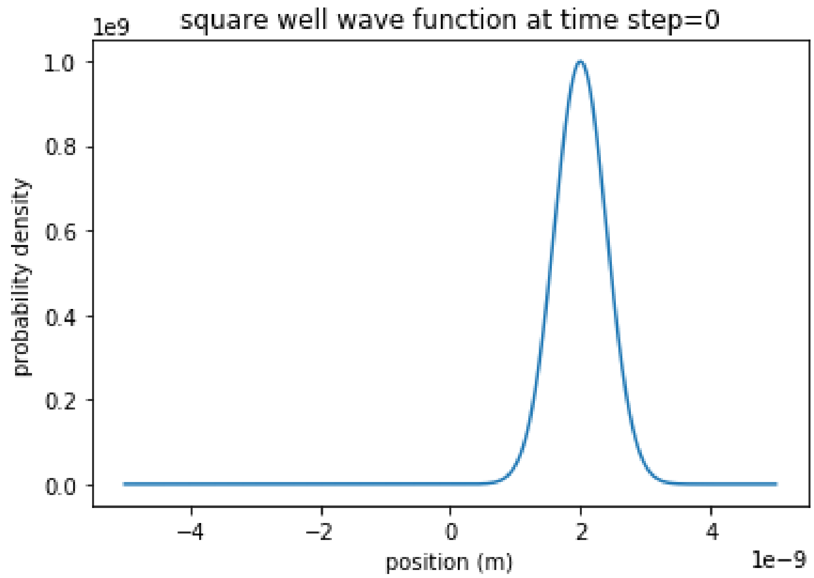
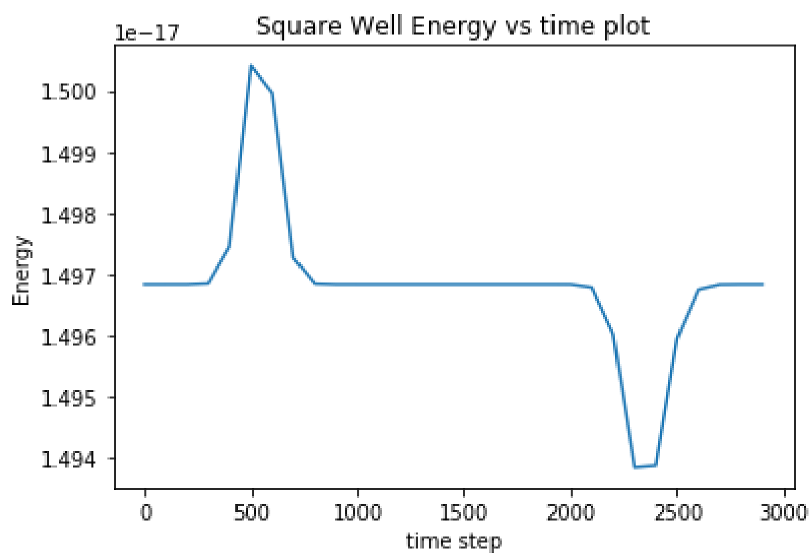
1 Solving the time-dependent Schrödinger equation with the Crank-Nicolson scheme

In this section we will find a solution to the Time-dependent Schrödinger equation, $ih\frac{\partial\Psi}{\partial t} = \mathbf{H}\Psi$ using the Crank-Nicolson, and then plot $\Psi^*(x,t)\Psi(x,t)$ for three different potential wells:
(1) Square well: V(x)=0
(2) Harmonic oscillator: V(x)=$\frac{1}{2}mw^2x^2$
(3) Double well: V(x)=$V_0(\frac{x^2}{x_1^2} - 1)^2$
We will also plot the energy vs Time and Position vs Time graphs for the Square potential well.

1.a

first we will plot the normalized wave function in the square well at the beginning of the time duration (time= 0 * 10^{-18} seconds) and then we will plot the energy vs time plot over the whole time duration we want to consider:
side-note: Time = timestep * 10^{-18} seconds.

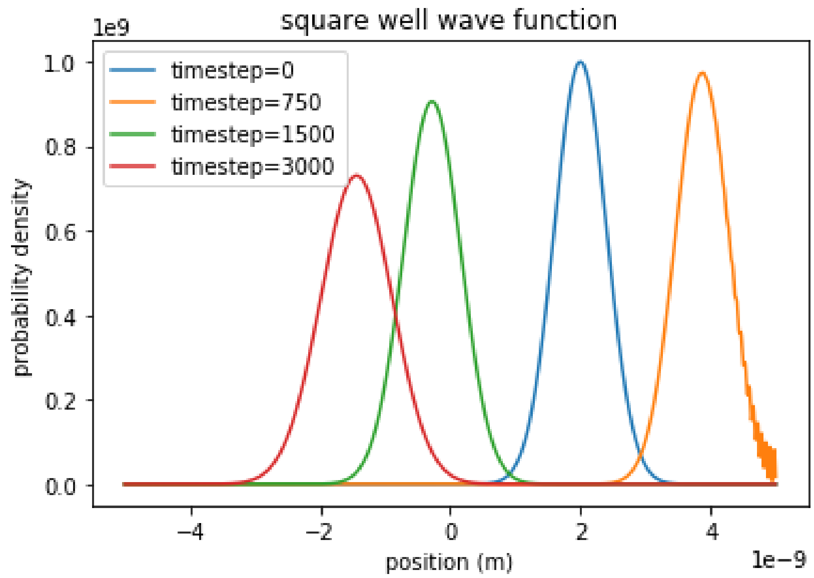


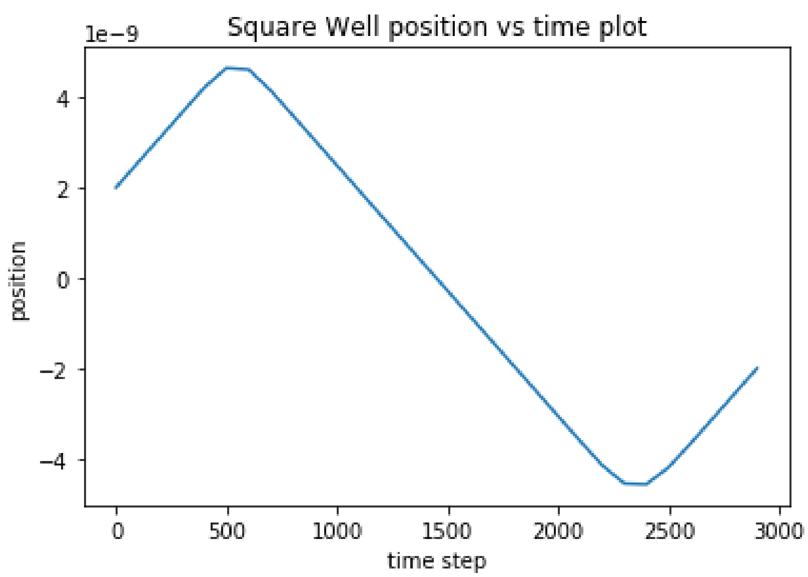


The energy is measured in Joules in this graph. Please have mercy :c
The energy stays constant until it makes contact with the wall, and the energy fluctuates as the wave function makes contact with the wall. Thus the Expected position conforms to the Ehrenfest theorem quote mentioned in the handout because The expected position follows the expected classical trajectory of an object bouncing from wall to wall.

1.b

Now we will plot the wave functions in the square well for timesteps=0, 750, 1500, and 3000 to observe the motion of the wavefunction over time:

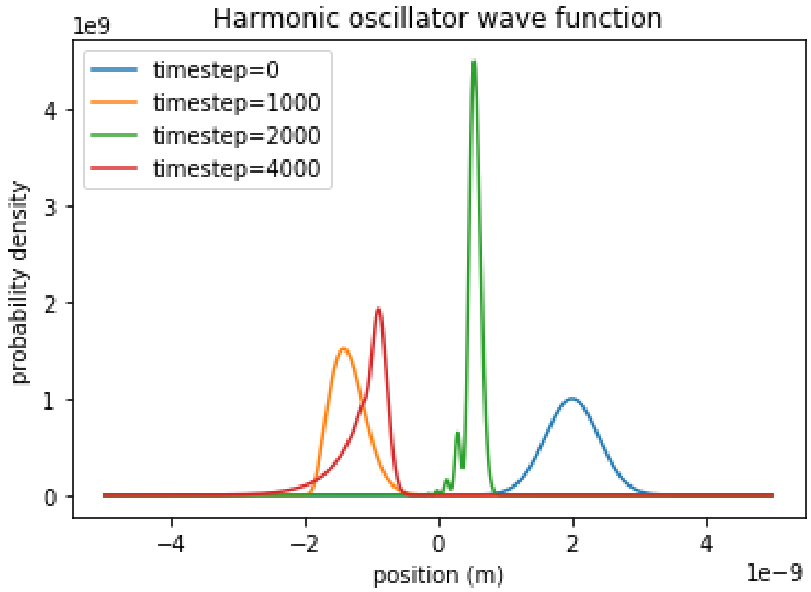




The position is measured in meters in this graph. Please have mercy :c
from the Position vs Time graph, it is clear that the wave function bounces from wall to wall, and the wave function graph shows that each bounce lowers the peak of the wave function.

1.c

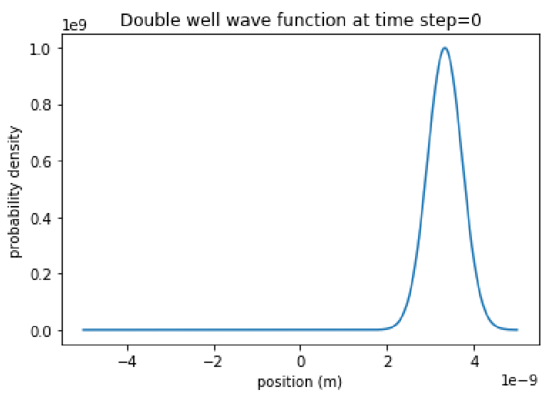
Now we will plot the wave functions in the harmonic oscillator well for timesteps=0, 1000, 2000, and 4000 to observe the motion of the wavefunction over time:

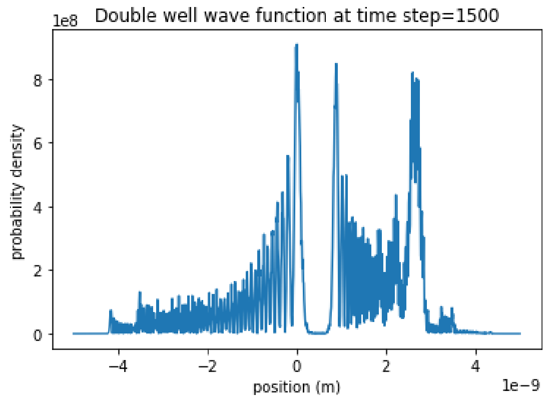


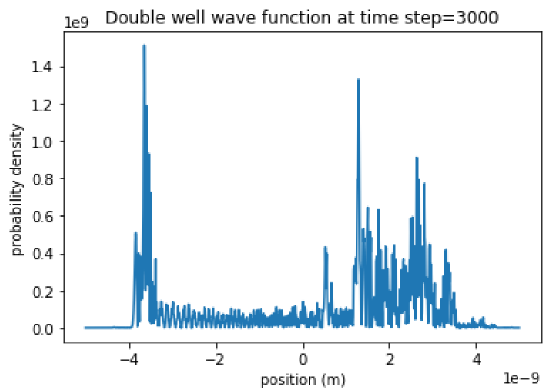
again the wave function seems to move back and forth along the x-axis but the peak of the wavefunction varies much more than in the square well

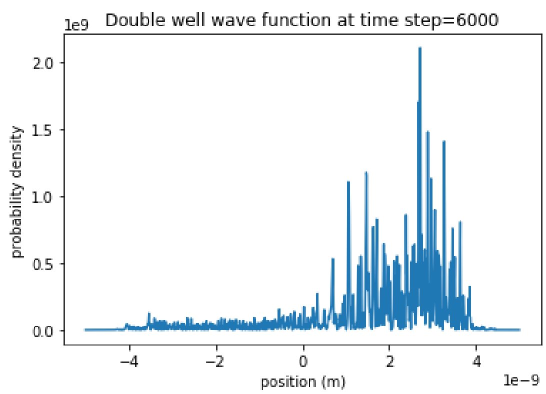
1.d

Now we will plot the wave functions in the double well for timesteps=0, 1500, 3000, and 6000 to observe the motion of the wavefunction over time:









The wave function looks like it is quantum tunnelling through the potential double well located between the walls of the infinite potential well.

2 Resonant EM cavity

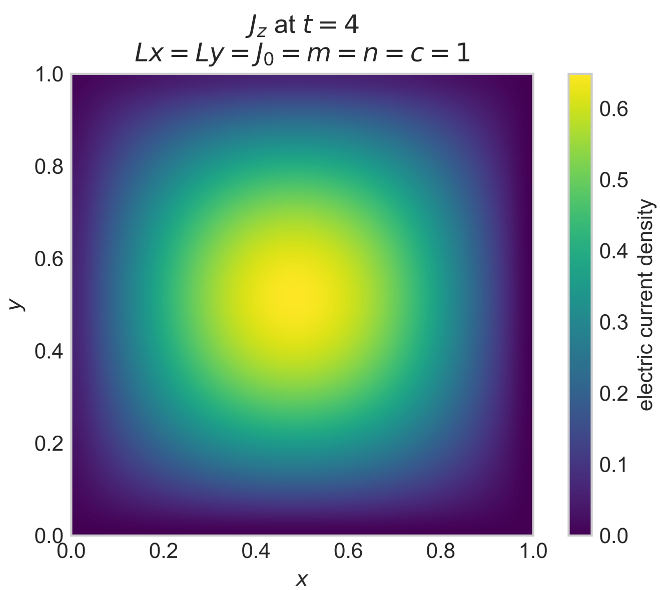
In this question Resonant EM cavity equations will be solved using Crank-Nicolson method.

2.a

The decomposition in eqns. (10 of manual) satisfy the boundary conditions of $E_z, H_x andH_y$ because $pandq$ in the equations correspond to $xandy$, so we should be getting zeros at the walls when we have sine functions, which is stated in the boundary conditions.

2.b

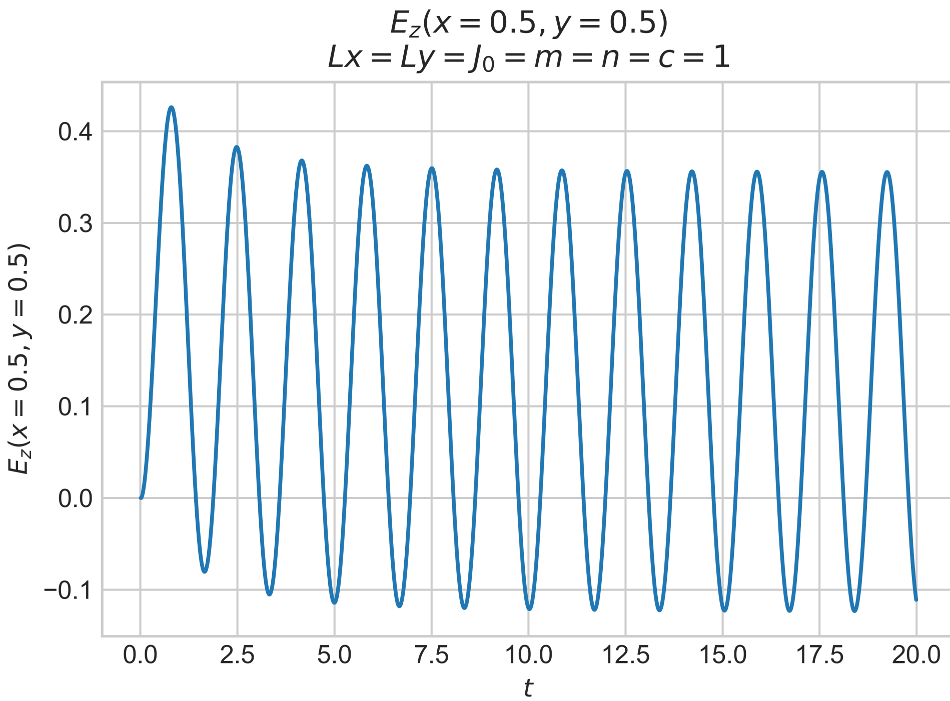
This part lays the ground for what is going to come up in the next parts. To demonstrate the $J_z(x, y, t)$, values of $T = N\tau = 20, \tau = 0.01, Lx = Ly = J0 = m = n = c = 1, P = 32$. Below is the figure:

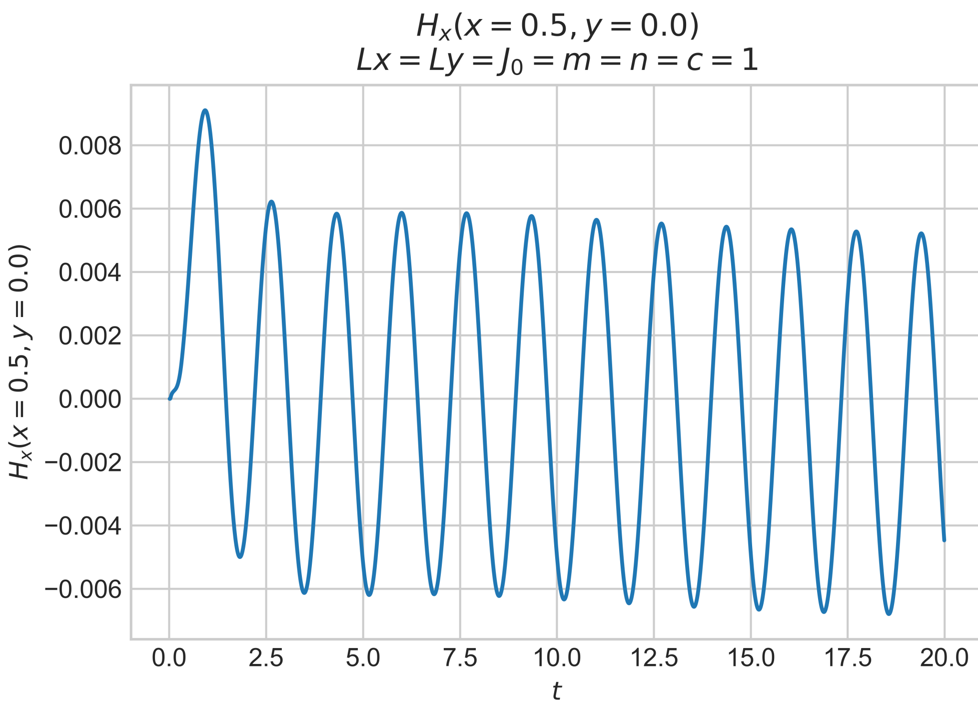


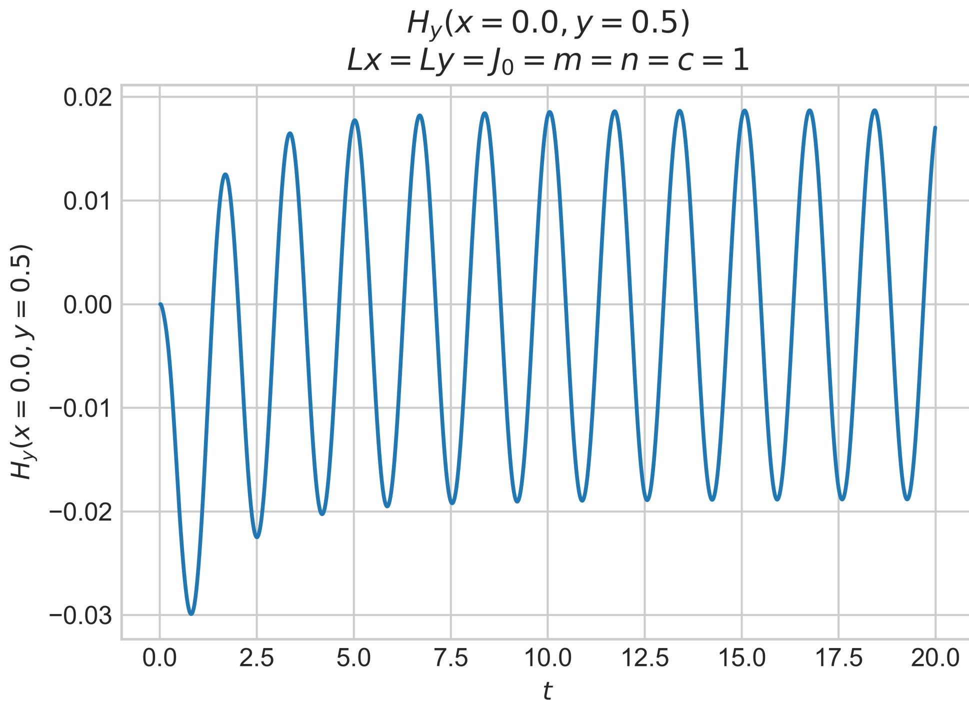
Also, in order to figure out what kind of DFT to use, equation 10 in the manual should be investigated. Looking at it, it can be seen that; DST in both x and y directions for E_z and J_z, DST in x direction and DCT in y direction for H_x, DCT. in x direction and DST in x direction for H_y. And, of course, their appropriate inverse DFTs will be used. In the cases of H_x and H_y, we have different treatment of the two directions so seperate functions that follow the same logic of the dcst.py file that was given with the manual was used. For the other two, there is no need to write new 2D DFT functions and what's inside dcst.py can be used.

2.c

With the driving frequency $\omega = 3.75$, the fields over time are evolved, then ploted the traces: $Hx(x = 0.5, y = 0.0)$, $Hy(x = 0.0, y = 0.5)$, and $Ez(x = 0.5, y = 0.5)$ as a function of time. Below are the figures:



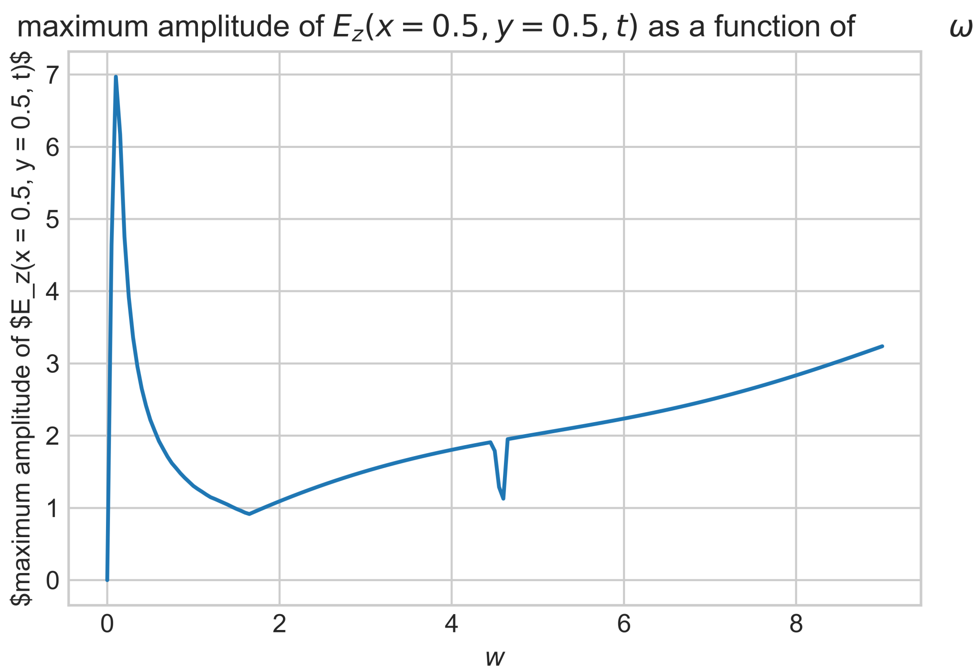

$H_x(x = 0.5, y = 0.0)$
$Lx = Ly = J_0 = m = n = c = 1$
0.008
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
$H_x(x = 0.5, y = 0.0)$
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
t



Some as can be seen there are oscillatory behaviours. This is expected since the driving current density, J_z, was oscillatory.

2.d

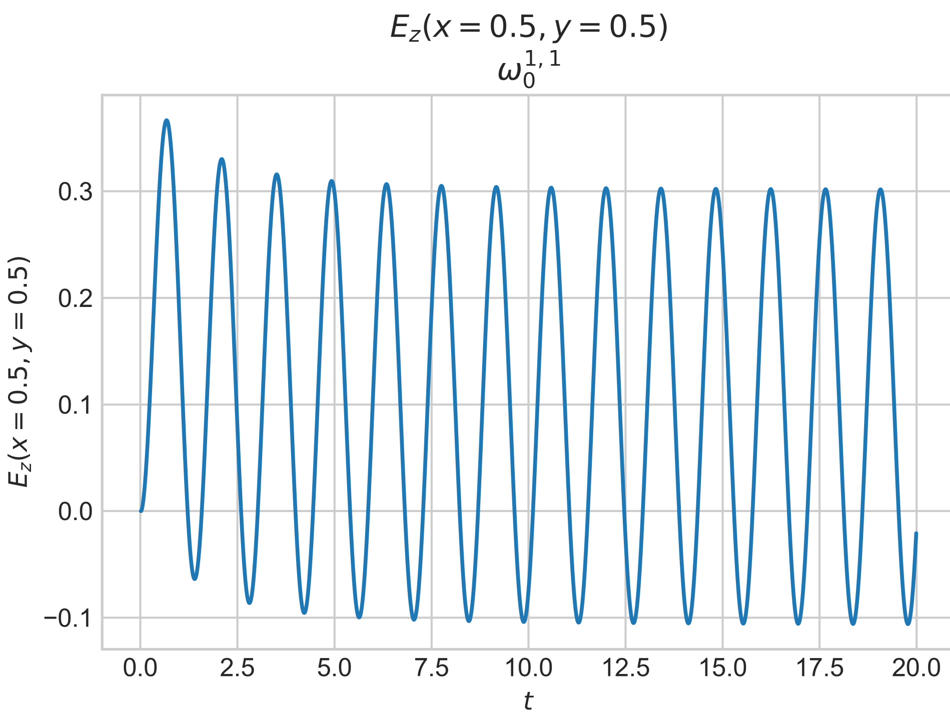
In this part, ω is varied, and the maximum amplitudes of $Ez(x = 0.5, y = 0.5, t)$ is plotted as a function of ω. Below is the figure:

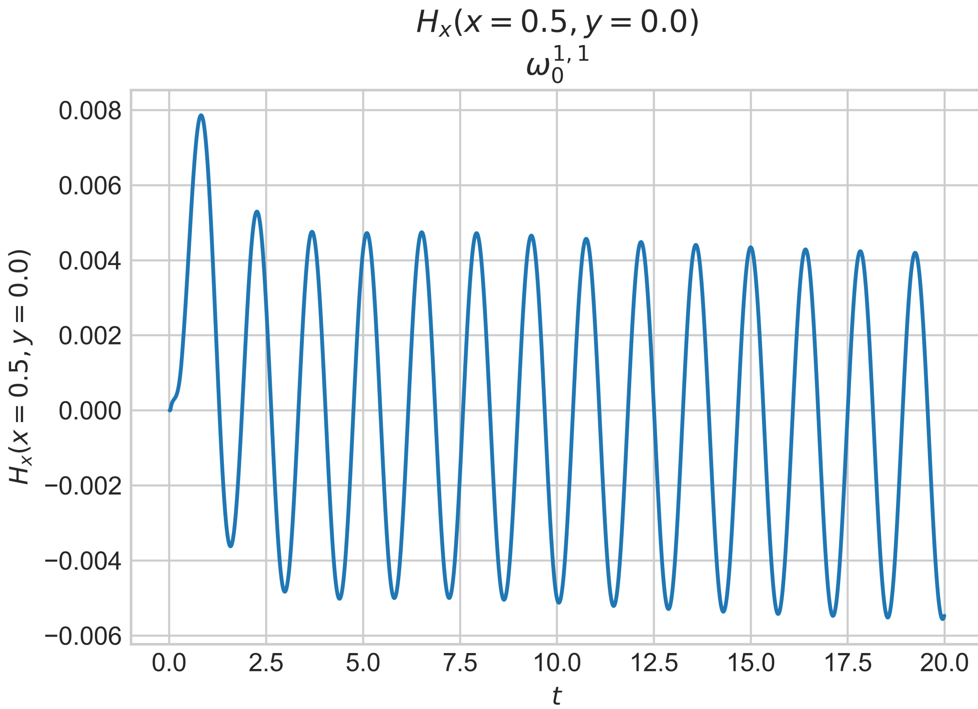


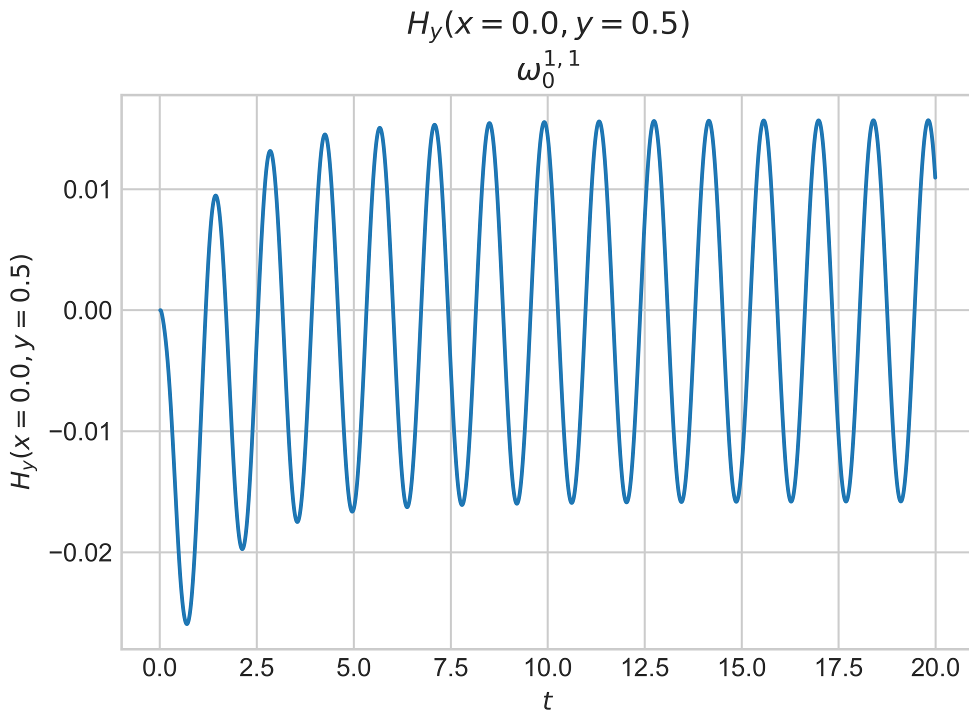
As can be seen, there is point at $\omega = 1.65$ and max amplitude of $Ez(x = 0.5, y = 0.5, t)$ as 0.91549947. This tells us the ω at which we have the least energy. There is one more drop after $\omega = 4$ but its value is more than this. According to the equation $\omega = \pi * c * \sqrt{(nL_x)^{-2} + (mL_y)^{-2}}$, and assuming n and m are same, $\omega = 0.91549947$ corresponds $n \simeq 0.0018$

2.e

From the part 2.d we have the expression for $\omega_0^{m,n}$ Taking $\omega = \omega_0^{1,1}$, the same traces as in part 2.c are plotted. Below are the figures:


$E_z(x = 0.5, y = 0.5)$
$\omega_0^{1,1}$
$E_z(x = 0.5, y = 0.5)$
0.3
0.2
0.1
0.0
−0.1
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
t


$H_x(x = 0.5, y = 0.0)$
$\omega_0^{1,1}$
0.008
0.006
0.004
0.002
0.000
−0.002
−0.004
−0.006
$H_x(x = 0.5, y = 0.0)$
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
t



When compared to the figure of part **??**, where we had $\omega = 3.75$, we see that the amplitudes have changed for the fields changed. However, the general pattern is similar. To note, in this part, we have $\omega = \pi * c * \sqrt{(nL_x)^{-2} + (mL_y)^{-2}} = 4.44$. So the change is normal as this is the deriving frequency that affects the value of J_z. And since the amplitudes of the fields in the cavity changed the energy should change as well.