PHY407 (Lab 9: Partial Differential equations, Pt. II)

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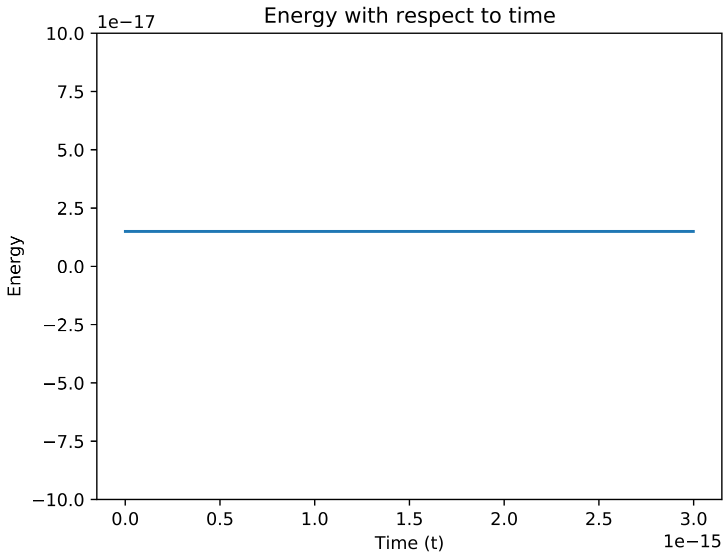
Contents

Work Allocation:
Utkarsh: Question 1
Aslesha: Question 2

Question 1: Time-dependent Schrödinger (Crank-Nicolson scheme)

(a) We used the given parameters to code the Crank-Nicolson method.



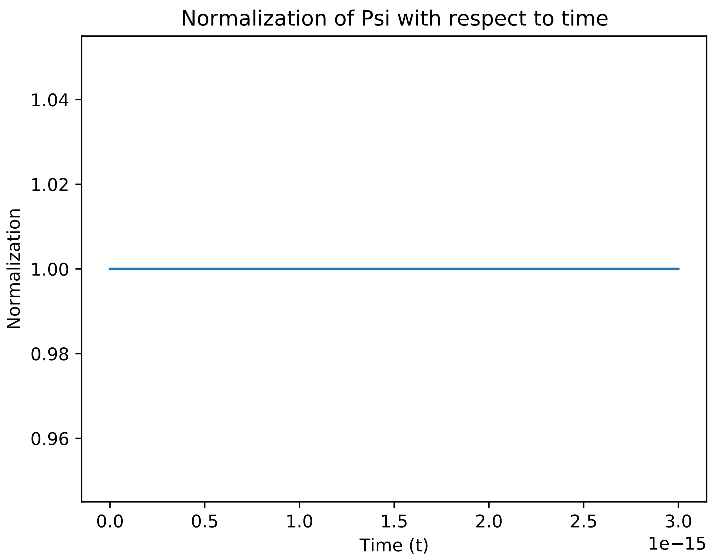


Figure 1: It can be observed that energy remains constant through out the loop. From this we know we are not breaking any conservation of energy laws.

Figure 2: We observe that normalization stays constant at 1 indicating that psi remains normalized throughout the loop

(b) This part of the code asks us to describe the behaviour of the wave function. We decided to use the probability density plots instead of the real value of psi since we though it would result in a cleaner shape. With reference to the out of context quote about Ehrenfest Theorem, we notice that the expectation of the position follows classical trajectories while the wave-function is localized in position space. This was observed at almost all times except when $t = 1.45$

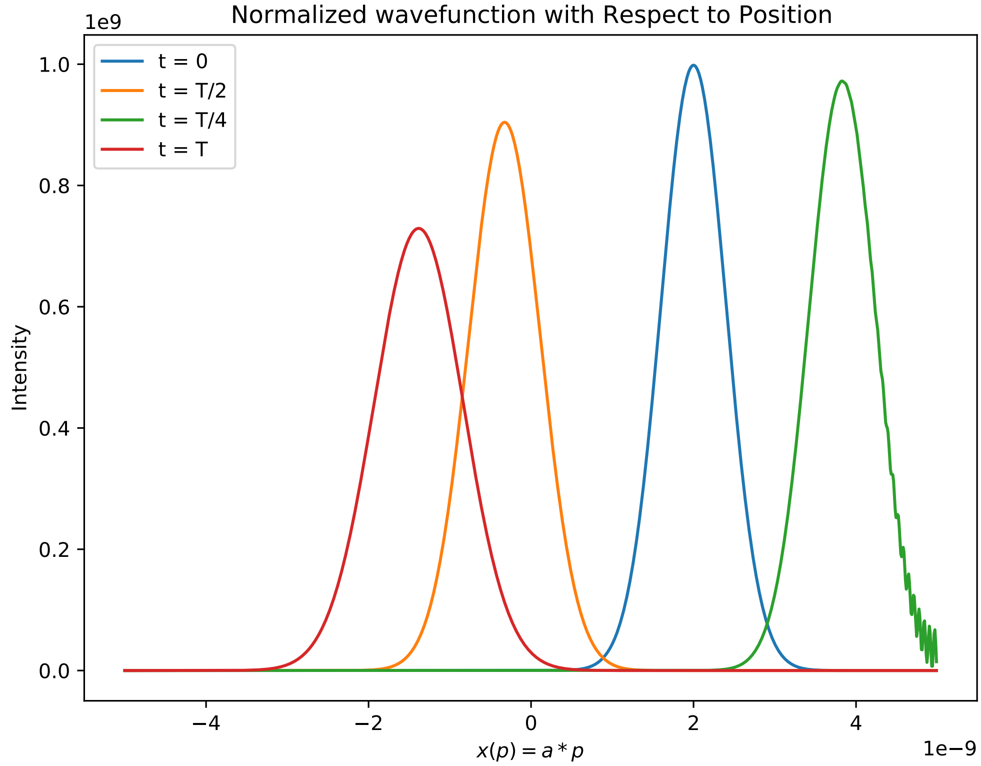


Figure 3: We noticed by observation that psi bounces from wall to wall with some level of convolution at each ends of the wall. We also notices the amplitude of psi changing as we traversed through the loop.

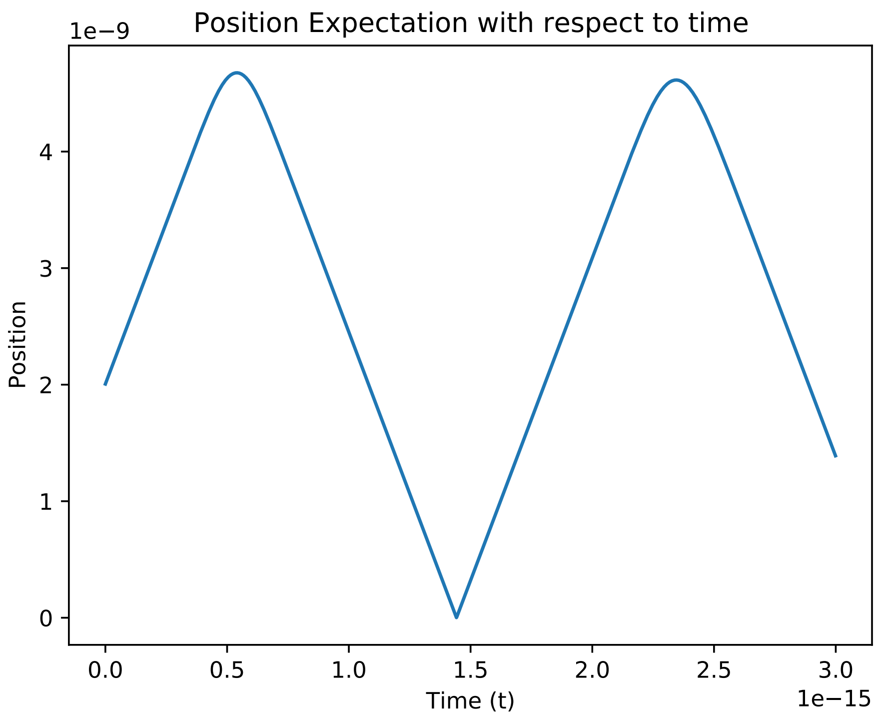


Figure 4: The expectation of position followed classical predictions except near $t = 1.45$ where a sharp change in position (which is non-classical) can be observed.

```
PSEUDOCODE:
# define constants as required in Q1a
# Define a checker for normalization
# Define value of normalization constant
# Define position expectation computer
# Compute psi without psi0
# Compute psi0
# Compute psi initially
# Define square well potential
# Define Quantum Harmonic Oscillator potential
# Define double well potential
# Define H_D() Matrix
# Define energy expectation
# Set initial time step
# Set initial value of psi
# Set expectation of position data
# Set normalization data
# Set energy expectation data
# Set total time to iterate
# Define Identity Matrix
# Compute Lmatrix and Rmatrix
```

```
# Set current psi to initial psi
# Crank-Nicolson loop
    # compute v and solve for new psi
    # Append values of expectations as required.
    # Save psi's for T, T/2, T/4
    # Update time step
    # Update psi for next loop

# Set time array for plotting purposes
# Plot real value of psi
# Plot all psi's evolved in time.
# Plot values of energy expectation
# Plot values of position expectation
# Plot values of normed data
```

All parts were run of this blueprint, hence pseudocode for parts c and d have been omitted.

(c) Here we are asked to repeat step (b) using a new quantum harmonic oscillator potential.

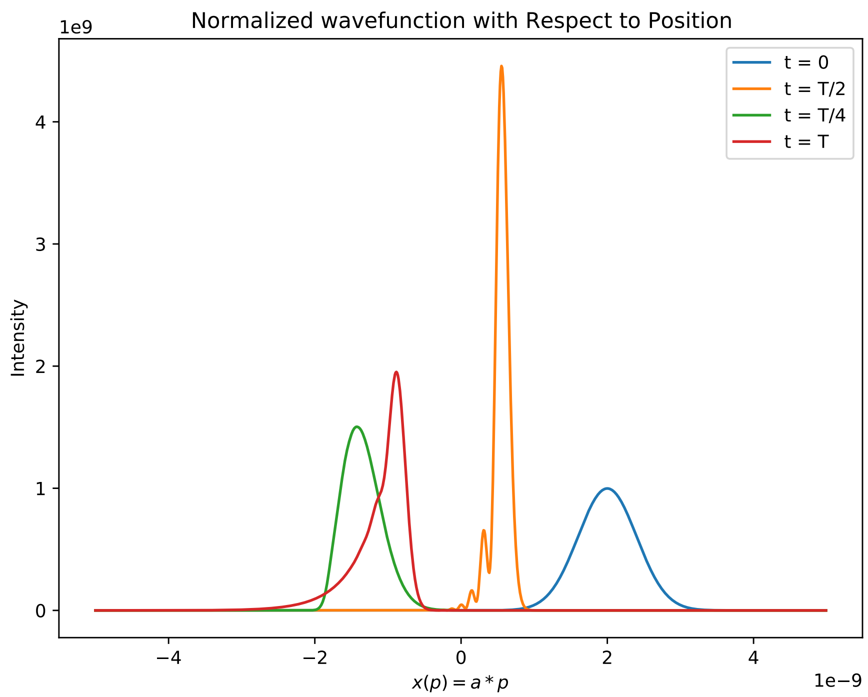


Figure 5: We noticed by observation that psi oscillates between the two boundaries. At certain points near the center, psi tends to behave analogous to a delta function potential.

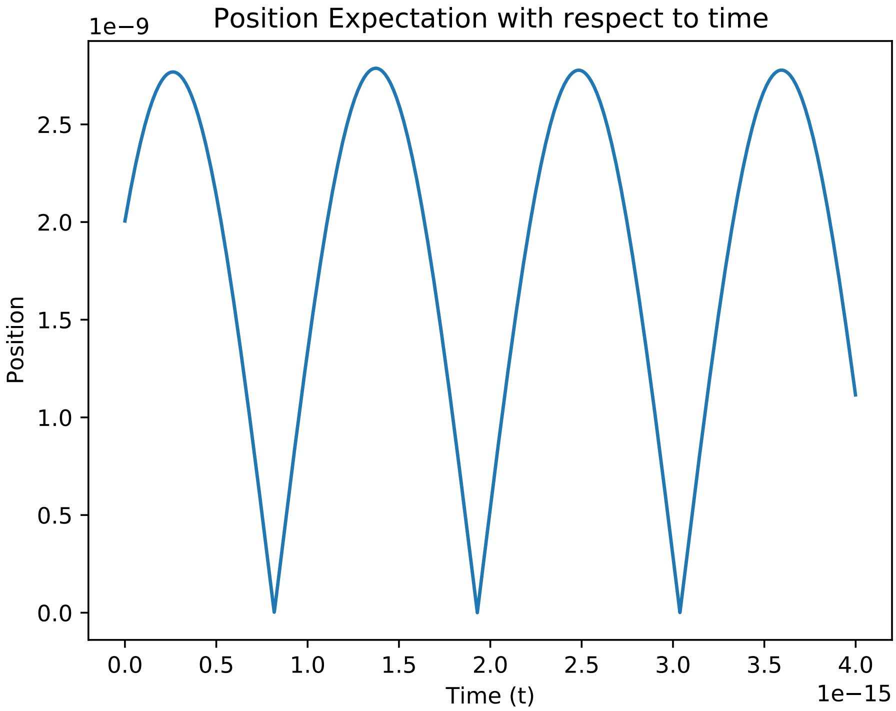


Figure 6: The expectation of position shows oscillatory behaviour as one would expect from a classical harmonic oscillator.

(d) Here we are asked to repeat steps (b) and (c) using a new quantum double well potential.

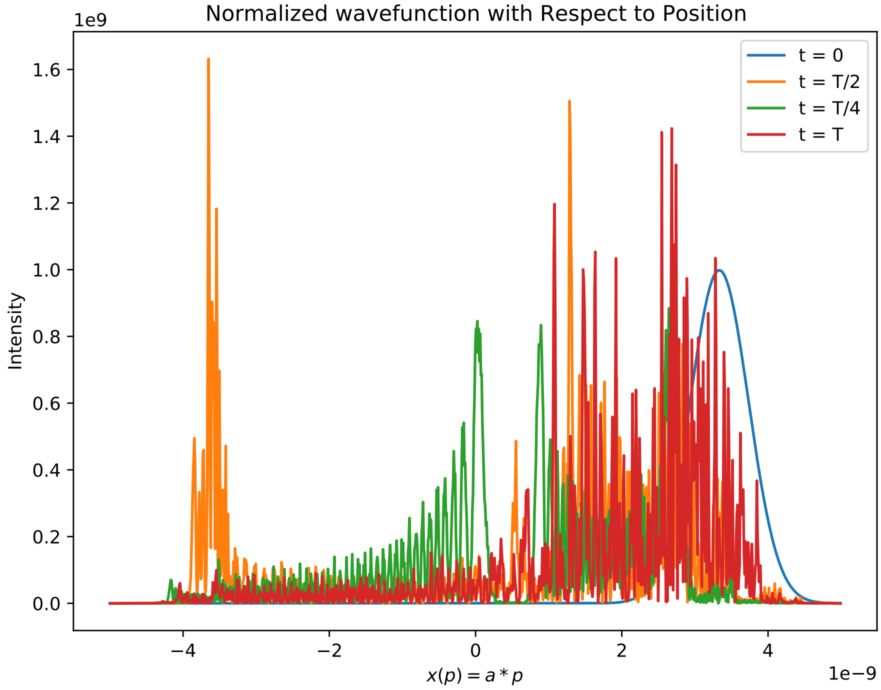


Figure 7: The plot observed here is far messier than the other plots. This is due to the nature of the double well. As psi bounces and tunnels through each well we observe different behaviours adding more and more noise to the final solution.

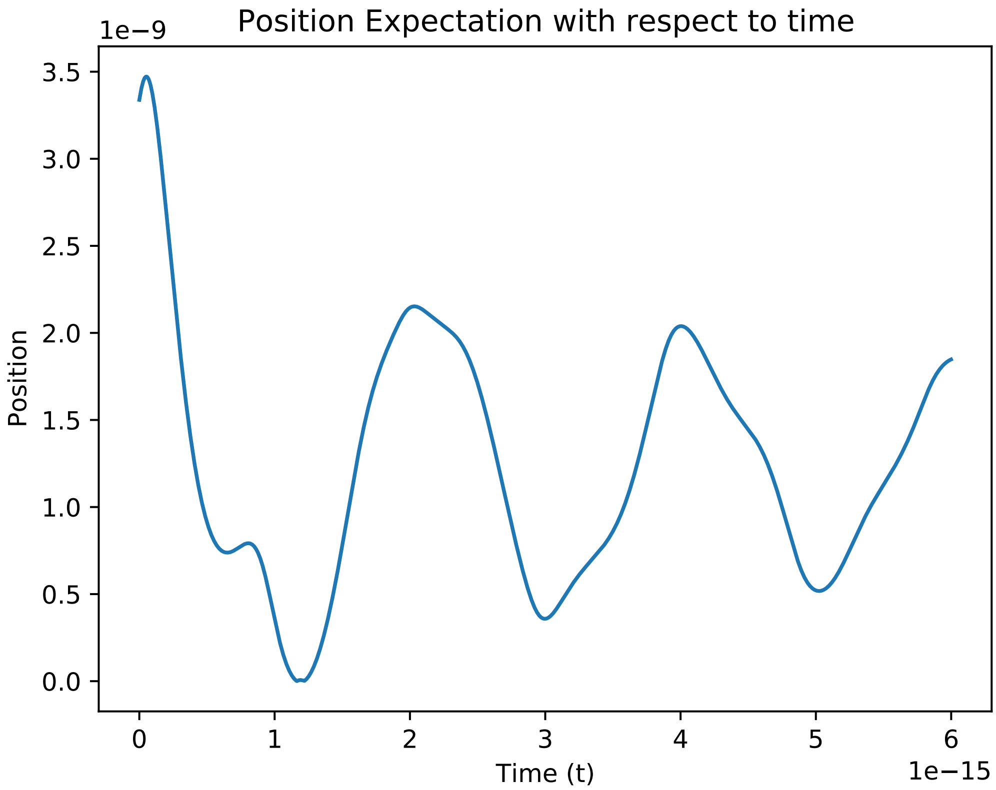


Figure 8: The expectation of position varies, but, this time we are unable to make predictions about the actual value since we do not know a common analytic solution to a double well potential.

Question 2: $\vec{E}$ and $\vec{B}$ in 2D Resonant Cavity

(a) First, we will explain why the decomposition in eqn.(10) given in the handout satisfies the boundary conditions of E_z, H_x and H_y.

(i) $E_z = 0$ at all the walls (which are located at $x = 0, L_x$ and $y = 0, L_y$).

At $x = 0$ or $y = 0$, either $p = 0$ or $q = 0$ respectively. So, we have at least one sin(0) inside the double summation in eqn. 10(a). Since $\sin(0) = 0$, we get $E_z = 0$ as we are summing over a bunch of zeros.

Similarly, at $x = L_x$ and $y = L_y$, we have $p = P$ and $q = P$ so substituting this into E_z we get:

$$\begin{aligned} E_z &= \sum_{q'=0}^{P}\sum_{p'=0}^{P} \hat{E}^n_{p',q'} \sin\left(\frac{Pp'\pi}{P}\right)\sin\left(\frac{Pq'\pi}{P}\right) \\ &= \sum_{q'=0}^{P}\sum_{p'=0}^{P} \hat{E}^n_{p',q'} \sin(p'\pi)\sin(q'\pi) \\ &= 0 \qquad\qquad (\text{as } \sin(k\pi) = 0, k \in \mathbf{Z}) \end{aligned}$$

(ii) $H_x = \partial_x H_y = 0$ at $x = 0, L_x$

At $x = 0$ we have, $p = 0$ and at $x = L_x$ we have, $p = P$ so, $\sin\left(\frac{pp'\pi}{P}\right)$ inside the summation of eqn.(10b) equals to 0 in both the cases as in part (i). Hence, $H_x = 0$ at $x = 0, L_x$.

(iii) $H_y = \partial_y H_x = 0$ at $y = 0, L_y$

Similarly as in part(ii), at $y = 0$ we have, $q = 0$ and at $y = L_y$ we have, $q = P$ so, $\sin\left(\frac{qq'\pi}{P}\right)$ inside the summation of eqn.(10c) equals to 0 in both the cases. Hence, $H_y = 0$ at $y = 0, L_y$.

(b) In this section, we implement the code to compute the electric and magnetic fields by following the routine suggested in the handout. The functions to compute the 2D Fourier transforms (and their inverses) for eqns.(10) are given in `lab09_Q2_functions.py` file and the routine to compute the fields and plot the traces for part c, d and e are given in `lab09_Q2.py` file.

(c) In this section, we use the driving frequency $\omega = 3.75$ to evolve the fields over time, then plot the traces $H_x(x = 0.5, y = 0), H_y(x = 0, y = 0.5)$ and $E_z(x = 0.5, y = 0.5)$ as a function of time by using the code from part (b). The plot is visualized below:

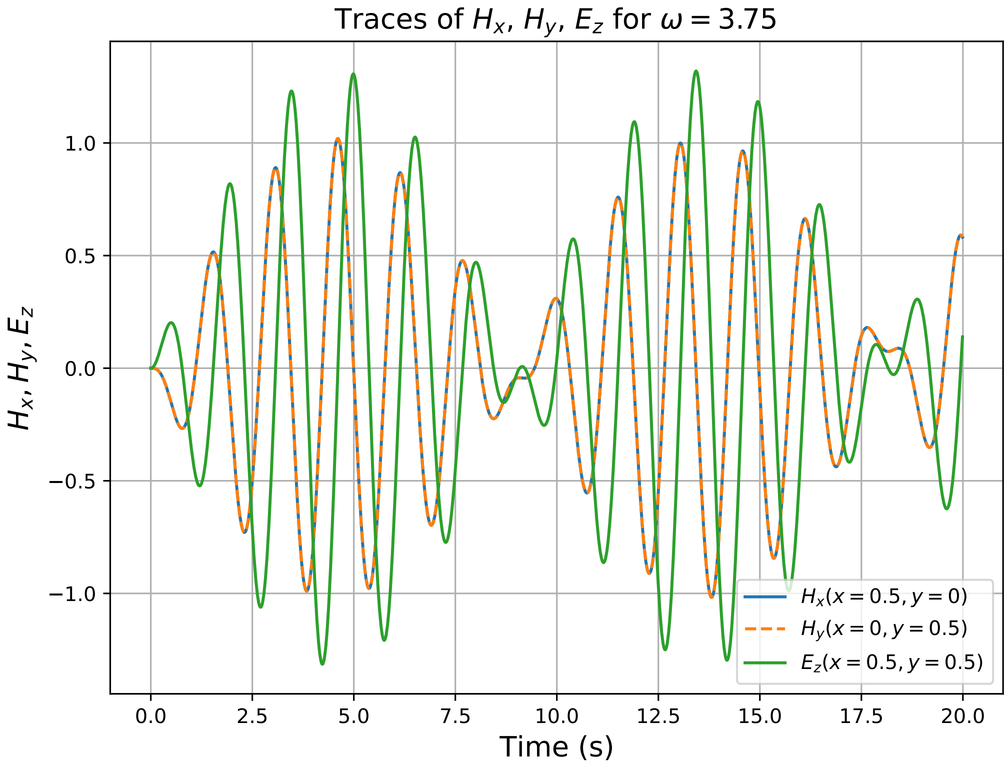


Figure 9: The plot showing the traces $H_x(x = 0.5, y = 0), H_y(x = 0, y = 0.5)$ and $E_z(x = 0.5, y = 0.5)$ as a function of time with driving frequency $\omega = 3.75$.

In fig. 9 we can see that the pattern of the formed traces resembles two interference patterns where one part oscillates at the driving frequency $\omega = 3.75$ and the other oscillates at the normal frequency $\omega_0^{1,1} \approx 4.44$ of the cavity. Since, the driving frequency is different from the natural frequency of the cavity, no resonance occurs.

(d) Now, we repeat the first question by allowing the driving frequency to uniformly vary between $\omega = 0$ to $\omega = 9$ and plot the maximum amplitude of $E_z(x = 0.5, y = 0.5, t)$ as a function of ω. This plot along with a plot of vertical line at normal frequency given by eqn.(21) is shown below:

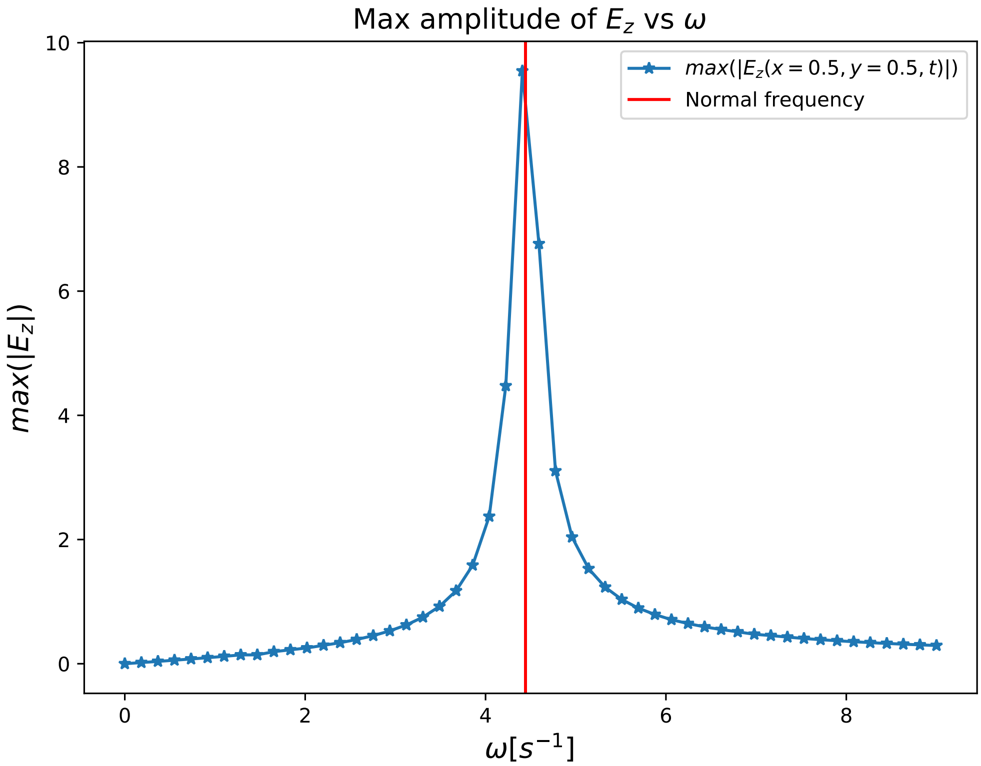


Figure 10: The plot showing the maximum amplitude of $E_z(x = 0.5, y = 0.5, t)$ as a function of ω which varies uniformly between $\omega = 0$ to $\omega = 9$.

The amplitude peaks at approximately 4.4. The normal frequency, $\omega_0^{1,1} \approx 4.44$ as given by eqn.21 where $m = n = 1$ in our setup. This approximately matches the frequency at which the amplitude peaks as shown in fig. 10.

(e) Finally, we take $\omega = \omega_0^{1,1}$ and plot $H_x(x = 0.5, y = 0), H_y(x = 0, y = 0.5)$ and $E_z(x = 0.5, y = 0.5)$ as a function of time. The plot is given below:

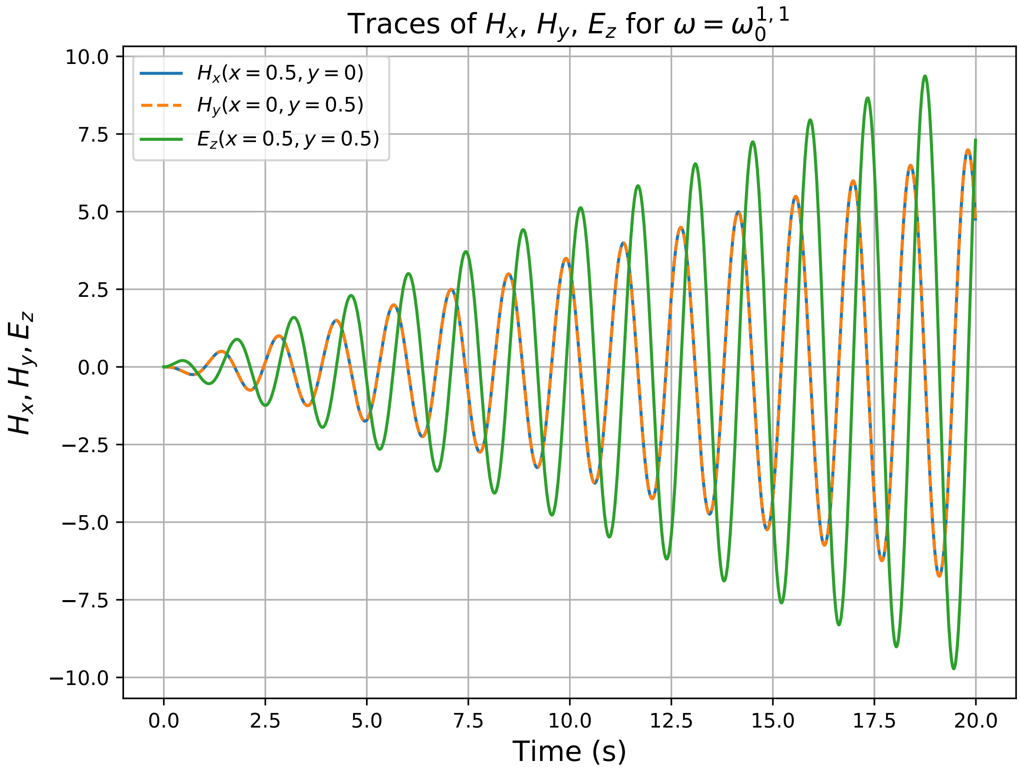


Figure 11: The plot showing the traces $H_x(x = 0.5, y = 0), H_y(x = 0, y = 0.5)$ and $E_z(x = 0.5, y = 0.5)$ as a function of time with driving frequency $\omega = \omega_0^{1,1}$.

In fig. 11 we see that the traces are represented by waves whose amplitude increases with increasing time. Here, the driving frequency matches the normal frequency (unlike in part c) of the cavity resulting in the resonance. The energy in the cavity is ever increasing as seen from fig. 11.