PHY407 Lab-09 Report

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[1] *Q2 - Simulating Resonant EM Cavity*
[2] *Q1 - Time Dependent Schrodinger Equation*

1. Q1 - TIME-DEPENDENT SCHRÖDINGER EQUATION

For the python code containing the functions used to solve the 1D time-dependent Schrödinger Equation, please refer to the file title `Lab09_Q1.py`

1.1. *Q1a - Crank-Nicolson method*

For this exercise, we first defined the (discretized) potential function, in this case an infinite potential well, which is defined as:

$$V_p(x) = \begin{cases} 0, & -\frac{L}{2} < x_p < \frac{L}{2} \\ \infty, & x < -\frac{L}{2}, x_p > \frac{L}{2} \end{cases} \tag{1}$$

where $L = 10^{-8}$ m is the width of our potential well, $p \in \{1, ..., P-1\}$ for $P = 1024$, $a = \frac{L}{P}$ is the discretized separation, $x_p = pa - \frac{L}{2}$ is the discretized positions we will used for the rest of this exercise.

Based on this discretized potential function, we defined the discretized Hamiltonian:

$$\mathbf{H}_D = \begin{bmatrix} B_1 & A & 0 & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ A & B_2 & A & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & A & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & A & B_{p-1} & A & 0 & \dots & \dots & \dots & \dots \\ \dots & \dots & 0 & A & B_p & A & 0 & \dots & \dots & \dots \\ \dots & \dots & \dots & 0 & A & B_{p+1} & A & 0 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & A & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & A & B_{P-2} & A \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & A & B_{P-1} \end{bmatrix} \tag{2}$$

where $A = -\frac{\hbar}{2m_e a}$, $B_p = V(x_p) - 2A$, and m_e is the electron mass.

Given the initial condition, we defined the initial (unnormalized) discretized wave function as:

$$\tilde{\Psi}(x_p, t=0) = \begin{pmatrix} \tilde{\Psi}_1(t=0) \\ \vdots \\ \tilde{\Psi}_{P-1}(t=0) \end{pmatrix} = \exp\left\{ -\frac{(x_p - x_0)^2}{4\sigma^2} + i\kappa x_p \right\} \tag{3}$$

where $x_0 = \frac{L}{5}$, $\sigma = \frac{L}{25}$, $\kappa = \frac{500}{L}$ is given. Next, we normalized the initial wavefunction by calculating

$$C = \int_{-\infty}^{\infty} \tilde{\Psi}^*(x, 0)\tilde{\Psi}(x, p)dx \tag{4}$$

and equate the normalized discretized wavefunction as

$$\Psi(x_p, t=0) = \frac{1}{\sqrt{C}}\tilde{\Psi}(x_p, t=0) \tag{5}$$

After which, we defined a time array to loop-over, with time-step $\tau = 10^{-18}$ s to be integrated for $N = 3000$ steps. From this, we can define the matrices needed for Crank-Nicolson needed to solve the linear system of equations:

$$\mathbf{L} = (\mathbf{I}_{P-1} + i\frac{\tau}{2\hbar}\mathbf{H}_D) \tag{6}$$

$$\mathbf{R} = (\mathbf{I}_{P-1} - i\frac{\tau}{2\hbar}\mathbf{H}_D) \tag{7}$$

where $\mathbf{I}_{P-1}$ is the identity matrix of size $P-1$. Finally, for each time step n, we can solve the next time step $n+1$ with:

$$\Psi^{n+1} = \mathbf{L}^{-1}\mathbf{R}\Psi^n \tag{8}$$

1.2. *Q1b - Wave Packet and Expectation value of Position*

By implementing the method described in part (a), we integrated and solve the Schrödinger equation of an electron in an infinte potential well from $t = 0$ s to $t = T = 3 \times 10^{-15}$ s for 3000 steps. We plotted the (real part of) the wave packet of the electron at $t = 0, \frac{T}{4}, \frac{T}{2}, \frac{3T}{4}, T$ in the following figure.

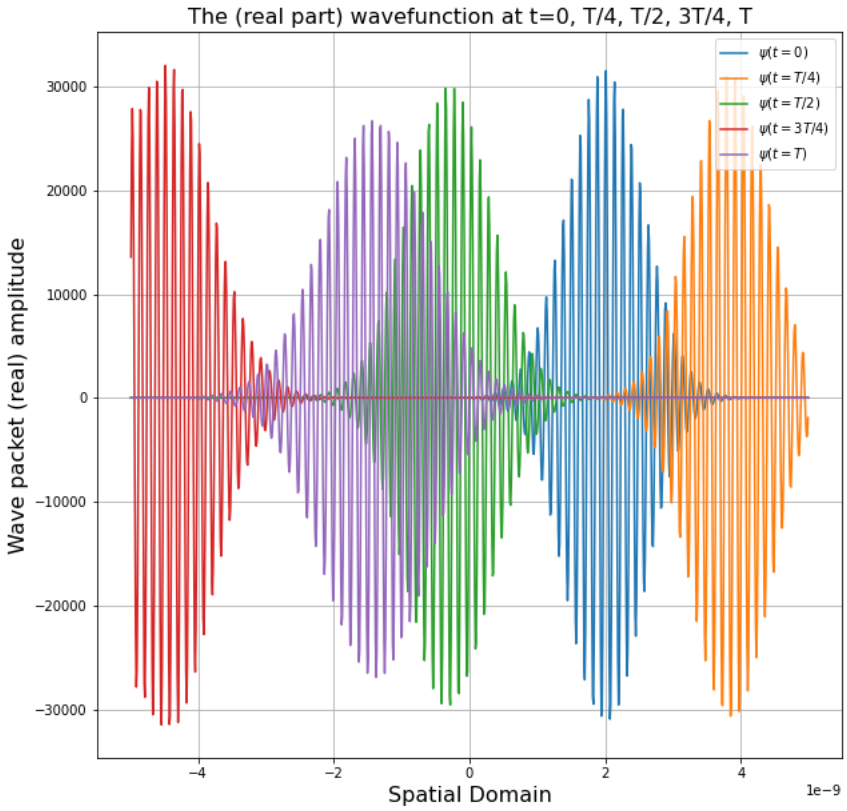

Figure 1: The electron wave packet in the infinite potential well (within $(-\frac{L}{2}, \frac{L}{2})$) as a function of time. The blue packet represents the initial state at $t = 0$; the orange packet represents the state at $t = \frac{T}{4}$; the green packet represents the state at $t = \frac{T}{2}$; the red packet represents the state at $t = \frac{3T}{4}$; the purple packet represents the state at $t = T$.

Subsequently, we calculated the position expectation value as a function of time using the integral:

$$\langle X \rangle(t) = \int_{-\infty}^{\infty} \Psi^*(x,t) x \Psi(x,t) dx \tag{9}$$

where in the program we simply used Simpson's method to evaluate the integral from $-\frac{L}{2}$ to $\frac{L}{2}$ (since $\Psi = 0$ inside the wall anyway). We then obtained the following graph:

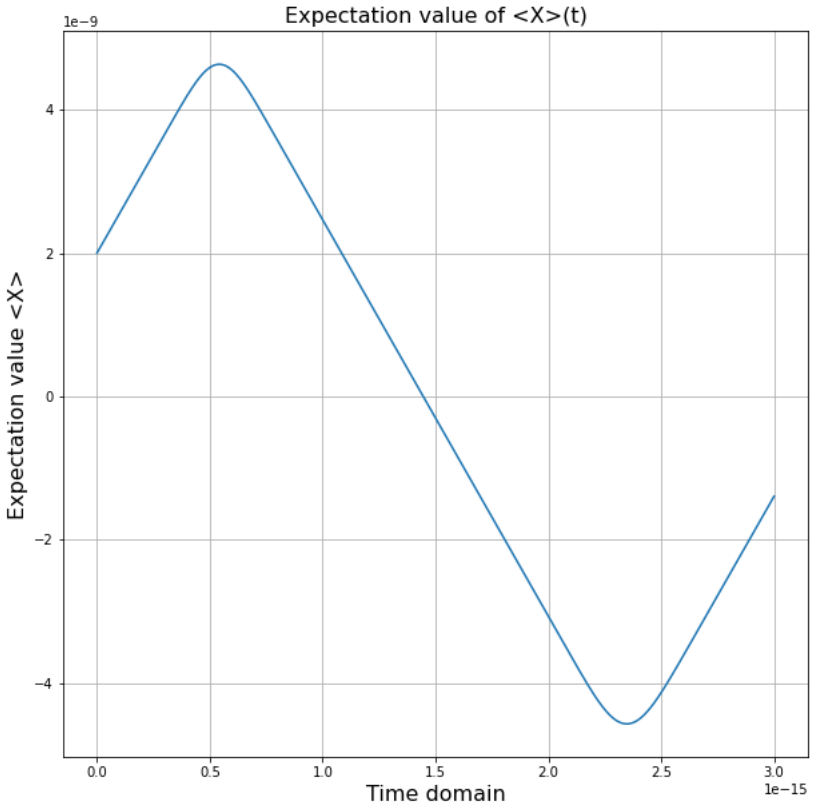

Figure 2: The "trajectory" or mean position value of the electron in the potential well as a funciton of time

From Figure 5 and 2 we can see that the wavepacket first moves to the right and hit the wall at around $t = \frac{T}{2}$ and bounces back to the left, and again hit the wall on the left at around $t = \frac{3T}{4}$ and bounces to the right. We can also see that the wave packet becomes more disperse over time.

1.3. *Q1c - Energy and Normalization Validation*

In order to validate our code, we calculated the energy in the system to check if it stays as constant over time using the integral:

$$E(t) = \int_{-\infty}^{\infty} \Psi^*(x,t)\mathbf{H}_D\Psi(x,t)dx \tag{10}$$

where the integrand is a scalar that sums up the value at each discretized points p, so the integral simply just becomes integrad $*a$. We also calculate the normalization condition

$$C = \int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx \tag{11}$$

at each time step to ensure it equals to 1. These 2 quantities are plotted in the graph below.

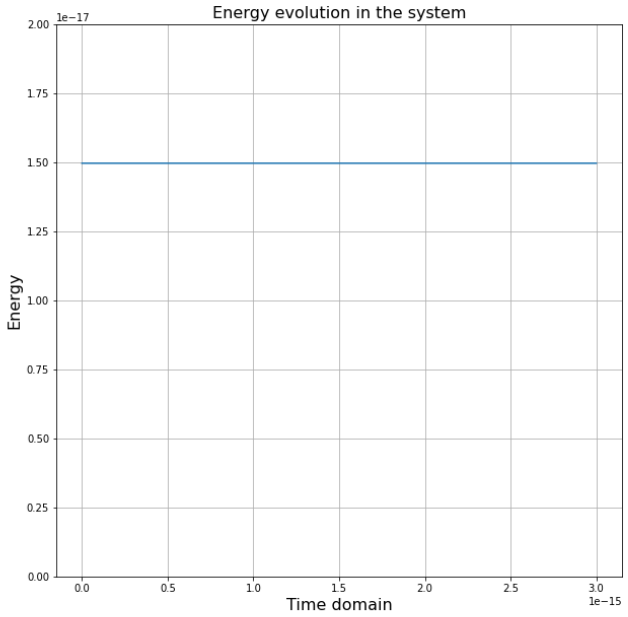

Figure 3: The expected energy value in the electron wave packet as a function of time. As we can see, energy remains constant over the numerical integration.

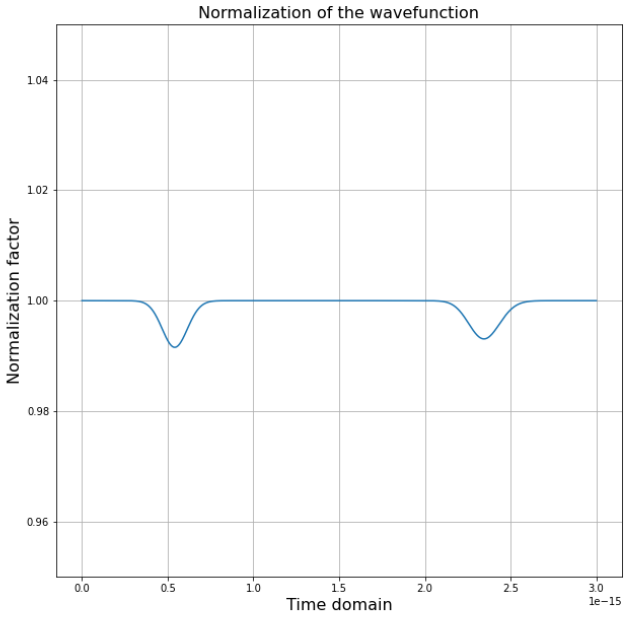

Figure 4: The normalization quantity in Eq.11 over the numerical integration. As we can see, it equals to 1 at most of the time, except there are 2 bumps that corresponds to when the wave packet hit the potential wall and is bouncing back, where the numerical derivation isn't perfect as expected.

2. Q2 - SIMULATING RESONANT EM CAVITY

For the python code containing the spectral method used to solve the PDE's of this system please refer to the python script titled `Lab09_Q2.py` Where we also provide an animation of the oscillating E-field.

2.1. *Q2a - Testing 2-Dimensional Fourier Transform Algorithm*

In the spectral method relies heavily on the ability to recover original signals from a function in Fourier-space. Therefore, before we implement the spectral method to solve the resonant EM cavity system we need to test we that we can recover 2-dimensional signals from an inverse Fourier transform. In order to test our 2D Fourier transform algorithm we generated a 2 dimensional Gaussian with mean 0 in x and y and standard deviation of 1 in both x and y directions.

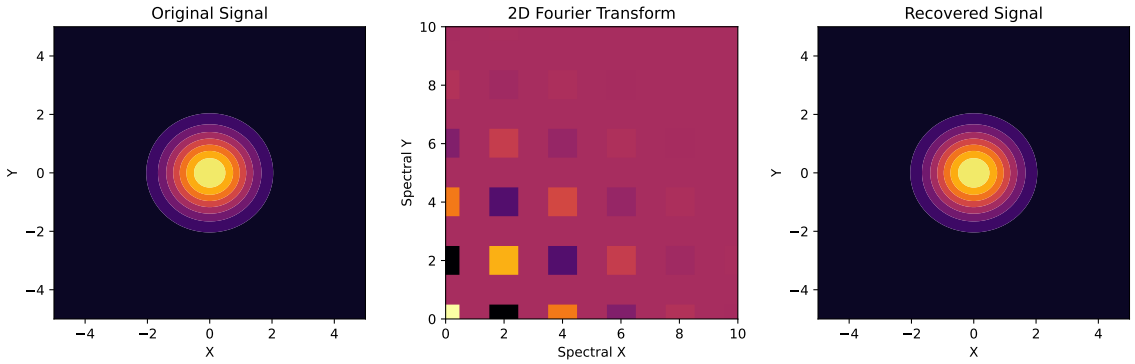

Figure 5: Graphical representation of testing 2-dimensional Fourier transform algorithm, where left most panel is the original Gaussian generated by the program. Middle panel is the same Gaussian function represented in Fourier space. Right-most panel is the recovered Gaussian through an inverse 2D Fourier on the middle panel. The residuals between the original and recovered function were of order $10^{-18} - 10^{-19}$ which is smaller than machine precision which implies the signals are numerically identical

For the print-out of the residuals between the original Gaussian and the recovered one please refer to the python script `Lab09_Q2.py`. Now that we have the 2D Fourier algorithm working we can continue to solve the resonant EM cavity system.

2.2. *Q2b - Simulating System Through Spectral Method*

We can express the electric field and magnetic fields within an cavity through Maxwell's equation where $H_x = cB_x$ and $H_y = -cB_y$ are representative of the magnetic field by a factor of c and we describe the electric current density as $J_z = -\mu_0 c^2 j_z$

$$\begin{aligned} \frac{\partial H_x}{\partial t} + c\frac{\partial E_z}{\partial y} &= 0 \\ \frac{\partial H_y}{\partial t} + c\frac{\partial E_z}{\partial x} &= 0 \\ \frac{\partial E_z}{\partial t} + c\frac{\partial H_y}{\partial x} + c\frac{\partial H_x}{\partial y} &= J_z \end{aligned} \tag{12}$$

Where we drive the current density through the following analyical expression.

$$J_z(x, y, t) = J_0 \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi y}{L_y}\right) \sin(\omega t) \tag{13}$$

The boundary conditions of this system are that the tangential electric field and the normal magnetic field must be zero at the conducting walls. These boundary conditions can be satisfied explicitly by using the Fourier transforms

that allow for zeros at the boundaries as follows.

$$(E_z)^n_{p,q} = \sum_{q'=0}^{P}\sum_{p'=0}^{P} \hat{E}^n_{p',q'} \sin\left(\frac{pp'\pi}{P}\right)\sin\left(\frac{q'q\pi}{P}\right) \tag{14}$$

$$(H_x)^n_{p,q} = \sum_{q'=0}^{P}\sum_{p'=0}^{P} \hat{X}^n_{p',q'} \sin\left(\frac{pp'\pi}{P}\right)\cos\left(\frac{q'q\pi}{P}\right) \tag{15}$$

$$(H_y)^n_{p,q} = \sum_{q'=0}^{P}\sum_{p'=0}^{P} \hat{Y}^n_{p',q'} \cos\left(\frac{pp'\pi}{P}\right)\sin\left(\frac{q'q\pi}{P}\right) \tag{16}$$

$$(J_z)^n_{p,q} = \sum_{q'=0}^{P}\sum_{p'=0}^{P} \hat{J}^n_{p',q'} \sin\left(\frac{pp'\pi}{P}\right)\sin\left(\frac{q'q\pi}{P}\right) \tag{17}$$

With these Fourier transforms we are insuring the solutions zero where we want them to zero. Taking $m = n = J_0 = L_x = L_y = 1$, $P = 32$ is the total number of spatial grids, $T = 20\,\mathrm{s}$ is the total time of the simulation $\Delta t = 0.01$ is the time step and the driving angular frequency is $\omega = 3.75$. We can solve for the z-component of the electric field and the x,y components of H.

The spectral procedure is as follows, discretize x, y and t given by the specifications of the problem, then we define $J_z(x, y, t)$ for all x and y at all later times. With these data cube created we can take its Fourier transform by noting the symmetry over x and y as stated in eq.17. Then we define the H_x, H_y, and E_z through the initial conditions and then take their Fourier transform at $t = 0$. Then once we have these inital states we can evolve them through the Crank-Nicolson scheme

$$\hat{E}^{n+1}_{p,q} = \frac{(1 - p^2D_x^2 - q^2D_y^2)\hat{E}^n_{p,q} + 2qD_y\hat{X}^n_{p,q} + 2pD_x\hat{Y}^n_{p,q} + \Delta t\hat{J}^n_{p,q}}{1 + p^2D_x^2 + q^2D_y^2} \tag{18}$$

$$\hat{X}^{n+1}_{p,q} = \hat{X}^n_{p,q} - qD_y(\hat{E}^{n+1}_{p,q} + \hat{E}^n_{p,q}) \tag{19}$$

$$\hat{Y}^{n+1}_{p,q} = \hat{Y}^n_{p,q} - qD_x(\hat{E}^{n+1}_{p,q} + \hat{E}^n_{p,q}) \tag{20}$$

Once we have the time evolution of these quantities in Fourier space we can recover the solution for E_z, H_x, and H_y by taking their inverse Fourier's by noting the symmetries in eq.14 to eq.17. Now we can look at traces of $H_x(x = 0.5, y = 0, t)$ which is the magnetic field mid-way through the boundary along the x-axis. Similarly, we look at the traces for $H_y(x = 0, y = 0.5, t)$ and $E_z(x = 0.5, y = 0.5, t)$. The results in Figure 6 are consistent with the

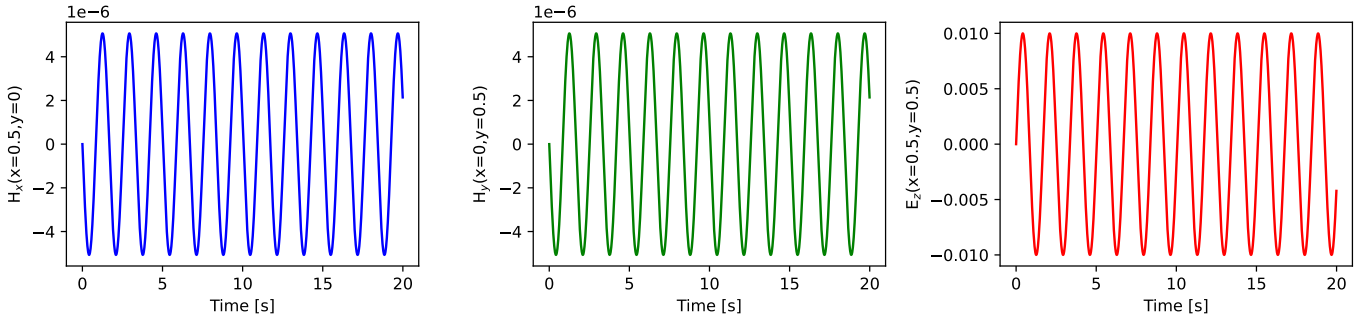

Figure 6: Left-most figure and center figure represent the oscillating magnetic fields midway through the boundary of the cavity. The right-most figure represents the oscillating electric field at the center of the cavity. We notice a phase difference of $\pi/2$ which what we expect the phase difference between the electric and magnetic fields to be.

animations of the electric and magnetic field where we see the field oscillate with respect to different positions within the cavity.

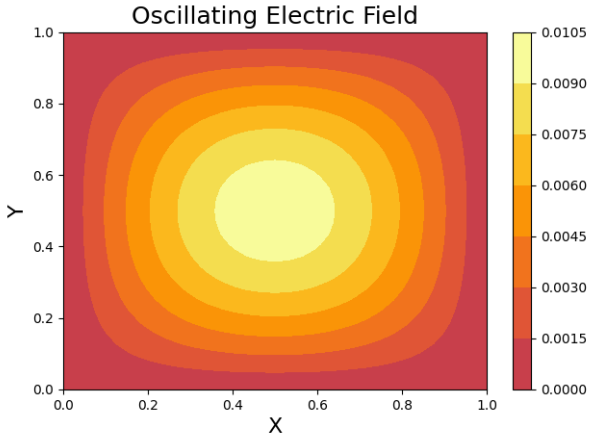

Figure 7: Electric field induced by driven current density. We see solution satisfies boundary conditions for the dimensions of the cavity.

2.3. *Q2c - Physical Interpretation*

The patterns in Figure 6 show oscillatory behaviour of the two fields which appear to be off phase. This makes sense because a changing electric field induces an magnetic field. Snippets of the simulations are shown in Figure 7

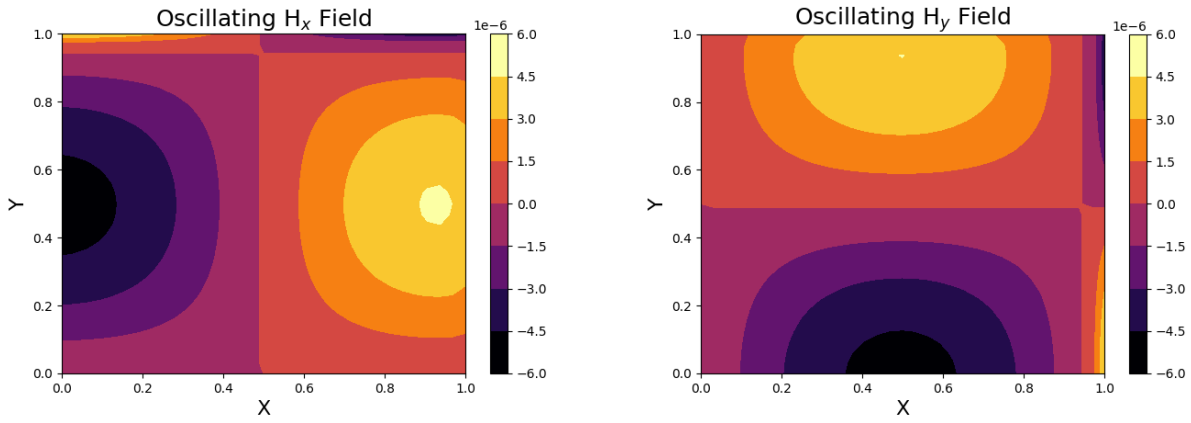

Figure 8: Left-most figure is the x-component of the scaled magnetic field. Right-most figure is the y-component of the scaled magnetic field. We see that both solutions satisfy the boundary conditions.

We see that the osciallating current density induces an osciallting electric field which in turn also induces an oscillating magnetic field. The animation indicate that these oscillation occur on a Gaussian-like object which oscillate from positive to negative values.