

PHY407 Lab-09 ReportRAINA IRONS¹¹ Wrote and solved Q1, Q2**QUESTION 1 - TIME-DEPENDENT SCHRODINGER EQUATION**

Consider a particle in an infinite square well of length $L = 10^{-8}\text{m}$ with mass $m_e = 9.109 \times 10^{-31}\text{kg}$. We will construct initial condition

$$\psi(x, t = 0) = \psi_0 e^{-\frac{(x-x_0)^2}{4\sigma^2} + ikx} \quad (1)$$

With $\sigma = L/25$, $\kappa = 500/L$, $x_0 = L/5$. Note that this initial condition follows a Gaussian, and we should expect such shape when plotting.

PART (A)

The Crank-Nicholson method follows an intermediate point of the FTCS method and implicit equation. Combining the two equations through an average, the Crank-Nicholson method for the Schrodinger equation is,

$$\psi(x, t + \tau) - \tau \frac{i\hbar}{4ma^2} [\psi(x+a, t + \tau) + \psi(x-a, t + \tau) - 2\psi(x, t + \tau)] = \psi(x, t) + \tau \frac{i\hbar}{4ma^2} [\psi(x+a, t) + \psi(x-a, t) - 2\psi(x, t)] \quad (2)$$

This can be written in vector notation as,

$$\vec{A}\psi(x, t + \tau) = \vec{B}\psi(t) \quad (3)$$

The discretized Hamiltonian can be broken into two matrices (following Ex.9 in the textbook) A and B .

$$\vec{A} = \begin{pmatrix} a_1 & a_2 & 0 & 0 & \dots \\ a_2 & a_1 & a_2 & 0 & \dots \\ 0 & a_2 & a_2 & a_1 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \quad \vec{B} = \begin{pmatrix} b_1 & b_2 & 0 & 0 & \dots \\ b_2 & b_1 & b_2 & 0 & \dots \\ 0 & b_2 & b_2 & b_1 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \quad (4)$$

Where \vec{A}, \vec{B} are tri-diagonal matrices with

$$a_1 = 1 + \tau \frac{i\hbar}{2ma^2} \quad a_2 = -\tau \frac{i\hbar}{4ma^2} \quad b_1 = 1 - \tau \frac{i\hbar}{2ma^2} \quad b_2 = \tau \frac{i\hbar}{4ma^2} \quad (5)$$

We solve the equation

$$\vec{\mathbf{v}} = \vec{B}\psi \quad (6)$$

In Equation 3, then solve the linear system $\vec{A}\vec{x} = \vec{\mathbf{v}}$. We can then loop over this method in time for the specified interval.

PART (B)

Looping over the time interval from our initial condition of the wave-function, we get the Figure 1 for various time intervals in the well.

PART (C)

We can see at a glance these wave-functions do not appear to be normalized, as the combinations of the heights and widths do not appear to integrate to one. I was not able to get the normalization factor (my own fault), but a segment in the textbook argues that the linearity of the wave-function causes the normalization constant to be canceled out on both sides of the equation and plays no part in the solution (pg. 451).

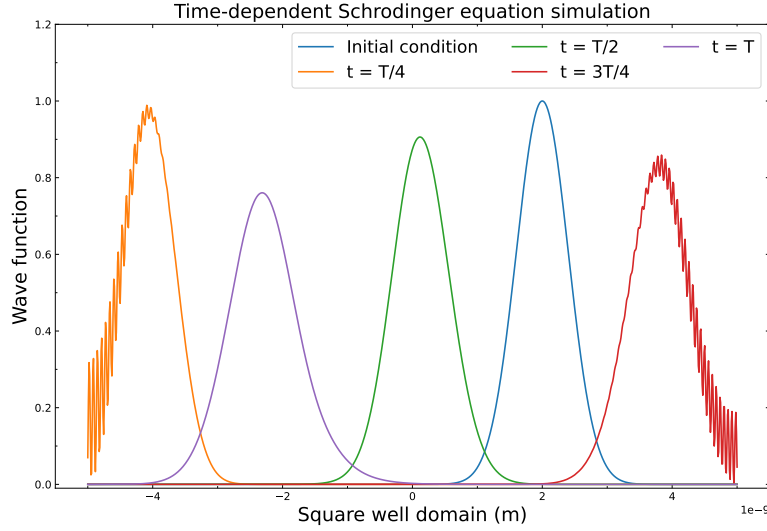


Figure 1: The initial condition on our wave-function has a Gaussian shape, and "bounces" off the right wall of the well and travels back towards the right.

QUESTION 2 - RESONANT EM CAVITY

We have a two-dimensional resonance cavity with conducting walls of size $L_x \times L_y$. We excite the cavity with a z

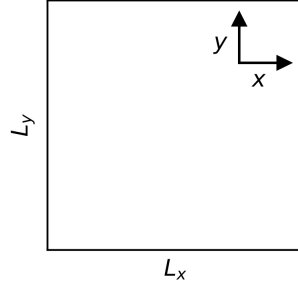


Figure 2: Two-dimensional resonance cavity.

directed alternating current of frequency ω . Our goal is to calculate the electric and magnetic field patterns excited within the cavity by the current pattern.

PART (A)

We can test the 2D Fourier transforms and their inverses by transforming a two dimensional array and then recovering it. For this we choose a simple even function, $x^2 + y^2$.

PART (B)

With our Fourier functions working, we can now implement our oscillating current in the z direction in the cavity. We begin with initial conditions $J_z = H_x = H_y = E_z = 0$, where J_z is the current density in the z direction, H are scaled magnetic fields, and E_z is the electric field in the z direction. These electric and magnetic fields follow Maxwell's

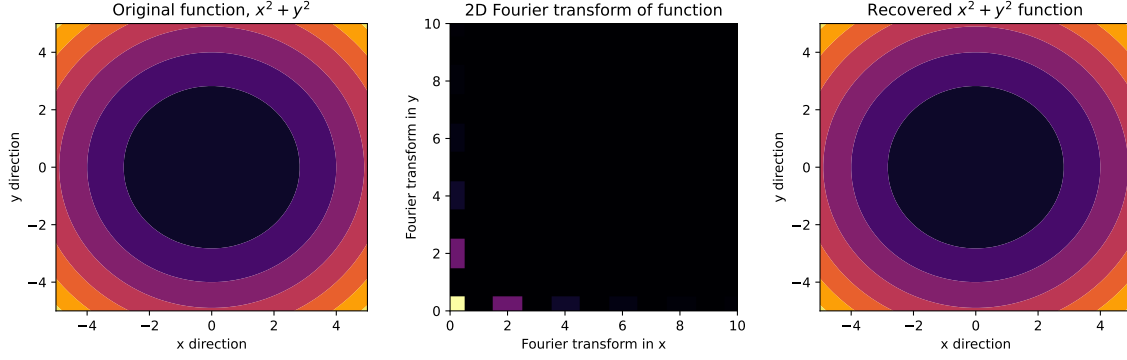


Figure 3: The even function $x^2 + y^2$ function was passed through the Fourier and inverse Fourier transforms to test the validity of our functions.

equations,

$$\begin{aligned} \frac{\partial H_x}{\partial t} + c \frac{\partial E_z}{\partial y} &= 0 \\ \frac{\partial H_y}{\partial t} + c \frac{\partial E_z}{\partial x} &= 0 \\ \frac{\partial E_z}{\partial t} + c \frac{\partial H_y}{\partial x} + c \frac{\partial H_x}{\partial y} &= J_z \end{aligned} \quad (7)$$

Where c is the speed of light, and μ_0 is the vacuum permeability. We use a Fourier transform to simplify the original PDE's for the Crank-Nicholson method.

$$(Ez)p, q^n = \sum q' = 0^P \sum p' = 0^P \hat{E}_{p',q'}^n \sin\left(\frac{pp'\pi}{P}\right) \sin\left(\frac{q'q\pi}{P}\right) \quad (8)$$

$$(Hx)p, q^n = \sum q' = 0^P \sum p' = 0^P \hat{X}_{p',q'}^n \sin\left(\frac{pp'\pi}{P}\right) \cos\left(\frac{q'q\pi}{P}\right) \quad (9)$$

$$(Hy)p, q^n = \sum q' = 0^P \sum p' = 0^P \hat{Y}_{p',q'}^n \cos\left(\frac{pp'\pi}{P}\right) \sin\left(\frac{q'q\pi}{P}\right) \quad (10)$$

$$(Jz)p, q^n = \sum q' = 0^P \sum p' = 0^P \hat{J}_{p',q'}^n \sin\left(\frac{pp'\pi}{P}\right) \sin\left(\frac{q'q\pi}{P}\right) \quad (11)$$

In doing so, we get the following plots for the scaled magnetic field in the x and y direction, as well as the electric field in the z direction.

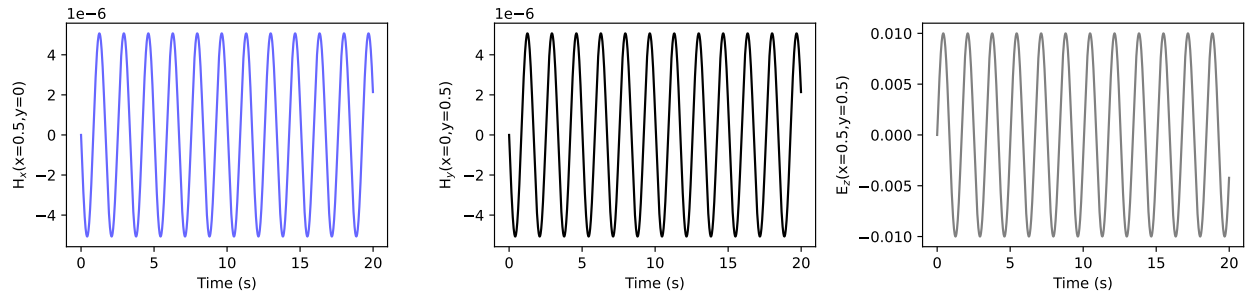


Figure 4: We see each field oscillates over time. The magnetic fields in the x and y direction oscillate in response to the alternating electric field. We see that the two fields are out of phase with one another, which makes physical sense and affirms our plots.

PART (C)

Although it is not obvious how the electric field should behave given the Fourier transformed function, Equations ??, we do get a response that makes physical sense for our magnetic field, which is the response to the changing electric field, for it to be out of phase with the changing E-field.