Quant2D

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1 2D time-dependent Schrödinger equation

$$\hat{H}\psi(x,y,t) = i\hbar\partial_t\psi(x,y,t) \tag{1}$$

In this problem the potential is only function of x and y coordinates, then: $\hat{H} = \frac{\hbar^2}{2m}(\partial_x\psi + \partial_y\psi) + V(x,y)$, and the equation will result as:

$$\frac{\hbar^2}{2m}(\partial_x\psi + \partial_y\psi) + V(x,y) = i\hbar\partial_t\psi(x,y,t) \tag{2}$$

2 Implicit method

Using a 2-point formula for the first time derivative and a 3-point formula for the second space derivatives:

$$\begin{aligned}\partial_t\psi &= \frac{\psi(t+\Delta t) - \psi(t)}{\Delta t} \\ \partial_x\psi &= \frac{\psi(x+\Delta x) - 2\psi(x) + \psi(x-\Delta x)}{(\Delta x)^2}\end{aligned} \tag{3}$$

Now evolving the partial time derivative forward and backward half a step of time for $\psi(t)$ and $\psi(t+\Delta t)$ respectively and equalizing the $\psi(t+\frac{\Delta t}{2})$ terms:

$$(1 + \frac{\Delta t}{2\hbar}i\hat{H})\psi_{i,j}^{k+1} = (1 - \frac{\Delta t}{2\hbar}i\hat{H})\psi_{i,j}^{k} \tag{4}$$

Where $\psi_{i,j}^k = \psi(x_i, y_j, t_k)$.

Other way to express it might be:

$$\hat{A}\psi_{i,j}^{k+1} = \hat{B}\psi_{i,j}^{k} = \overline{\psi}_{i,j}^{k} \tag{5}$$

Where $\hat{A}$ and $\hat{B}$ are two tridiagonal matrices and being $\psi_{i,j}^k$ the wave function at the current time and $\psi_{i,j}^{k+1}$ the wave function after one step of time.

As $\hat{A}$ and $\hat{B}$ are tridiagonal they can be defined using their three diagonals:

$$\hat{A} = \begin{cases} A_{sup} = r \\ A_{diag} = 1 - 4r + \frac{idt}{2\hbar}V(x,y) \\ A_{inf} = r \end{cases}$$

$$\hat{B} = \begin{cases} B_{sup} = -r \\ B_{diag} = 1 + 4r - \frac{idt}{2\hbar}V(x,y) \\ B_{inf} = -r \end{cases}$$

Both deduced from (3) and (4).

The solution $\psi_{i,j}^{k+1}$ is found using the tridiagonal matrix algorithm or Thomas algorithm. As this algorithm was made to solve a tridiagonal system of equations and in this specific problem $\overline{\psi}$ is matrix-shaped, first will evolve for x and then for y.

3 Some results for now

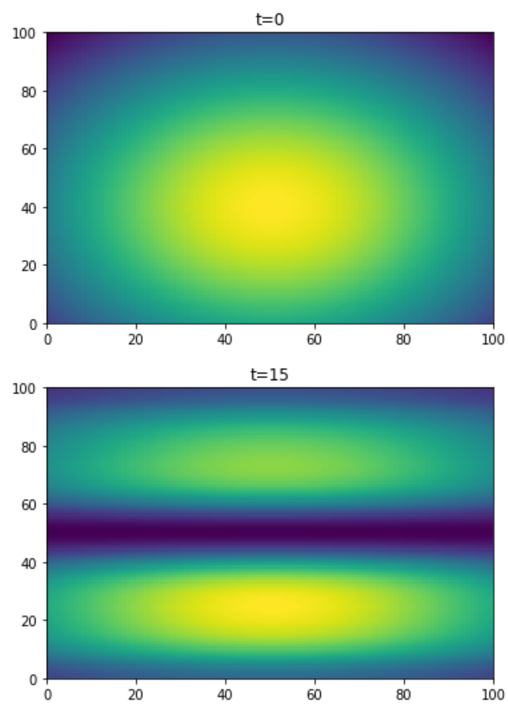

Figure 1: Sample of tunneling effect

Figure generated using a Gaussian distribution centered at $(\frac{2L}{5}, \frac{L}{2})$ with a potential barrier through $x = \frac{L}{2}$. The first picture is the initial density of probability that comes from the initial wave function. The picture below is the representation of this same system after 15 units of time. This sample has been made being $\Delta t = 0.15$ the time step and $\Delta x = 0.1$ the space step. The last picture is the system after 100 time iterations.