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