Time Evolution of a 2D Gaussian Wave Packet

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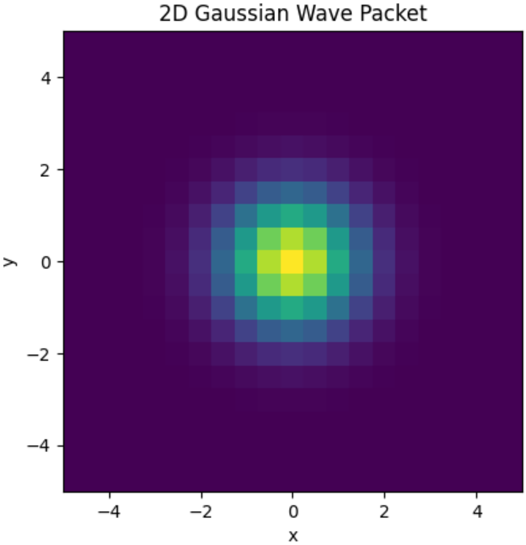
2D Gaussian Wave Packet

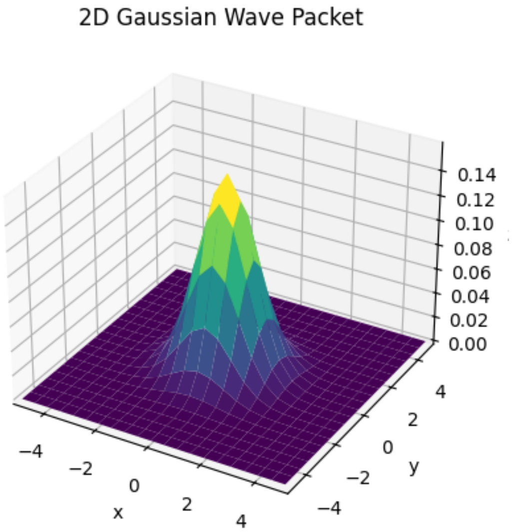
$$\Psi(x, y, t) = A \exp\left[-\frac{1}{2\sigma_x^2}(x - x_0)^2 - \frac{1}{2\sigma_y^2}(y - y_0)^2 + i(k_x x + k_y y - \omega t)\right]$$

- Parameters: σ_x, σ_y, x_0, y_0, k_x, k_y.
- Discretization. $\delta x, \delta t = 0.5, 0.5$

Plots at $t = 0$



Plots at $t = 0$


2D Gaussian Wave Packet
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
−4
−2
0
2
4
x
−4
−2
0
2
4
y

Schroedinger Equation in two dimensions

$$i\frac{\partial\psi(x,y,t)}{\partial t} = -\nabla^2\psi(x,y,t) + V(x,y,t)\,\psi(x,y,t)\,.$$

- Choice of Potential : Infinite square well, parabolic potential

Parabolic Potential

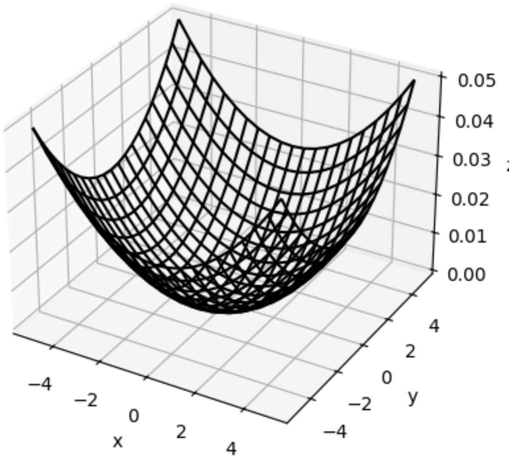


Figure: Time evolution of the 2D Gaussian wave packet.

Numerical Methods

- Crank-Nicolson Method.
- Finite Difference Method.
- Why these methods for the simulation?

Crank nicholson

Consider the time derivative of ψ as a function of F discretized on the 2D plane.

- Forward euler method: $\frac{\psi_{i,j}^{n+1} - \psi_{i,j}^{n}}{\Delta t} = F_{i,j}^{n}$.
- Backward euler method: $\frac{\psi_{i,j}^{n+1} - \psi_{i,j}^{n}}{\Delta t} = F_{i,j}^{n+1}$.
- $\frac{\psi_{i,j}^{n+1} - \psi_{i,j}^{n}}{\Delta t} = \frac{1}{2}\left[F_{i,j}^{n+1} + F_{i,j}^{n}\right]$.

Crank nicholson

$$\frac{\partial\psi(x,y,t)}{\partial t} = \frac{\psi_{i,j}^{n+1} - \psi_{i,j}^{n}}{\Delta t}$$

$$\frac{\partial^2\psi(x,y,t)}{\partial x^2} = \frac{1}{2(\Delta x)^2}\left[(\psi_{i,j+1}^{n+1} - 2\psi_{i,j}^{n+1} + \psi_{i,j-1}^{n+1}) + (\psi_{i,j+1}^{n} - 2\psi_{i,j}^{n} + \psi_{i,j-1}^{n})\right]$$

$$\frac{\partial^2\psi(x,y,t)}{\partial y^2} = \frac{1}{2(\Delta y)^2}\left[(\psi_{i-1,j}^{n+1} - 2\psi_{i,j}^{n+1} + \psi_{i+1,j}^{n+1}) + (\psi_{i-1,j}^{n} - 2\psi_{i,j}^{n} + \psi_{i+1,j}^{n})\right]$$

$$V(x,y,z)\,\psi(x,y,z) = \frac{1}{2}\left[V_{i,j}^{n+1}\psi_{i,j}^{n+1} + V_{i,j}^{n}\psi_{i,j}^{n}\right]$$

Let $r_x = -\frac{\Delta t}{2i(\Delta x)^2}\ , \quad r_y = -\frac{\Delta t}{2i(\Delta y)^2}\ .$

Crank nicholson

$$-r_y\psi^{n+1}_{i+1,j} - r_y\psi^{n+1}_{i-1,j} + a_{i,j}\psi^{n+1}_{i,j} - r_x\psi^{n+1}_{i,j+1} - r_x\psi^{n+1}_{i,j-1}$$

$$= r_y\psi^{n}_{i+1,j} + r_y\psi^{n}_{i-1,j} + b_{i,j}\psi^{n}_{i,j} + r_x\psi^{n}_{i,j+1} + r_x\psi^{n}_{i,j-1}$$

Switch to matrix form

$$Ax = b$$

.

Crank nicholson

$$
\mathbf{A} \cdot \mathbf{x} = \begin{pmatrix}
a_{00} & -r_x & 0 & 0 & \cdots & 0 & -r_y & 0 & 0 & \cdots \\
0 & & & & & & & & & \\
-r_x & a_{10} & -r_x & 0 & \cdots & & 0 & -r_y & 0 & \cdots \\
0 & & & & & & & & & \\
0 & -r_x & a_{20} & -r_x & & & & & -r_y & \\
0 & 0 & -r_x & \ddots & \ddots & & & & & \ddots \\
\vdots & \vdots & & \ddots & & & & & & \\
0 & & & & & & & & & \\
-r_y & 0 & & & & & & & & \\
0 & -r_y & & & & & & & & \\
0 & 0 & -r_y & & & & & & & \ddots \\
\vdots & \vdots & & \ddots & & & & & \ddots & \ddots \\
-r_x & & & & & & & & & \\
0 & 0 & & & & & & & & -r_x \\
a_{(N-1),(N-1)} & & & & & & & & &
\end{pmatrix}
\begin{pmatrix}
\psi_{0,0}^{n+1} \\
\psi_{1,0}^{n+1} \\
\psi_{2,0}^{n+1} \\
\vdots \\
\psi_{i,j}^{n+1} \\
\vdots \\
\psi_{(N-1),(N-1)}^{n+1}
\end{pmatrix}.
$$

Crank nicholson

$$
\mathbf{b} = \begin{pmatrix}
b_0 & r_x & 0 & 0 & \cdots & 0 & r_y & 0 & 0 & \cdots \\
0 \\
r_x & b_1 & r_x & 0 & \cdots & & 0 & r_y & 0 & \cdots \\
0 \\
0 & r_x & b_2 & r_x & & & & & r_y & \\
0 & 0 & r_x & \ddots & \ddots & & & & & \ddots \\
\vdots & \vdots & & \ddots & & & & & & \\
0 & & & & & & & & & \\
r_y & 0 & & & & & & & & \\
0 & r_y & & & & & & & & \\
0 & 0 & r_y & & & & & & & \ddots \\
\vdots & \vdots & & \ddots & & & & & \ddots & \ddots \\
r_x \\
0 & 0 & & & & & & & & r_x \\
b_{(N-3)(N-1)}
\end{pmatrix}
\begin{pmatrix}
\psi_0^n \\ \psi_1^n \\ \psi_2^n \\ \vdots \\ \psi_k^n \\ \vdots \\ \psi_{(N-3)(N-1)}^n
\end{pmatrix}
$$

Finite difference algorithm

Time evolution operator : $\psi(t+\Delta t) = U(\Delta t)\psi(t)$ where $U(\Delta t) = e^{-i\tilde{H}\Delta t}$.
So, $\psi_{i,j}^{n+1} = U(\Delta t)\psi_{i,j}^{n}$ and $\psi_{i,j}^{n-1} = U^{-1}(\Delta t)\psi_{i,j}^{n}$ where $U^{-1}(\Delta t) = e^{i\tilde{H}\Delta t}$

$$\psi^{n+1} = \psi^{n-1} + \left[e^{-i\tilde{H}\Delta t} - e^{i\tilde{H}\Delta t}\right]\psi^{n}$$

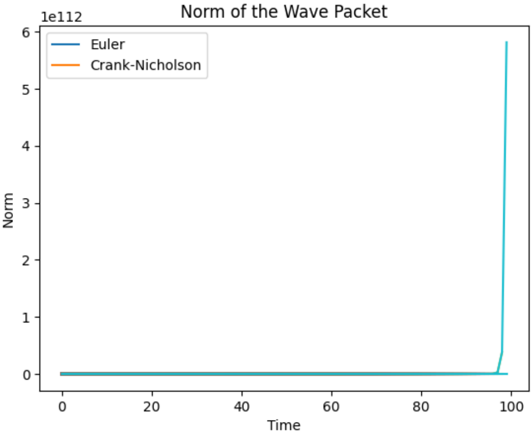
$$\frac{\partial^2\psi}{\partial x^2} \simeq -\frac{1}{2}\left[\psi_{i+1,j}^{n} + \psi_{i-1,j}^{n} - 2\psi_{i,j}^{n}\right]$$

Finite difference algorithm

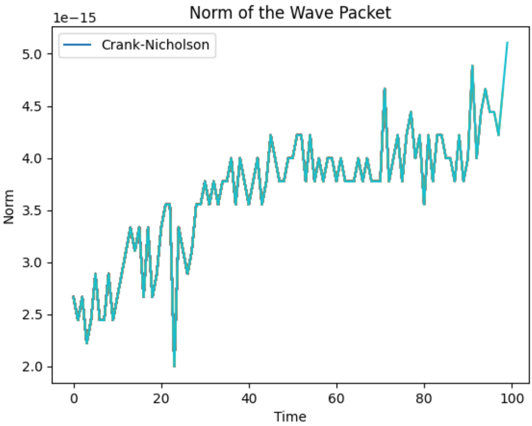
$$\psi_{i,j}^{n+1} = \psi_{i,j}^{n-1} - 2i\left[\left(4\alpha + \frac{1}{2}\Delta t V_{i,j}\right)\psi_{i,j}^{n} - \alpha\left(\psi_{i+1,j}^{n} + \psi_{i-1,j}^{n} + \psi_{i,j+1}^{n} + \psi_{i,j-1}^{n}\right)\right]$$

where $\alpha = \Delta t / 2(\Delta x)^2$

Euler algorithm



Euler algorithm



Conclusions

- Crank Nicholson matrix size scales quadratically unlike the 1D case.
- Not a tridiagonal matrix.
- Tried to save it as a sparse matrix but no considerable improvement.
- Finite difference method sidesteps matrix operations entirely.
- Finite difference - misnomer?