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Project 5: "Schrödinger's double slit" / double-slit in a box

- Q: How many has taken a course on QM? (not needed)
- Topics:
  - PDEs in # 2+1 dim
  - Crank-Nicolson (implicit scheme)
  - Working with complex numbers
  - Some matrix considerations ..
  - Probability
- Schr. eq:

$$i\hbar \frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle$$

(Energy operator)

- In position space, for single particle, two dim:

$$i\hbar \frac{\partial}{\partial t}\psi(x,y,t) = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\psi(x,y,t) + V(x,y,t)\psi(x,y,t)$$

(kinetic energy + potential energy)

- Born rule:

$$p(x,y;t) = |\psi(x,y,t)|^2 = \psi^*(x,y,t)\,\psi(x,y,t)$$

(Prob density)

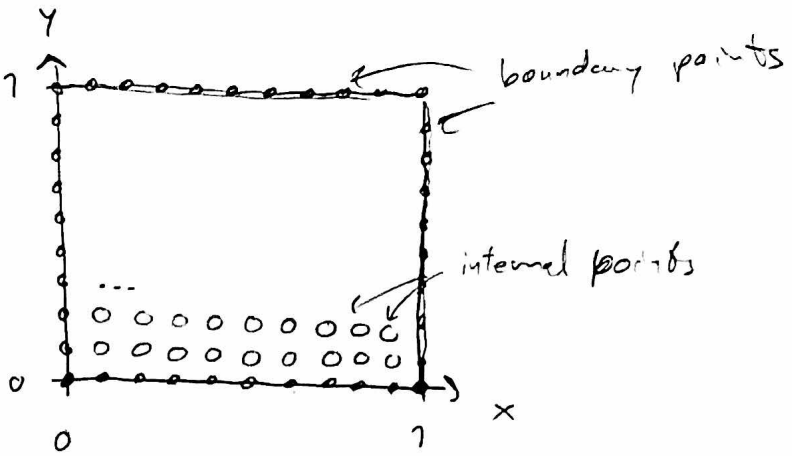
$$\left[\text{Prob}(\text{particle in } x\in[a,b],\ y\in[c,d]) = \int_a^b\int_c^d \psi^* \times \psi \, dx\, dy\right]$$

- Our case: All dim.less! General form of the diff eq.

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

Now a time-indep. potential

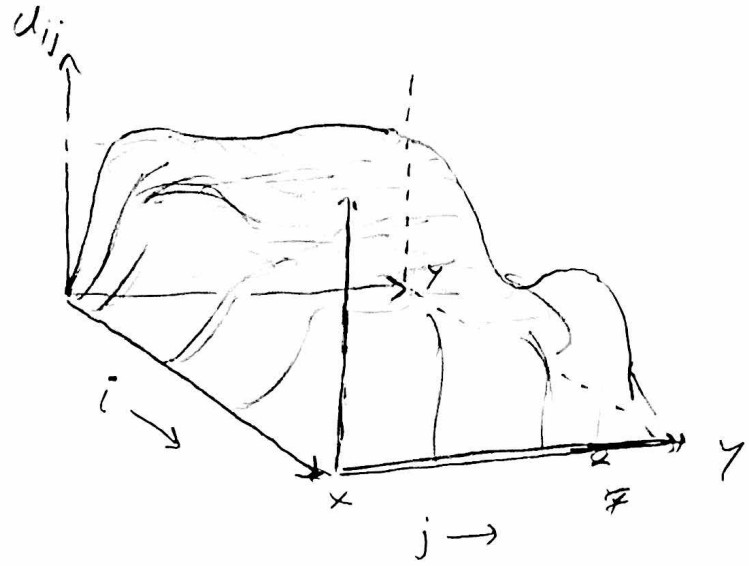
- Our box:



  - $x \in [0,1]$, $y \in [0,1]$
  - $\Delta x = \Delta y = h$
  - M points in each direction (incl boundary points)
    - ↳ $M-1$ steps
    - ↳ $M-2$ internal points

  - $X \to x_i = ih$ (Normally $x_i = x_0 + ih$, but $x_0 = 0$)
  - $Y \to y_j = jh$ $\quad i,j = 0,1,2,\ldots,M-1$
  - $u(x,y,t) \to u(x_i, y_j, t_n) = u_{ij}^n$ ← Notation!
  - $V(x,y) \to V_{ij}$

- u_{ij} and v_{ij} are functions on the xy plane



- We'll use conservation of probability as a consistency check.

- v_{ij} is fixed in time
- But for u_{ij} one entire grid of values for each timestep → one matrix per timestep

- In this project we will need to swap between matrix and vector representation of our solution:

- Entire state: $( ) =$

$$\begin{bmatrix} u_{00} & u_{01} & \cdots & u_{0,M-1} \\ u_{10} & u_{11} & & \\ u_{20} & & \text{internal points} & \\ \vdots & & & \\ u_{M-1,0} & \cdots & & u_{M-2,M-2} \end{bmatrix}$$

Needed for the C-N method.

- Internal part →

$$\begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1,M-2} \\ u_{21} & & & \\ \downarrow & & & \\ u_{M-2,1} & & & \end{bmatrix}$$

as matrix

$\longleftrightarrow$

$$\begin{bmatrix} \begin{pmatrix} u_{11} \\ u_{21} \\ \vdots \\ u_{M-2,1} \end{pmatrix} \\ \begin{pmatrix} u_{12} \\ u_{22} \\ \vdots \\ u_{M-2,2} \end{pmatrix} \\ \vdots \end{bmatrix}$$

as vector