Project 5 - FYS4150
The Schrödinger equation

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Abstract
Supporting material may be found in the following GitHub repository: https://github.com/Vikenes/FYS4150/tree/main/project5.

NOMENCLATURE

Basics

$x \in [0, 1]$; $x \to x_i = ih$ with $i = 0, 1, \ldots, M-1$.

$y \in [0, 1]$; $y \to y_j = jh$ with $j = 0, 1, \ldots, M-1$.

$\mathbf{x} = (x,\, y)$; $\mathbf{x} \to \mathbf{x}_{i,j} = h(i, j)$ with $i, j \in [0, M-1]$.

$t \in [0, T]$; $t \to t_n = n\Delta t$ with $n = 0, 1 \ldots, N_t - 1$.

$u(t, \mathbf{x}) \to u(t_n, \mathbf{x}_{i,j}) \equiv u^{(n)}_{i,j}$.

$U^{(n)}$ is a matrix with elements $u^{(n)}_{i,j}$.

$v(\mathbf{x}) \to v(\mathbf{x}_{i,j}) \equiv v_{i,j}$.

V is a matrix with elements $v_{i,j}$.

NB

M is the number of points along x and y axis.

$M - 1$ is the number of steps.

$M - 2$ is the number of internal points (excluding boundary points).

Dirichlet boundary conditions

$u(t, \mathbf{x}_{0,j}) = u(t, x\!=\!0, y) = 0.$

$u(t, \mathbf{x}_{M-1,j}) = u(t, x\!=\!1, y) = 0.$

$u(t, \mathbf{x}_{i,0}) = u(t, x, y\!=\!0) = 0.$

$u(t, \mathbf{x}_{i,M-1}) = u(t, x, y\!=\!1) = 0.$

I. INTRODUCTION

Blah blah

For a single, non-relativistic particle with mass m_P in a two-dimensional potential $V(t, \mathbf{x})$, the Schrödinger equation reads[1]

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\Psi(t, \mathbf{x}) = -\frac{\hbar^2}{2m_\mathrm{P}}\nabla^2\Psi(t, \mathbf{x}) + V(t, \mathbf{x})\Psi(t, \mathbf{x}). \tag{1}$$

For a set of initial and boundary conditions, the partial differential equation (PDE) describes the temporal and spatial evolution of the complex-valued function $\Psi(t, \mathbf{x})$ related to the quantum state of the aforementioned particle. In such a case, at a time t, the probability density for an experimentalist to locate the particle at $\mathbf{x}$ ("for detecting ..." is better, but I don't want to copy Anders) is large P or small p???

$$P(\mathbf{x};\, t) = |\Psi(t, \mathbf{x})|^2 = \Psi^*(t, \mathbf{x})\Psi(t, \mathbf{x}), \tag{2}$$

originating from the Born rule; fill me

In this paper we will consider a dimensionless time-independent potential, i.e. we let $V(t, \mathbf{x}) \to v(\mathbf{x})$. The specifics of the scaling do not concern us in this paper, and we simply rewrite equation (1) to the dimensionless equation

$$\mathrm{i}\frac{\partial}{\partial t}u(t, \mathbf{x}) = -\nabla^2 u(t, \mathbf{x}) + v(\mathbf{x})u(t, \mathbf{x}), \tag{3}$$

where we substituted $\Psi(t, \mathbf{x}) \to u(t, \mathbf{x})$. In equation (3) all variables are dimensionless. When demanding the proper normalisation on $u(t, \mathbf{x})$, it follows that the Born rule now takes the form of

$$p(\mathbf{x};\, t) = |u(t, \mathbf{x})|^2 = u^*(t, \mathbf{x})u(t, \mathbf{x}). \tag{4}$$

Should maybe rephrase this paragraph.

II. METHODS

choose one of these:

$$u(t\!=\!0, \mathbf{x}) = \exp\left\{-(\mathbf{x} - \mathbf{x}_\mathrm{c})^\mathrm{T}\Sigma^{-1}(\mathbf{x} - \mathbf{x}_\mathrm{c}) + \mathrm{i}\mathbf{p}^\mathrm{T}(\mathbf{x} - \mathbf{x}_\mathrm{c})\right\}; \quad \Sigma = \mathrm{diag}(\boldsymbol{\sigma}^2) \tag{5}$$

[1] In position space, that is. Should we comment on this?

$$u(t\!=\!0,\mathbf{x}) = \exp\left\{-\frac{(x-x_\mathrm{c})^2}{2\sigma_x^2} - \frac{(y-y_\mathrm{c})^2}{2\sigma_y^2} + \mathrm{i}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}_\mathrm{c})\right\} \tag{6}$$

III. RESULTS

IV. DISCUSSION

V. CONCLUSION

Appendix A: Discretisation

Suppose you have the (1+1)-dimensional PDE $\partial u/\partial t = F$ where $u = u(t,x)$ and $F = F(t,x,u,\partial u/\partial x\,,\partial^2 u/\partial x^2\,)$. The Crank-Nicolson scheme reads ref

$$\frac{u_i^{(n+1)} - u_i^{(n)}}{\Delta t} = \frac{1}{2}\left(F_i^{(n+1)} - F_i^{(n)}\right), \tag{A1}$$

where $u_i^{(n)} = u(n\Delta t, i\Delta x)$ and $F_i^{(n)}$ is F evaluated for i,n and $u_i^{(n)}$. In our (2+1)-dimensional case where $u = u(t,\mathbf{x})$ we have

$$\frac{\partial u}{\partial t} = F(t,\mathbf{x},u,\nabla^2 u) = \mathrm{i}\left(\nabla^2 u - v(\mathbf{x})u\right), \tag{A2}$$

and this approach translates to

$$\frac{u_{i,j}^{(n+1)} - u_{i,j}^{(n)}}{\Delta t} = \frac{1}{2}\left(F_{i,j}^{(n+1)} - F_{i,j}^{(n+1)}\right) \tag{A3}$$

where $u_{i,j}^{(n)} = u(n\Delta t, \mathbf{x}_{i,j})$, $\mathbf{x}_{i,j} = h(i,j)$, and $F_{i,j}^{(n)}$ is the right-hand side of equation (A2), explicitly:

$$F_{i,j}^{(n)} = \mathrm{i}\left(\left[\frac{\partial^2 u}{\partial x^2}\right]_{i,j}^{(n)} + \left[\frac{\partial^2 u}{\partial y^2}\right]_{i,j}^{(n)} - v_{i,j}u_{i,j}^{(n)}\right)\;; \tag{A4}$$

We can approximate the two spatial double derivatives (correct way to say?) according to (Don't know what this approximation is called):

$$\left[\frac{\partial^2 u}{\partial x^2}\right]_{i,j}^{(n)} \approx \frac{1}{h^2}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right)^{(n)}\;; \tag{A5a}$$

$$\left[\frac{\partial^2 u}{\partial y^2}\right]_{i,j}^{(n)} \approx \frac{1}{h^2}\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right)^{(n)}\;; \tag{A5b}$$

Define $r \equiv \frac{\mathrm{i}\Delta t}{2h^2}$. Further, let

$$\begin{aligned}\mathcal{A}^{(n)} = {} & r\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right)^{(n)} \\ & + r\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right)^{(n)} \\ & - \frac{\mathrm{i}\Delta t}{2} v_{i,j}\, u_{i,j}^{(n)}.\end{aligned} \tag{A6}$$

Equation (A3) becomes:

$$u_{i,j}^{(n+1)} - \mathcal{A}^{(n+1)} = u_{i,j}^{(n)} + \mathcal{A}^{(n)}\,; \tag{A7}$$

The final discretisation (A7) is valid for any step in time within the time range ($n \in [0, N_t - 2]$) and all internal points on the grid ($i,j \in [1, M-2]$).