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 $n = 0, 1 \ldots, N_t - 1$.

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

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

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

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 $\mathcal{V}(t,\mathbf{x})$, the Schrödinger equation reads[1]

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

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 $\mathcal{V}(t,\mathbf{x}) \to v(\mathbf{x})$. 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.

HUSK:

* Noe om diffraction
* Noe om hva vi forventer å se med og uten slits

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

II. METHODS

We will use the Schrödinger equation to simulate a particle inside a two-dimensional quadratic box of size L^2. The use of periodic boundary conditions gives rise to the confinement of the particle or something like that. We will place two or more walls inside the box to create one or more slits. The specifics of such configurations is elaborated in section II D. A position inside if the box is called $\mathbf{x} = (x, y)$ and a time $t \in$, all unit less. Now $x, y \in [0,\, L]$ and $t \in [0,\, T]$ if we let T be the time we simulate for. In this paper, we will use $L = 1$.

A. Numerical scheme

How to solve etc.

1. Discretisation

We discretise the position $\mathbf{x} \to \mathbf{x}_{i,j} = (x_i, y_j) = h(i, j)$, where h is the spatial separation between two points on the grid. We consider M points in each direction, giving $i, j \in [0,\, M)$. The lattice is then made up of $(M-2) \times (M-2)$ internal points and boundary points. The time points become $t \to t_n = n\Delta t$, $n \in [0, N_t)$, where Δt is the time step size and $N_t = T/\Delta t$ is the number of time points. Further, we find the wave function as

$$u(t, \mathbf{x}) \to u(t_n, \mathbf{x}_{i,j}) \equiv u_{i,j}^{(n)}, \tag{5}$$

and subsequently the probability density,

$$p(\mathbf{x};\, t) \to p(\mathbf{x}_{i,j};\, t_n) \equiv p_{i,j}^{(n)}. \tag{6}$$

The potential is discretised as $v(\mathbf{x}) \to v(\mathbf{x}_{i,j}) \equiv v_{i,j}$.

2. Implementation

In order to solve equation (3) numerically on a discretised grid, as explained above, we use the Crank-Nicolson approximation. A derivation of this is given in appendix A. It allows us to express the time evolution of the system as:

$$u_{i,j}^{(n+1)} - \mathcal{F}_{i,j}^{(n+1)} = u_{i,j}^{(n)} + \mathcal{F}_{i,j}^{(n)}, \tag{7}$$

where

$$\begin{aligned} \mathcal{F}_{i,j}^{(n)} = \quad & r\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right)^{(n)} \\ & + r\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right)^{(n)} \\ & - \frac{\mathrm{i}\Delta t}{2} v_{i,j}\, u_{i,j}^{(n)}, \end{aligned} \tag{8}$$

and we have defined $r \equiv \frac{\mathrm{i}\Delta t}{2h^2}$. This time evolution is valid for any time step with the time range $n \in [0, N_t - 2]$. Its spatial validity is restricted to the internal points of the grid; $i, j \in [1, M-2]$. For the boundary points we impose the Dirichlet boundary conditions (stated in the nomenclature).

If we define

$$\mathbf{u}^{(n)} \equiv [u_{1,1}^{(n)}, \ldots, u_{M-2,1}^{(n)}, \ldots u_{1,M-2}^{(n)}, \ldots u_{M-2,M-2}^{(n)}], \tag{9}$$

to be the column vector of shape $((M-2)^2 \times 1)$ that contains all $u_{i,j}^{(n)}$ values for the internal points on the grid.

is this necessary? $u_k^{(n)}$ is the k-th element of $\mathbf{u}^{(n)}$ where $k = (j-1)\cdot(M-2) + (i-1)$ is valid for the internal points.

This, combined with the boundary conditions allows us to rewrite equation (7) into a matrix equation of the form:

$$A\mathbf{u}^{(n+1)} = B\mathbf{u}^{(n)}, \tag{10}$$

where A and B are special matrices, explained in appendix some appendix reference goes here. We are now able to evolve the system in time by solving equation (10) in a time loop by dividing it into two steps:

$$\begin{aligned} \mathbf{b} &= B\mathbf{u}^{(n)} \\ A\mathbf{u}^{(n+1)} &= \mathbf{b}, \end{aligned} \tag{11}$$

where we solve for $u^{(n+1)}$. When solving equation (11) we can use the structure of A to our advantage. A arise from a boundary value problem. We could use direct methods, such as Gaussian elimination or LU-decomposition to find A^{-1}. It could be beneficial to find this inverse since we solve for many time instances without changing A. We could also use iterative methods such as the Jacobi method or Gauss-Seidel. A is by construction diagonally dominant[2], we are thus guaranteed convergence with the Jacobi method More here?. However, noticing that the vast majority of the entries in A are zeros, we represent it numerically as a *sparse matrix*, only saving the indices and values of non-zero entries. We thus use a build in solver in Armadillo to solve equation (11) this citation should perhaps not be here[**?**].

B. Simulation

When simulating a system, we have to evolve it in time, and thus initialise it with an initial state.

[2] See appendix ref to appendix about A and B

1. Initial wave packet

The initialisation is done by imposing the following initial condition.

$$u(t=0,\mathbf{x}) = \exp\{-(\mathbf{x}-\mathbf{x}_c)^T\Sigma^{-1}(\mathbf{x}-\mathbf{x}_c) + i\mathbf{p}^T(\mathbf{x}-\mathbf{x}_c)\};$$
$$\Sigma = \mathrm{diag}(\boldsymbol{\sigma}^2) \tag{12}$$

check how thourough you need to be when defining the variables in the above equation This initial state is normalised such that $\langle \mathbf{u}^{(0)} | \mathbf{u}^{(0)} \rangle = 1$, so that the initial probability starts out normalised to 1. rewrite thsi, make it clearer.

2. Slit configuration

To create a single slit, we need *two* objects with the property that the particle cannot propagate through it. Said objects are to have a separation between them, a *slit*, perpendicular to the dominating motion of the particle Pls send help, cannot write proper sentences any more:. A natural choice for the shape is the rectangular with the longer side parallel to the slit, (Some theory about interference??) hence the name "wall". Three such walls give rise to two slits, etcetera.

To give the Schrödinger equation information about these walls, we simply create a very large potential in the walls. These potential barriers will resemble concrete (mener egt ikke betong, men konkrete... hva er ordet??) walls in the sense that the particle will have to navigate around it in order to get through to the other side.

In particular, we will set up a number of such walls in the middle of our box, the separation between which is the aperture, aligned perpendicular to the initial momentum $\mathbf{p}$ in equation (12). We will make sure that the slit setup is symmetric around the box centre in both directions.

3. Artificial detector screen

To reduce the dimensionality of the problem, we can assume to measure a particle with a detector screen at some horisontal position $x = x_{sc}$ and time $t = t_{sc}$, so that the screen spans of the vertical axis y. With a smart choice of pairing (t_{sc} & x_{sc}), we can safely assume that the particle is located somewhere along this line. Thus, it makes sense to consider a normalised one-dimensional probability function $p_{x=x_{sc}}(y;\, t_{sc})$ (read: probability of y given $x = x_{sc}$, at $t = t_{sc}$) such that

$$p^{\mathrm{tot}}_{x=x_{sc}}(t=t_{sc}) = \sum_{j\in[0,M)} p_{x=x_{sc}}(y_j;\, t_{sc}) = 1. \tag{13}$$

Do we have to explain how we find this?

4. Simulation parameters

Simulation parameters ??	
Spatial step size (h)	$5.0 \cdot 10^{-3}$
Temporal step size (Δt)	$2.5 \cdot 10^{-5}$
Total time (T)	$*$
Slit configuration (following section **??**)	
Number of slits (#slits)	$*$
Number of identical walls	#slits $+ 1 \geq 2$
Wall dimensions; width$\times$height	0.02×0.05
Wall centre position	$(0.5, \sim 0.5)$[a]
Slit aperture (separation between walls)	0.05
Potential inside barrier (v_0)	$1.0 \cdot 10^{10}$
Initial wave packet (the Gaussian in equation (12))	
Centre position ($\mathbf{x}_c$)	(0.25, 0.50)
Spatial extent ($\boldsymbol{\sigma}$)	$(0.05, *)$
Momentum ($\mathbf{p}$)	(200, 0)
Vertical screen (following section **??**)	
Horisontal position (x_{sc})	0.8
Time point (t_{sc})	0.002

[a] Slit setup symmetric around $y = 0.5$.

TABLE I: Numerical values for static simulation parameters. Simulation-specific values are denoted "$*$".

Simulation name (label[a])		#slits	T	$\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_y$
1. No slits	(*NS*)	0	0.008	0.05
2. Double-slit (1)	(*DS1*)	2	0.008	0.10
3. Double-slit (2)	(*DS2*)	2	0.002	0.20
4. Single-slit	(*SS*)	1	0.002	0.20
5. Triple-slit	(*TS*)	3	0.002	0.20

[a] Prefix to look for in link to animations etc.

TABLE II: Supplement to table I. Additional information about the simulations considered in this paper.

III. RESULTS

What to name these sections?
Maybe put links to animations here?

A. Sanity check

The first simulation[3], where there are no slits, is run with parameters according to tables I and II (*NS*). By

[3] Animation available here.

rights, at any time t, the probabilities $p(\mathbf{x}_{i,j};\, t)$ should sum up to one, as the particle is present inside the box. As a sanity check, we plot

$$\left|1 - p^{\text{tot}}(t)\right|; \quad p^{\text{tot}}(t) = \sum_{i,j\in[0,M)} p(\mathbf{x}_{i,j};\, t) \tag{14}$$

as a function of time in figure 1, where we see that the deviation ($\sim 10^{-14}$) is close to machine precision.

The next simulation[4] we consider has a double-slit barrier and a somewhat broader initial wave packet in the vertical direction (*DS1* in table II). We perform the same sanity check as above and once again get deviations of order 10^{-14}, also shown in figure 1.

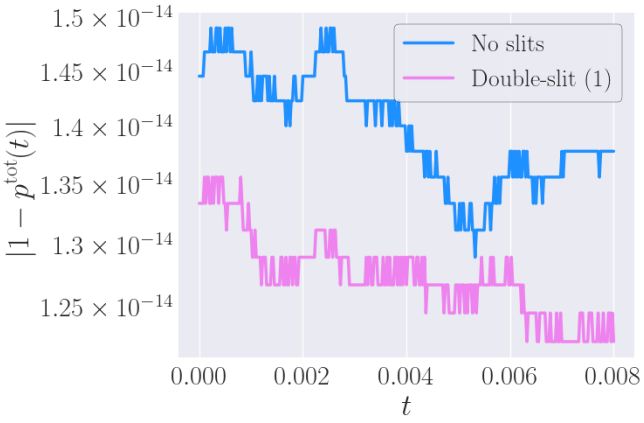


FIG. 1: *NS* & *DS1*: The total probability's deviation from the theoretical value, following equation (15), as function of time, for the two initial experiments. The vertical axis is logarithmic.

B. Two-dimensional problem

We change the settings of our simulations so that they are only run for a fourth of the duration and with an even larger initial wave packet. Still two slits considered, our third simulation[5] is run with parameters in accordance with I and II (*DS2*). Snapshots of the probability distribution $p(\mathbf{x};\, t)$ at $t = 0,\ T/2$ and T, $T = 0.002$, are presented in figure 2a. In addition, the real and imaginary part of $u(t, \mathbf{x})$ at the same time points are presented in figures 2b and 2c, respectively.

The scaling of the colour maps is such that the colour bars in figure 2 follow

$$Q(\mathbf{x};\, t_n) \to \frac{Q(\mathbf{x};\, t_n)}{\max|Q(\mathbf{x};\, t_n)|}, \tag{15}$$

where $Q(\mathbf{x};\, t_n)$ is the spatial distribution of a quantity at time $t = t_n$. Still not sure about this...

[4] Animation available here.
[5] Animation available here.

C. One-dimensional problem

Using the same parameters, we run two additional simulations[6] (*SS* and *TS*), except that we vary the number of slits (see tables I and II). In the following, we study the system further by removing a dimension.

Take note of the dotted vertical line in the right panel of figure 2a. Following the method described in section II E, we find the probability density along this screen for detecting the particle. Is this clear? The distribution for this particular experiment is plotted as a function of y in figure 3a. The same screen is used for the single- and triple-slit experiments, resulting in the graphs in figures 3b and 3c, respectively.

IV. DISCUSSION

The sanity check represented by the graphs figure 1 indicates that our solution is stable for $t \leq 0.008$, which is satisfying.

FILL ME

The animations (found here) show very different behaviours for *NS* and *DS1*. From the former to the ladder, we can clearly see the effect of introducing slits and how the probability distribution navigates around the barriers.

The first experiment, for which the initial wave packet is circular, shows the expected behaviour as this is analytically solvable (Should check this solution). As the particle propagates in the x-direction, we can see the dispersive behaviour of the probability density in the y-direction. In other words, the initially narrow spatial probability distribution gets broader over time.

The second experiment starts out with a somewhat larger wave packet, being more spread out in the y-direction. It propagates to the double-slit where it is split in several "pieces". After hitting the walls and being bounced back, the slits make sure to divide the blobs into even more blobs. More here

Comment on boundary conditions

FILL ME

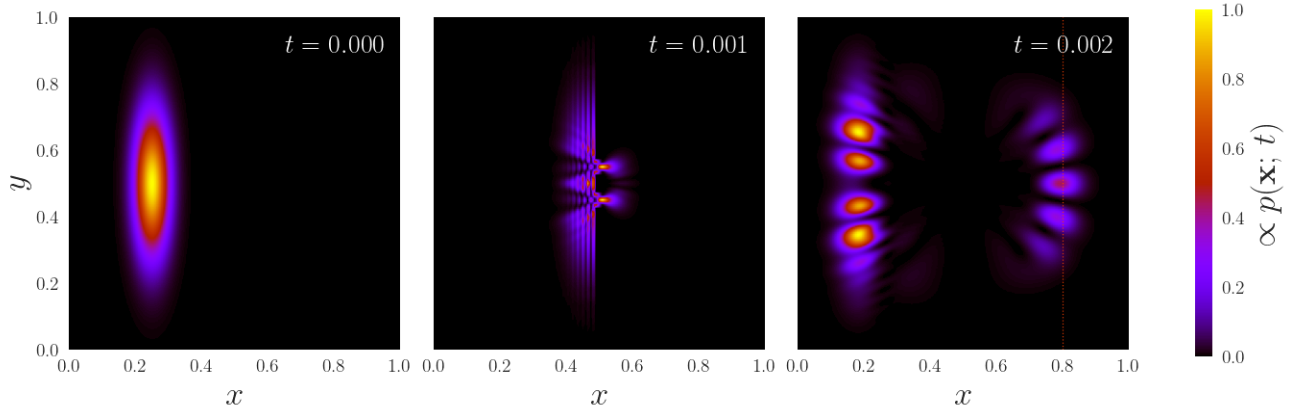
The probability density

V. CONCLUSION

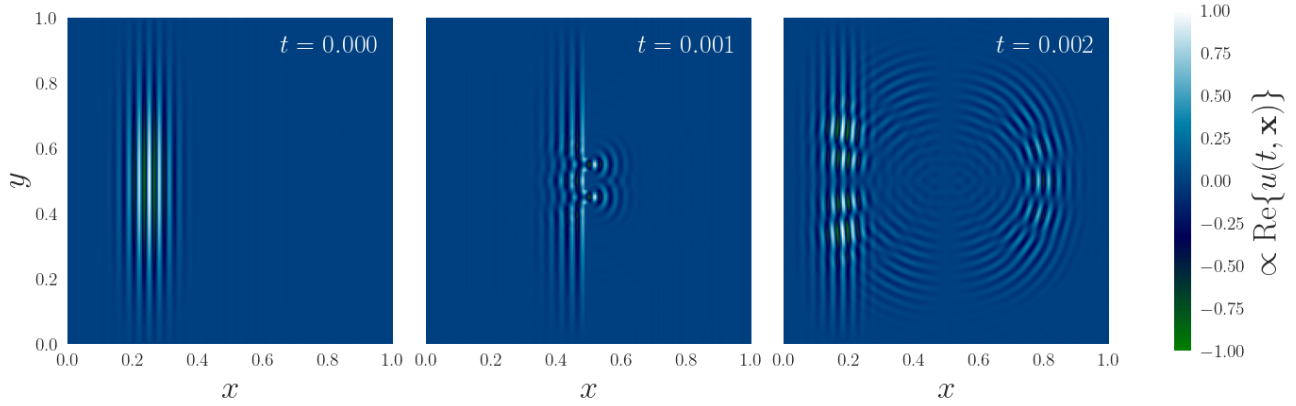
SUPPORTING MATERIAL

We recommend visiting our github repository for supporting material.

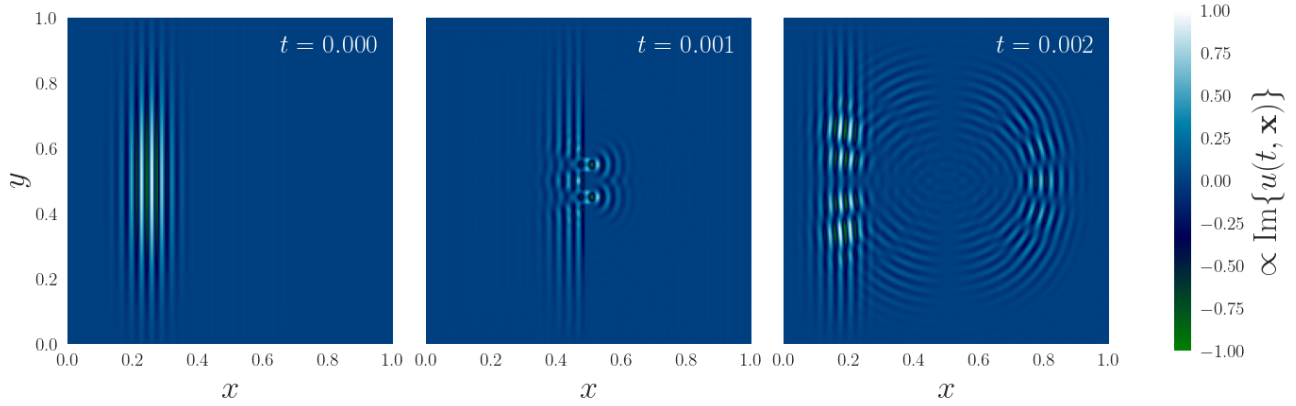
[6] Animations available here and here.



(a) *DS2*: Snapshots representing the evolution of the probability density. The dotted vertical line represents the screen we consider in figure 3. The yellow areas are where we are most likely to detect the particle at the relevant time, whereas in the dark areas we are very unlikely to find it.



(b) *DS2*: Snapshots representing the evolution of the real part of the wave function in space.



(c) *DS2*: Snapshots representing the evolution of the imaginary part of the wave function in space.

FIG. 2: Colour maps showing the solution of the Schrödinger equation for the *DS2* setup at times $t = 0.000, 0.001, 0.002$. The walls that set up the slits are illustrated by the green rectangles. Each map have been scaled using the absolute maximum of the quantity at the current time point. Idk how to explain

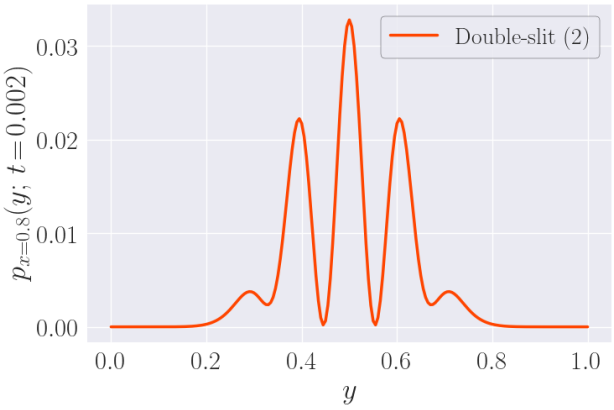
Code availability

The code that was used to produce the results can be found here.

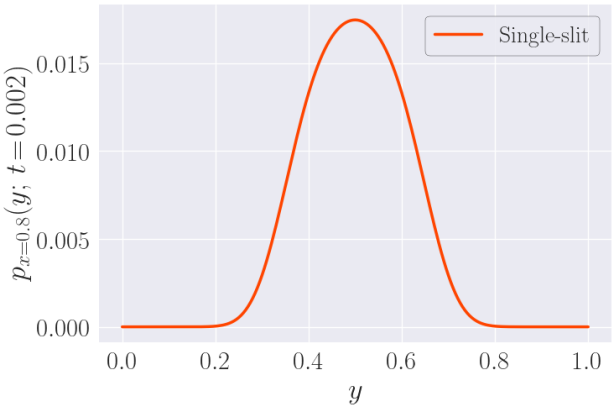
Animations

We present animations of the evolution of the probability density with proper colour bars for all simulations.

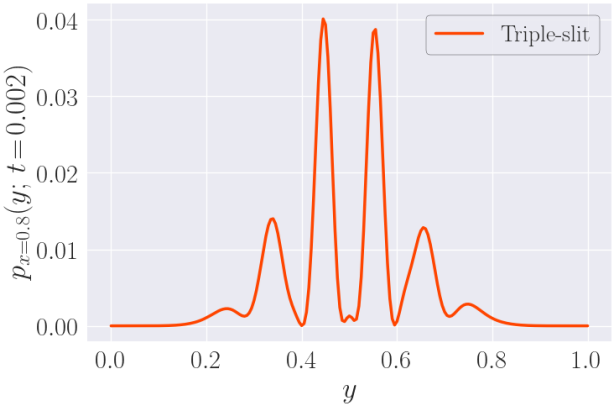
ref to readme for explanations??



(a) *DS2*: The probability density along the y-axis for the double-slit (2) experiment.



(b) *SS*: The probability density along the y-axis for the single-slit experiment.



(c) *TS*: The probability density along the y-axis for the triple-slit experiment.

FIG. 3: The amplitude for detecting the particle at vertical positions y at time $t = 0.002$ given that it is located at horisontal position $x = 0.8$, that is the quantity $p_{x=0.8}(y;\, 0.002)$ obeying equation (14), for simulations with one, two and three slits, but otherwise equal parameters.

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

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

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

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

Equation (A3) becomes:

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

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 ($i,j \in [1, M-2]$).

Appendix B: A and B matrices

In order to generalise the Crank-Nicolson approximation to the Schrödinger equation as a matrix equation $A\mathbf{u}^{(n+1)} = B\mathbf{u}^{(n)}$, that satisfy the Dirichlet boundary conditions on a discretised grid, we require A and B to take specific forms. We need both of them to be square matrices with dimensions $((M-2)^2 \times (M-2)^2)$, with vectors $\mathbf{a}$ and $\mathbf{b}$ as diagonal. These are given by:

$$\begin{aligned} a_k &= 1 + 4r + \frac{\mathrm{i}\Delta t}{2} v_{i,j} \\ b_k &= 1 - 4r - \frac{\mathrm{i}\Delta t}{2} v_{i,j}, \end{aligned} \tag{B1}$$

where r is still $r \equiv \frac{\mathrm{i}\Delta t}{2h^2}$. We fill the matrices A and B with $\pm r$-values along the first and third super- and subdiagonal; A with $-r$ and B with $+r$. The $(M-2)$-th element along the first super- and subdiagonal for each matrix must be zero. For demonstrative purposes, if $(M-2) = 3$, A and B would look like the following:

$$A = \begin{bmatrix} a_0 & -r & 0 & -r & 0 & 0 & 0 & 0 & 0 \\ -r & a_1 & -r & 0 & -r & 0 & 0 & 0 & 0 \\ 0 & -r & a_2 & 0 & 0 & -r & 0 & 0 & 0 \\ -r & 0 & 0 & a_3 & -r & 0 & -r & 0 & 0 \\ 0 & -r & 0 & -r & a_4 & -r & 0 & -r & 0 \\ 0 & 0 & -r & 0 & -r & a_5 & 0 & 0 & -r \\ 0 & 0 & 0 & -r & 0 & 0 & a_6 & -r & 0 \\ 0 & 0 & 0 & 0 & -r & 0 & -r & a_7 & -r \\ 0 & 0 & 0 & 0 & 0 & -r & 0 & -r & a_8 \end{bmatrix} \tag{B2}$$

$$B = \begin{bmatrix} b_0 & r & 0 & r & 0 & 0 & 0 & 0 & 0 \\ r & b_1 & r & 0 & r & 0 & 0 & 0 & 0 \\ 0 & r & b_2 & 0 & 0 & r & 0 & 0 & 0 \\ r & 0 & 0 & b_3 & r & 0 & r & 0 & 0 \\ 0 & r & 0 & r & b_4 & r & 0 & r & 0 \\ 0 & 0 & r & 0 & r & b_5 & 0 & 0 & r \\ 0 & 0 & 0 & r & 0 & 0 & b_6 & r & 0 \\ 0 & 0 & 0 & 0 & r & 0 & r & b_7 & r \\ 0 & 0 & 0 & 0 & 0 & r & 0 & r & b_8 \end{bmatrix} \tag{B3}$$