Path-Integrals and Quantum-Walks in Multi-Slit Systems

A thesis submitted towards partial fulfilment of
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by

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Certificate

This is to certify that this thesis entitled "Path-Integrals and Quantum-Walks in Multi-slit systems" submitted towards the partial fulfillment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research Pune represents original research carried out by "Aravind HV" at "Center for High Energy Physics, Indian Institute of Science, Bangalore", under the supervision of "Prof. Aninda Sinha" during the academic year 2013-2014.

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Abstract

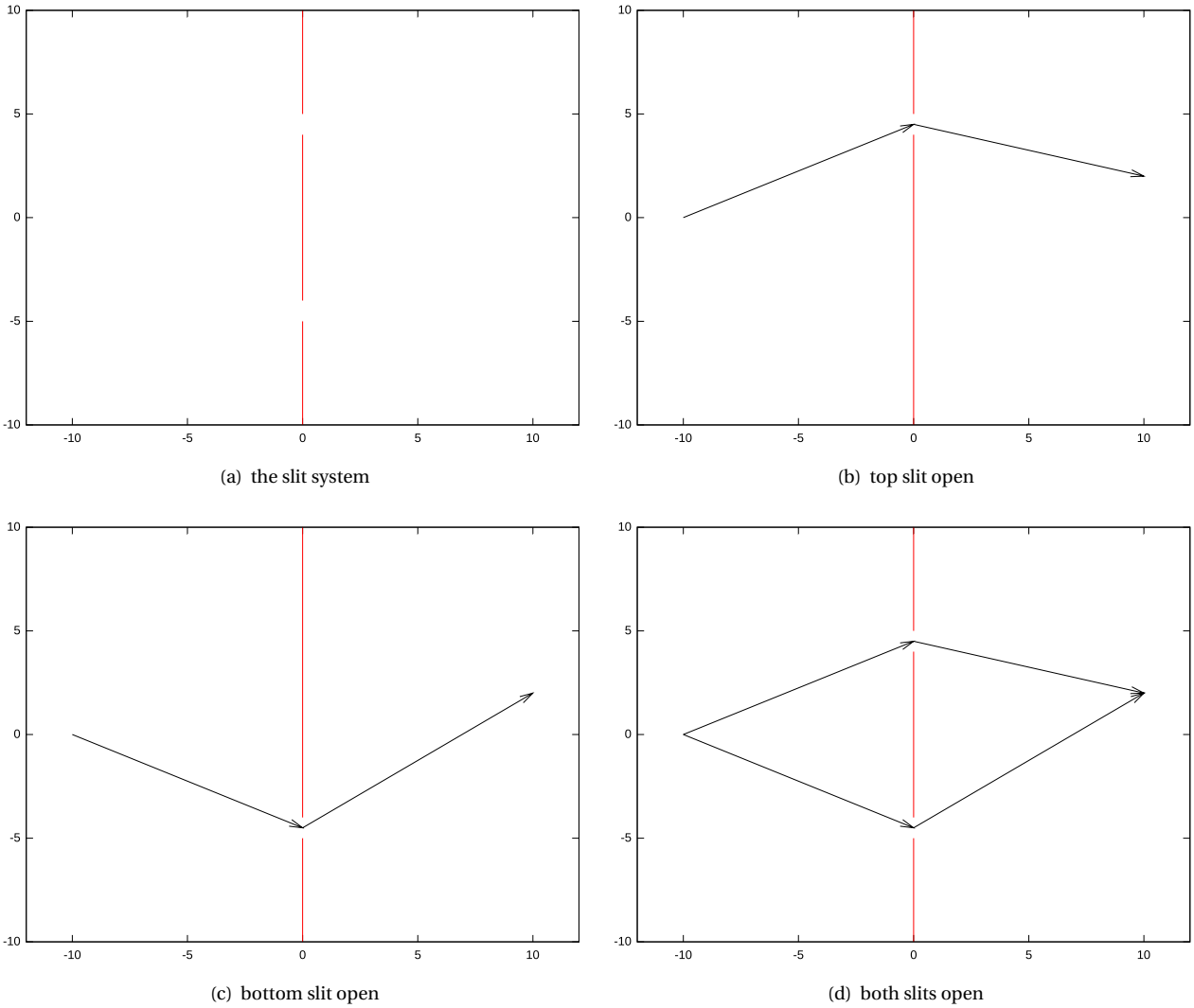
We examine the double and triple slit systems and their analysis using the popular superposition principle. This approach is only approximately true as the boundary conditions are different in each case. We define a quantity which can be used to quantify the deviation of the actual solution from those obtained from naive superposition principle and present two methods which can be used to obtain solutions and measure their deviation using the defined parameter. We then compare the two methods in the domain where they are expected to match.

Contents

Chapter 1

1 Introduction and Statement of the problem

We are familiar with the superposition principle for the solutions of the wave equation and it's application to obtain approximate solutions of the wave equation in the case of multi-slit interference systems (the pattern on the screen can be treated as an interference between the two waves that are emerging from the slits treated as sources). But this argument is only approximately valid as we cannot apply the superposition principle since this is a problem with different boundary conditions [1], [2], [3], [4]. In this chapter, we use the Feynman path integral formulation [5] of quantum mechanics to review the current understanding of the Young's double slit experiment for electrons [2].



(a) the slit system

(b) top slit open

(c) bottom slit open

(d) both slits open

Figure 1: illustration of different cases

The configuration in Fig.1(d) is not a superposition of the 2 configurations described in Fig.1(b) and Fig.1(c) as the boundary conditions are different. Just as an example, it can also allow paths (Feynman paths) as shown in Fig.2 which would not be accounted for in the superposition principle.

$$\begin{aligned} \psi_{ab} &\neq \psi_a + \psi_b \\ \text{Def}: \quad \rho &= \psi_{ab} - (\psi_a + \psi_b) \end{aligned}$$

(We can define similar parameter even for other waves).

Intuitively, we know that ρ is small as the deviations from 0 come only due to paths which pass through both the slits. But it is not possible to measure this quantity experimentally by any known way for quantum mechanical waves or for high frequency light, although it is possible to do the same for microwaves, sound waves and other waves where

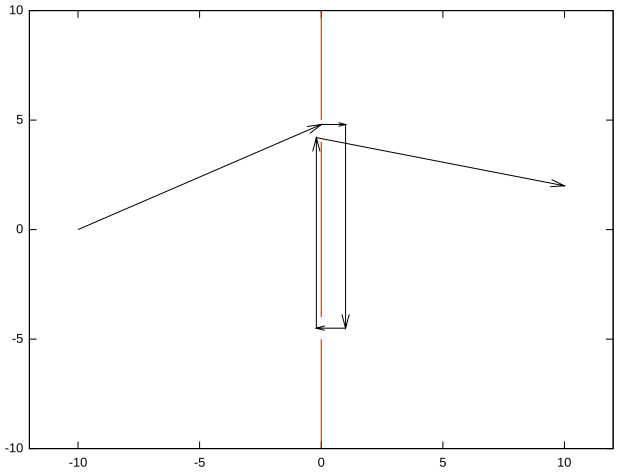


Figure 2: Paths excluded from $\psi_a + \psi_b$

we can actually measure the wave solution. **From this point on-wards, we will refer to ρ (and other paths which deviate significantly from straight lines) as "Non-Classical contributions" [2] (in the sense of Feynman paths, as these paths are not close to the classical paths which extremise the action) although we observe non-zero ρ even in the case of classical waves like sound or water waves.**. We now try to find a quantity which we can use to quantify "Non-Classical contributions" in cases where we are not allowed to measure the actual wave function. For this we consider the three slit setup [6], [7].

1.1 Quantifying "Non-Classical contributions" using intensities

For a 3 slit set up, we define:

ψ_a := Wave function when the top slit is open.
ψ_b := Wave function when the middle slit is open.
ψ_c := Wave function when the bottom slit is open.
ψ_{ab} := Wave function when both the top and the middle slits are open.
ψ_{bc} := Wave function when both the bottom and the middle slits are open.
ψ_{ca} := Wave function when both the top and the bottom slits are open.
ψ_{abc} := Wave function when all three slits are open.

$$
\begin{aligned}
\phi_a &:= |\psi_a|^2 \\
\phi_b &:= |\psi_b|^2 \\
\phi_c &:= |\psi_c|^2 \\
\text{Def: } \phi_{ab} &:= |(\psi_a + \psi_b)|^2 \\
&= |\psi_a|^2 + |\psi_b|^2 + 2\,\mathrm{Re}(\psi_a \bar{\psi}_b) \\
&= \phi_a + \phi_b + 2\Phi_{ab} \\
\text{with: } \Phi_{ab} &:= \mathrm{Re}(\psi_a \bar{\psi}_b) = \tfrac{\phi_{ab} - \phi_a - \phi_b}{2} \\
\text{Def: } \phi_{bc} &:= |(\psi_b + \psi_c)|^2 \\
&= |\psi_b|^2 + |\psi_c|^2 + 2\,\mathrm{Re}(\psi_b \bar{\psi}_c) \\
&= \phi_b + \phi_c + 2\Phi_{bc} \\
\text{with: } \Phi_{bc} &:= \mathrm{Re}(\psi_b \bar{\psi}_c) = \tfrac{\phi_{bc} - \phi_b - \phi_c}{2} \\
\text{Def: } \phi_{ca} &:= |(\psi_c + \psi_a)|^2 \\
&= |\psi_c|^2 + |\psi_a|^2 + 2\,\mathrm{Re}(\psi_c \bar{\psi}_a) \\
&= \phi_c + \phi_a + 2\Phi_{ca} \\
\text{with: } \Phi_{ca} &:= \mathrm{Re}(\psi_c \bar{\psi}_a) = \tfrac{\phi_{ca} - \phi_c - \phi_a}{2} \\
\text{Def: } \phi_{abc} &:= |(\psi_a + \psi_b + \psi_c)|^2 \\
&= |\psi_a|^2 + |\psi_b|^2 + |\psi_c|^2 + 2\,\mathrm{Re}(\psi_a \bar{\psi}_b) + 2\,\mathrm{Re}(\psi_b \bar{\psi}_c) + 2\,\mathrm{Re}(\psi_c \bar{\psi}_a) \\
&= \phi_a + \phi_b + \phi_c + \phi_{ab} - \phi_a - \phi_b + \phi_{bc} - \phi_b - \phi_c + \phi_{ca} - \phi_c - \phi_a \\
\Rightarrow \quad \phi_{abc} &= \phi_{ab} + \phi_{bc} + \phi_{ca} - \phi_a - \phi_b - \phi_c
\end{aligned}
$$

$$
\Rightarrow \quad \frac{\phi_{abc} - \phi_{ab} - \phi_{bc} - \phi_{ca} + \phi_a + \phi_b + \phi_c}{\phi_{abc}(\vec{c})} = 0 \tag{1}
$$

$\big($Here, $\vec{c}$ is the position of the center of the screen$\big)$.

Now, let us define [1]:

$$\text{Def}: \quad \kappa \quad := \quad \frac{|\psi_{abc}|^2 - (|\psi_{ab}|^2 + |\psi_{bc}|^2 + |\psi_{ac}|^2) + (|\psi_a|^2 + |\psi_b|^2 + |\psi_c|^2)}{|\psi_{abc}(\vec{c})|^2} \tag{2}$$

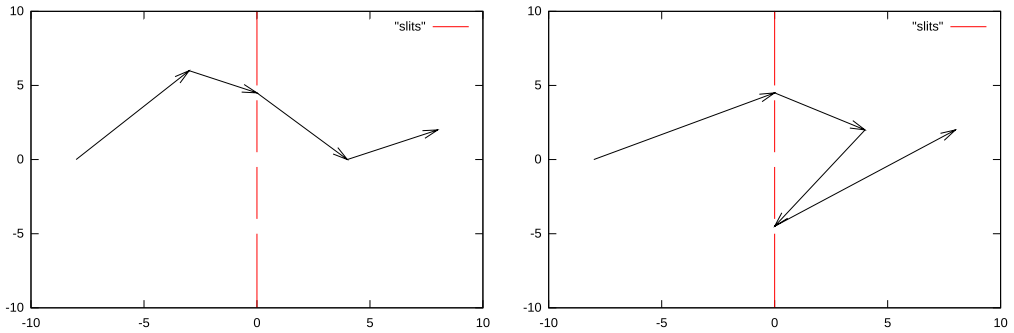
(The definition can be generalized using set theory for larger slit systems as shown in [1])
Naive super-position principle ($\psi_{abc} \equiv \psi_a + \psi_b + \psi_c$) yields $\kappa = 0$ (eq.1). We expect $\kappa \neq 0$ due to "Non-Classical contributions", at the same time the non-zeroness of κ (eq.2) is only due to certain subset of all the non-classical contributions, refer to (Section 2.1). In Chapter 2.2, we analyze a way which we can use to quantify the non-zeroness of κ (eq.2).

Chapter 2

2 Estimation of κ using the path-integral formulation of quantum mechanics:

2.1 Analyzing "Non-Classical contributions"

We now analyze the "Non-Classical contributions" and see which of those contribute to κ (eq.2), consider the paths as shown in Fig.3 Clearly, the path as shown in (Fig.3(a)) does not extremise the classical action and hence is a "Non-



(a) A Non Classical Contribution

(b) Yet another Non Classical Contribution (here, the figure is intended to demonstrate a path which just touches the slit plane and goes towards the screen)

Figure 3: illustration of nonclassical contributions

Classical Path", but such paths are part of ψ_a and hence by (eq.1) do not contribute to κ (eq.2), only paths which pass through at least 2 slits at least once (like Fig.2, Fig.3(b)) contribute to κ (eq.2).

2.2 Direct approach for a solution:

For simplicity, let us consider the interference experiment with non-relativistic particles and choose to work in three spatial dimensions. Assuming a steady source, the quantum mechanical Hamiltonian of the system is expected to be constant with respect to time, this allows us to use the familiar time variable separation technique (Section 6.1.2), the same method can also be applied to the wave equation (Maxwell's equation), refer (Section 2.3.1).

$$\begin{aligned} \bar{H}\vec{\psi} &= E\vec{\psi} \\ \Rightarrow \quad \frac{-\hbar^2}{2m}\nabla^2\psi(\vec{r}) &= E\psi(\vec{r}) \end{aligned}$$

2.2.1 Boundary conditions for the system

To accurately model the slit system, we assume that the slit plane is an infinitely large and infinitesimally thick plane at $x = 0$ which is perfectly absorbing (Robin's boundary condition):

$$\begin{aligned} \text{(absorbing boundary)} \quad \overrightarrow{\nabla\psi(\vec{r})} &= i\vec{k}\psi(\vec{r}) \\ \text{where:} \quad |\vec{k}| &= k \\ \text{and} \quad \vec{k} &= -k\hat{n} \end{aligned}$$

where $\hat{n}$ is normal to the slit plane.

We also need the solution to satisfy the Sommerfeld radiation condition([8], [9]) to avoid getting "particle in a box" like solutions, this ensures that the system is radiating and there is a constant flux of field being radiated to infinity. For this, ψ should satisfy

$$\begin{aligned} \lim_{r\to\infty} r\left(\frac{\partial\psi}{\partial r} - ik\psi\right) &= 0 \\ \text{here:} \quad r &= |\vec{r}| \end{aligned}$$

We can now proceed to solving the PDE using some of the typical numerical methods like finite element method, boundary element method [10] and finite difference method [11]. These methods are computationally very demanding (as they involve solving a huge simultaneous linear system) and hence hard to implement when the wavelength is small compared to other length scales in the problem (like the case of optical light or electrons).

2.3 Approximate solution using the path integral approach

An alternative was proposed by [2], we present a discussion on the same below. This method is based on the Feynman path integral formalism [5], we use the Green's function of the Helmholtz's equation as propagator (eq.**??**). Consider the system as shown in Fig.4, let $\vec{r}_S$ be the position of source S and $\vec{r}_P$ position of a point P where we wish to

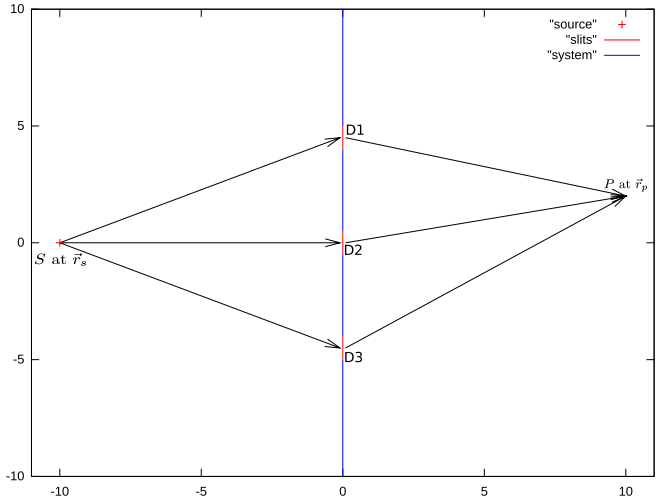


Figure 4: the Three slit system

know the solution u, $D1$ is a 2-dimensional surface which represents the top slit, similar conventions are used for $D2$ and $D3$. We can write the solution, $u(\vec{r}_P)$ as: (here, G is the Green's function)

$$\begin{aligned} \text{define}: \quad D &= D1 \cup D2 \cup D3 \\ u(\vec{r}_P) &= \int_D G(\vec{r}_S - \vec{r}_m) G(\vec{r}_m - \vec{r}_P) d\vec{r}_m \\ &\quad \big(\text{Here, } \vec{r}_m \text{ is the parameter used for integration}\big) \end{aligned} \tag{3}$$

(In writing these relations, we have assumed the stationary phase approximation and the approximation of using the free particle Green's function [2])
Similar method can be used to calculate the solution for other permutations (when less than 3 slits are open). But if we calculate κ (eq.2) using these solutions then we end up with $\kappa = 0$ (similar to eq.1) as:

$$\int_{D1\cup D2} G(\vec{r}_S - \vec{r}_m) G(\vec{r}_m - \vec{r}_P) = \int_{D2} G(\vec{r}_S - \vec{r}_m) G(\vec{r}_m - \vec{r}_P) d\vec{r}_m + \int_{D1} G(\vec{r}_S - \vec{r}_m) G(\vec{r}_m - \vec{r}_P) d\vec{r}_m \tag{4}$$

To get a good estimate for κ (eq.2), we need to perform the integration to a higher order (to account for paths as shown in: Fig.3(b)), hence we also need to include terms like:

$$\int_{r_n \in D2} \int_{\vec{r}_m \in D1} G(\vec{r}_S - \vec{r}_m) G(\vec{r}_m - \vec{r}_n) G(\vec{r}_n - \vec{r}_P) d\vec{r}_m d\vec{r}_n \tag{5}$$

(Here again, $\vec{r}_m$ and $\vec{r}_n$ are parameters used for integration)
as correction to the previous integral, this includes contributions from paths which pass through the slit plane twice. These paths are the most dominant contribution to κ (eq.2). We can proceed to get even higher order corrections in the same way but we can see from (Section 2.4) that the second order corrections are very small, hence third order corrections are expected to be even smaller.

We now proceed to integrate the above expression numerically as there exists no known analytical method. The only computational step involved in this method is numerical integration and hence is much more efficient than other methods when the wavelength is small. This method can be easily generalized for the wave (Section 2.3.1) and diffusion equations.

2.3.1 Path integral like approach for the wave equation:

We now consider the wave equation and present an approach which can be used to estimate the value of κ (eq.2)

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2}\right)\psi = 0 \quad \big(\text{With speed of the wave, } c = 1\big)$$

We now assume the source is in steady state so this allows us to perform variable separation.

$$\psi = X(\vec{r})T(t)$$

Where $\vec{r}$ is the vector corresponding to position coordinate, so:

$$\begin{aligned} X(\vec{r})T''(t) + (\nabla^2 X(\vec{r}))T(t) &= 0 \\ \Rightarrow \quad X(\vec{r})T(t)\frac{T''(t)}{T(t)} + \frac{(\nabla^2 X(\vec{r}))}{X(\vec{r})}X(\vec{r})T(t) &= 0 \\ \Rightarrow \quad \frac{T''(t)}{T(t)} &= K \\ \text{and} \quad \frac{(\nabla^2 X(\vec{r}))}{X(\vec{r})} &= K \end{aligned}$$

This gives us a solution of the form $T(t) = e^{\sqrt{K}t}$, if we want a situation where the source amplitude is constant in time, then we want $\sqrt{K}$ to be imaginary, so:

$$\text{define}: \quad K := -k^2 \quad \text{where} \quad k \in \mathbb{R}$$

This gives:

$$T(t) = e^{ikt} \tag{6}$$

$$\text{and} \quad (\nabla^2 + k^2)X(\vec{r}) = 0 \tag{7}$$

This is the Helmholtz equation and being a special case of the wave equation, we can use Huygens' principle [12] for this equation (a detailed analysis of the method presented can be found in [13], [14]).

NOTE: Many of the statements in Section 2.2 (like (eq.3) and (eq.5)) and this Section are only valid in spaces of odd spatial dimensions (please refer [12]). We will now be working in three spatial dimensions.

$$\text{define}: \quad G(\vec{r}) = \frac{ke^{ik|\vec{r}|}}{2\pi i|\vec{r}|}$$

This is the green's function (see section 59 of ref. [14]) for the free (in unbounded $\mathbb{R}^3$) Helmholtz equation in 3 dimensions. If we have a point source at $\vec{r}_0$ then the solution at $\vec{r}_2$ is given by $G(\vec{r}_0 - \vec{r}_2)$, the Huygens' principle states that:

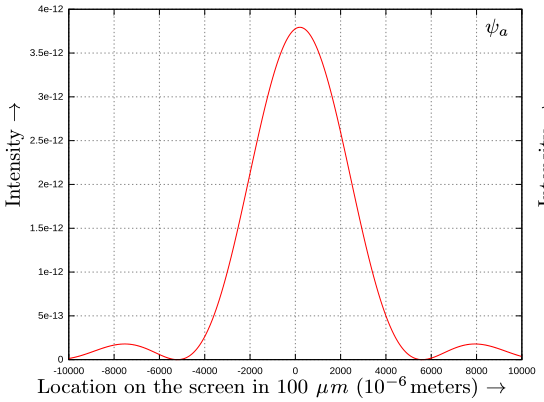
$$G(\vec{r}_0 - \vec{r}_2) = \int\int_D G(\vec{r}_0 - \vec{r}_1)G(\vec{r}_1 - \vec{r}_2)d^2\vec{r}_1 \tag{8}$$

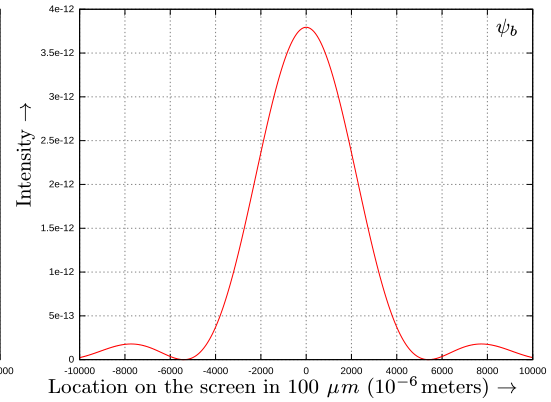
Where D is the 2 dimensional surface. This provides us an approximate way to obtain the solution as a function of position. We can now proceed as we did in (Section 2.3)

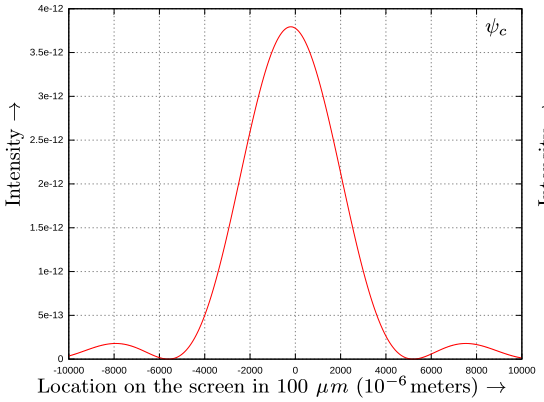
2.4 Sample Results

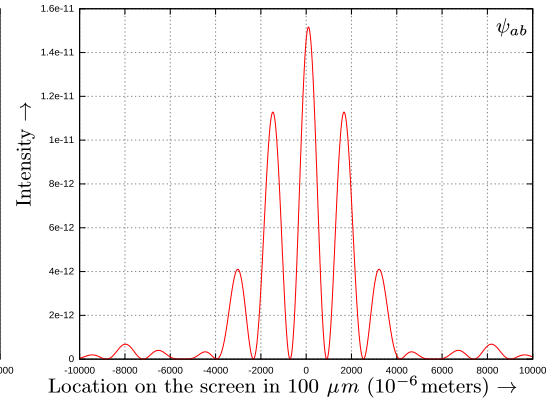
The results for all 7 cases and κ are given in the following order: $\psi_a, \psi_b, \psi_c, \psi_{ab}, \psi_{bc}, \psi_{ac}, \psi_{abc}, \kappa$
The following parameters were used for the calculation:

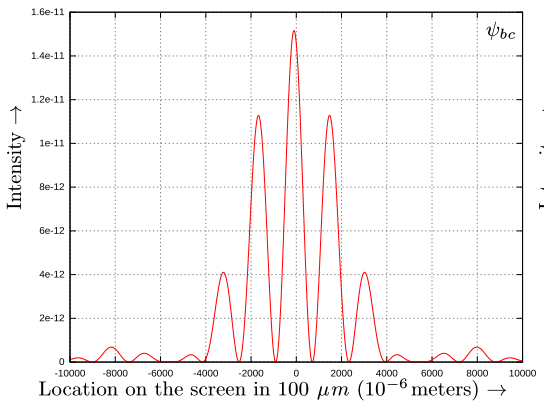
$$\begin{aligned} \text{Distance between source and slit plane} &: 20cm \\ \text{Distance between slit plane and screen} &: 20cm \\ \text{Inter-slit distance} &: 100\mu m \\ \text{Slit width} &: 30\mu m \\ \lambda &: 810nm \end{aligned}$$

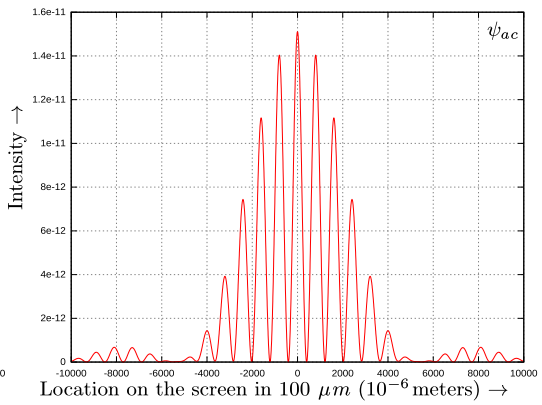

ψ_a
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →

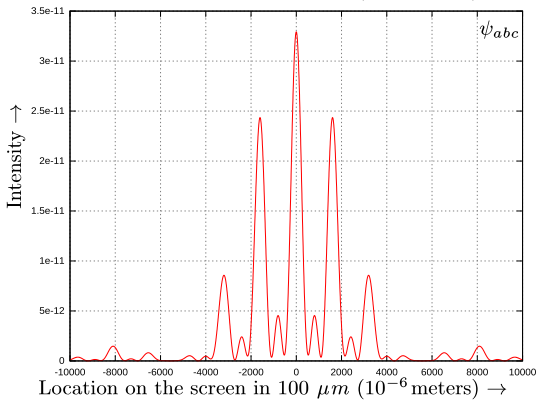

ψ_b
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →

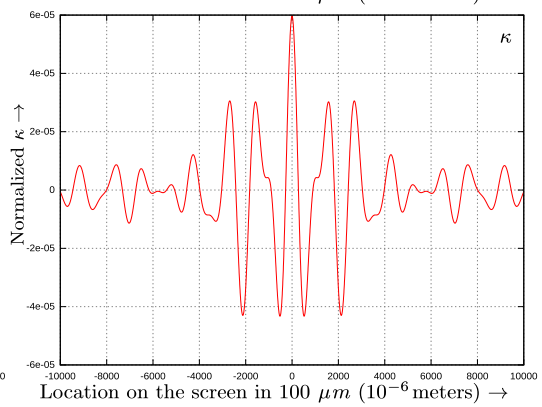

ψ_c
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →


ψ_{ab}
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →


ψ_{bc}
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →


ψ_{ac}
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →


ψ_{abc}
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →


κ
Normalized κ →
Location on the screen in 100 μm (10^{-6} meters) →

Chapter 3

3 The finite difference method for numerical solutions to the diffusion equation (statistical limit of random walk):

The method presented in the previous chapter uses several approximations which may not always hold (time independent Hamiltonian, stationary phase), in this chapter ([15], [16]) we explore more direct methods of solving the complete time dependent equations to get answers to higher accuracy (in real experiments, the Hamiltonian cannot be time independent and the sources are not perfectly steady), this method also has the disadvantage that the method is much more intensive than the one discussed in the previous chapter.

The most simple way of obtaining approximate numerical solutions to the diffusion equation is by discretising the derivative:

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \frac{1}{D}\nabla^2\psi \\ \text{In 1 space dimension:} & \\ \frac{\psi(t+h,x)-\psi(t,x)}{h} &= \frac{1}{D}\left(\frac{\psi(t,x+h)+\psi(t,x-h)-2\psi(t,x)}{h^2}\right) \\ \Rightarrow \quad \psi(t+h,x) &= \psi(t,x)+\left(\frac{\psi(t,x+h)+\psi(t,x-h)-2\psi(t,x)}{Dh}\right) \\ &= \psi(t,x)\left(1-\frac{2}{Dh}\right)+\frac{\psi(t,x+h)+\psi(t,x-h)}{Dh} \end{aligned}$$

(the fact that we are using the same number, h for discretising both space and time is just for convenience and can be avoided, later we will present a formulation which takes them to be different.)

We will now consider a random walk on a 1 dimensional lattice with 3 choices for each turn:
Probability to move 1 lattice step forward: $\frac{1}{Dh}$
Probability to move 1 lattice step backward: $\frac{1}{Dh}$
Probability to remain in the same lattice point: $1-\frac{2}{Dh}$

If we initially start with large number of particles executing the above random walk and density given as a function of the lattice point: $\rho(x)$, then this random walk satisfies the discretised diffusion equation. This provides the motivation for us to find a similar approach for the Schrodinger's equation (which is just a diffusion equation with an imaginary constant of diffusion).

We first define a matrix which will be useful throughout. We can treat the discretised form of the functions as a column matrix:

$$\text{define}: \quad \vec{\psi}(t) := \begin{pmatrix} \cdots \\ \psi(t,x-h) \\ \psi(t,x) \\ \psi(t,x+h) \\ \cdots \end{pmatrix}$$

This enables us to write the time evolution of $\vec{\psi}$ as:

$$\vec{\psi}(t+h) = \left(\mathbb{I}+\frac{\bar{M}}{Dh}\right)\vec{\psi}(t)$$

Here $\bar{M}$ is an infinitely large matrix (assuming $\vec{\psi}$ is an infinite dimensional vector) with diagonal elements -2, 1 on both sides of the diagonal and 0 everywhere else, $\mathbb{I}$ is the infinitely large identity matrix. $\left(\mathbb{I}+\frac{\bar{M}}{Dh}\right)$ is the transition matrix corresponding to the time evolution operator, $\bar{H}$:

$$\begin{aligned} \bar{H} &:= \left(\mathbb{I}+\frac{\bar{M}}{Dh}\right) \\ \text{so}: \quad \vec{\psi}(t+h) &= \bar{H}\vec{\psi}(t) \end{aligned}$$

Note: We are still dealing with the diffusion equation and hence the solution directly represents the probability (without the need for a norm) and $\bar{H}$ just represents the operator required to obtain a solution at a slightly later time, with the solution at an earlier time.

Consider the quantity: $\sum_{x=-\infty}^{x=+\infty}\psi(t,x)$, this will be equal to $\sum_{x=-\infty}^{x=+\infty}\psi(t+h,x)$

This is the statement that the number of particles are the same for all time or that there are no sources or sinks in a free diffusion equation.

3.1 Boundary conditions:

We again employ perfectly absorbing boundary conditions [17] for the diffusion equation at the slit planes and treat the whole system as if it were enclosed in a perfectly absorbing rectangle Fig.1(a)

$$\psi(t,\vec{x}) \quad = \quad 0 \quad \text{when} \quad \vec{x}\in\partial\Omega$$

Where the region corresponding to the interior of the system is Ω and the walls including the opaque parts of the slit planes belong to $\partial\Omega$. Due to this boundary conditions the total number of particles need not be conserved.

3.2 Quantum walks and unitary finite difference methods

3.2.1 1-D Schrodinger's equation:

Repeating the above procedure, we get:

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \\ \frac{\partial\psi}{\partial t} &= \frac{i\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} \\ \psi_x(t+\Delta t) &= \psi_t(x)+\frac{i\hbar}{2m}\frac{\Delta t}{(\Delta x)^2}[\psi_t(x+\Delta x)+\psi_t(x-\Delta x)-2\psi_t(x)] \end{aligned}$$

Now we will consider the coordinates to be discrete and ψ_t to be a vector in the index x. Also define the second derivative to be the matrix operator:

$$M := \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & -1 & 2 & -1 & 0 & \dots \\ \dots & 0 & -1 & 2 & -1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

So the equation now becomes

$$\begin{aligned} \psi_x(t+\Delta t) &= \psi_x(t)-\frac{i\hbar}{2m}\frac{\Delta t}{(\Delta x)^2}M_{x,\bar{x}}\psi_{\bar{x}}(t) \quad \text{(here, } \bar{x} \text{ index is summed over)} \\ \text{define:} \quad C &:= \frac{\hbar}{2m}\frac{\Delta t}{(\Delta x)^2} \\ \text{we now observe:} & \quad \text{By application of the method as described for the diffusion equation,} \\ |\psi(t+\Delta t)|^2 &= |\psi(t)|^2+O(\Delta t^2) \end{aligned} \tag{9}$$

So the time evolution operator as obtained from using the naive method from the diffusion equation does not produce a unitary evolution operator for the Schrodinger's equation.

Note: even-though $O(\Delta t^2)$ is small, the value of $|\psi|^2$ increase each step (interval of Δt) of the iteration and hence errors add up very fast. so we wish to avoid the approximation at this step.

To get a unitary evolution, we resort to methods as discussed in [18], [19]. Now if we relax the bound on Δt and Δx and let them be finite, we get:

$$\begin{aligned} \vec{\psi}(t+\Delta t) &= e^{-iC\bar{M}}\vec{\psi}(t) \\ & \quad \text{(here we have dropped the index notation and used } \vec{\psi} \text{ and } \bar{M} \text{ instead)} \end{aligned}$$

now $e^{-iC\bar{M}}$ is a difficult term to evaluate so we try to find good approximations for it,

$$\begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & -1 & 2 & -1 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & -1 & 2 & -1 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & -1 & 2 & -1 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & -1 & 2 & -1 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & -1 & 2 & -1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & 1 & -1 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & -1 & 1 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 1 & -1 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & -1 & 1 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & 1 & -1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$
$$+ \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & -1 & 1 & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 1 & -1 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & -1 & 1 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 1 & -1 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & -1 & 1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

now the first matrix on the right hand side will be addressed as $\bar{M}_0$ and second matrix as $\bar{M}_1$, so

$$\begin{aligned} \vec{\psi}(t+\Delta t) &= e^{-iC(\bar{M}_0+\bar{M}_1)}\vec{\psi}(t) \\ &\approx e^{-iC\bar{M}_0}e^{-iC\bar{M}_1}\vec{\psi}(t) \end{aligned}$$

by doing this, we are neglecting terms of higher order in C, which is small (refer Section 3.3), but more importantly t

we now notice a few interesting properties,

$$\begin{aligned} \bar{M}_0^2 &= 2\bar{M}_0 \\ \bar{M}_1^2 &= 2\bar{M}_1 \end{aligned}$$

now consider,

$$\begin{aligned} e^{-iC\bar{M}_0} &= 1 + (-iC\bar{M}_0) + \frac{(-iC\bar{M}_0)^2}{2!} + \frac{(-iC\bar{M}_0)^3}{3!} + \dots \\ &= 1 + (-2iC)\frac{\bar{M}_0}{2} + \frac{(-2iC)^2\frac{\bar{M}_0}{2}}{2!} + \frac{(-2iC)^3\frac{\bar{M}_0}{2}}{3!} + \dots \\ &= 1 - \frac{\bar{M}_0}{2} + \frac{\bar{M}_0}{2} + (-2iC)\frac{\bar{M}_0}{2} + \frac{(-2iC)^2\frac{\bar{M}_0}{2}}{2!} + \frac{(-2iC)^3\frac{\bar{M}_0}{2}}{3!} + \dots \\ &= 1 - \frac{\bar{M}_0}{2} + \frac{\bar{M}_0}{2}e^{-2iC} = 1 - \frac{\bar{M}_0}{2}(1 - e^{-2iC}) \\ \Rightarrow \quad e^{-iC\bar{M}_0} &= 1 - \frac{\bar{M}_0}{2}(1 - e^{-2iC}) \end{aligned}$$

similarly,

$$\Rightarrow \quad e^{-iC\bar{M}_1} = 1 - \frac{\bar{M}_1}{2}(1 - e^{-2iC})$$

so, define:

$$U_0 := 1 - \frac{\bar{M}_0}{2}(1 - e^{-2iC}) \tag{11}$$

$$U_1 := 1 - \frac{\bar{M}_1}{2}(1 - e^{-2iC}) \tag{12}$$

The final evolution operator is a product of the two. Note: since we have decided to bear with the error involved in neglected the second order (in C) terms, it does not matter in what order we take the product but we have to preserve the order through after deciding since U_0 and U_1 do not commute.

$$
\begin{aligned}
P &:= U_0U_1 = 1-\frac{(M_0+M_1)}{2}K+\frac{M_0M_1}{2}K^2 \\
\text{where}: \quad K &:= (1-e^{-2iC}) \\
\Rightarrow \quad P &= 1-\frac{\bar{M}}{2}K+\frac{M_0M_1}{2}K^2 \\
\text{with}: \quad \bar{M}_0\psi_x &= \psi_x-\psi_{x+(-1)^x} \\
\bar{M}_1\psi_x &= \psi_x-\psi_{x-(-1)^x} \\
\bar{M}_0\bar{M}_1\psi_x &= \psi_x-\psi_{x+(-1)^x}-\bar{M}_0\psi_y \\
\text{with}: \quad y &= x-(-1)^x \\
\bar{M}_0\bar{M}_1\psi_x &= \psi_x-\psi_{x+(-1)^x}-\psi_{x-(-1)^x}-\psi_{x-2(-1)^x} \qquad (13)
\end{aligned}
$$

Here $\bar{M}$, $\bar{M}_0$ & $\bar{M}_1$ are "infinitely" large matrices, this gives a picture of 1-D unbounded quantum walk. Here we employ the same absorbing boundary conditions as described in the diffusion equation (Section 3.1).

3.2.2 Massless 1-D Dirac Equation:

We now consider 1-D Dirac equation:

$$
\begin{aligned}
\sqrt{-p_0^2+p_1^2} &= m \\
\Rightarrow \quad (-\alpha^0p_0+\alpha^1p_1)^2 &= m^2 \\
(\alpha^0)^2p_0^2+(\alpha^1)^2p_1^2 &= -p_0^2+p_1^2 \\
\Rightarrow \quad (\alpha^0)^2 &= -1 \\
(\alpha^1)^2 &= 1 \\
\alpha^0\alpha^1+\alpha^1\alpha^0 &= 0 \\
\text{consider}: \quad \alpha^0 &= i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
(\alpha^0)^2 &= -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
\text{consider}: \quad \alpha^1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
(\alpha^1)^2 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
\alpha^0\alpha^1 &= i\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\
\alpha^1\alpha^0 &= i\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}
\end{aligned}
$$

Now we choose to consider mass-less particles,

$$
\begin{aligned}
\alpha^0p_0\psi &= \alpha^1p_1\psi \\
\frac{\partial\psi}{\partial t} &= \alpha^1\alpha^0\frac{\partial\psi}{\partial x} \\
\begin{pmatrix} \frac{\partial\psi_\uparrow}{\partial t} \\ \frac{\partial\psi_\downarrow}{\partial t} \end{pmatrix} &= i\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \frac{\partial\psi_\uparrow}{\partial x} \\ \frac{\partial\psi_\downarrow}{\partial x} \end{pmatrix} \\
\begin{pmatrix} \psi_\uparrow(t+\partial t) \\ \psi_\downarrow(t+\partial t) \end{pmatrix} &= \begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix}+i\frac{\partial t}{\partial x}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\bar{M}\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix} \\
\begin{pmatrix} \psi_\uparrow(t+\partial t) \\ \psi_\downarrow(t+\partial t) \end{pmatrix} &= \begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix}+\begin{pmatrix} 0 & -i\frac{\partial t}{\partial x}\bar{M} \\ i\frac{\partial t}{\partial x}\bar{M} & 0 \end{pmatrix}\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix} \\
&= \left[\begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & \bar{\mathrm{I}} \end{pmatrix}+i\frac{\partial t}{\partial x}\begin{pmatrix} 0 & -\bar{M} \\ \bar{M} & 0 \end{pmatrix}\right]\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix}
\end{aligned}
$$

Where $\bar{M}$ is the differentiation matrix

$$\bar{M} = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & -1 & 1 & 0 & 0 & \dots \\ \dots & 0 & -1 & 1 & 0 & \dots \\ \dots & 0 & 0 & -1 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

Now, in order to make the derivative symmetric W.R.T x coordinate, we redefine the discrete derivative as:

$$\begin{aligned} f'(x) &= \frac{\left(\frac{f(x+\partial x)-f(x)}{\partial x} + \frac{f(x)-f(x-\partial x)}{\partial x}\right)}{2} \quad \text{(average of LHD \& RHD)} \\ \Rightarrow \quad f'(x) &= \frac{f(x+\partial x)-f(x-\partial x)}{2\partial x} \end{aligned}$$

Now the Matrix,

$$\bar{M} = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & 1 & 0 & 0 & 0 & \dots \\ \dots & -1 & 0 & 1 & 0 & 0 & \dots \\ \dots & 0 & -1 & 0 & 1 & 0 & \dots \\ \dots & 0 & 0 & -1 & \ddots & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \ddots & \dots \end{pmatrix}$$

$$\text{therefore}: \quad \bar{M} = \bar{M}_0 + \bar{M}_1$$

$$\text{where}: \quad \bar{M}_0 = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & 1 & 0 & 0 & 0 & \dots \\ \dots & -1 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 1 & 0 & \dots \\ \dots & 0 & 0 & -1 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

$$\bar{M}_1 = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & 0 & 0 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 1 & 0 & 0 & \dots \\ \dots & 0 & -1 & 0 & 0 & 0 & \dots \\ \dots & 0 & 0 & 0 & 0 & 1 & \dots \\ \dots & 0 & 0 & 0 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

now, $\bar{M}_0$ and $\bar{M}_1$ have the property:

$$\begin{aligned} \bar{M}_0^2 &= -\bar{\mathrm{I}} \\ \bar{M}_1^2 &= -\bar{\mathrm{I}} \end{aligned}$$

$$
\begin{aligned}
\text{Define}: \quad \bar{C} &:= \begin{pmatrix} 0 & -\bar{M} \\ \bar{M} & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\bar{M}_0 \\ \bar{M}_0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -\bar{M}_1 \\ \bar{M}_1 & 0 \end{pmatrix} \\
\bar{C}_0 &:= \begin{pmatrix} 0 & -\bar{M}_0 \\ \bar{M}_0 & 0 \end{pmatrix} \\
\bar{C}_1 &:= \begin{pmatrix} 0 & -\bar{M}_1 \\ \bar{M}_1 & 0 \end{pmatrix} \\
\text{again, we can notice:} \quad \bar{C}_0^2 &= \begin{pmatrix} -\bar{M}_0^2 & 0 \\ 0 & -\bar{M}_0^2 \end{pmatrix} = \begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & \bar{\mathrm{I}} \end{pmatrix} = \bar{\mathrm{I}} \\
\text{similarly}: \quad \bar{C}_1^2 &= \bar{\mathrm{I}} \\
\text{We wish to evaluate} \quad :- \quad e^{i\bar{C}\frac{\partial t}{\partial x}} &\approx e^{i\bar{C}_0\frac{\partial t}{\partial x}} e^{i\bar{C}_1\frac{\partial t}{\partial x}} \\
&= \left[\left\{ \bar{\mathrm{I}} - \frac{\left(\bar{C}_0\frac{\partial t}{\partial x}\right)^2}{2!} + \frac{\left(\bar{C}_0\frac{\partial t}{\partial x}\right)^4}{4!} \ldots \right\} + i \left\{ \bar{C}_0\frac{\partial t}{\partial x} - \frac{\left(\bar{C}_0\frac{\partial t}{\partial x}\right)^3}{3!} \ldots \right\} \right] [\ldots] \\
&= \left[\bar{\mathrm{I}} \left\{ 1 - \frac{\left(\frac{\partial t}{\partial x}\right)^2}{2!} + \frac{\left(\frac{\partial t}{\partial x}\right)^4}{4!} \ldots \right\} + i\bar{C}_0 \left\{ \frac{\partial t}{\partial x} - \frac{\left(\frac{\partial t}{\partial x}\right)^3}{3!} \ldots \right\} \right] [\ldots] \\
&= \left[\cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} + i\sin\left(\frac{\partial t}{\partial x}\right)\bar{C}_0 \right] \left[\cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} + i\sin\left(\frac{\partial t}{\partial x}\right)\bar{C}_1 \right] \\
\text{define}: \quad \bar{U}_0 &:= \begin{pmatrix} \cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} & 0 \\ 0 & \cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} \end{pmatrix} + \begin{pmatrix} 0 & -i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_0 \\ i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_0 & 0 \end{pmatrix} \\
\Rightarrow \quad \bar{U}_0 &= \begin{pmatrix} \cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} & -i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_0 \\ i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_0 & \cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} \end{pmatrix} \\
\text{similarly}: \quad \bar{U}_1 &= \begin{pmatrix} \cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} & -i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_1 \\ i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_1 & \cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} \end{pmatrix}
\end{aligned}
$$

Now, we consider how these operators act on the wave-functions,

$$
\begin{aligned}
\bar{U}_0\vec{\psi} &= \begin{pmatrix} \cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} & -i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_0 \\ i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_0 & \cos\left(\frac{\partial t}{\partial x}\right)\bar{\mathrm{I}} \end{pmatrix} \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \\
&= \begin{pmatrix} \cos\left(\frac{\partial t}{\partial x}\right)\psi_\uparrow - i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_0\psi_\downarrow \\ \cos\left(\frac{\partial t}{\partial x}\right)\psi_\downarrow + i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_0\psi_\uparrow \end{pmatrix} \\
\text{similarly}: \quad \bar{U}_1\vec{\psi} &= \begin{pmatrix} \cos\left(\frac{\partial t}{\partial x}\right)\psi_\uparrow - i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_1\psi_\downarrow \\ \cos\left(\frac{\partial t}{\partial x}\right)\psi_\downarrow + i\sin\left(\frac{\partial t}{\partial x}\right)\bar{M}_1\psi_\uparrow \end{pmatrix}
\end{aligned}
$$

we now consider $\bar{M}\psi$,

$$
\begin{aligned}
(\bar{M}_0)_{x,\tilde{x}}\psi_{\tilde{x}} &= (-1)^{(\tilde{x})}\psi_{[\tilde{x}+(-1)^{(\tilde{x})}]} \\
(\bar{M}_1)_{x,\tilde{x}}\psi_{\tilde{x}} &= (-1)^{(\tilde{x}+1)}\psi_{[\tilde{x}+(-1)^{(\tilde{x}+1)}]}
\end{aligned}
$$

3.2.3 Maxwell's equation:

We will use some of the methods discussed in [20]

$$\vec{\nabla}\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$
$$\vec{\nabla}\times\vec{B} = \frac{1}{c^2}\frac{\partial\vec{E}}{\partial t}$$
$$\overline{(\vec{\nabla}\times)} = \begin{pmatrix} 0 & \frac{-\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & \frac{-\partial}{\partial x} \\ \frac{-\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{-\partial}{\partial x} \\ 0 & \frac{\partial}{\partial x} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \frac{\partial}{\partial y} \\ 0 & 0 & 0 \\ \frac{-\partial}{\partial y} & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & \frac{-\partial}{\partial z} & 0 \\ \frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\bar{M}_1 := \frac{1}{dx}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\bar{M}_x \\ 0 & \bar{M}_x & 0 \end{pmatrix}^2$$
$$\Rightarrow \quad \bar{M}_1 = -\bar{M}_x^2\frac{1}{dx^2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\bar{M}_2 := \frac{1}{dy}\begin{pmatrix} 0 & 0 & \bar{M}_y \\ 0 & 0 & 0 \\ -\bar{M}_y & 0 & 0 \end{pmatrix}$$
$$\Rightarrow \quad \bar{M}_2^2 = -\bar{M}_y^2\frac{1}{dy^2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\bar{M}_3 := \frac{1}{dz}\begin{pmatrix} 0 & -\bar{M}_z & 0 \\ \bar{M}_z & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\Rightarrow \quad \bar{M}_3^2 = -\bar{M}_z^2\frac{1}{dz^2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
:

(Here $\bar{M}_x, \ldots$ are the derivative matrices as was defined and used in the previous cases)

$$\bar{M}_x = \bar{M}_y = \bar{M}_z = \begin{pmatrix} \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & -1 & 0 & 1 & 0 & 0 & \ldots \\ \ldots & 0 & -1 & 0 & 1 & 0 & \ldots \\ \ldots & 0 & 0 & -1 & 0 & 1 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}$$

(Note: $\bar{M}_x, \bar{M}_y, \bar{M}_z$ act on different spatial component of $\vec{v}$)

$$\text{note}: \quad \bar{M}_x^T = -\bar{M}_x$$

and so on. The results used here are same as the ones used for Dirac Equation

$$\text{Therefore}: \quad \overline{(\vec{\nabla}\times)}^T = \begin{pmatrix} 0 & \frac{\bar{M}_z^T}{\partial z} & \frac{-\bar{M}_y^T}{\partial y} \\ \frac{-\bar{M}_z^T}{\partial z} & 0 & \frac{\bar{M}_x^T}{\partial x} \\ \frac{\bar{M}_y^T}{\partial y} & \frac{-\bar{M}_x^T}{\partial x} & 0 \end{pmatrix} = \overline{(\vec{\nabla}\times)}$$
$$\text{consider}: \quad \vec{v} := \begin{pmatrix} E_x \\ E_y \\ E_z \\ c^2B_x \\ c^2B_y \\ c^2B_z \end{pmatrix}$$
$$\vec{v}(t+\partial t) = \vec{v}(t) + \begin{pmatrix} 0 & \overline{\nabla\times} \\ -\overline{\nabla\times} & 0 \end{pmatrix}\vec{v}(t)\partial t$$
$$\text{define}: \quad \bar{H} = \begin{pmatrix} 0 & \overline{\nabla\times} \\ -\overline{\nabla\times} & 0 \end{pmatrix}$$
$$\bar{H}^\dagger = \bar{H}^T = \begin{pmatrix} 0 & -\overline{\nabla\times} \\ \overline{\nabla\times} & 0 \end{pmatrix} = -\bar{H}$$
$$\Rightarrow \quad e^{\bar{H}t} \text{ is unitary}$$

$$
\begin{aligned}
\bar{H} &= \begin{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} & -\begin{pmatrix} 0 & \frac{-\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & \frac{-\partial}{\partial x} \\ \frac{-\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & \frac{-\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & \frac{-\partial}{\partial x} \\ \frac{-\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\bar{M}_z}{\partial z} & -\frac{\bar{M}_y}{\partial y} \\ 0 & 0 & 0 & -\frac{\bar{M}_z}{\partial z} & 0 & \frac{\bar{M}_x}{\partial x} \\ 0 & 0 & 0 & \frac{\bar{M}_y}{\partial y} & -\frac{\bar{M}_x}{\partial x} & 0 \\ 0 & -\frac{\bar{M}_z}{\partial z} & \frac{\bar{M}_y}{\partial y} & 0 & 0 & 0 \\ \frac{\bar{M}_z}{\partial z} & 0 & -\frac{\bar{M}_x}{\partial x} & 0 & 0 & 0 \\ -\frac{\bar{M}_y}{\partial y} & \frac{\bar{M}_x}{\partial x} & 0 & 0 & 0 & 0 \end{pmatrix} \\
\bar{H}_{xe} &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\bar{M}_{xe}}{\partial x} \\ 0 & 0 & 0 & 0 & -\frac{\bar{M}_{xe}}{\partial x} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\bar{M}_{xe}}{\partial x} & 0 & 0 & 0 \\ 0 & \frac{\bar{M}_{xe}}{\partial x} & 0 & 0 & 0 & 0 \end{pmatrix} \\
&= \frac{\bar{M}_{xe}}{\partial x} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} := \frac{\bar{M}_{xe}\bar{N}_{xe}}{\partial x} \\
\bar{N}^2_{xe} &= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \\
\bar{H}^2_{xe} &= \frac{\bar{M}^2_{xe}}{\partial x^2}\bar{N}^2_{xe} \\
&= -\frac{\bar{\mathrm{I}}}{\partial x^2}\bar{N}^2_{xe} \\
&= -\frac{\bar{\mathrm{I}}}{\partial x^2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \\
\bar{H}^{2n}_{xe} &= \left[\frac{\bar{\mathrm{I}}}{\partial x^2} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \right]^n
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{(-1)^n \bar{\mathrm{I}}}{\partial x^{2n}} \begin{pmatrix} 0&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \end{pmatrix} \\
&:= \frac{(-1)^n \bar{\mathrm{I}} \bar{P}_{xe}}{\partial x^{2n}} \\
\text{define:}\quad \bar{P}_{xe} &= \begin{pmatrix} 0&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \end{pmatrix} \\
\bar{H}^{2n+1}_{xe} &= \frac{(-1)^n \bar{M}_{xe} \bar{N}_{xe}}{\partial x^{2n+1}} \\
\bar{H}^{2n}_{xe} &= \frac{(-1)^n \bar{P}_{xe}}{\partial x^{2n}} \\
e^{\partial t H_{xe}} &= \bar{\mathrm{I}}_{6\times 6} + \bar{H}_{xe}\partial t + \frac{\bar{H}^3_{xe}}{3!}\partial t^3 + \frac{\bar{H}^5_{xe}}{5!}\partial t^5 + \ldots + \frac{\bar{H}^2_{xe}}{2!}\partial t^2 + \frac{\bar{H}^4_{xe}}{4!}\partial t^4 + \frac{\bar{H}^6_{xe}}{6!}\partial t^6 + \ldots \\
e^{\partial t H_{xe}} &= \bar{\mathrm{I}}_{6\times 6} + \left[\sum_{n=0}^{n=\infty}\left(\frac{\bar{H}^{2n+1}_{xe}\partial t^{2n+1}}{(2n+1)!}\right)\right] + \left[\sum_{n=1}^{n=\infty}\left(\frac{\bar{H}^{2n}_{xe}\partial t^{2n}}{(2n)!}\right)\right] \\
e^{\partial t H_{xe}} &= \bar{\mathrm{I}}_{6\times 6} + \bar{M}_{xe}\bar{N}_{xe}\left[\sum_{n=0}^{n=\infty}\left(\frac{(-1)^n}{\partial x^{2n+1}}\frac{\partial t^{2n+1}}{(2n+1)!}\right)\right] + \bar{P}_{xe}\left[\sum_{n=1}^{n=\infty}\left(\frac{(-1)^n}{\partial x^{2n}}\frac{\partial t^{2n}}{(2n)!}\right)\right] \\
e^{\partial t H_{xe}} &= \bar{\mathrm{I}}_{6\times 6} + \bar{M}_{xe}\bar{N}_{xe}\sin\left(\frac{\partial t}{\partial x}\right) + \bar{P}_{xe}\left[\cos\left(\frac{\partial t}{\partial x}\right) - 1\right] \\
e^{\partial t H_{xe}} &= \begin{pmatrix} 1&0&0&0&0&0 \\ 0&\cos\left(\frac{\partial t}{\partial x}\right)&0&0&0&0 \\ 0&0&\cos\left(\frac{\partial t}{\partial x}\right)&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&0&0&\cos\left(\frac{\partial t}{\partial x}\right)&0 \\ 0&0&0&0&0&\cos\left(\frac{\partial t}{\partial x}\right) \end{pmatrix} \\
&\quad + \begin{pmatrix} 0&0&0&0&0&0 \\ 0&0&0&0&0&\bar{M}_{xe}\sin\left(\frac{\partial t}{\partial x}\right) \\ 0&0&0&0&-\bar{M}_{xe}\sin\left(\frac{\partial t}{\partial x}\right)&0 \\ 0&0&0&0&0&0 \\ 0&0&-\bar{M}_{xe}\sin\left(\frac{\partial t}{\partial x}\right)&0&0&0 \\ 0&\bar{M}_{xe}\sin\left(\frac{\partial t}{\partial x}\right)&0&0&0&0 \end{pmatrix} \\
\bar{U}_{xe} := e^{\partial t H_{xe}} &= \begin{pmatrix} 1&0&0&0&0&0 \\ 0&\cos\left(\frac{\partial t}{\partial x}\right)&0&0&0&\bar{M}_{xe}\sin\left(\frac{\partial t}{\partial x}\right) \\ 0&0&\cos\left(\frac{\partial t}{\partial x}\right)&0&-\bar{M}_{xe}\sin\left(\frac{\partial t}{\partial x}\right)&0 \\ 0&0&0&1&0&0 \\ 0&0&-\bar{M}_{xe}\sin\left(\frac{\partial t}{\partial x}\right)&0&\cos\left(\frac{\partial t}{\partial x}\right)&0 \\ 0&\bar{M}_{xe}\sin\left(\frac{\partial t}{\partial x}\right)&0&0&0&\cos\left(\frac{\partial t}{\partial x}\right) \end{pmatrix} \\
\text{Similarly:}\quad \bar{U}_{ye} &= \begin{pmatrix} \cos\left(\frac{\partial t}{\partial x}\right)&0&0&0&0&\bar{M}_{ye}\sin\left(\frac{\partial t}{\partial x}\right) \\ 0&1&0&0&0&0 \\ 0&0&\cos\left(\frac{\partial t}{\partial x}\right)&-\bar{M}_{ye}\sin\left(\frac{\partial t}{\partial x}\right)&0&0 \\ 0&0&-\bar{M}_{ye}\sin\left(\frac{\partial t}{\partial x}\right)&\cos\left(\frac{\partial t}{\partial x}\right)&0&0 \\ 0&0&0&0&1&0 \\ \bar{M}_{ye}\sin\left(\frac{\partial t}{\partial x}\right)&0&0&0&0&\cos\left(\frac{\partial t}{\partial x}\right) \end{pmatrix} \\
&\ldots
\end{aligned}
$$

similarly all other operators can be solved, this method is unconditionally stable and better than other simpler methods like finite difference time domain.

3.3 Higher order corrections

During the simplification, we had used the approximation $e^{(M_1+M_2)t} \approx e^{M_1 t} e^{M_2 t}$ and neglected the higher order corrections. The expression accurate to second order turns out to be [21]: $e^{M_1 \frac{t}{2}} e^{M_2 t} e^{M_1 \frac{t}{2}} := S(\Delta t)$, so:

$$\begin{aligned} e^{(M_1+M_2)t} &= S(\Delta t) + O(\Delta t^3) \\ \text{we now let:} \quad S_3(\Delta t) &= S(s\Delta t)S((1-2s)\Delta t)S(s\Delta t) \end{aligned}$$

We now evaluate the third order term $O(\Delta t^3)$ using the Baker-Campbell Hausdorff formula and and solve for s such that the terms go to 0, we can then repeat this procedure recursively to obtain terms to arbitrary orders. For third order, s turns out to be [21]: $\frac{1}{2-(2)^{\frac{1}{3}}}$

3.4 Estimation of error:

There are two main approximations we have used in this method, we first look at the approximation involved due to numerical differentiation using Taylor series:

$$\begin{aligned} f(x+h) - f(x) &= f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \frac{f''''(x)h^4}{4!} + \frac{f'''''(x)h^5}{5!} + \dots \\ f(x-h) - f(x) &= -f'(x)h + \frac{f''(x)h^2}{2!} - \frac{f'''(x)h^3}{3!} + \frac{f''''(x)h^4}{4!} - \frac{f'''''(x)h^5}{5!} + \dots \\ &\text{(adding the 2 equations)} \\ f''(x) &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \frac{f''''(x)h^4}{4!} + \dots \\ &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^4) \end{aligned}$$

Using the 2nd order expression from the previous section (3.3), we get the overall error to be 4th order in space and 3rd order in time.

$$\begin{aligned} e^{i\Delta t \nabla^2} &= e^{i\Delta t (M_1+M_2+O(\Delta x)^4)} = e^{i\Delta t \frac{(M_1+M_2)}{2}} e^{i\Delta t (O(\Delta x)^4) I} e^{i\Delta t \frac{(M_1+M_2)}{2}} + O(\Delta t^3) \\ &\text{Note: identity matrix } I \text{ commutes with every matrix and hence the middle exponent can be moved.} \\ &= e^{i\Delta t (M_1+M_2)} e^{i\Delta t (O(\Delta x)^4) I} + O(\Delta t^3) \\ &\approx e^{i\Delta t (M_1+M_2)} I(1 + i\Delta t (O(\Delta x)^4)) + O(\Delta t^3) \\ &= e^{i\Delta t (M_1+M_2)} + e^{i\Delta t (M_1+M_2)} i\Delta t (O(\Delta x)^4) + O(\Delta t^3) \end{aligned}$$

Using the parameters which will be discussed later, $\Delta x \approx \frac{1}{4000}$ and $\Delta t \approx 4 \times 10^{-6}$, we will assume that the coefficients appearing next to the terms are identity just to get an approximate order of magnitude of the error ($O(\Delta x^4) \approx \Delta x^4$) the relative error of the operator in each step comes out to be:

$$\begin{aligned} \Delta t \Delta x^4 + O(\Delta t^3) e^{-i\Delta t (M_1+M_2)} &= \Delta t \Delta x^4 + \Delta t^3 (1 - i\Delta t (M_1+M_2)) \\ &\approx \Delta t \Delta x^4 + \Delta t^3 + \Delta t^4 i (M_1+M_2) \end{aligned}$$

In the last step, we have assumed that errors always add, this gives us a better estimate of the worst case error, hence the sign flip. the term $\Delta t^4 i(M_1+M_2)$ is difficult to evaluate and also an order higher in Δt compared to the second term, also note that Δt is chosen to be much smaller than Δx hence, with some precaution, we can further drop $\Delta t^4 i(M_1+M_2)$, hence the final error term we get turns out to be: $\Delta t \Delta x^4 + \Delta t^3$, this gives us an error estimate of 10^{-18} at each step, but when we integrate this from 0 to $\frac{1}{\Delta t}$, and assume an estimate for the errors propagating along x at each step of the integration to be $\approx \Delta x$ we end up with much higher error due to the repeated approximation at each step, this gives an error of $\approx 10^{-9}$ this turns out to be an optimistic case where we had implicitly assumed that $O(\Delta x) \approx \Delta x$ and similarly for Δt, clearly these approximations break down with increasing frequency.

3.5 Advantages and disadvantages

As could be seen from the derivation (eq.10), since we obtained the final evolution operator by exponentiating a Hermitian matrix(eq.10), it is guaranteed to be unitary, so they provide an unconditionally stable (as shown in eq.9, finite difference method cannot conserve probability for finitely large discretization steps. but eq.10 guarantees the time evolution to be unitary irrespective of the discretization step size.) method for solving the Schrodinger, Dirac and Maxwell's equations (some of the more popular methods like finite difference time domain methods for solving the Maxwell's equations and symplectic integration for simulating Hamiltonian dynamics are not unconditionally stable (the size of discretization steps need to satisfy certain conditions or inequalities)).

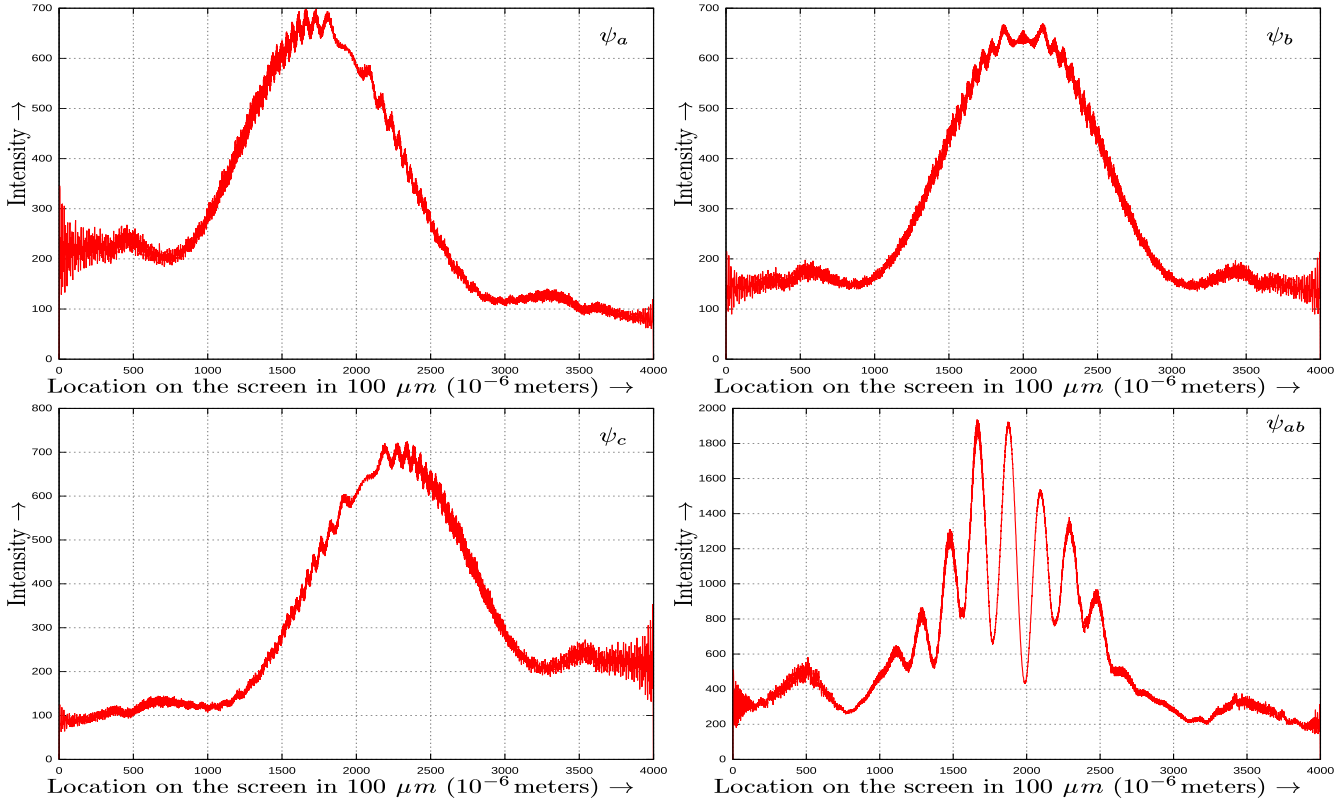
Care has to be taken when extending this method for other PDEs as the main advantage of this method (unconditional stability) may not hold (as can be seen from (Section 6.2.1: Massive Dirac Equation) and (Section 6.2.2: general wave equation)) if we are not exponentiating a Hermitian matrix.

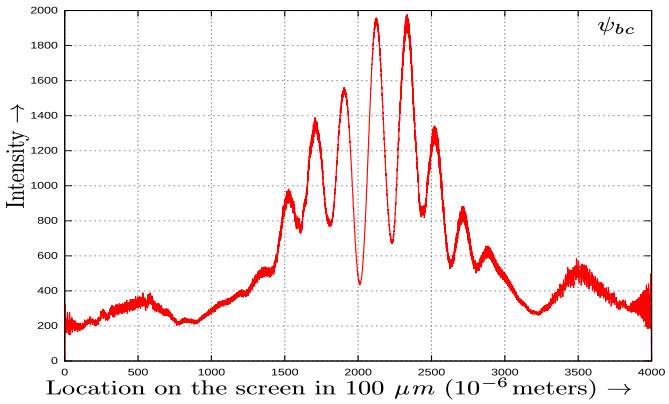
3.6 Sample results from these calculations:

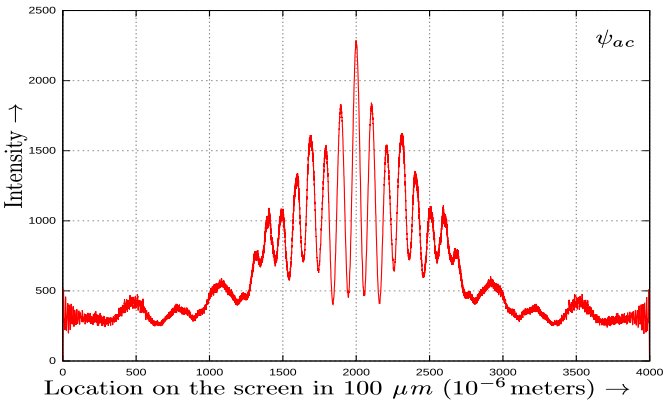
As highlighted in the previous chapter (Section 2.2), the kind of methods presented in this chapter do not work well when the length scales involved are much larger than the wavelength due the high computational memory and processing requirements (this can be seen from [18], [4]) and hence we are restricted to the cases where the wavelengths are large.

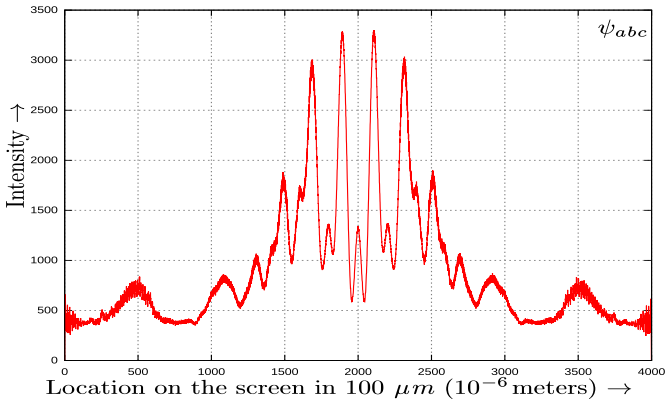
The values for various parameters used during this simulation are as follows:

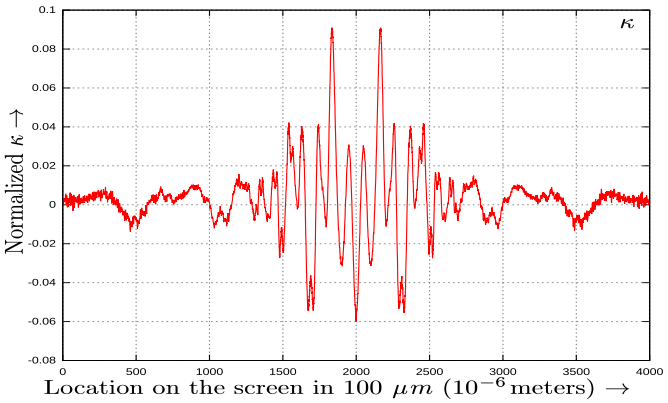
$$\begin{aligned} \text{Wavelength}: \quad \lambda &= 4\times10^{-4}m \\ \text{Distance between source and slit}: \quad l_1 &= 4\times10^{-2}m \\ \text{Distance between slit and screen}: \quad l_2 &= 16\times10^{-2}m \\ \text{Slit width}: \quad w &= 11\times10^{-4}m \\ \text{Inter-slit distance}: \quad d &= 50\times10^{-4}m \end{aligned}$$




ψ_{bc}
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →


ψ_{ac}
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →


ψ_{abc}
Intensity →
Location on the screen in 100 μm (10^{-6} meters) →


κ
Normalized κ →
Location on the screen in 100 μm (10^{-6} meters) →

Chapter 4

4 Comparison of the path-integral approach with the quantum-walk method

It does not make much sense in comparing the actual intensities between the methods presented in the previous two chapters as the cases are completely different (please refer Section 4.1). So we now try and find the limits where they correspond to each other. For this we need a parameter which can effectively quantify the difference between the two methods and preferably be independent of the intensity of the sources, by definition (eq.2), κ is independent of the intensities of the sources (due to the denominator) and it is exactly the parameter we were interested in so far. From this point onwards we will use κ (eq.2) as the main parameter to quantify the two methods.

4.1 Issues to be considered for comparing the two methods:

1. The method presented in (Chapter 2) involved the assumption of steady state, hence the first step in determining the domain in which both the methods are valid is to have a steady source in the method presented in (Chapter 3). This also forces us to run the simulations for a very long time (as the solution should reach steady state).

2. For the method presented in the (Chapter 3), we choose to work in two spatial dimensions to avoid high computational requirements, but the method presented in (Chapter 2) does not work for two spatial dimensions (please look at the note before eq.**??** of Section 2.3.1). Hence we use large slit height (perpendicular to the plane of the Figure 4) compared to slit widths.

3. Even after restricting to two spatial dimensions, the amount of computational power required for the complete simulation (using the method presented in Chapter 3) is huge (similar to the methods presented in [18], [4]) so this method is applicable only when the wavelength of the radiation used is not too small compared with the length scales of the system. This further restricts the domain in which both the methods are practically applicable.

4.2 Details of the simulation:

We will now try and compare the two methods in the domain where they can be compared, the method presented in (Chapter 3) allows us to obtain $\psi(t,x,y)$ given $\psi(t_0,x,y)$, the source can be treated as $\psi_i(t,x,y)$ which is localized in a small neighborhood around the point where we want the source to be and 0 everywhere else, here i represents the time when we want to introduce the wave-function of the source.

A steady source can be modeled by adding $\psi_i(t,x,y)$ at each iteration (time step) to the solution, so each iteration will look like (we will be using the conventions as defined in eq.10 and eq.13):

$$\begin{aligned}\vec{\psi}(t+\Delta t) &= \bar{M}_0\bar{M}_1\vec{\psi}(t)+\vec{\psi}_s\\ &\quad \text{Since we have assumed the source is steady, } \vec{\psi}_s := \vec{\psi}_i(t) \text{ is a constant with time}\end{aligned}$$

4.2.1 Modeling the detector:

The simplest way to model the detector is to graph $|\psi(t,x,y)|^2$ as a function of detector position as was followed so far. Practically though, a particle once detected at the screen will contribute to all future observations of the pattern on the screen, hence we should actually consider the time integral of the solution:

$$\int_{t\in[0,t_f]}\int_{x\in\left[s_x-\frac{\Delta x}{2},s_x+\frac{\Delta x}{2}\right]}\int_{y\in S_y}|\psi(t,x,y)|^2\,dx\,dy\,dt$$

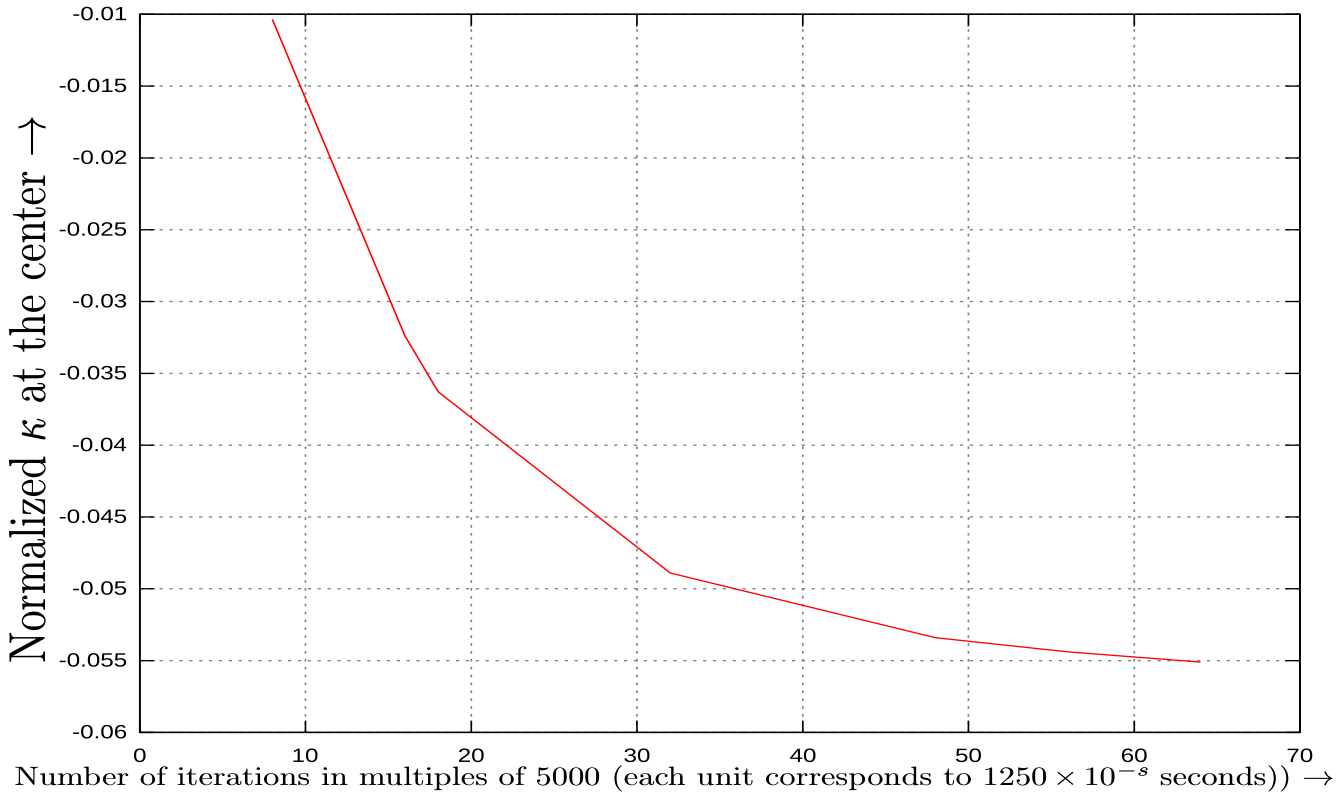
where:

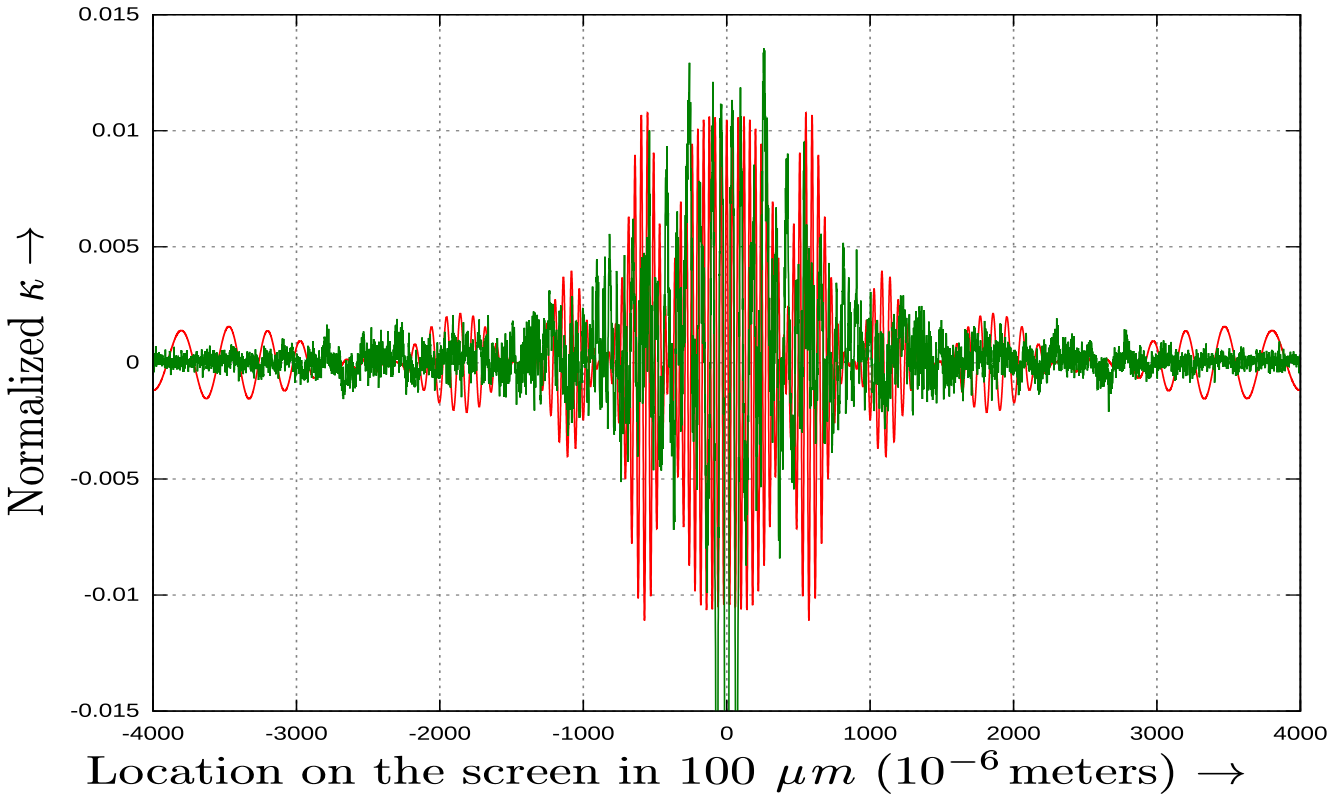
$$\begin{aligned}t_f &:= \text{total time that the simulation was run for.}\\ s_x &:= x \text{ coordinate of the screen.}\\ \Delta x &:= \text{the discretisation steps used in the simulation for } x \text{ coordinate.}\\ \Delta y &:= \text{the discretisation steps used in the simulation for } y \text{ coordinate.}\\ S_y &:= \text{the span of the detector in } y \text{ coordinate, unlike } s_x \text{ which was a single number, this is a set.}\end{aligned}$$

(The issues presented so far were considered in obtaining the results presented in Section 3.6)

4.3 Results:

We will now present the results of the comparison.





This graph was evaluated using the parameters:

$$\begin{aligned}
\text{Wavelength:} \quad \lambda &= 4 \times 10^{-4} m \\
\text{Slit width:} \quad w &= 20 \times 10^{-4} m \\
\text{Inter-slit distance:} \quad d &= 200 \times 10^{-4} m \\
\text{distance between source and slit:} \quad l_1 &= 2000 \times 10^{-4} m \\
\text{distance between slit and screen:} \quad l_2 &= 2000 \times 10^{-4} m
\end{aligned}$$

Chapter 5

5 Conclusion and Discussion

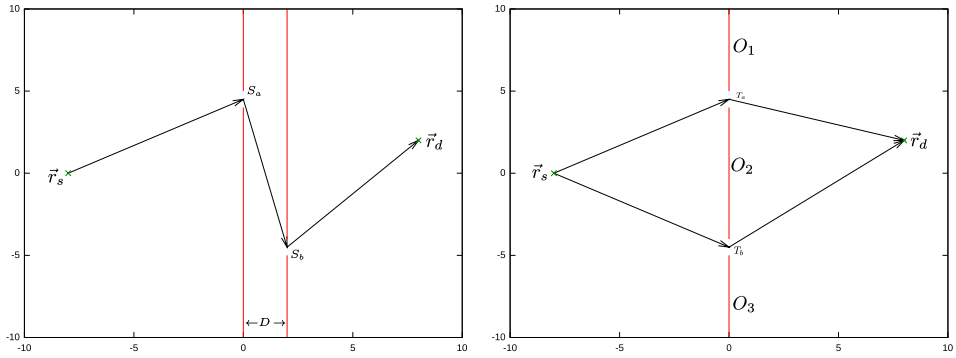
We have presented two detailed methods in which some of the interesting property of the multi-slit interference system can be analyzed, this also provides a fertile ground for testing various alternative theories in the foundations of quantum mechanics [1]. In reference [6] the κ parameter was used as a measure of the presence or absence of higher order interference in quantum mechanics as per reference [1]. the error bound in the experiment was higher than the accuracy required to be able to comment on the current theory. a more precise version of the same experiment could serve as a perfect table top demo of the current theory. As pointed out in [2], it would be interesting to perform this experiment in the microwave domain, which is currently underway at RRI.

6 Appendices:

6.1 Appendix to chapter 2:

6.1.1 Babinet's principle

Consider the system as shown as shown in Fig.5(a)



(a) 2D cross-section of the system, the slit planes extend to infinity and S_a, S_b are sets representing the transparent portions

(b) figure denoting the domains used for the integration

Figure 5: figures illustrating the system considered for Babinet's principle

The contribution to $\vec{r}_d$ due to a source at $\vec{r}_s$ is given by: (please note: through this section, the definition (eq.**??**) is used for G)

$$\psi(\vec{r}_d) = \int_{\vec{r}_1 \in S_a} \int_{\vec{r}_2 \in S_b} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_2) G(\vec{r}_2 - \vec{r}_d) d\vec{r}_1 d\vec{r}_2$$

With, $\lim D \to 0$, this reduces to the integral of second order corrections (eq.5).

For the simple case of double slit diffraction (without the higher order correction), the Babinet's principle states that the sum of the pattern due to slits and slots (opaque portions of the slit plane) give identity (no slit plane), consider the system as shown in Fig.5(b) (Here the slit plane extends till infinity, T_a and T_b represents the transparent parts of the slit plane and O_1, O_2, O_3 represent the opaque parts of the slit plane, also $T_a \bigcap O_2 = \phi$ and so on for other domains). We now have (to first order):

$$\begin{aligned} G(\vec{r}_s - \vec{r}_d) = & \int_{\vec{r}_1 \in O_1} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 + \int_{\vec{r}_1 \in O_2} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 \\ & + \int_{\vec{r}_1 \in O_3} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 + \int_{\vec{r}_1 \in T_a} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 \\ & + \int_{\vec{r}_1 \in T_b} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 \end{aligned}$$

So, in case we were to flip the transparent and opaque parts of the slit plane, then (to first order):

$$\begin{aligned} \psi(\vec{r}_d) = & \int_{\vec{r}_1 \in O_1} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 + \int_{\vec{r}_1 \in O_2} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 \\ & + \int_{\vec{r}_1 \in O_3} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 \\ \psi(\vec{r}_d) = & G(\vec{r}_s - \vec{r}_d) - \left(\int_{\vec{r}_1 \in T_a} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 + \int_{\vec{r}_1 \in T_b} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_d) d\vec{r}_1 \right) \end{aligned} \quad (14)$$

We now wish to evaluate this to second order, we consider a situation similar to (Fig.5(a)) except the opaque and transparent portions are flipped as shown in Fig.6.

We again let $\lim D \to 0$, this gives us the second order corrections:

$$\Psi_2(\vec{r}_d) = -\int_{\vec{r}_1 \in S_a} \int_{\vec{r}_2 \in S_b} G(\vec{r}_s - \vec{r}_1) G(\vec{r}_1 - \vec{r}_2) G(\vec{r}_2 - \vec{r}_d) (d\vec{r}_1)(d\vec{r}_2)$$

and similarly for the other slit.

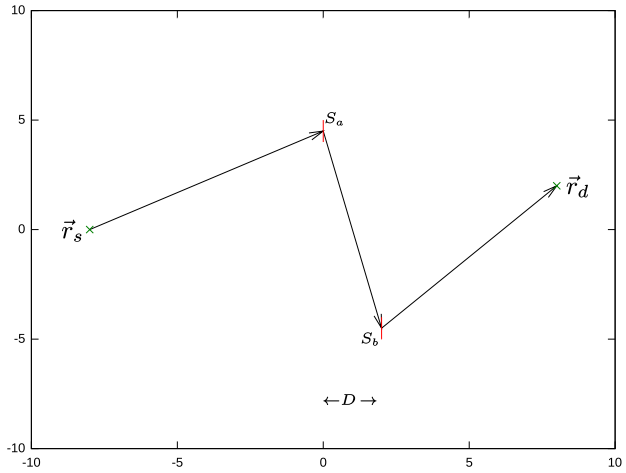


Figure 6: Figure depicting the portion which needs to be subtracted for obtaining the second order corrections

And the complete wave function accurate to second order is given by:

$$\begin{aligned}\psi(\vec{r}_d) &= G(\vec{r}_s-\vec{r}_d)-\left(\int_{\vec{r}_1\in T_a} G(\vec{r}_s-\vec{r}_1)G(\vec{r}_1-\vec{r}_d)d\vec{r}_1+\int_{\vec{r}_1\in T_b} G(\vec{r}_s-\vec{r}_1)G(\vec{r}_1-\vec{r}_d)d\vec{r}_1\right)\\ &-\left(\int_{\vec{r}_1\in S_a}\int_{\vec{r}_2\in S_b} G(\vec{r}_s-\vec{r}_1)G(\vec{r}_1-\vec{r}_2)G(\vec{r}_2-\vec{r}_d)(d\vec{r}_1)(d\vec{r}_2)\right)\\ &-\left(\int_{\vec{r}_2\in S_a}\int_{\vec{r}_1\in S_b} G(\vec{r}_s-\vec{r}_1)G(\vec{r}_1-\vec{r}_2)G(\vec{r}_2-\vec{r}_d)(d\vec{r}_1)(d\vec{r}_2)\right)\end{aligned}$$

6.1.2 Diffusion and Schrodinger's equations:

The Diffusion (heat) equation is given by:

$$\frac{\partial\psi}{\partial t} = \frac{1}{D}\nabla^2\psi$$

The Schrodinger's equation is just a diffusion equation with an imaginary coefficient of diffusion $D=\frac{i}{\hbar^2}$

$$\begin{aligned}\text{assume}: \quad \psi &= X(\vec{x})T(t)\\ \Rightarrow \quad \frac{\partial\psi}{\partial t}-\frac{1}{D}\nabla^2\psi &= X(\vec{x})T'(t)-\frac{T(t)}{D}\nabla^2X(\vec{x}) = 0\\ 0 &= X(\vec{x})T(t)\left(\frac{T'(t)}{T(t)}-\frac{1}{D}\frac{\nabla^2X(\vec{x})}{X(\vec{x})}\right)\end{aligned}$$

Now, we can easily see that this equation too reduces to the Helmholtz's equation. We can thus use the same method as presented in Section 2.2 and Section 2.3 to solve for steady state interference solutions even in the case of Schrodinger's equation.

6.2 Appendix to Chapter 3:

6.2.1 Massive Dirac Equation:

$$
\begin{aligned}
(-\alpha^0 p_0 + \alpha^1 p_1)\psi &= m\psi \\
-i\alpha^0\hbar\frac{\partial\psi}{\partial t} + i\alpha^1\hbar\frac{\partial\psi}{\partial x} &= m\psi \\
i\hbar\frac{\partial\psi}{\partial t} + i\alpha^0\alpha^1\hbar\frac{\partial\psi}{\partial x} &= m\alpha^0\psi \\
\frac{-i}{\hbar}i\hbar\frac{\partial\psi}{\partial t} &= \frac{-i}{\hbar}m\alpha^0\psi + \frac{-i}{\hbar}i\alpha^0\alpha^1\hbar\frac{\partial\psi}{\partial x} \\
\frac{\partial\psi}{\partial t} &= \frac{-im}{\hbar}\alpha^0\psi + \alpha^0\alpha^1\frac{\partial\psi}{\partial x} \\
\psi(t+\partial t) &= \psi(t) + \frac{-im}{\hbar}\alpha^0\psi\partial t + \alpha^0\alpha^1\frac{\partial\psi}{\partial x}\partial t \\
\psi(t+\partial t) &= \bar{1}\psi(t) + \frac{-im\partial t}{\hbar}\alpha^0\psi + \frac{\partial t}{\partial x}\alpha^0\alpha^1\bar{M}\psi \\
&= \begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix}\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix} + \begin{pmatrix} \frac{m\frac{\partial t}{\partial x}}{\hbar}\bar{1} & 0 \\ 0 & -\frac{m\frac{\partial t}{\partial x}}{\hbar}\bar{1} \end{pmatrix}\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix} + \begin{pmatrix} 0 & i\frac{\partial t}{\partial x}\bar{M} \\ -i\frac{\partial t}{\partial x}\bar{M} & 0 \end{pmatrix}\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix} \\
&\quad \text{(Where } \bar{M} \text{ is the usual differentiation matrix)} \\
\psi(t+\partial t) &= \left[\begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix} + \begin{pmatrix} \frac{m\frac{\partial t}{\partial x}}{\hbar}\bar{1} & i\frac{\partial t}{\partial x}\bar{M} \\ -i\frac{\partial t}{\partial x}\bar{M} & -\frac{m\frac{\partial t}{\partial x}}{\hbar}\bar{1} \end{pmatrix}\right]\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\psi(t+\partial t) &= \left[\begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix} + \begin{pmatrix} \frac{m\frac{\partial t}{\partial x}}{\hbar}\bar{1} & i\frac{\partial t}{\partial x}\bar{M} \\ -i\frac{\partial t}{\partial x}\bar{M} & -\frac{m\frac{\partial t}{\partial x}}{\hbar}\bar{1} \end{pmatrix}\right]\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix} \\
\text{Def:}\quad \bar{C} &:= \begin{pmatrix} \frac{m\frac{\partial t}{\partial x}}{\hbar}\bar{1} & i\frac{\partial t}{\partial x}\bar{M} \\ -i\frac{\partial t}{\partial x}\bar{M} & -\frac{m\frac{\partial t}{\partial x}}{\hbar}\bar{1} \end{pmatrix} \\
\bar{C} &= \frac{m\frac{\partial t}{\partial x}}{\hbar}\begin{pmatrix} \bar{1} & 0 \\ 0 & -\bar{1} \end{pmatrix} + i\frac{\partial t}{\partial x}\begin{pmatrix} 0 & \bar{M}_0 \\ -\bar{M}_0 & 0 \end{pmatrix} + i\frac{\partial t}{\partial x}\begin{pmatrix} 0 & \bar{M}_1 \\ -\bar{M}_1 & 0 \end{pmatrix} \\
\psi(t+\partial t) &= e^{\bar{C}}\begin{pmatrix} \psi_\uparrow(t) \\ \psi_\downarrow(t) \end{pmatrix} \\
&\quad \text{(Similar to the case without mass, define)} \\
\bar{C}_0 &= i\frac{\partial t}{\partial x}\begin{pmatrix} 0 & \bar{M}_0 \\ -\bar{M}_0 & 0 \end{pmatrix} \\
\bar{C}_1 &= i\frac{\partial t}{\partial x}\begin{pmatrix} 0 & \bar{M}_1 \\ -\bar{M}_1 & 0 \end{pmatrix} \\
\text{(Extra):}\quad \bar{C}_2 &= \frac{m\frac{\partial t}{\partial x}}{\hbar}\begin{pmatrix} \bar{1} & 0 \\ 0 & -\bar{1} \end{pmatrix}
\end{aligned}
$$

Now two of the above terms can be simplified as in the previous case, we only have to deal with $\bar{C}_2$

$$
\begin{aligned}
\text{define:}\quad \bar{M}_3 &:= \begin{pmatrix} \bar{1} & 0 \\ 0 & -\bar{1} \end{pmatrix} \\
\bar{M}_3^2 &= \begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix} \\
e^{\bar{C}_2} &= \left(1 + \frac{\left(\frac{m\frac{\partial t}{\partial x}}{\hbar}\right)^2}{2!} + \frac{\left(\frac{m\frac{\partial t}{\partial x}}{\hbar}\right)^4}{4!} + \ldots\right)\begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix} + \left(\frac{\left(\frac{m\frac{\partial t}{\partial x}}{\hbar}\right)}{1!} + \frac{\left(\frac{m\frac{\partial t}{\partial x}}{\hbar}\right)^3}{3!} + \ldots\right)\begin{pmatrix} \bar{1} & 0 \\ 0 & -\bar{1} \end{pmatrix} \\
&= \cosh\left(\frac{m\frac{\partial t}{\partial x}}{\hbar}\right)\begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix} + \sinh\left(\frac{m\frac{\partial t}{\partial x}}{\hbar}\right)\begin{pmatrix} \bar{1} & 0 \\ 0 & -\bar{1} \end{pmatrix}
\end{aligned}
$$

Now two of the above terms can be simplified as in the previous case, we only have to deal with $\bar{C}_2$

$$
\begin{aligned}
\text{define}: \quad \bar{M}_3 &:= \begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & -\bar{\mathrm{I}} \end{pmatrix} \\
\bar{M}_3^2 &= \begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & \bar{\mathrm{I}} \end{pmatrix} \\
e^{\bar{C}_2} &= \left(1 + \frac{\left(m\frac{\partial t}{\partial x}\right)^2}{2!} + \frac{\left(m\frac{\partial t}{\partial x}\right)^4}{4!} + \ldots\right)\begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & \bar{\mathrm{I}} \end{pmatrix} + \left(\frac{\left(m\frac{\partial t}{\partial x}\right)}{1!} + \frac{\left(m\frac{\partial t}{\partial x}\right)^3}{3!} + \ldots\right)\begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & -\bar{\mathrm{I}} \end{pmatrix} \\
&= \cosh\left(\frac{m\frac{\partial t}{\partial x}}{\hbar}\right)\begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & \bar{\mathrm{I}} \end{pmatrix} + \sinh\left(\frac{m\frac{\partial t}{\partial x}}{\hbar}\right)\begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & -\bar{\mathrm{I}} \end{pmatrix}
\end{aligned}
$$

This term is not unitary and hence it does not make sense to use this method to simulate Dirac's Equation with mass. There are other methods which give unitary evolution (and does not involve exponentiating a matrix [22]) and hence can be used to effectively apply this method to obtain an approximate solution to the time dependent Dirac equation (although the analysis presented in Section 3.4 and Section 3.3 are not applicable). At this point we are done with the discretization of the Dirac's equation.

6.2.2 Wave Equation:

Just like the previous case, it turns out that naive application of this method for the wave equation gives evolution operators which are not unitary:

$$
\begin{aligned}
\text{consider}: \quad \frac{\partial^2\psi}{\partial t^2} &= c^2\nabla^2\psi \\
\text{define}: \quad \phi &:= \frac{\partial\psi}{\partial t} \\
\text{define}: \quad \vec{v} &:= \begin{pmatrix} \phi \\ \psi \end{pmatrix} \\
\text{so}: \quad \frac{\partial\phi}{\partial t} &= c^2\nabla^2\psi \\
\frac{\partial\psi}{\partial t} &= \phi \\
\Rightarrow \quad \frac{\partial\vec{v}}{\partial t} &= \bar{H}\vec{v} \\
\text{where}: \quad \bar{H} &= \begin{pmatrix} 0 & c^2\nabla^2 \\ \bar{\mathrm{I}} & 0 \end{pmatrix} \\
\text{so}: \quad \vec{v}(t+\Delta t) &= e^{\bar{H}\Delta t}\vec{v}(t) \\
\text{discretizing}: \quad \bar{H} &= \begin{pmatrix} 0 & -c^2\bar{M}_e \\ \bar{\mathrm{I}} & 0 \end{pmatrix} + \begin{pmatrix} 0 & -c^2\bar{M}_o \\ \bar{\mathrm{I}} & 0 \end{pmatrix} \\
\text{define}: \quad \bar{H}_e &:= \begin{pmatrix} 0 & -c^2\bar{M}_e \\ \bar{\mathrm{I}} & 0 \end{pmatrix} \\
\text{define}: \quad \bar{H}_o &:= \begin{pmatrix} 0 & -c^2\bar{M}_o \\ \bar{\mathrm{I}} & 0 \end{pmatrix} \\
\text{with}: \quad \bar{M} &:= \begin{pmatrix} \ldots & -2 & 1 & 0 & 0 & \ldots \\ 0 & 1 & -2 & 1 & 0 & \ldots \\ 0 & 0 & 1 & -2 & 1 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix} \\
\bar{M} &:= -\bar{M}_e - \bar{M}_o \quad \left(- \text{ sign is chosen so that } \bar{M}_e^2 = 2M_e\right)
\end{aligned}
$$

At this point, getting the random walk is very similar to the usual cases we have worked till now.

$$
\begin{aligned}
\bar{H}^2 &= \begin{pmatrix} 0 & c^2\bar{M} \\ \bar{\mathrm{I}} & 0 \end{pmatrix}\begin{pmatrix} 0 & c^2\bar{M} \\ \bar{\mathrm{I}} & 0 \end{pmatrix} = c^2 M\begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & \bar{\mathrm{I}} \end{pmatrix} \\
\text{so}: \quad H_e^2 &= -c^2 M_e\begin{pmatrix} \bar{\mathrm{I}} & 0 \\ 0 & \bar{\mathrm{I}} \end{pmatrix} \\
\bar{U}_e &= e^{\bar{H}_e\Delta t} \\
&= \bar{\mathrm{I}} + \bar{H}_e\Delta t + \frac{(\bar{H}_e\Delta t)^2}{2!} + \frac{(\bar{H}_e\Delta t)^3}{3!} + \frac{(\bar{H}_e\Delta t)^4}{4!} + \ldots \\
&= \bar{\mathrm{I}} + \frac{(\bar{H}_e\Delta t)^2}{2!} + \frac{(\bar{H}_e\Delta t)^4}{4!} + \ldots + \frac{(\bar{H}_e\Delta t)}{1} + \frac{(\bar{H}_e\Delta t)^3}{3!} + \frac{(\bar{H}_e\Delta t)^5}{5!} + \ldots \\
&= \bar{\mathrm{I}} + \frac{(\Delta t)^2(-c^2M_e)}{2!} + \frac{(\Delta t)^4(c^4M_e^2)}{4!} + \ldots + \bar{H}_e\Delta t\left(\bar{\mathrm{I}} + \frac{(\Delta t)^2(-c^2M_e)}{3!} + \frac{(\Delta t)^4(c^4M_e^2)}{5!} + \ldots\right) \\
&= \left(\bar{\mathrm{I}} + \sum_{n=1}^{n=\infty}\frac{(-\Delta t^2c^2)^nM_e^n}{(2n)!}\right) + \bar{H}_e\Delta t\left(\bar{\mathrm{I}} + \sum_{n=1}^{n=\infty}\frac{(-c^2\Delta t^2)^n\bar{M}_e^n}{(2n+1)!}\right) \\
&= \left(\bar{\mathrm{I}} + \sum_{n=2}^{n=\infty}\frac{(-\Delta t^2c^2)^n2^{n-1}M_e}{(2n)!} + \frac{(-\Delta t^2c^2)M_e}{2}\right) + \bar{H}_e\Delta t\left(\bar{\mathrm{I}} + \sum_{n=2}^{n=\infty}\frac{(-c^2\Delta t^2)^n2^{n-1}\bar{M}_e}{(2n+1)!} + \frac{(-c^2\Delta t^2)\bar{M}_e}{3!}\right) \\
&= \bar{\mathrm{I}} + M_e\sum_{n=1}^{n=\infty}\frac{(-\Delta t^2c^2)^n2^{n-1}}{(2n)!} + \bar{H}_e\Delta t\left(\bar{\mathrm{I}} + \bar{M}_e\sum_{n=1}^{n=\infty}\frac{(-c^2\Delta t^2)^n2^{n-1}}{(2n+1)!}\right) \\
&= \bar{\mathrm{I}} + \frac{M_e}{2}\sum_{n=1}^{n=\infty}\frac{(-2\Delta t^2c^2)^n}{(2n)!} + \bar{H}_e\Delta t\left(\bar{\mathrm{I}} + \frac{\bar{M}_e}{2}\sum_{n=1}^{n=\infty}\frac{(-2c^2\Delta t^2)^n}{(2n+1)!}\right) \\
&= \bar{\mathrm{I}} + \frac{M_e}{2}\left(\sum_{n=1}^{n=\infty}\frac{(-1)^n\left(\sqrt{2}\Delta tc\right)^{2n}}{(2n)!}\right) + \bar{H}_e\Delta t\left(\bar{\mathrm{I}} + \frac{\bar{M}_e}{2}\left(\sum_{n=1}^{n=\infty}\frac{(-1)^n\left(\sqrt{2}c\Delta t\right)^{2n}}{(2n+1)!}\right)\right) \\
&= \bar{\mathrm{I}} + \frac{M_e}{2}\left(\sum_{n=0}^{n=\infty}\frac{(-1)^n\left(\sqrt{2}\Delta tc\right)^{2n}}{(2n)!} - 1\right) \\
&\quad + \bar{H}_e\Delta t\left(\bar{\mathrm{I}} + \frac{\bar{M}_e}{2\left(\sqrt{2}c\Delta t\right)}\left(\sum_{n=0}^{n=\infty}\frac{(-1)^n\left(\sqrt{2}c\Delta t\right)^{2n+1}}{(2n+1)!} - \left(\sqrt{2}c\Delta t\right)\right)\right) \\
U_e &= \bar{\mathrm{I}} + \bar{\mathrm{I}}\frac{M_e\left[\cos\left(\sqrt{2}\Delta tc\right) - 1\right]}{2} + \bar{H}_e\Delta t\left(\bar{\mathrm{I}} + \frac{\bar{M}_e\left[\sin\left(\sqrt{2}c\Delta t\right) - \left(\sqrt{2}c\Delta t\right)\right]}{2\left(\sqrt{2}c\Delta t\right)}\right) \\
U_o &= \bar{\mathrm{I}} + \bar{\mathrm{I}}\frac{M_o\left[\cos\left(\sqrt{2}\Delta tc\right) - 1\right]}{2} + \bar{H}_o\Delta t\left(\bar{\mathrm{I}} + \frac{\bar{M}_o\left[\sin\left(\sqrt{2}c\Delta t\right) - \left(\sqrt{2}c\Delta t\right)\right]}{2\left(\sqrt{2}c\Delta t\right)}\right) \\
&= \begin{pmatrix} \bar{\mathrm{I}} & \frac{M_o\left[\cos\left(\sqrt{2}\Delta tc\right)-1\right]}{2} \\ \frac{M_o\left[\cos\left(\sqrt{2}\Delta tc\right)-1\right]}{2} & \bar{\mathrm{I}} \end{pmatrix} \\
&\quad + \begin{pmatrix} 0 & -c^2\bar{M}_e\Delta t \\ \bar{\mathrm{I}}\Delta t & 0 \end{pmatrix}\left(\bar{\mathrm{I}} + \frac{\bar{M}_o\left[\sin\left(\sqrt{2}c\Delta t\right) - \left(\sqrt{2}c\Delta t\right)\right]}{2\left(\sqrt{2}c\Delta t\right)}\right)
\end{aligned}
$$

This again fails to provide us with an operator which is unitary. If we consider the specific case of Maxwell's equations, we will get a unitary evolution using similar approach.

6.3 Quantum Mechanics ↔ Fluid Dynamics Correspondence, attributing a particle nature to the random walk:

This correspondence is due to the De Broglie–Bohm theory [23], here we present a derivation of the correspondence [24]

We start from the time dependent Schrodinger's Equation:

$$
\begin{aligned}
i\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \\
\text{(We now perform the substitution)}: \quad \psi &= \sqrt{\rho}e^{\frac{iS}{\hbar}} \quad := \quad e^F \\
\text{where}: \quad F &= \frac{1}{2}\log_e(\rho) + \frac{iS}{\hbar} \\
\frac{\partial F}{\partial t} &= \frac{1}{2}\frac{1}{\rho}\frac{\partial\rho}{\partial t} + \frac{i}{\hbar}\frac{\partial S}{\partial t} \\
\overrightarrow{\nabla F} &= \frac{1}{2}\frac{\overrightarrow{\nabla\rho}}{\rho} + \frac{i}{\hbar}(\overrightarrow{\nabla S}) \\
\nabla\cdot(\overrightarrow{\nabla F}) &= \frac{1}{2}\frac{\nabla\cdot(\overrightarrow{\nabla\rho})}{\rho} - \frac{1}{2}\frac{(\overrightarrow{\nabla\rho})^2}{\rho^2} + \frac{i}{\hbar}\nabla\cdot(\overrightarrow{\nabla S}) \\
\nabla^2 F &= \frac{1}{2}\frac{\nabla^2\rho}{\rho} - \frac{1}{2}\frac{(\overrightarrow{\nabla\rho})^2}{\rho^2} + \frac{i}{\hbar}\nabla^2 S \\
\text{substituting}: \quad i\hbar\frac{\partial e^F}{\partial t} &= -\frac{\hbar^2}{2m}\nabla\cdot(\overrightarrow{\nabla e^F}) + Ve^F \\
i\hbar e^F\frac{\partial F}{\partial t} &= -\frac{\hbar^2}{2m}\nabla\cdot(e^F\overrightarrow{\nabla F}) + Ve^F \\
i\hbar e^F\frac{\partial F}{\partial t} &= -\frac{\hbar^2}{2m}[(\overrightarrow{\nabla e^F})\cdot\overrightarrow{\nabla F} + e^F(\nabla^2 F)] + Ve^F \\
i\hbar e^F\frac{\partial F}{\partial t} &= -\frac{\hbar^2}{2m}[e^F(\overrightarrow{\nabla F})^2 + e^F(\nabla^2 F)] + Ve^F \\
i\hbar\frac{\partial F}{\partial t} &= -\frac{\hbar^2}{2m}(\overrightarrow{\nabla F})^2 - \frac{\hbar^2}{2m}(\nabla^2 F) + V \\
i\hbar\left(\frac{1}{2}\frac{1}{\rho}\frac{\partial\rho}{\partial t} + \frac{i}{\hbar}\frac{\partial S}{\partial t}\right) &= -\frac{\hbar^2}{2m}\left(\frac{1}{2}\frac{\overrightarrow{\nabla\rho}}{\rho} + \frac{i}{\hbar}(\overrightarrow{\nabla S})\right)^2 \\
&\quad -\frac{\hbar^2}{2m}\left(\frac{1}{2}\frac{\nabla^2\rho}{\rho} - \frac{1}{2}\frac{(\overrightarrow{\nabla\rho})^2}{\rho^2} + \frac{i}{\hbar}\nabla^2 S\right) + V \\
i\hbar\frac{1}{2}\frac{1}{\rho}\frac{\partial\rho}{\partial t} + i\hbar\frac{i}{\hbar}\frac{\partial S}{\partial t} &= -\frac{\hbar^2}{2m}\left(\frac{\overrightarrow{\nabla\rho}}{2\rho}\right)^2 + \frac{\hbar^2}{2m}\left(\frac{(\overrightarrow{\nabla S})}{\hbar}\right)^2 \\
&\quad -\frac{\hbar^2}{2m}\frac{i(\overrightarrow{\nabla S})\cdot(\overrightarrow{\nabla\rho})}{\hbar\rho} - \frac{\hbar^2}{2m}\frac{1}{2}\frac{\nabla^2\rho}{\rho} \\
&\quad +\frac{\hbar^2}{2m}\frac{1}{2}\frac{(\overrightarrow{\nabla\rho})^2}{\rho^2} - \frac{\hbar^2}{2m}\frac{i}{\hbar}\nabla^2 S + V \\
\frac{i\hbar}{2\rho}\frac{\partial\rho}{\partial t} - \frac{\partial S}{\partial t} &= -\frac{\hbar^2(\overrightarrow{\nabla\rho})^2}{8m\rho^2} + \frac{\hbar^2}{4m}\frac{(\overrightarrow{\nabla\rho})^2}{\rho^2} + \frac{(\overrightarrow{\nabla S})^2}{2m} \\
&\quad -\frac{\hbar}{2m}\frac{i(\overrightarrow{\nabla S})\cdot(\overrightarrow{\nabla\rho})}{\rho} - \frac{\hbar^2}{4m}\frac{\nabla^2\rho}{\rho} - \frac{i\hbar}{2m}\nabla^2 S + V
\end{aligned}
$$

$$
\begin{aligned}
\text{imaginary}: \quad 0 &= \frac{(\overrightarrow{\nabla S})\cdot(\overrightarrow{\nabla\rho})}{m} + \frac{\rho\nabla^2 S}{m} + \frac{\partial\rho}{\partial t} \\
\text{imaginary}: \quad 0 &= \frac{\vec{\nabla}\cdot[\rho\overrightarrow{\nabla S}]}{m} + \frac{\partial\rho}{\partial t} \\
\text{real}: \quad 0 &= \frac{\partial S}{\partial t} - \frac{\hbar^2(\overrightarrow{\nabla\rho})^2}{8m\rho^2} + \frac{\hbar^2(\overrightarrow{\nabla\rho})^2}{4m\rho^2} + \frac{(\overrightarrow{\nabla S})^2}{2m} \\
&\quad -\frac{\hbar^2}{4m}\frac{\nabla^2\rho}{\rho} + V \\
\text{real}: \quad 0 &= \frac{\partial S}{\partial t} + \frac{\hbar^2(\overrightarrow{\nabla\rho})^2}{8m\rho^2} - \frac{\hbar^2}{4m}\frac{\nabla^2\rho}{\rho} + \frac{(\overrightarrow{\nabla S})^2}{2m} + V \\
\text{real}: \quad 0 &= \frac{\partial S}{\partial t} - \frac{\hbar^2}{4m}\left(\frac{\nabla^2\rho}{\rho} - \frac{\overrightarrow{\nabla\rho^2}}{2\rho^2}\right) + \frac{(\overrightarrow{\nabla S})^2}{2m} + V
\end{aligned}
$$

$$
\begin{aligned}
\text{digression}: \quad \frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} &= \frac{1}{\sqrt{\rho}}\nabla\cdot\left(\frac{1}{2\sqrt{\rho}}\overrightarrow{\nabla\rho}\right)\\
\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} &= \frac{1}{\sqrt{\rho}}\left(\frac{1}{2}\overrightarrow{(\nabla(\rho)^{-1/2})}\cdot\overrightarrow{\nabla\rho}+\frac{1}{2}\rho^{-1/2}\nabla^2\rho\right)\\
\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} &= \frac{1}{\sqrt{\rho}}\left(\frac{-1}{4}(\rho)^{-3/2}(\overrightarrow{\nabla\rho})^2+\frac{1}{2}\rho^{-1/2}\nabla^2\rho\right)\\
\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} &= \frac{1}{2}\left(\frac{\nabla^2\rho}{\rho}-\frac{\overrightarrow{\nabla\rho}^2}{2\rho^2}\right)
\end{aligned}
$$

$$
\begin{aligned}
\text{substituting in}: \quad 0 &= \frac{\partial S}{\partial t}-\frac{\hbar^2}{4m}\left(\frac{\nabla^2\rho}{\rho}-\frac{\overrightarrow{\nabla\rho}^2}{2\rho^2}\right)+\frac{(\overrightarrow{\nabla S})^2}{2m}+V\\
0 &= \frac{\partial S}{\partial t}+\frac{(\overrightarrow{\nabla S})^2}{2m}+V-\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} \qquad (15)\\
0 &= \frac{\vec{\nabla}\cdot[\rho\overrightarrow{\nabla S}]}{m}+\frac{\partial\rho}{\partial t} \qquad (16)
\end{aligned}
$$

Now, (eq.15) is very similar to the Hamilton-Jacobi equation from classical mechanics [25]. Hence we identify S with the action function, $S=\int L\,dt$, where L is the Lagrangian.

$$
\begin{aligned}
\overrightarrow{\nabla S} &= \vec{p} = m\vec{v} \quad \text{(here, } \vec{p} \text{ is the momentum of the particle and } \vec{v} \text{ its velocity.)}\\
\frac{\partial S}{\partial t} &= H \quad \text{(here, H is the hamiltonian function.)}\\
V &\Rightarrow \text{potiental}\\
\text{define}: \quad Q &:= -\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} \quad \text{(this will be referred to as the quantum potential henceforth)}
\end{aligned}
$$

Using the above results, (eq.16) can be recast as:

$$
\begin{aligned}
0 &= \frac{\vec{\nabla}\cdot[\rho\overrightarrow{\nabla S}]}{m}+\frac{\partial\rho}{\partial t} = \frac{\vec{\nabla}\cdot[\rho\vec{p}]}{m}+\frac{\partial\rho}{\partial t} = \vec{\nabla}\cdot\left(\rho\frac{\vec{p}}{m}\right)+\frac{\partial\rho}{\partial t} = \vec{\nabla}\cdot(\rho\vec{v})+\frac{\partial\rho}{\partial t} = 0\\
\Rightarrow \quad 0 &= \vec{\nabla}\cdot(\rho\vec{v})+\frac{\partial\rho}{\partial t} \quad \text{(This is nothing but the continuity equation from fluid dynamics.)}
\end{aligned}
$$

So, the system of two equations,

$$
\begin{aligned}
0 &= \frac{\vec{\nabla}\cdot[\rho\overrightarrow{\nabla S}]}{m}+\frac{\partial\rho}{\partial t}\\
0 &= \frac{\partial S}{\partial t}+\frac{(\overrightarrow{\nabla S})^2}{2m}+V-\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}
\end{aligned}
$$

should be equivalent to the Schrodinger's equation and can be interpreted as describing a fluid flowing with no pressure and viscosity but under the influence of the quantum potential Q in addition to the potential V, so we can now cast these equations in a more familiar form (we now consider only a free particle with no potential):

$$
\begin{aligned}
\left(\frac{\partial\vec{v}}{\partial t}+(\vec{v}\cdot\vec{\nabla})\vec{v}\right) &= \overrightarrow{\nabla\left(\frac{\hbar^2}{2m^2}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}\right)} \quad \rightarrow \quad \text{(Navier-Stokes equation with } V=0\text{)}\\
\frac{\partial\rho}{\partial t}+\vec{\nabla}\cdot(\rho\vec{v}) &= 0 \quad \rightarrow \quad \text{(Continuity equation)}\\
&\quad \text{(at this point, } \rho \text{ is the mass density instead of the number density)}
\end{aligned}
$$

the stream-lines of this fluid flow will give the "Bohmian trajectories".

6.3.1 Sample results from the correspondence:

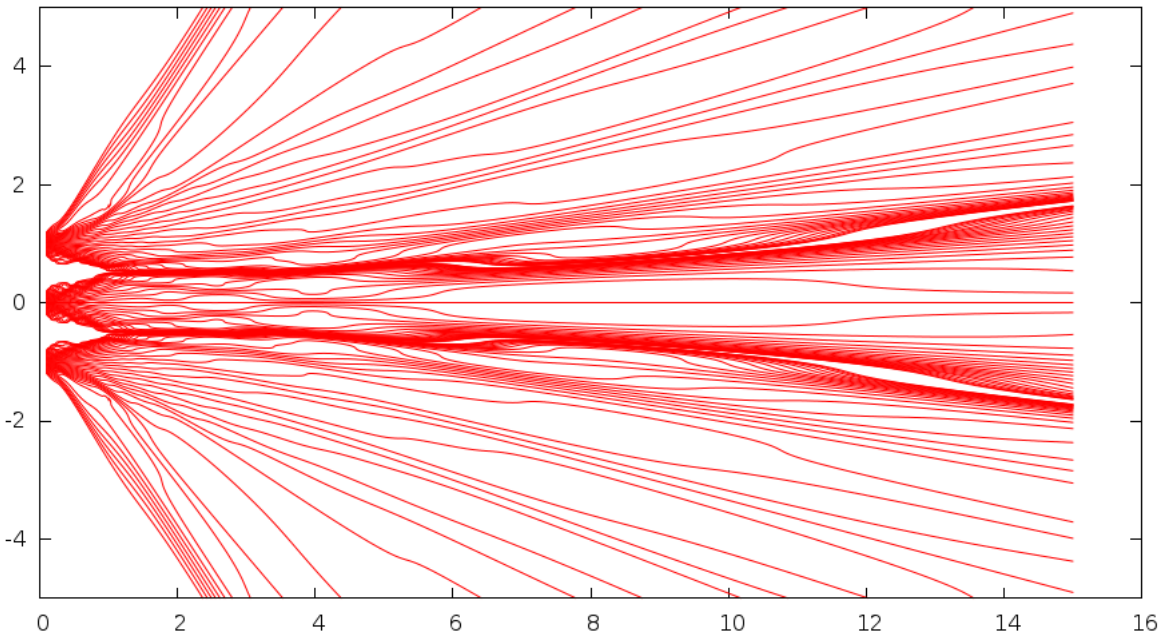


Figure 7: Stream lines for the triple slit interference system.

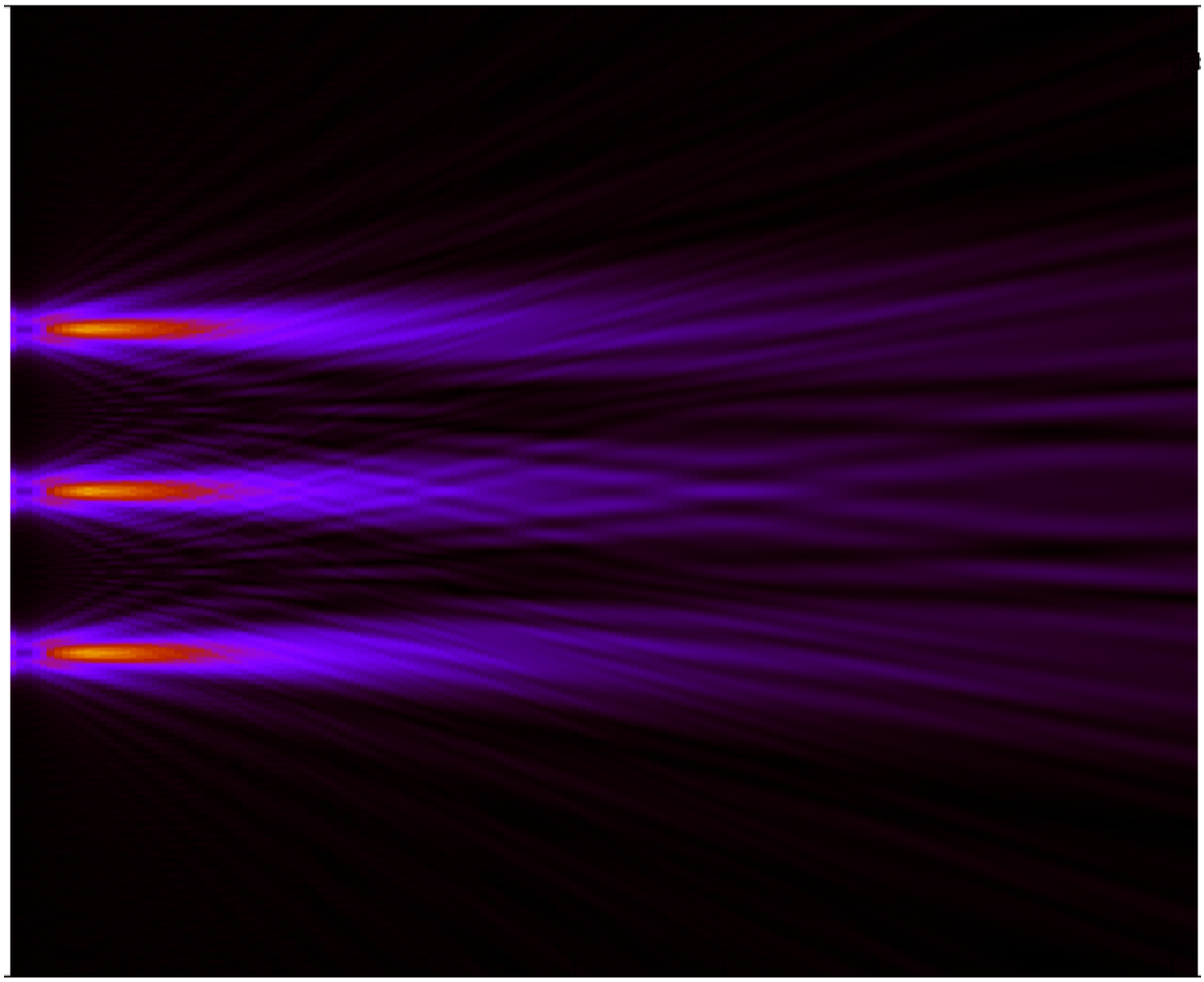


Figure 8: Density of the fluid flow for the triple slit system.

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