

An attempt at obtaining stationary solutions to nonlinear Schrödinger's equation via a pseudo-spectral method

A REPORT

submitted in partial fulfilment of the requirements

for the award of the dual degree of

Bachelor of Science-Master of Science

in

PHYSICS

by

CHIRAG ADWANI

(18077)

Under the guidance of

DR YANA NEC

*Thompson Rivers University,
Kamloops, BC, Canada*

DR AUDITYA SHARMA

*Indian Institute of Science
Education and Research, Bhopal*



IISERB

DEPARTMENT OF PHYSICS
INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH
BHOPAL
BHOPAL, MADHYA PRADESH, INDIA - 462066

April 2023



भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान भोपाल
Indian Institute of Science Education and Research Bhopal
(Estb. By MHRD, Govt. of India)

CERTIFICATE

This is to certify that **Chirag Adwani**, BS-MS (Physics), has worked on the project entitled ‘**An attempt at obtaining stationary solutions to nonlinear Schrödinger’s equation via a pseudo-spectral method**’ under my supervision and guidance. The content of this report is original and has not been submitted elsewhere for the award of any academic or professional degree.

April 2023
IISER Bhopal

Dr Yana Nec
*Thompson Rivers
University, Kamloops,
BC, Canada*

Dr Auditya Sharma
*Indian Institute of
Science Education and
Research, Bhopal*

Committee Member

Signature

Date

_____	_____	_____
_____	_____	_____
_____	_____	_____

ACADEMIC INTEGRITY AND COPYRIGHT DISCLAIMER

I hereby declare that this project is my own work and, to the best of my knowledge, it contains no materials previously published or written by another person, or substantial proportions of material which have been accepted for the award of any other degree or diploma at IISER Bhopal or any other educational institution, except where due acknowledgement is made in the document.

I certify that all copyrighted material incorporated into this document is in compliance with the Indian Copyright Act (1957) and that I have received written permission from the copyright owners for my use of their work, which is beyond the scope of the law. I agree to indemnify and save harmless IISER Bhopal from any and all claims that may be asserted or that may arise from any copyright violation.

April 2023
IISER Bhopal

Chirag Adwani

ACKNOWLEDGEMENT

I wish to express immense, heartfelt gratitude towards my supervisor Dr Yana Nec (TRU, Kamloops, BC, Canada) for her able guidance, invaluable insights and constant support throughout the project. I am sincerely indebted to her for unending belief in me and for investing her time in helping me become a better researcher and an even better person. I would also like to thank my co-guide Dr Auditya (IISERB) for all his support and insights which have aided me in the completion of this project. I would like to extend a special thanks to Prof Jeremy Upsal from the University of Washington for his inputs in the project.

I want to thank my dear friends (in no particular order of importance) Padu, Kavin, Paras, Chandu, Bhavz, Mansi, Mishika, Saksham, Shivan, Hemakshi, Aarya and Samidha for their constant love and support, even during very tough times. I want to extend a special thanks to all my colleagues for providing me with support whenever I have needed it and for providing me with a huge room to grow both professionally and socially. I would like to especially thank my loving sister Suman and my parents for their constant support in my pursuit of a career in Sciences. I would also like to thank Dr Sheereen K Bajpai (IISERB) and the student counselling cells at IISER Bhopal and TRU for all their help. I am also grateful to the existence of caffeine, without which, writing this thesis would have been impossible.

Finally, I would like to thank MITACS for providing me with an opportunity to work under the guidance of Dr Yana on the same topic, in person at the Thomson Rivers University. My four month stay in Canada was financially aided by a MITACS scholarship of CA\$8,896 for the first three months, and by a generous scholarship of CA\$1,667 from Dr Yana Nec and TRU, for the last month, for which I am immensely grateful.

Chirag Adwani

ABSTRACT

The concept of derivatives with non-integral orders has been studied for centuries and has found numerous applications in physics and engineering. Recently, there has been growing interest in exploring fractional versions of popular differential equations. This study aims at finding stationary solutions to the fractional generalisation of the Nonlinear Schrödinger equation. Analytical stationary solutions to the nonlinear Schrödinger equation (NLSE) exist and are well known in literature [1] to have their amplitudes related to the Jacobi elliptic trigonometric functions. However, the spectrum of linearisation around the Jacobi elliptic solution is known to be purely imaginary, making it impossible to obtain the solution with direct numerical attempts. We present a novel approach attempting to stabilise the numerical scheme and obtaining the Jacobi elliptic solutions by replacing the NLSE with a pair of coupled (auxiliary) PDEs inspired by the Gierer-Meinhardt (GM) model, which is known to have stable spike-type solutions that have negative real parts in their stability spectrum[2]. The stable nature of the solution persists even when the Laplacian is replaced with a derivative of a non-integral order[3], which makes it a suitable inspiration for our purposes. Results of the numerical trial of the auxiliary PDE approach are presented. We use a pseudo-spectral scheme based on Fourier transforms to simplify the problem from a system of partial differential equations to ordinary differential equations and to allow for generalisation to non-integral order derivatives. Despite extensive experimentation with various parameters, our method fails to converge to the Jacobi elliptic solutions. Lastly, we also present a comprehensive review of the literature on fractional calculus, the Nonlinear Schrödinger equation and the stability analysis of stationary solutions to the NLSE.

LIST OF SYMBOLS OR ABBREVIATIONS

$\operatorname{sn}(x, k)$	Jacobi elliptic sine function in x with elliptic modulus k
$\operatorname{sgn}(x)$	The <i>sign</i> function. $= +1$ if $x > 0$, $= -1$ if $x < 0$ and $= 0$ if $x = 0$
$\Gamma(x)$	The gamma function
NLSE	The Nonlinear Schrödinger Equation
fNLSE	The Nonlinear Schrödinger Equation of a fractional order
GL	The Ginzburg-Landau Equation
CCGL	Complex Cubic Ginzburg-Landau Equation
AB2	Two-step explicit Adams-Basforth scheme
CN	Crank-Nicolson method
FT	Fourier Transform
DFT	Discrete Fourier Transform
FFT	The Fast Fourier Transform

LIST OF FIGURES

2.1	The (analytical) trivial phase Jacobi elliptic sine solution to the NLSE for $k = 0.8$	26
2.2	Obtained outputs of an attempt to directly solve the NLSE.	30
4.1	Obtained outputs of a numerical implementation of the auxiliary PDE method.	40
4.2	Obtained solution for $\tau_0 = 0.035$ at different values of t	41

Contents

Certificate	ii
Academic Integrity and Copyright Disclaimer	iii
Acknowledgement	iv
Abstract	v
List of Symbols or Abbreviations	vi
List of Figures	vii
1 Introduction and motivation	10
1.1 Dispersion relations	11
1.2 The Nonlinear Schrödinger equation	12
1.3 Fractional calculus	15
1.4 The fNLSE	21
2 Theoretical background	24
2.1 Stationary solutions to the NLSE	24
2.2 Stability analysis	27
2.3 Numerical Schemes	29
3 Approach and Methodology	33
3.1 The Gierer-Meihardt model	33
3.2 The auxiliary PDE method	35
3.3 Implementation of Numerics	37
4 Results	39
5 Conclusion and Future prospects	42

Appendices

A	Fourier Transforms	45
A.1	Definitions	45
A.2	Properties of Fourier Transforms	46
A.3	Discrete Fourier Transforms	47
B	The Jacobi elliptic trigonometric functions	49
	Bibliography	53

Chapter 1

Introduction and motivation

There exists an idea of extending the definitions of (“usual”) derivatives of integer order n to any arbitrary real (or even complex) order α . This extension can at first be demanded with the same motivation that extensions to the natural number system were demanded – purely to appease the curiosity. For instance, if we were only aware of the integer number system, one may ask “Is there a number that can be added to itself n times, to give 1?”, allowing us to discover the multiplicative inverses and then eventually, the rationals. From there, one may ask “Is there a number that can be multiplied to itself twice, to give the answer 2?”, allowing us to expand our knowledge even beyond the rationals.

The extensions arising from mathematical curiosities have allowed us to answer and explain a number of phenomena. The length of the hypotenuse of a right triangle with unit base and perpendicular could only be represented with a symbol *after* people accepted that numbers could exist beyond rationals. Roots to quadratic equations like $x^2 + 1 = 0$ could only be given when numbers beyond the reals were accepted to exist. The argument, of course, does not apply only to number systems. The Gamma function $\Gamma(x)$ was discovered as an extension of the integer operator known as the factorial and has also seen many applications throughout mathematics. A number of applications of fractional derivatives also exist, as we shall see in a later section. A common prescription to obtaining applications of fractional derivatives involves extending the equations governing well-established systems to their fractional counterparts. This has been a successful method in helping us explain naturally occurring phenomena like anomalous diffusion [3, 4] and Lévy flights. With this motivation, we shall explore the extension of the nonlinear Schrödinger equation involving fractional derivatives.

The Nonlinear Schrödinger equation(NLSE) is a canonical equation of nonlinear dynamics, which describes the time evolution of a wave travelling in a dispersive

medium. The dynamics of such systems is characterised by *dispersion relations*. These relations will prove useful while motivating important questions this project aims to answer.

1.1 Dispersion relations

At the heart Quantum Mechanics, just like any other branch of Physics, is a differential equation. The equation, termed as the Schrödinger's equation, is a model for one of many ways of describing quantum mechanical systems. Particularly, it describes the time-evolution of the quantum state of a particle. It was first postulated by Erwin Schrödinger, after whom the equation has been named, in 1925. In its usual form, the Schrödinger's equation (1.1.1) is a *linear* differential equation with its structure similar to that of the diffusion equation: consisting of a single derivative in the time variable and double derivative in spatial variables,

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t), \quad (1.1.1)$$

where $\psi(x,t)$ is the *wavefunction* of the particle and $V(x,t)$ is the *potential* that represents the environment that the particle is in. The Schrödinger's equation is intended to be a representative of quantum mechanics that is analogous to Newtonian mechanics. Which is to say that it must follow the classical energy-momentum relation

$$E = \frac{p^2}{2m} + V, \quad (1.1.2)$$

where E is the total energy of the system and p is the momentum. It is clear that the system is totally nonrelativistic. Relations such as (1.1.2) are often termed as *dispersion relations*. The term *dispersion relation* originates from optics, where in that context, it is the relation between the wave number k and the frequency ω . The dispersion relation for *usual* optical systems, i.e., the systems that follow the free wave equation

$$\frac{1}{c^2} \frac{\partial^2 u(x,t)}{\partial t^2} = \frac{\partial^2 u(x,t)}{\partial x^2}, \quad (1.1.3)$$

can be obtained by taking the Fourier transform on both sides in all space and time variables (refer chapter A) to get

$$\begin{aligned} \frac{1}{c^2} \mathcal{F} \left\{ \frac{\partial^2 u(x, t)}{\partial t^2} \right\}_{x \rightarrow k, t \rightarrow \omega} &= \mathcal{F} \left\{ \frac{\partial^2 u(x, t)}{\partial x^2} \right\}_{x \rightarrow k, t \rightarrow \omega}, \\ \implies \frac{1}{c^2} \omega^2 \hat{u} &= k^2 \hat{u}. \end{aligned}$$

Where $\hat{u} \equiv \mathcal{F}\{u\}$. We have used the property (A.2) of Fourier transforms to get from the first expression above, to the second. This gives us the relation $\omega = ck$ that we know from optics.

Similarly, if we take Fourier transforms on both sides of the Schrödinger's equation (1.1.1) with $V = 0$, we get

$$\begin{aligned} i\hbar \mathcal{F} \left\{ \frac{\partial \psi(x, t)}{\partial t} \right\}_{x \rightarrow k, t \rightarrow \omega} &= -\frac{\hbar^2}{2m} \mathcal{F} \left\{ \frac{\partial^2 \psi(x, t)}{\partial x^2} \right\}_{x \rightarrow k, t \rightarrow \omega} \\ \implies \hbar \omega \hat{\psi} &= \frac{\hbar^2 k^2}{2m} \hat{\psi}. \end{aligned}$$

Where again, we have $\hat{\psi} \equiv \mathcal{F}\{\psi\}$. If we now remember the De-Broglie relations $E = \hbar \omega$ and $p = \hbar k$, we see that we have arrived at the dispersion relation (1.1.2).

In general, one may obtain the dispersion relations of a system if the basic equations governing the system are known. However, It is quite often the case that the dispersion relations are easier to experimentally obtain or to be realised through physical arguments, than the basic equations themselves. And once we have a dispersion relation governing our system, we may derive the basic equations that the system would follow, instead of going the other way around. The whole prescription of looking at experimental data, finding the dispersion relations and then coming up with a basic equation of the system provides us with a *phenomenological* method of doing physics. As stated earlier, we will motivate the Nonlinear Schrödinger equation(NLSE) and even the fractional Nonlinear Schrödinger equation(fNLSE), using dispersion relations.

1.2 The Nonlinear Schrödinger equation

The Nonlinear Schrödinger equation has been an equation of great physical and mathematical interest for the past 60 years. The essence of NLSE can be found in the works of Ginzburg and Landau(1950) in their study of macroscopic superconductivity. However, it was not until mid-1960s that the wider applicability of

the NLSE started coming into the focus. The NLSE has found applicability in a very diverse set of fields[5], including nonlinear optics [6], plasma physics [7], fluid dynamics, magnetic spin waves, etc. **Generally speaking, it has been found that most weakly nonlinear, dispersive, energy-conserving systems lead to the NLSE, in an appropriate limit.** Let us take a closer look at how the NLSE appears in nonlinear optical systems.

Optical fibre technology has brought about a paradigm shift in data transmission technology. It allows for transmission with a much larger bandwidth and over significantly longer distances as compared to the electric cables. However, as is with any new technology, it came with its own set of limitations. Dispersion and nonlinearity are amongst some serious limitations of optical fibres [8].

Dispersion originates from the frequency dependence of the refractive index. The different spectral components of the signal propagate at different speeds, and as a result, arrive at different times at their destination. This results in pulse broadening and distortion.

Fibre nonlinearity is due to the so-called Kerr effect, where the refractive index develops a dependence on the intensity of the beam passing through it. In the presence of dispersion and Kerr nonlinearity, the refractive index of the material is given by

$$n(\omega, E) = n_0(\omega) + n_2|E|^2, \quad (1.2.1)$$

where ω and E represent the frequency and the electric field of the electromagnetic wave, respectively; $n_0(\omega)$ is the linear, frequency-dependent part of the refractive index; and the constant n_2 is referred to as the Kerr coefficient. It is typically of the order $10^{-22} \text{ m}^2/\text{W}$. Despite its small value, the nonlinearity can cause effects to accumulate over large distances and result in significant pulse broadening during propagation. Note that if we have a modulated wave, as is often the case with signal propagation, E will represent the amplitude of the carrier wave.

The following is a sketch of the derivation. A detailed and comprehensive treatment can be found in [6] along with relevant references cited therein. We use the motivation from the previous section to write down the dispersion relation for a wave propagating through a medium with refractive index given by (1.2.1):

$$k(\omega, E) = \frac{\omega}{c} (n_0(\omega) + n_2|E|^2), \quad (1.2.2)$$

where c denotes the speed of light in vacuum. The Taylor series expansion of $k(\omega, E)$

around $\omega = \omega_0$ up to second order in ω yields

$$k - k_0 = k'(\omega_0)(\omega - \omega_0) + \frac{k''(\omega_0)}{2}(\omega - \omega_0)^2 + \frac{\omega_0 n_2}{c}|E|^2, \quad (1.2.3)$$

where the prime ($'$) denotes derivative in ω and $k_0 = k(\omega_0)$. And now, exactly in the opposite way as in the previous section, we replace $k - k_0$ and $\omega - \omega_0$ with their corresponding inverse Fourier operator equivalents $\iota\partial/\partial z$ and $\iota\partial/\partial t$, respectively. We also then let the whole expression operate on E , to obtain

$$\iota \left(\frac{\partial E}{\partial z} + k'(\omega_0) \frac{\partial E}{\partial t} \right) - \frac{k''(\omega_0)}{2} \frac{\partial^2 E}{\partial t^2} + \nu |E|^2 E = 0, \quad (1.2.4)$$

where $\nu \in \mathbb{R}$ is an appropriate constant, defined by collecting all the constants in front of the cubic term. We may identify $k'(\omega_0) = 1/v_g$, where v_g is the group velocity of a given travelling wave.

To obtain the dimensionless version of (1.2.4), we first introduce retarded time coordinate $t_{ret} = t - z/v_g$. Assume that t_* , z_* and P_* are the characteristic time, distance and power of the system, respectively. If we choose $z_* = 1/\nu P_*$ and $t_*^2 = z_* | -k''(\omega_0) |$ and move to the dimensionless coordinates $t' = t/t_*$, $z' = z/z_*$ and $q = E/\sqrt{P_*}$, we arrive at the NLSE

$$\iota \frac{\partial q}{\partial z} + \frac{\text{sgn}(-k''(\omega_0))}{2} \frac{\partial^2 q}{\partial t^2} + |q|^2 q = 0. \quad (1.2.5)$$

There are now two cases of physical interest depending on the sign of $-k''(\omega_0)$. When $-k''(\omega_0) > 0$, we obtain what is termed as the *defocusing NLSE*, and the resulting dispersion in this case is “normal”. While $-k''(\omega_0) < 0$ results in the *focusing NLSE* and “anomalous” dispersion. Unless specifically mentioned, we will restrict our analysis to the defocusing NLSE, even after we change the form of the Laplacian in the following sections. Hence, the equation of our interest is

$$\iota q_t = -\frac{1}{2} q_{xx} + q|q|^2. \quad (1.2.6)$$

There has been an extensive amount of research on the solutions of the NLSE and their properties[1]. The NLSE is known to be a completely integrable system. In the context of this project, we would be interested in separable solutions of the type

$$\Psi(x, t) = e^{-i\omega t} \phi(x),$$

where ω is a real constant. We are specifically interested in a class of periodic

solutions in x , where the amplitude $\phi(x)$ is expressed in terms of the Jacobi elliptic sine function $\text{sn}(x, k)$ (refer Appendix B):

$$\Psi(x, t) = k \text{sn}(x, k) e^{-\frac{t}{2}(1+k^2)}, \quad (1.2.7)$$

where $k \in [0, 1)$ is called the *elliptic modulus*. $\text{sn}(x, k)$ is a periodic function with the period $T(k) = 4K(k)$, and $K(k)$ is the elliptic integral of first kind. We will take a deeper look at the NLSE and the Jacobi elliptic solutions in the next chapter, where we also discuss the stability spectrum of these solutions.

Finally, we would like to point out the resemblance between the Nonlinear Schrödinger equation (NLSE) and the complex cubic Ginzburg-Landau (CCGL) [5] equation, which appears in the context of pattern formation processes in nonlinear media:

$$\psi_t = g\psi + (a + ib)\nabla^2\psi - (d + ic)|\psi|^2\psi, \quad (1.2.8)$$

where ψ is complex. $g > 0$ is known as the *gain coefficient*. $a > 0$ and $b \in \mathbb{R}$ are coefficients controlling the diffusion and dispersion processes. $c \in \mathbb{R}$ and $d > 0$ account for the nonlinear dissipations. In the $|a| \ll |b|$ and $|d| \ll |c|$ limit, we can see that the CCGL equation becomes the NLSE. So, the NLSE also makes its appearance in the theory of pattern formation.

In summary, the above discussion has highlighted the immense physical and mathematical significance of the Nonlinear Schrödinger equation (1.2.6). In a later section, we will introduce a generalisation of the NLSE based on the concept of *fractional derivatives*, which extends the conventional integer-order derivatives to derivatives of arbitrary real order α . This idea falls under the realm of *fractional calculus*, which is the subject matter of the next section.

1.3 Fractional calculus

The notion of fractional derivatives has existed for centuries, originally appearing in the works of Leibniz in 1695. However, it was only after more than a century later, in 1823, that a practical application of *fractional calculus* was found. Niels Abel published his treatment of the famous tautochrone problem in 1823, at an age of 21, where he used fractional derivatives to find the solution [9]. That stood as the sole example of an application of fractional derivatives, for almost an entire century, that is up until the early 1920s, when Oliver Heaviside, an autodidact, found the application of fractional derivatives in his works on the theory of transmission lines

[10].

Even though there was a steady progress in the subject on the side of mathematical exploration, it was not until the works of Mandelbrot on fractal geometry in the early 1980s [11, 12] that the topic started to gain the interest of physicists too. Fractional derivatives started appearing in the contexts of fractional Brownian motion [13] and anomalous diffusion processes [14]. Since then, fractional versions of various, physically important differential equations have come to light and raised fundamental questions about the physical nature of the systems governed by those equations. For instance, N. Laskin (2002) [15] presented a fractional version of the Schrödinger equation and also proved, in the same article, that the fractional Schrödinger operator was Hermitian. Goldfain (2006) [16] demonstrated that fractional dynamics in Minkowski spacetime mimics that of free fields in curved Riemannian spacetime. An approach to quantise fractional free fields was also given in the same article. A quantisation description for fractional free Klein-Gordon type fields has also been addressed in literature [17]. Fractional calculus thus presents us with a scope to gain novel physical insights and develop innovative methodologies and approaches.

There is a multitude of definitions of fractional derivatives in the literature [9, 10], which are all used depending on the context they are required in. Most definitions require that we identify derivatives and anti-derivatives as inverse operators of each other. That is, if we define the anti-derivative (or integration) operator as

$${}_a I_x(f) := \int_a^x f(x_0) dx_0,$$

then we must identify this as the inverse of derivative operator ${}_a \mathfrak{D}_x$,

$${}_a \mathfrak{D}_x^{-1} \equiv {}_a I_x.$$

In the above notation the superscript on the right denotes the order of the operator, the subscript to the left denotes the lower limit of the integral in the definition of the operator and the subscript on the right denotes the independent variable that the operator is defined with. Now, if we look at higher order anti-derivative operators, ${}_a I_x^n$ for $n \in \mathbb{N}$, we see that it assumes the form of a repeated integral

$${}_a I_x^n(f) = \int_a^x dx_{n-1} \int_a^{x_{n-1}} dx_{n-2} \cdots \int_a^{x_2} dx_1 \int_a^{x_1} f(x_0) dx_0,$$

where we assume that the function f is of a sufficiently regular behaviour for all required integer integrals and derivatives to exist. The above repeated integral can be written in terms of a single integral using the **Cauchy's formula for repeated**

integrals.

Theorem 1.1 (Cauchy's formula for repeated integrals). *For a continuous, real function f , the n^{th} repeated integral*

$${}_a I_x^n(f) = \int_a^x dx_{n-1} \int_a^{x_{n-1}} dx_{n-2} \cdots \int_a^{x_2} dx_1 \int_a^{x_1} f(x_0) dx_0,$$

equals the single integral

$${}_a I_x^n(f) = \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} f(t) dt.$$

Proof. The proof follows from mathematical induction.

For $n = 1$, the formula reads

$${}_a I_x^1(f) = \frac{1}{(0)!} \int_a^x (x-t)^0 f(t) dt = \int_a^x f(t) dt = \int_a^x f(x_0) dx_0,$$

which satisfies the base case without much effort, if we incorporate the extension of the factorial to have $0! = 1$. Next, assume that the hypothesis holds for $k \in \mathbb{N}$. We also note that

$$\frac{d}{dx} \left[\frac{1}{k!} \int_a^x (x-t)^k f(t) dt \right] = \frac{1}{(k-1)!} \int_a^x (x-t)^{k-1} f(t) dt. \quad (1.3.1)$$

using the Leibniz Integral rule¹. Now,

$$\begin{aligned} {}_a I_x^{k+1}(f) &= \int_a^x dx_k \int_a^{x_k} dx_{k-1} \int_a^{x_{k-1}} dx_{k-2} \cdots \int_a^{x_2} dx_1 \int_a^{x_1} f(x_0) dx_0 \\ &= \int_a^x dx_k \frac{1}{(k-1)!} \int_a^{x_k} (x_k-t)^{k-1} f(t) dt \quad (\text{from induction hypothesis}) \\ &= \int_a^x dx_k \frac{d}{dx_k} \left[\frac{1}{k!} \int_a^{x_k} (x_k-t)^k f(t) dt \right] \quad (\text{from equation (1.3.1)}) \\ &= \frac{1}{k!} \int_a^x (x-t)^k f(t) dt, \end{aligned} \quad (1.3.2)$$

which completes the proof. □

¹The Leibniz Integral rule for differentiating an input function with an integral sign:

$$\frac{d}{dx} \left(\int_{a(x)}^{b(x)} g(x, t) dt \right) = g(x, b(x))b'(x) - g(x, a(x))a'(x) + \int_{a(x)}^{b(x)} \frac{\partial}{\partial x} g(x, t) dt.$$

We can then write an expression for a higher order anti-derivative as

$${}_a\mathfrak{D}_x^{-n}(f) = {}_aI_x^n(f) = \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} f(t) dt, \quad (1.3.3)$$

where $n \in \mathbb{N}$. The above expression provides us with an approach of defining integrals of more general orders. If we allow the formula to hold for any $\alpha \in \mathbb{R}$ and replace the factorial with its analytic continuation, $\Gamma(\alpha)$, we can define the **Riemann-Liouville fractional Integral**:

Definition 1.2 (The Riemann-Liouville fractional integral). For $\alpha \in \mathbb{R}$, the Riemann-Liouville fractional integral can be defined as

$${}_a\mathfrak{D}_x^{-\alpha}(f) = {}_aI_x^\alpha(f) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1} f(t) dt,$$

where the constant a is the lower bound of the integration domain and needs to be specified a priori.

Now, we again emphasise the fact that the integration operators and the derivative operators conceptually are the inverses of each other², allowing us to write

$$\begin{aligned} \mathfrak{D}^\alpha &= \mathfrak{D}^m \mathfrak{D}^{-(m-\alpha)}, \quad m \in \mathbb{N} \\ &= \frac{d^m}{dx^m} I^{m-\alpha} \end{aligned} \quad (1.3.4)$$

where we dropped the subscripts for convenience. We shall make the choice $m = \lceil \alpha \rceil$, which denotes the smallest integer $\geq \alpha$. The above may be interpreted as a definition of a fractional derivative of order α , wherein we are required to first compute a Riemann-Liouville fractional integral of the order $(m - \alpha)$, and then take the usual derivative of order m . It must be noted that when α is an integer, $\lceil \alpha \rceil$ will be the same as α and we will just be left with computing the usual derivative (i.e. we want to identify the integral operator of order 0, ${}_aI_x^0$, with the identity operator so that $\mathfrak{D}^m \equiv d^m/dx^m$, for all $m \in \mathbb{N}$). Thus, we arrive at the **Riemann-Liouville definition of a fractional derivative**:

Definition 1.3 (Riemann-Liouville fractional derivative). For $\alpha \in \mathbb{R}$ and $m = \lceil \alpha \rceil$, the Riemann-Liouville fractional derivative can be defined as

$${}_a\mathfrak{D}_x^\alpha(f) = \frac{d^m}{dx^m} {}_aI_x^{m-\alpha}(f) = \frac{d^m}{dx^m} \frac{1}{\Gamma(m-\alpha)} \int_a^x (x-t)^{m-\alpha-1} f(t) dt,$$

²Note that this is not exactly the case! A beautiful discussion on this is given in [10]. However, it is beyond the scope of this thesis.

where again the constant a that defines the domain, will have to be specified a priori.

One may also have given a definition of fractional derivatives by inverting the order in which the derivative and integral operators appear in equation (1.3.4). This gives us the **Caputo fractional derivative**.

Definition 1.4 (Caputo fractional derivative). For $\alpha \in \mathbb{R}^+$ and $m = \lceil \alpha \rceil$, the Caputo fractional derivative can be defined as

$${}_a^C \mathfrak{D}_x^\alpha(f) = {}_a I_x^{m-\alpha} \frac{d^m}{dx^m}(f) = \frac{1}{\Gamma(m-\alpha)} \int_a^x (x-t)^{m-\alpha-1} f^{(m)}(t) dt,$$

where once again, the constant a will have to be specified a priori. We introduce the left superscript in ${}_a^C \mathfrak{D}_x^\alpha$ to distinguish the Caputo derivative (1.4) from the Riemann-Liouville derivative (1.3). One of the eminent advantages of the Caputo derivative is that the derivative of a constant function is 0, which is not the case for the RL derivative and which may pose problems in contexts where this feature important, such as equilibria of dynamical systems.

It can be noted that the above definitions of fractional derivatives suggest that the fractional operators are **nonlocal**. Which means that the fractional derivative of a function f at a point x in its domain, is dependent upon the shape of the function elsewhere in the domain too (this is also the reason why we have been carrying the left subscript in our notation). This is quite visibly the case for the Riemann-Liouville and Caputo fractional derivatives as they are both dependent on the computation of an integral involving the function itself, over the whole domain. So, if the function (or its derivative in the case of Caputo) were to be modified continuously elsewhere, it would affect the value of derivative of non-integral order α , at the point x . However, for integer values of α , the derivative completely loses its property of nonlocality and such a change will not make a difference in the value of derivative at the point x . There are many such interesting properties of fractional derivatives beyond the scope of this discussion.

Both Riemann-Liouville and Caputo derivatives provide us with plausible definitions of the fractional derivatives. However, they are not the most practical when it comes to numerical implementations. One will not only have to worry about using a good quadrature rule to carry out the integration process, but also a good scheme to compute the derivative. We will also have to worry about the cases for which α is an integer, separately.

It may be noted that the above definitions were developed based on generalisations of the properties of the usual, integer order derivatives. Specifically, both arise

from the composition property of derivatives exploited in (1.3.4). One may look for other such properties of usual derivatives to generalise and thence define fractional derivatives. To this end, we recall the Fourier transform property of derivatives

Property 1.1 (Fourier transform property of derivatives). For a derivative operator d^m/dx^m of integer order m in the variable x , the following relation holds true for a Fourier-transformable function

$$\mathcal{F}\left\{\frac{d^m}{dx^m}f(x)\right\}_{x \rightarrow \xi} = (\iota\xi)^m \mathcal{F}\{f(x)\}_{x \rightarrow \xi}, \quad (1.3.5)$$

where \mathcal{F} denotes the Fourier transform.

It is desirable to define a similar property for non-integral orders. This is where the **Riesz fractional derivative** comes to the rescue [18].

Definition 1.5 (Riesz fractional derivative). For $\alpha \in \mathbb{R}^+$, we define the Riesz fractional derivative as the Riemann-Liouville derivative with $a = -\infty$,

$${}_{-\infty}\mathfrak{D}_x^\alpha(f) = \frac{d^m}{dx^m} {}_{-\infty}I_x^{m-\alpha}(f) = \frac{d^m}{dx^m} \frac{1}{\Gamma(m-\alpha)} \int_{-\infty}^x (x-t)^{m-\alpha-1} f(t) dt. \quad (1.3.6)$$

It can be proven that the Riesz fractional derivative as defined above, possesses the following Fourier transform property:

$$\mathcal{F}\{{}_{-\infty}\mathfrak{D}_x^\alpha(f)\} := (\iota\xi)^\alpha \mathcal{F}\{f(x)\},$$

However, using this as the Fourier transform for derivatives of any order $\alpha \neq 2, \alpha > 0$ will bring in another issue as the derivative operator itself does not possess the reflection symmetry $x \mapsto -x$. This symmetry is essential to keep the expression of the derivative real, under a Fourier transform. The Riemann-Liouville and the Caputo derivative also do not possess this symmetry either, whilst all highest order derivatives of popular equations (like ∇^2, ∇^4 , etc.) always do seem to possess it. To obtain a definition of a fractional derivative that has this symmetry, we will first make a variable shift in 1.3.6

$${}_{\infty}\mathfrak{D}_x^\alpha(f) = \frac{d^m}{dx^m} {}_xI_\infty^{m-\alpha}(f) = \frac{d^m}{dx^m} \frac{1}{\Gamma(m-\alpha)} \int_x^\infty (t-x)^{m-\alpha-1} f(t) dt, \quad (1.3.7)$$

the Fourier transform of which, would look like

$$\mathcal{F}\{{}_{\infty}\mathfrak{D}_x^\alpha(f)\} = (-\iota\xi)^\alpha \mathcal{F}\{f(x)\}.$$

This allows us to define fractional Laplacian, which possesses reflection symmetry (note that we omit $\alpha = 2m + 1, m \in \mathbb{Z}$ as that would correspond to the case which should typically *not* possess the reflection symmetry that we are trying to achieve.):

Definition 1.6 (The fractional Laplacian). For $\alpha \in \mathbb{R}^+, \alpha \neq 2m + 1, m \in \mathbb{Z}$, we define the fractional Laplacian $(-(-\nabla^2)^{\alpha/2})$ as

$$-(-\nabla^2)^{\alpha/2}(f) := \left(-\frac{-\infty \mathfrak{D}_x^\alpha + \infty \mathfrak{D}_x^\alpha}{2 \cos(\alpha\pi/2)} \right) (f) \quad (1.3.8)$$

Now, if we keep in mind the fact that

$$|\xi|^\alpha = \frac{(\iota\xi)^\alpha + (-\iota\xi)^\alpha}{2 \cos(\alpha\pi/2)},$$

the fractional Laplacian will possess the following Fourier transform property

$$\mathcal{F}\{ -(-\nabla^2)^{\alpha/2}(f) \} = -\frac{(\iota\xi)^\alpha + (-\iota\xi)^\alpha}{2 \cos(\alpha\pi/2)} \mathcal{F}\{f(x)\} = -|\xi|^\alpha \mathcal{F}\{f(x)\}.$$

Hence, we now have a reflection symmetric fractional derivative. This also gives us a fairly straightforward way to implement fractional derivatives numerically. In contrast to Riemann-Liouville, Caputo and Riesz derivatives, we would only need to perform a Fourier transform, and then invert it after multiplying by some factors, to implement the fractional Laplacian numerically. This process can be achieved with a far greater efficiency, owing to the existence of Fast Fourier Transforms (FFTs).

The ability to implement fractional derivatives numerically, allows us to investigate a wide range of previously unexplored problems. The specific problem that we shall be interested in, is the fractional generalisation of the Nonlinear Schrödinger equation, as discussed at the end of the previous section. We will take a closer look at the motivations to investigate this problem, in the next section.

1.4 The fractional Nonlinear Schrödinger equation (fNLSE)

In the previous section, we saw that fractional derivatives have historically been used to provide a generalisation for equations governing various branches of physics and engineering, allowing us to explain a wide variety of novel physical phenomena [5]. The fractional generalisation has been particularly successful in explaining large classes of diffusion-related phenomena. For instance, in the case of free diffusion

processes, whenever one finds a deviation from Fick's law of diffusion³, fractional calculus might be employed [4]. The aesthetic similarity between the diffusion equation and the Schrödinger equation has been a motivation for enquiries on fractional quantum mechanics and fractional *linear* Schrödinger equations of various types [15, 19, 20]. We have seen in section 1.2 that similarities exist between the Complex Cubic Ginzburg-Landau (CCGL) equation and the Nonlinear Schrödinger equation, and because there are fractional generalisations of the CCGL [4, 21], there is motivation to look at the fractional generalisation of the Nonlinear Schrödinger equation as well.

The Nonlinear Schrödinger equation was introduced in section 1.2, wherein a sketch of a derivation of the NLSE was also given. We can follow a similar process to derive the fractional Nonlinear Schrödinger equation as well, by essentially replacing the dispersion relation (1.2.3) by the following (as done in [21]):

$$k = \omega k' + |\omega|^\alpha \frac{k''}{2} + \nu |E|^2, \quad (1.4.1)$$

where $\alpha \in \mathbb{R}$. The next step in the derivation was to replace the powers of ω with their inverse Fourier operator equivalents. We can recall that the equivalent of $|\omega|^\alpha$ would be the fractional Laplacian (definition 1.6), multiplied by a factor of -1 . If we then keep following the rest of the derivation exactly as in the above section, we will arrive at the fractional Nonlinear Schrödinger equation:

$$i \frac{\partial \Psi(x, t)}{\partial t} = -\frac{1}{2} \mathfrak{D}_x^\alpha \Psi(x, t) + \Psi(x, t) |\Psi(x, t)|^2, \quad (1.4.2)$$

where $\Psi(x, t)$ is a complex valued function and $\alpha \in \mathbb{R}^+$, $\alpha \neq 2m + 1$, $m \in \mathbb{Z}$ is the order of the fractional Laplacian ($\mathfrak{D}_x^\alpha = -(-\nabla^2)^{\alpha/2}$). The $\alpha = 2$ case corresponds to the usual nonlinear Schrödinger equation (1.2.6). Thus, we are now at a place where we can establish the objectives of this project.

Objective 1. An objective of this project is to make an attempt at numerically obtaining stationary solutions of the nonlinear Schrödinger's equation of a fractional order (fNLSE) (1.4.2).

To make an approach towards achieving objective 1, we may first attempt to

³The usual Fickian diffusion processes will have the Mean Square Displacement (MSD) linearly proportional to t :

$$\langle r^2(t) \rangle \propto t.$$

However, various types of 'anomalous' diffusion processes have emerged over the years that have $\langle r^2(t) \rangle \propto t^\gamma$, where γ can be ≤ 1 . Fractional calculus has been highly successful in explaining such processes[4].

obtain the Jacobi elliptic solutions (1.2.7) of the usual NLSE ($\alpha = 2$), that were introduced in section (1.2). Once we have a working scheme to obtain the Jacobi elliptic solutions, we may proceed to generalise the algorithm to work for fractional order derivatives. However, to achieve our intended generalisation, we will try to obtain the Jacobi elliptics by using the Fourier transform property (1.3.5) of derivatives in the numerical implementation, as it is the closest to the definition of Riesz fractional derivatives. Doing so will also aid us in another way; as after we transform the Laplacian, we would only be left to solve an ordinary Initial Value Problem in t , as compared to a partial differential equation in two variables that we started off with. Thus, we have

Objective 2. To attain objective 1, we will first aim to obtain the Jacobi elliptic solutions (1.2.7) numerically using a scheme that utilises the Fourier transform property 1.3.5 of derivatives.

In this chapter, we presented an introduction to the NLSE, its stationary solutions, and the various places that it arises in literature. An elaborate discussion on fractional derivatives was also given, wherein we saw various definitions of the fractional derivatives, before eventually settling for the one that is most useful to us: the Riesz fractional derivative. We remarked the recent upsurge in the interest in fractional derivatives, due to various discoveries of its usefulness being made across many branches of Physics and Engineering. Finally, we established the objectives 1 and 2, of the project. In the subsequent chapters, we will make progress towards achieving those objectives by first studying the Jacobi elliptic stationary solutions of NLSE, in greater depth and then developing schemes to obtain them numerically.

Chapter 2

Theoretical background

In chapter 1, the (defocusing) NLSE was introduced as an equation governing the amplitude of a wave in dispersive media. It was established that the equation has a class of stationary solutions related to the Jacobi elliptic functions. In this chapter, we will look at the Jacobi elliptic solutions in a greater detail: how they arise and whether they can be obtained numerically or not. While answering the latter, we will see what happens to perturbations around stationary solutions of the NLSE. This chapter will also present the first numerical trial done towards a primary objective of the project (2), which is to obtain the Jacobi elliptic numerically.

2.1 Stationary solutions to the NLSE

The (defocusing) NLSE is given by

$$i\Psi_t = -\frac{1}{2}\Psi_{xx} + \Psi|\Psi|^2, \quad (2.1.1)$$

where $\Psi(x, t)$ is intensity of the carrier wave propagating in a dispersive medium. We aim to look for separable solutions of the type

$$\Psi(x, t) = e^{-i\omega t}\phi(x), \quad (2.1.2)$$

where $\omega \in \mathbb{R}$ is a constant. Plugging this into (2.1.1), we obtain an equation for $\phi(x)$

$$\omega\phi(x) = -\frac{1}{2}\phi_{xx} + \phi(x)|\phi(x)|^2. \quad (2.1.3)$$

Decomposing the solution further, we write $\phi(x)$ as an amplitude and a phase

$$\phi(x) = R(x)e^{i\theta(x)},$$

where both $R(x)$ and $\theta(x)$ are now real-valued functions. Plugging this into (2.1.3) and separating the real and imaginary parts, we get the differential equations for $R(x)$ and $\theta(x)$

$$R_x\theta_x + \frac{1}{2}R\theta_{xx} = 0, \quad (2.1.4a)$$

$$R_{xx} = 2R^3 - 2\omega R + R\theta_x^2. \quad (2.1.4b)$$

Equation (2.1.4a) can be solved right away by noting that it implies

$$\begin{aligned} \frac{\theta_{xx}}{\theta_x} &= \frac{-2R_x}{R} \\ \implies \ln(\theta_x) &= -2\ln(R) + c_1, \\ \implies \theta &= \int_0^x \frac{c}{R^2(y)} dy, \end{aligned} \quad (2.1.5)$$

where c_1 and c are some integration constants. Plugging this in (2.1.4b)

$$R_{xx} = 2R^3 - 2\omega R + \frac{c^2}{R^3}. \quad (2.1.6)$$

Equation (2.1.6) can be solved using standard techniques of elliptic integration [1], and it can be shown that $R(x)$ is given by

$$R^2(x) = k^2 \operatorname{sn}^2(x, k) + b, \quad (2.1.7)$$

where $\operatorname{sn}(x, k)$ is the *Jacobi elliptic sine function*, $k \in [0, 1)$ is the *elliptic modulus* and b is another real constant. A discussion on Jacobi elliptic functions can be found in Appendix B. The Jacobi sine function $\operatorname{sn}(x, k)$ is a periodic function with the period $T(k) = 4K(k)$, where $K(k)$ is the elliptic integral of the first kind

$$K(k) = \int_0^{\pi/2} \frac{dy}{\sqrt{1 - k^2 \sin^2 y}}.$$

For (2.1.7), we also have

$$\omega = \frac{1}{2}(1 + k^2) + \frac{3}{2}b, \quad c^2 = b(b + 1)(b + k^2). \quad (2.1.8)$$

Noting that $R(x)$, $\theta(x)$ and all of the associated constants must be real, we get $b \geq 0$ (to keep c in \mathbb{R}). If we choose to look at the solution with $b = c = 0$, $\omega = \frac{1}{2}(1 + k^2)$, we will get a class of solutions with $\theta(x) = 0$, i.e., the trivial phase solutions:

$$\Psi(x, t) = k \operatorname{sn}(x, k) e^{-\frac{t}{2}(1+k^2)}, \quad (2.1.9)$$

up to symmetry transformations permitted by the original equation (2.1.1). Fig-

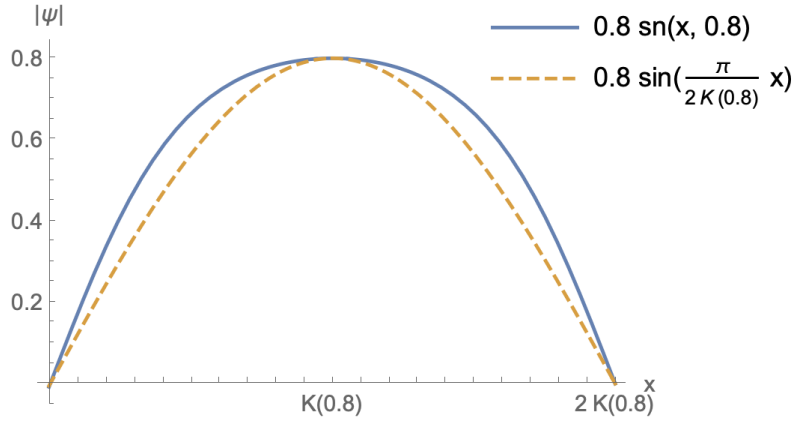


Figure 2.1: The Jacobi elliptic sine solution to the NLSE for $k = 0.8$.

ure 2.1 provides an example of a trivial phase solution (2.1.9) for $k = 0.8$. Only the amplitude $|\psi(x)|$ has been plotted in the figure as a function of x , alongside a scaled sine function. We can see that the Jacobi sine function bears a striking resemblance to the regular sine function, except for a flatter top.

To this end, we recall that an objective of the project is to solve the NLSE (2.1.1) numerically and obtain the Jacobi elliptic solution (2.1.9) as a stationary solution of the system (i.e. we see where the solution is tending towards, in the large t limit). Furthermore, we place emphasis on employing a scheme that involves performing a Fourier transform on the Laplacian. This is done with the intention of facilitating the generalisation to fractional derivatives that we eventually plan to pursue. Doing this also helps us in transforming a partial differential equation in two variables (say x and t , just like in our case), into an ordinary differential equation in just one variable (in our case, t), thus greatly reducing the complexity of the problem. We can then use standard numerical integration techniques for ODEs to progress in t and then eventually invert the Fourier transform to reach to the solution. However, it turns out that there is a fundamental issue in trying to directly use numerical integration methods on (2.1.1), owing to the stability of its solutions.

Numerical implementations inherently introduce perturbations to the system being analysed, that are outside of our control. These perturbations can be attributed

to several factors [22], including the discrete nature of the implementation, limitations in the floating point representation system, errors caused by truncation and rounding off, and inaccuracies that arise when reading or writing data to the disk. Hence, the qualitative nature of stationary solutions becomes important when we wish to obtain them numerically. The stability of a solution is determined, as we will see in the next section, by its *linearisation spectrum*. It is essential that the solution we are trying to obtain be *stable*, meaning that small perturbations near them decay to zero. In order to determine whether a solution is stable or not, certain conditions must be met, which we will explore further. We will also discuss the aforementioned issue associated with obtaining stationary solutions of the NLSE.

2.2 Stability analysis

The notion of stability of stationary solutions falls under the realm of qualitative stability analysis of differential equations. The idea involves linearising the system around a stationary solution, and then analysing how the perturbations evolve over time, while being restricted to only the first order terms. To see how this process works out for our problem, we first transform (2.1.1) to incorporate solutions of the type

$$\Psi(x, t) = e^{-i\omega t} \psi(x, t).$$

Using this, we get that $\psi(x, t)$ follows

$$i\psi_t = -\omega\psi - \frac{1}{2}\psi_{xx} + \psi|\psi|^2. \quad (2.2.1)$$

Stationary solutions will, by definition, have $\psi_t \equiv 0$. Remember that in the previous section, we had shown that such solutions exist for the NLSE. Now, we introduce perturbations to these solutions, in the following manner

$$\psi(x, t) = e^{i\theta(x)}(R(x) + \epsilon u(x, t) + i\epsilon v(x, t)) + \mathcal{O}(\epsilon^2), \quad (2.2.2)$$

where $u(x, t)$ and $v(x, t)$ are real-valued functions, and $|\epsilon| \ll 1$. $R(x)$ and $\theta(x)$ are the same as in (2.1.2). Note that because there are no restrictions on u or v as functions of space and time, the above form represents the most general perturbation. Any changes in the phase can be factored inside. Substituting (2.2.2) in (2.2.1) and

dropping any terms of order ϵ^2 or higher, we get

$$e^{i\theta}(\iota\epsilon u_t - \epsilon v_t) = -\omega e^{i\theta}(R + \epsilon u + \iota\epsilon v) - \frac{1}{2}[(Re^{i\theta})_{xx} + \epsilon(ue^{i\theta})_{xx} + \iota\epsilon(v e^{i\theta})_{xx}] \\ + e^{i\theta}(R^3 + 3\epsilon R^2 u + \iota\epsilon R^2 v). \quad (2.2.3)$$

From here, we collect all the order zero terms in ϵ and realise that they give us back (2.1.3), vanishing thereby. Next, we separately collect the real and imaginary parts of $\mathcal{O}(\epsilon)$ terms to get

$$\frac{\partial}{\partial t} \begin{pmatrix} u \\ v \end{pmatrix} = \mathcal{L} \begin{pmatrix} u \\ v \end{pmatrix} = J \begin{pmatrix} L_+ & S \\ -S & L_- \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}, \quad (2.2.4a)$$

where L_+ , L_- and S are linear operators given by

$$L_+(\cdot) = -\frac{1}{2}\partial_x^2(\cdot) + \left(3R^2(x) - \omega + \frac{c^2}{2R^4(x)}\right)(\cdot), \quad (2.2.4b)$$

$$L_-(\cdot) = -\frac{1}{2}\partial_x^2(\cdot) + \left(R^2(x) - \omega + \frac{c^2}{2R^4(x)}\right)(\cdot), \quad (2.2.4c)$$

$$S(\cdot) = \frac{c}{R(x)}\partial_x \left(\frac{(\cdot)}{R(x)}\right), \quad (2.2.4d)$$

and

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (2.2.4e)$$

In equation (2.2.4a), we can separate the variables and consider solutions of the form

$$\begin{pmatrix} u(x, t) \\ v(x, t) \end{pmatrix} = e^{\lambda t} \begin{pmatrix} U(x) \\ V(x) \end{pmatrix}, \quad (2.2.5)$$

essentially reducing the system to an eigenvalue problem

$$\mathcal{L} \begin{pmatrix} U \\ V \end{pmatrix} = \lambda \begin{pmatrix} U \\ V \end{pmatrix}. \quad (2.2.6)$$

By looking at equations (2.2.5) and (2.2.6), we can conclude that the spectrum of \mathcal{L} (denoted $\sigma(\mathcal{L})$) is what determines the stability of the solutions. Negative real parts in an eigenvalue would imply stability in that eigenspace, and vice versa. And in case the real part happens to be zero, i.e. the eigenvalue is purely imaginary, the

perturbations would neither grow nor die out to zero.

The stability spectrum of Jacobi elliptic solution has been extensively studied in the 2011 article by Bottman et al [1] and references cited therein. All the numerical and analytical enquiries suggest that the Jacobi elliptic solution has a purely imaginary spectrum. Consequently, although small perturbations around the solution remain small forever, they never approach zero. An illustration of this fact is given in fig. 2.2. Even for large times, the solution does not appear to converge to the Jacobi elliptic (orange), denoted by ψ_{JE} , as small perturbations seem to persist. The obtained numerical solution (blue), denoted as ψ_{num} , deviates away from ψ_{JE} and then returns closer to it periodically, as can be seen from the first four panels of the figure. The graph of relative error in the last panel confirms this behaviour as the error oscillates with an approximately constant amplitude over time. This output establishes that we cannot obtain the Jacobi elliptic solution by tackling the problem head on, just as we expected from theory.

To obtain the solution here, we performed a Fourier transform on the Laplacian in (2.1.1) as we had emphasised earlier;

$$\iota \frac{d\hat{\psi}}{dt} = -\frac{1}{2}q^2\hat{\psi} + \mathcal{F}\{\psi|\psi|^2\}, \quad (2.2.7)$$

where $\hat{\psi} := \mathcal{F}\{\psi\}$ and q is the transform variable. We then use a combination of two different numerical integration algorithms to progress in time. The nonlinear terms were integrated by the explicit two-step Adams-Bashforth scheme, while the linear terms were progressed using the implicit Crank-Nicolson method. A description of these methods can be found in the next section (2.3). Finally, we invert the Fourier transform to obtain the solution.

The computation was carried out in Wolfram Mathematica (v12.0.0.0) on a Mac OS X x86 (64-bit) platform. Number of points in the spatial domain, `npts`, was set to 101. While the time variable ran from `tmin = 0` to `tmax = 10`, in steps of `dt = 0.0001`. The plots were obtained using Mathematica's default `Plot[]` and `ListPlot[]` commands.

2.3 Numerical Schemes

In the previous section, we saw how Fourier transforming the Laplacian turns the partial differential equation (2.1.1) into a first order ordinary differential equation (2.2.7). It is still, however, not analytically solvable, just like most differential equations known to humanity. Nonetheless, for most practical applications, numerical

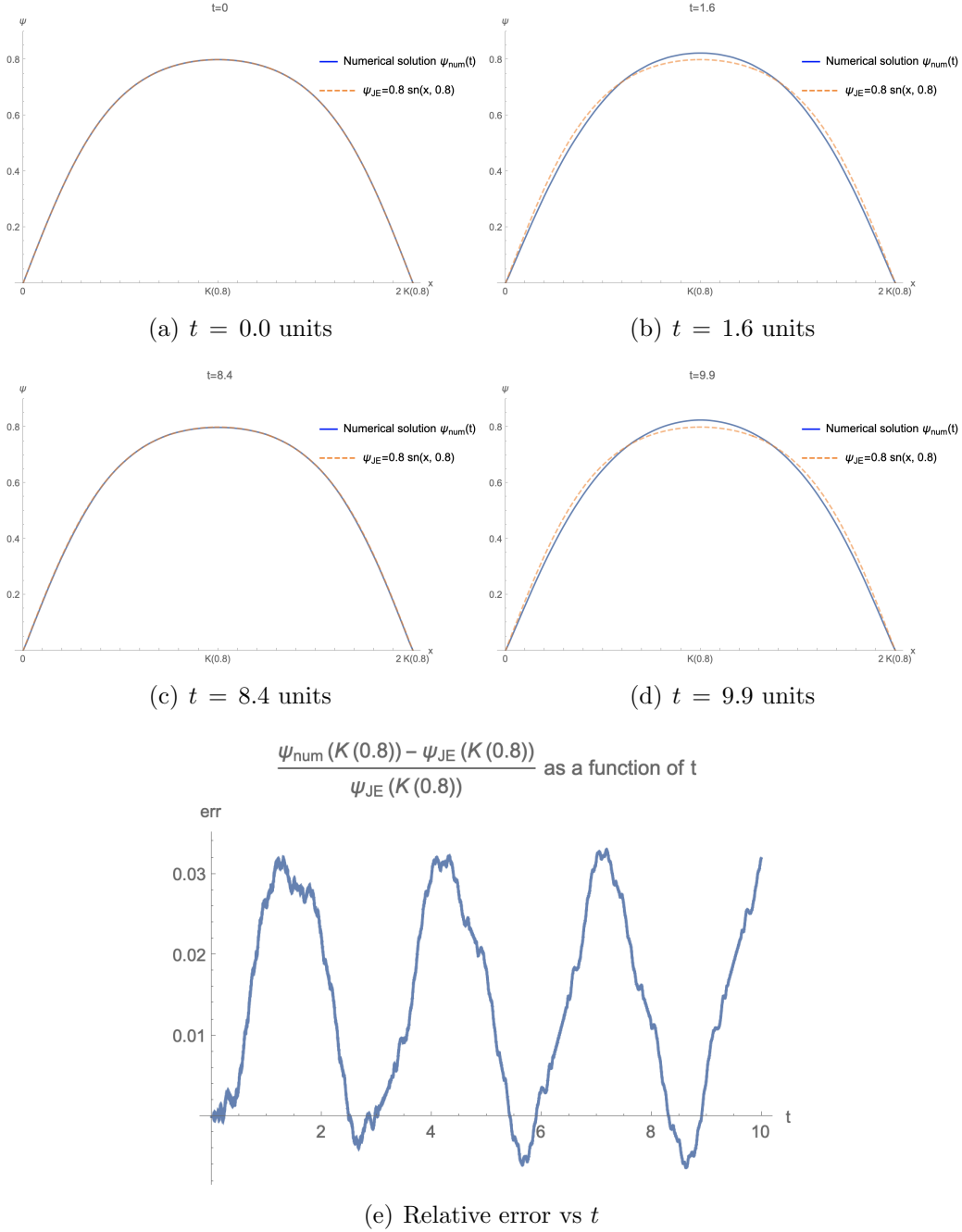


Figure 2.2: Time progression of the numerical solution ψ_{num} obtained from a direct implementation of the NLSE, plotted alongside the Jacobi elliptic solution $\psi_{\text{JE}} = 0.8 \operatorname{sn}(x, 0.8)$, which is also taken as the initial conditions for the computation of ψ_{num} . The spatial domain ranges from $x = 0$ to $x = 2K(0.8)$, where $K(0.8)$ is the complete elliptic integral of the first kind with elliptic modulus $k = 0.8$. Panels (a)-(d) shows the time progression of ψ_{num} . Panel (e) shows the relative error $(\psi_{\text{num}} - \psi_{\text{JE}}) / \psi_{\text{JE}}$ at the mid point of the domain, $x = K(0.8)$.

approximations to the solutions are sufficient. Hence, over the years, algorithms to obtain those numerical solutions have been developed. All of the algorithms focus on

approximating the shape of the solution at discrete steps, given an initial condition and an integrand.

The algorithms for finding numerical solutions to first order ordinary differential equations can be broadly categorised into two types: linear multistep methods and predictor-corrector methods. The predictor-corrector methods, like the famous Runge-Kutta methods, calculate intermediate steps between the current and next step in order to approximate the next step. However, these methods do not make use of any information from any of the previous steps. Linear multistep methods, on the other hand, use one or more previously computed steps to approximate the next step. Although both algorithms can give accurate solutions up to an arbitrary order, linear multistep methods require us to evaluate the integrand only once per step, whereas the predictor-corrector methods access the integrand for as many times as the number of intermediate steps. The choice of method to be used, depends on the specific requirements of the problem at hand.

For our specific problem, the integrand is the right-hand side of (2.2.7). The expression involves computation of a Fourier transform. Computing the Fourier transform at multiple intermediate steps, including the repeated evaluation of the integrand, would entail prohibitive computational cost. Hence, we will rely exclusively on linear multistep methods. There are two methods that must be pointed out, which would be utilised, in combination, for all numerical implementations in this project:

- Second order Adams-Bashforth (AB2) method,
- Trapezoidal rule or the Crank-Nicolson (CN) method.

Let us first give a precise definition of multistep methods [22]:

Definition 2.1 (*m*-step multistep methods). Given the initial value problem (IVP)

$$y' = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha, \quad (2.3.1)$$

an *m*-step multistep method approximates the solution y_{i+1} at t_{i+1} , as

$$\begin{aligned} y_{i+1} = & a_{m-1} y_i + a_{m-2} y_{i-1} + \cdots + a_0 y_{i-m+1} \\ & + h [b_m f(t_{i+1}, y_{i+1}) + b_{m-1} f(t_i, y_i) + \cdots + b_0 f(t_{i-m+1}, y_{i-m+1})], \end{aligned} \quad (2.3.2)$$

for $i = m - 1, m, \dots, N - 1$. Here, $a_0, a_1, \dots, a_{m-1}, b_0, b_1, \dots, b_m$ are constants and h is the grid spacing $(b - a)/N$.

If $b_m = 0$, the method is termed *explicit* as the next step is explicitly given by only the terms that come before it. And similarly, if $b_m \neq 0$, the method is termed *implicit* as the equation for y_{i+1} is implicit in it. Generally, implicit methods have better accuracy than their explicit counterparts, since they are stable.

The aforementioned AB2 and CN methods are different types of multistep methods. Their corresponding definitions are as follows. The second order Adams-Bashforth (AB2) is an explicit, two-step method given by

Definition 2.2 (Two-step Adams-Bashforth method).

$$y_{n+1} = y_n + \frac{h}{2}[3f(t_i, y_i) - f(t_{i-1}, y_{i-1})],$$

where $i = 1, 2, \dots, N - 1$. The local truncation error for this algorithm is $\mathcal{O}(h^2)$.

The trapezoidal rule is an implicit, two-step method given by

Definition 2.3 (Trapezoidal rule).

$$y_{n+1} = y_n + \frac{h}{2}[f(t_{i+1}, y_{i+1}) + f(t_i, y_i)],$$

where $i = 1, 2, \dots, N - 1$. The local truncation error for this algorithm is $\mathcal{O}(h^3)$.

This rule is equivalent to the implicit Crank-Nicolson (CN) scheme, when applied to our initial value problem (2.3.1). Hence, we may use the names exchangeably.

To conclude, it has been established that stationary solutions to the NLSE exist in the form of Jacobi elliptic solutions (2.1.9) and that their stability spectrum is purely imaginary. As a consequence of the later, we saw that it is impossible to obtain them directly by using numerical integration techniques. So to acquire the Jacobi elliptic solution from the NLSE numerically, we seek an alternative system that differs from NLSE in concept, but remains sufficiently similar to enable a conversion to NLSE. In the following chapter, we will explore a potential candidate for the same.

Chapter 3

Approach and Methodology

In this chapter we shall present a candidate for stabilising the Jacobi elliptic solution. As we saw in the last chapter, we cannot hope to solve the NLSE directly and get the Jacobi elliptics. Hence, we instead replace the NLSE with a system of partial differential equations inspired by the well known Gierer-Meinhardt system. We shall also present the details of the numerical implementation for solving the system on a computer.

3.1 The Gierer-Meinhardt model and spike-type solutions

In 1972 Geirer and Meinhardt [23] introduced a model for reaction-diffusion system involving activators and inhibitors. The system has found applicability in biological pattern formation [24], cell differentiation [25], and pattern formation on the shells of sea animals [26]. The model is a system of coupled partial differential equations. In their dimensionless form the 1D equations at the limit of slow activator and fast inhibitor are [3, 27]

$$\partial_t a = \epsilon^2 \partial_x^2 a - a + \frac{a^p}{h^q}, \quad -1 < x < 1, \quad t > 0, \quad (3.1.1a)$$

$$\tau_0 \partial_t h = D \partial_x^2 h - \mu h + \frac{1}{\epsilon} \frac{a^m}{h^s}, \quad -1 < x < 1, \quad t > 0, \quad (3.1.1b)$$

$$\partial_x a(x = \pm 1, t), \quad \partial_x h(x = \pm 1, t), \quad a(x, 0) = a_0(x), \quad h(x, 0) = h_0(x). \quad (3.1.1c)$$

Here $a(x, t)$, $h(x, t)$ denote the activator and the inhibitor concentrations, respectively. Also ϵ , D , $\mu > 0$ and $\tau \geq 0$ are the activator diffusivity, inhibitor diffusivity, inhibitor decay rate and the reaction time constant, respectively. The exponents

(p, q, m, s) satisfy [3, 23, 27]

$$p > 1, \quad q > 0, \quad m > 0, \quad s \geq 0, \quad \frac{qm}{p-1} - (s+1) > 0. \quad (3.1.2)$$

The system has been known to have a stable (spike-type) stationary solution for $0 < \epsilon \ll 1$ and $0 < D < D_1(\epsilon) \sim \epsilon^2 e^{2/\epsilon}$ [2, 3, 27], for over two decades now, and is well studied in the literature. Moreover, the eigenvalues of the the system obtained by the linearisation of (3.1.1) around a stationary solution are proven to have negative real parts [2]. If we recall from the previous chapter, that is a property we desired the NLSE system to have, in order to obtain them numerically.

There also exists a generalisation of the above system to fractional derivatives, as studied in [3]:

$$\partial_t a = \epsilon^\gamma - (-\nabla^2)^{\gamma/2} a - a + \frac{a^p}{h^q}, \quad -1 < x < 1, \quad t > 0, \quad (3.1.3a)$$

$$\tau_0 \partial_t h = D \partial_x^2 h - \mu h + \frac{1}{\epsilon} \frac{a^m}{h^s}, \quad -1 < x < 1, \quad t > 0, \quad (3.1.3b)$$

$$\partial_x a(x = \pm 1, t), \quad \partial_x h(x = \pm 1, t), \quad a(x, 0) = a_0(x), \quad h(x, 0) = h_0(x), \quad (3.1.3c)$$

$$a(x, t) = a(x + 2k, t), \quad h(x, t) = h(x + 2k, t), \quad x \in \mathbb{R}, \quad t > 0, \quad k \in \mathbb{Z}. \quad (3.1.3d)$$

In [3], the range $1 \leq \gamma \leq 2$ of the order of fractional derivatives was explored. It was found that the spike type stationary solution still existed, although with slightly different properties. For $1 \leq \gamma < 2$, spike type stationary solution produced algebraically decaying tails, compared to an exponential decay in the $\gamma = 2$ case. The $1 \leq \gamma < 2$ solutions were also comparatively less stable, but were found to be stable nonetheless.

It must be noted that in (3.1.3d), we take values of x from all of \mathbb{R} to make sure that the fractional derivative can be evaluated. Fractional derivatives, as can be recalled from section (1.3), are nonlocal operators and require functions to be defined over the interval of their definition, which is \mathbb{R} for the above case. The functions $a(x, t)$ and $h(x, t)$ are made periodic to agree with the domain of interest. The Neumann boundary conditions (3.1.3c) makes sure that the function is smooth throughout.

For eqns. (3.1.3), one can find an equation that the spike-type solution follows by constructing an asymptotic expansion of the solution near the centre of the spike (the spike inner region). The analysis of the region eventually leads to the *ground state equation* $-(-\nabla^2)^{\gamma/2} u - u + u^p = 0$, which assumes a form similar to that of the NLSE. Now, if one tries to solve this equation directly using the same method

as in section 2.3, it is seen that the solution diverges very quickly. To stabilise the solution, a new system of augmented PDEs is introduced [3], which provides us with the conceptual basis for the process which we can use to stabilise our system.

The Gierer-Meinhardt system, hence, would be an excellent candidate to take an inspiration from, in order to construct a system that stabilises the Jacobi elliptic solutions. This can only prove useful though, if we are able to connect it to the NLSE. In the following section, a system of *auxiliary* coupled partial differential equations will be introduced, that will be of the similar form as system (3.1.1). This will be done in the hope to obtain a stable stationary solution from them and connect it to the Jacobi elliptic solution of the NLSE.

3.2 The auxiliary PDE method

Recall that the Nonlinear Schrödinger equation is given by

$$\iota \Psi_t = -\frac{1}{2} \Psi_{xx} + \Psi |\Psi|^2. \quad (3.2.1)$$

As in the section (2.2), we transform the NLSE to incorporate solutions of the type

$$\Psi(x, t) = e^{-i\omega t} \psi(x, t).$$

Hence, $\psi(x, t)$ satisfies

$$\iota \psi_t = -\omega \psi - \frac{1}{2} \psi_{xx} + \psi |\psi|^2,$$

and is known to have stationary solutions related to the Jacobi elliptic functions (2.1.9), which we are trying to obtain numerically. We expect $\omega = (1 + k^2)/2$, as in the Jacobi elliptic solution, cf. equation (2.1.8). To achieve this, we introduce the following system of auxiliary PDEs in two functions, ψ and ϕ :

$$\iota \frac{\partial \psi}{\partial t} + \omega_\psi \psi + \frac{1}{2} \frac{\partial^2}{\partial x^2} \psi - \frac{\psi |\psi|^2}{|\phi|^2} = 0, \quad (3.2.2a)$$

$$\iota \tau_0 \frac{\partial \phi}{\partial t} + \omega_\phi \phi + \frac{D}{2} \frac{\partial^2}{\partial x^2} \phi - \psi |\psi|^2 = 0. \quad (3.2.2b)$$

Next, following an identical construction for the Gierer-Meinhardt system [27], we assume an asymptotic expansion of ψ and ϕ in $1/D$, and take $D \gg 1$ to limit the analysis to linear terms. The expansions are as follows:

$$\psi \sim \psi_0 + \frac{\psi_1}{D} + \mathcal{O}\left(\frac{1}{D^2}\right), \quad \phi \sim \phi_0 + \frac{\phi_1}{D} + \mathcal{O}\left(\frac{1}{D^2}\right). \quad (3.2.3)$$

The following table contains the $\mathcal{O}(1)$ and $\mathcal{O}(D)$ terms for both eqs. (3.2.2a) and (3.2.2b):

	$\mathcal{O}(D)$	$\mathcal{O}(1)$
Equation (3.2.2a)	-	$\iota\partial_t\psi_0 + \omega_\psi\psi_0 + \frac{1}{2}\partial_x^2\psi_0 - \psi_0 \psi_0 ^2/ \phi_0 ^2 = 0$
Equation (3.2.2b)	$\partial_x^2\phi_0 = 0$	$\iota\tau_0\partial_t\phi_0 + \omega_\phi\phi_0 + \frac{1}{2}\partial_x^2\phi_1 - \psi_0 \psi_0 ^2 = 0$

Now, The $\mathcal{O}(D)$ term of eq. (3.2.2b) along with the no flux boundary condition implies that ϕ_0 is only $\phi_0(t)$, i.e., it is a constant function in x . $\mathcal{O}(1)$ term of equation (3.2.2b) at $t \rightarrow \infty$ implies

$$\frac{1}{2} \frac{\partial^2}{\partial x^2} \phi_1 = \psi_0 |\psi_0|^2 - \omega_\phi \phi_0,$$

on which we now impose the solvability condition, which yields

$$\phi_0 = \frac{1}{2K(k)\omega_\phi} \int_0^{2K(k)} \psi_0 |\psi_0|^2 dx, \quad (3.2.4)$$

where $(0, 2K(k))$ is the interval of integration, as per the definition of the inner product $\left(\langle u, v \rangle = \frac{1}{(b-a)} \int_b^a u \cdot v dx\right)$. $K(k)$ is the complete elliptic integral of the first kind, with elliptic modulus k . It is also the half-period of the Jacobi sine $\text{sn}(x, k)$.

Now, $\mathcal{O}(1)$ term of equation (3.2.2a) implies

$$\omega_\psi \psi_0 = -\frac{1}{2} \frac{\partial^2}{\partial x^2} \psi_0 + \frac{\psi_0 |\psi_0|^2}{|\phi_0|^2}.$$

Since ϕ_0 is just a constant at steady state, we can simplify the expression by substituting $\psi_0 = c\eta$ and make the equation independent of ϕ_0 by choosing $|c| = |\phi_0|$. This yields that η then must follow

$$\omega_\psi \eta = -\frac{1}{2} \frac{\partial^2}{\partial x^2} \eta + \eta |\eta|^2, \quad (3.2.5)$$

which is exactly the NLSE. Hence, we now have a method to connect the NLSE with the auxiliary system (3.2.2). Once we obtain a solution to the auxiliary system, we just need to normalise it with $c = |\phi_0|$ to get a solution to the NLSE, which we expect to be the Jacobi elliptic.

A numerical trial was attempted for the above problem, details of which will be discussed in the next section. It must be noted that the parameter values were chosen so that they closely resembled the ones from (3.1.1). We allowed ourselves to explore a wide range of values of τ_0 . Results of the numerical trial will be presented

in the next chapter. Before that, we discuss our numerical implementation of the problem.

3.3 Implementation of Numerics

The numerical schemes that were used to solve system (3.2.2), were once again a combination of two-step Adams-Bashforth and Crank-Nicholson algorithms. This is the same setup we followed in the direct numerical trial of the NLSE (figure 2.2) given in the previous chapter. We recall the equations governing the above schemes are as follows.

The two-step Adams-Bashforth scheme for an ODE of the shape $y' = f(y, t)$ is given by

$$y_{n+1} = y_n + \frac{h}{2} (3y'_n - y'_{n-1}), \quad (3.3.1)$$

and the Crank-Nicholson method, given by

$$y_{n+1} = y_n + \frac{h}{2} (y'_{n+1} + y'_n). \quad (3.3.2)$$

The subscript n denotes the evaluation of the term at n^{th} time step. We shall stick with this notation hereafter.

We start our approach, once again, by performing a Fourier transform on the Laplacian and turn our system into an ordinary differential equation in t . The Fourier transformed versions of equations (3.2.2a) and (3.2.2b) are:

$$\iota \frac{\partial \hat{\psi}}{\partial t} = -\omega_{\psi} \hat{\psi} - \frac{1}{2} q^2 \hat{\psi} + \mathcal{F} \left\{ \frac{\psi |\psi|^2}{|\phi|^2} \right\}, \quad (3.3.3a)$$

$$\iota \tau_0 \frac{\partial \hat{\phi}}{\partial t} = -\omega_{\phi} \hat{\phi} - \frac{D}{2} q^2 \hat{\phi} + \mathcal{F} \{ \psi |\psi|^2 \}, \quad (3.3.3b)$$

where hats denote Fourier transformed quantities and q is the transform variable. We choose to progress the nonlinear terms using the two-step Adams-Bashforth algorithm (3.3.1) and the remaining using Crank-Nicholson algorithm (3.3.2). Hence, using (3.3.3) as the integrand for (3.3.1) and (3.3.2), we get the following as the time-step progressions:

$$\begin{aligned} \iota\hat{\psi}_{n+1} = \iota\hat{\psi}_n + \frac{h}{2} \left[-\omega_\psi\hat{\psi}_{n+1} - \omega_\psi\hat{\psi}_n - \frac{1}{2}q^2\hat{\psi}_{n+1} - \frac{1}{2}q^2\hat{\psi}_n \right. \\ \left. + 3\mathcal{F}\left\{\frac{\psi|\psi|^2}{|\phi|^2}\right\}_n - \mathcal{F}\left\{\frac{\psi|\psi|^2}{|\phi|^2}\right\}_{n-1} \right], \end{aligned}$$

$$\begin{aligned} \iota\tau_0\hat{\phi}_{n+1} = \iota\tau_0\hat{\phi}_n + \frac{h}{2} \left[-\omega_\phi\hat{\phi}_{n+1} - \omega_\phi\hat{\phi}_n - \frac{D}{2}q^2\hat{\phi}_{n+1} - \frac{D}{2}q^2\hat{\phi}_n \right. \\ \left. + 3\mathcal{F}\left\{\psi|\psi|^2\right\}_n - \mathcal{F}\left\{\psi|\psi|^2\right\}_{n-1} \right]. \end{aligned}$$

Collecting like terms and simplifying, we get

$$\begin{aligned} \hat{\psi}_{n+1} = \frac{1}{\left(\iota + \frac{h}{4}q^2 + \frac{h}{2}\omega_\psi\right)} \left[\left(\iota - \frac{h}{4}q^2 - \frac{h}{2}\omega_\psi\right)\hat{\psi}_n + \right. \\ \left. \frac{h}{2} \left(3\mathcal{F}\left\{\frac{\psi|\psi|^2}{|\phi|^2}\right\}_n - \mathcal{F}\left\{\frac{\psi|\psi|^2}{|\phi|^2}\right\}_{n-1} \right) \right], \end{aligned}$$

$$\begin{aligned} \hat{\phi}_{n+1} = \frac{1}{\left(\iota\tau_0 + \frac{h}{4}q^2 + \frac{hD}{2}\omega_\phi\right)} \left[\left(\iota - \frac{hD}{4}q^2 - \frac{h}{2}\omega_\phi\right)\hat{\phi}_n + \right. \\ \left. \frac{h}{2} \left(3\mathcal{F}\left\{\psi|\psi|^2\right\}_n - \mathcal{F}\left\{\psi|\psi|^2\right\}_{n-1} \right) \right]. \end{aligned}$$

At the end, we shall invert the Fourier transform and normalise the solution according to the prescription given in section 3.2 and thereby recover a solution to the NLSE. As can be noted from the algorithms, we require values from the n^{th} and the $(n-1)^{\text{th}}$ step for the computation of the $(n+1)^{\text{th}}$ step. This is because we chose to use the two-step Adams-Bashforth method. However, this feature will imply that if the initial conditions are at $n = 1$, then we do not have enough previous steps to compute the step at $n = 2$. This problem is circumvented by progressing the nonlinear terms with the Euler algorithm at $n = 2$. This completes all the details that will be needed to implement a numerical trial to solve 3.2.2. We shall present the results of this numerical trial in the next chapter.

Chapter 4

Results

In the previous chapter we set up the details of the numerical trial for finding solutions to the auxiliary PDE system 3.2.2. We first converted the system of PDEs in x and t into ODEs in t , by performing a Fourier transform on the variable x . Then, we made use of a combination of AB2 and CN algorithms, resulting in an algorithm to progress in t . In this chapter, we shall present the solutions obtained from this setup for various parameter values.

In anticipation of the Jacobi elliptic solutions, we set up the initial conditions of the algorithm as the following

$$\psi_{n=1} = \nu k \operatorname{sn}(x, k), \quad (4.1)$$

$$\phi_{n=1} = \frac{1}{2K(k)\omega_\phi} \int_0^{2K(k)} \psi |\psi|^2 dx. \quad (4.2)$$

Here, $\nu \approx 1$ but $\neq 1$ as we do not wish to start exactly *at* the solution itself, but slightly away from it, in order to be able to observe a clear convergence towards the desired solution. We also choose $k = 0.8$, $D = 1000$, $\nu = \frac{0.5}{0.8}$ and $\omega_\phi = \omega_\psi = \frac{1}{2}(1+k^2)$, as in (2.1.8). The number of grid points in the spatial domain, `npts`, was set to 2^{10} while the time variable ran from `tmin` = 0 to `tmax` = 10, in steps of `dt` = 0.01. All of the computation was carried out in Wolfram Mathematica (v12.0.0.0) on a Mac OS X x86 (64-bit) platform. The plots were obtained using Mathematica's default `Plot[]` and `ListPlot[]` commands.

Figure 4.1 shows the output of the algorithm for different values of τ_0 . Even complex values of τ_0 were tried out. However, all of the obtained solutions are convergent to the trivial instead of the Jacobi elliptic, marked by the orange curves which implies that the given prescription has failed to stabilise the Jacobi elliptic solution and a different candidate is needed for the same. Nonetheless, certain values of τ_0 produced interesting evolution scenarios. One such case is listed in fig. 4.2

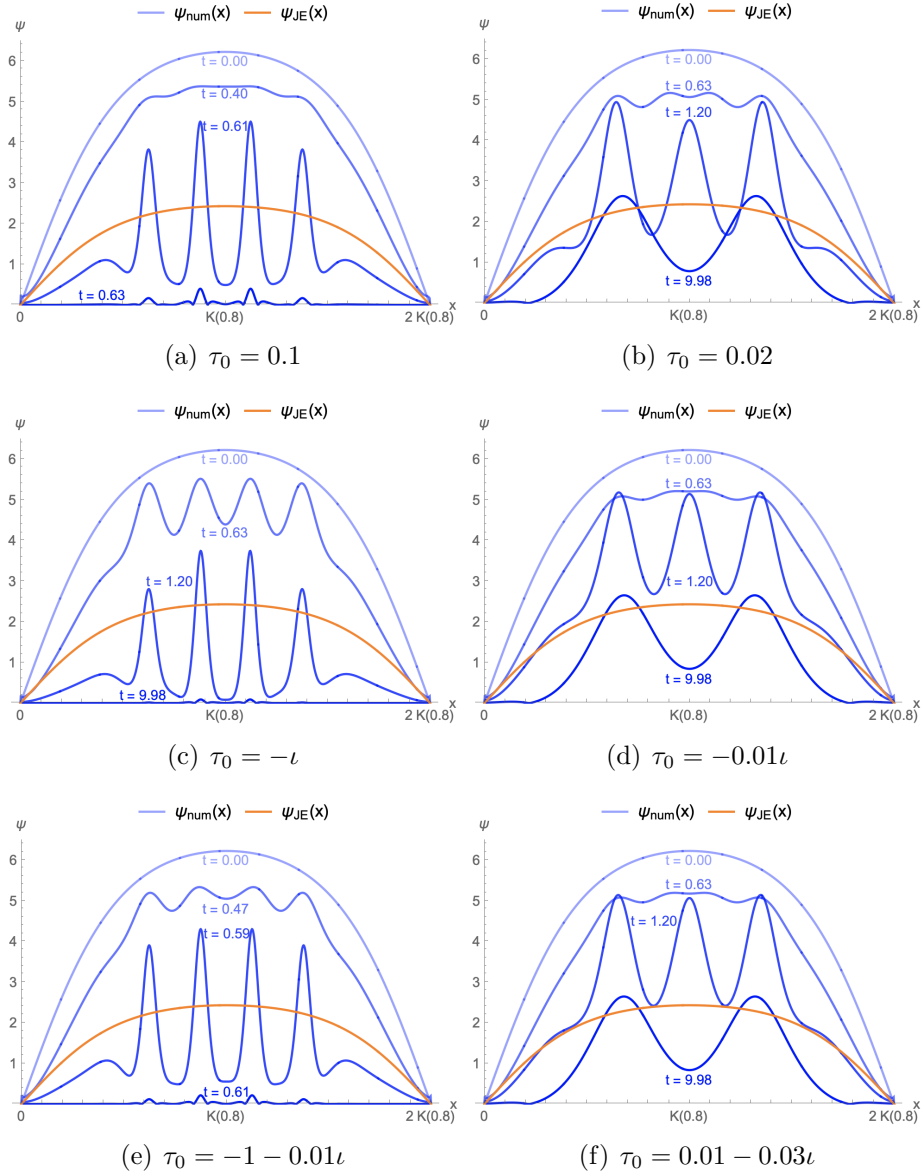


Figure 4.1: Obtained outputs for a numerical implementation of the auxiliary PDE method. Panels (a) - (f) show the evolution for different values of τ_0 . In each panel, $\psi_{\text{num}}(x, t)$ is shown in blue at different values of t , each indicated above their corresponding curves. The Jacobi elliptic solution $\psi_{\text{JE}}(x) = 0.8 \text{sn}(x, 0.8)$ is also displayed alongside in orange, for comparison. The spatial domain is $0 \leq x \leq 2K(0.8)$.

($\tau_0 = 0.035$). As can be clearly seen, the graph of $\psi_{\text{num}}(x, t)$ seems to converge to 0 by $t = 9.3$, before attaining large values again only to be seen going down to 0 by $t = 99.9$.

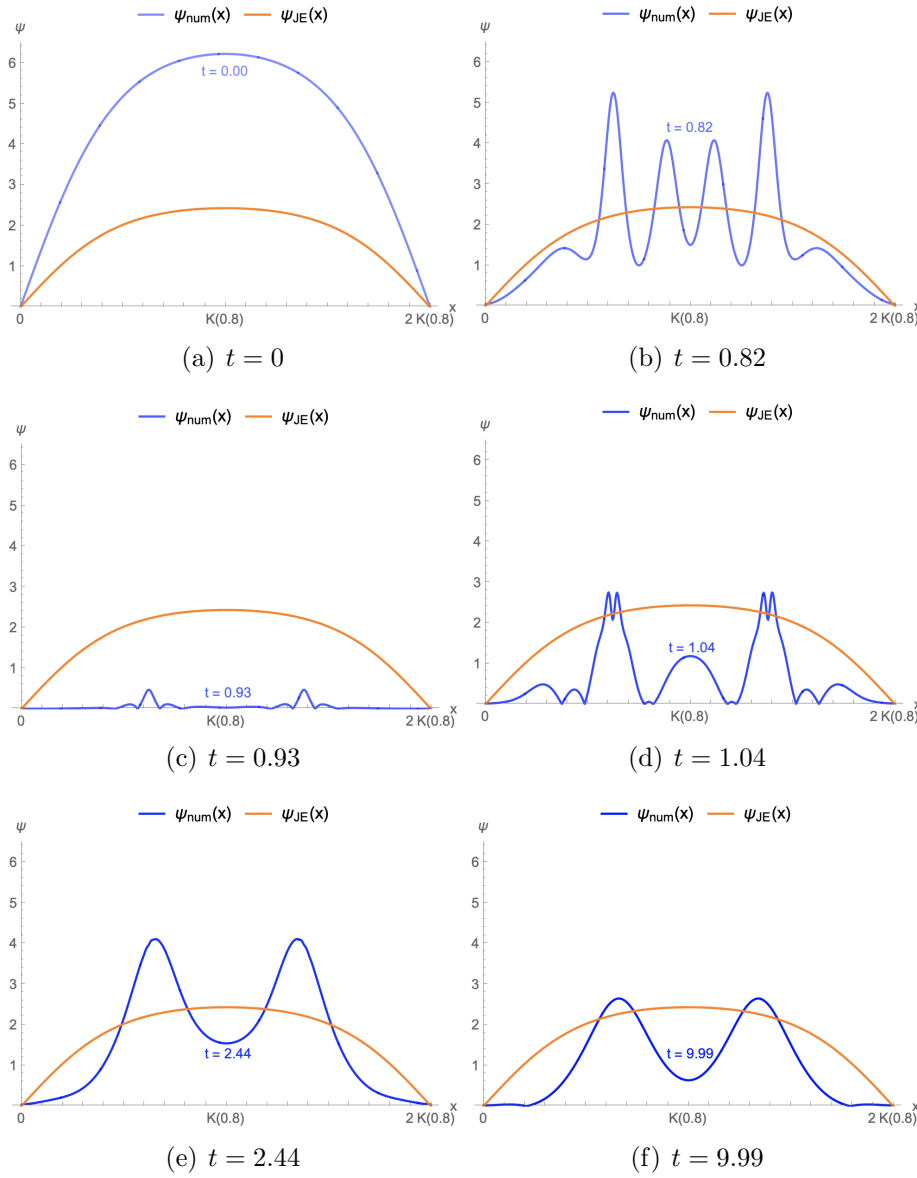


Figure 4.2: Panels (a)-(f) display the obtained solution (blue) $\psi_{\text{num}}(x, t)$ for $\tau_0 = 0.035$ at different values of t . The Jacobi elliptic solution $\psi_{\text{JE}}(x) = 0.8 \text{sn}(x, 0.8)$ is also displayed alongside in orange, for comparison. The spatial domain is $0 \leq x \leq 2K(0.8)$.

Hence, it is apparent from the results given in figs. 4.1 and 4.2 that achieving stabilisation via this scheme is unlikely. The NLSE must be sufficiently different from the GM model to elude this attempt.

Chapter 5

Conclusion and Future prospects

Although objectives 1 and 2 of the computational aspect of the project were not achieved in the allocated duration of this project, a wide range of topics in the field of dynamics were explored in review of the literature required for the project.

We came across multiple famous partial differential equation models like the nonlinear Schrödinger equation, the complex Ginzburg-Landau equation and the Gierer-Meinhardt system, all bearing tremendous usefulness in modelling of natural phenomena. An extensive discussion on the nonlinear Schrödinger equation was presented. The Jacobi elliptic solutions were introduced as stationary solutions of the NLSE and their (purely imaginary) linear stability spectrum was discussed.

We also presented an enquiry into the intriguing notion of fractional order derivatives, wherein we saw four out of a multitude of its plausible definitions that appear in literature. We also noted its immense success in various practical applications and the recent upsurge in the interest in exploring fractional versions of popular differential equations. This is where our interest in exploring the solutions to the nonlinear Schrödinger equation of a fractional order was conceived. To do that, we first wished to obtain the Jacobi elliptic solutions of the NLSE, numerically. However, the spectral nature of the Jacobi solutions prevented us from doing so directly. Hence, a novel scheme, inspired by the Gierer-Meinhardt system (3.1.1), was developed in hopes of stabilising the Jacobi elliptic solution. The scheme involved development of an auxiliary system of PDEs (3.2.2), which resembled the GM system. The auxiliary PDE system was then solved numerically for various values of different parameters.

A comprehensive investigation of an adequate range of parameters ν and τ_0 was made and all of them resulted in a convergence to the trivial solution. So, we are forced to conclude that the mentioned approach might require a much deeper numerical or, even better, an analytical insight to glean any details about the exis-

tence and/or the location of the basins of attraction of the stationary solutions of the auxiliary PDE system (3.2.2). Such a basin, of course, may not even exist as (3.2.2) merely bears resemblance to the well established Gierer-Meinhardt system (3.1.1) on visual grounds. A better auxiliary system may be found if one is able to circumvent the issue created by the imaginary factor ι on the LHS of the NLSE, while attempting to connect the NLSE and the Gierer-Meinhardt system (3.1.1) in a fashion similar to the approach in section (3.2). One can also search for better candidates for processes that can stabilise the Jacobi elliptic solution. Once a working algorithm for obtaining the Jacobi elliptic from the NLSE is found, one can generalise the process to obtain solutions to the fractional Nonlinear Schrödinger equation (fNLSE).

Appendices

Appendix A

Fourier Transforms

Fourier transform (FT) is one of many available types of integral transforms in mathematics. It converts a function of time (space) into a form that describes the frequencies (wave numbers) present in the original function (i.e. the *spectrum*). FTs have found applicability in various branches of mathematics, physics and engineering. In the context of this thesis, FTs have primarily been used as a tool to convert difficult-to-solve partial differential equations into ordinary differential equations, which are far easier to deal with. We shall take a look at the definition and some properties of FTs along with a brief introduction to Discrete Fourier Transforms.

A.1 Definitions

There are multiple conventions that are followed to define FTs, depending on the context. We shall stick to the convention that has the formulas of FT and the *inverse Fourier Transform* symmetric (as it makes the definitions easy to remember and follow).

Definition A.1 (Fourier Transform). The **Fourier Transform** $\hat{f}(\xi)$ of a function $f(x)$; $x, \xi \in \mathbb{R}$, is given by

$$\hat{f}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-i\xi x} dx \quad (\text{A.1.1})$$

provided that f is *Lebesgue-measurable* on the real line [28], i.e., $\int_{-\infty}^{\infty} |f(x)| dx < \infty$.

The inverse Fourier Transform can also be defined in a similar fashion

Definition A.2 (Inverse Fourier Transform). The **inverse Fourier Transform**

$f(x)$ of a function $\hat{f}(\xi)$; $x, \xi \in \mathbb{R}$, is given by

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \hat{f}(\xi) e^{i\xi x} d\xi \quad (\text{A.1.2})$$

The pair of functions f and \hat{f} is often termed as a *Fourier transform pair*. There are a few commonly used short-hand notations to denote FTs

$$\hat{f}(\xi) = \mathcal{F}\{f(x)\}_{x \rightarrow \xi} \quad \text{or simply} \quad \hat{f}(\xi) = \mathcal{F}\{f(x)\},$$

and similarly for Inverse FT

$$f(x) = \mathcal{F}^{-1}\{\hat{f}(\xi)\}_{\xi \rightarrow x} \quad \text{or} \quad f(x) = \mathcal{F}^{-1}\{\hat{f}(\xi)\}.$$

Note that Fourier Transforms may be defined in any number of space (and/or time) dimensions. **In the case where both space and time variables are present, it is customary to define the Fourier transform in a manner that treats the time variables distinctively from all spatial variables.** For instance, here is how one may define a FT in $3 + 1$ dimensions

Definition A.3 (Fourier Transform in $3 + 1$ dimensions). The **Fourier Transform** $\hat{f}(\mathbf{k}, \omega)$ of a function $f(\mathbf{x}, t)$; $\mathbf{x}, \mathbf{k} \in \mathbb{R}^3$; $t, \omega \in \mathbb{R}$, is given by

$$\hat{f}(\mathbf{k}, \omega) = \frac{1}{(2\pi)^2} \iint_{\mathbb{R}^4} f(\mathbf{x}, t) e^{-i(\mathbf{k} \cdot \mathbf{x} - \omega t)} d^3\mathbf{x} dt \quad (\text{A.1.3})$$

and similarly

Definition A.4 (Inverse Fourier Transform in $3 + 1$ dimensions). The **Inverse Fourier Transform** $f(\mathbf{x}, t)$ of a function $\hat{f}(\mathbf{k}, \omega)$; $\mathbf{x}, \mathbf{k} \in \mathbb{R}^3$; $t, \omega \in \mathbb{R}$, is given by

$$f(\mathbf{x}, t) = \frac{1}{(2\pi)^2} \iint_{\mathbb{R}^4} \hat{f}(\mathbf{k}, \omega) e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} d^3\mathbf{k} d\omega. \quad (\text{A.1.4})$$

It may be noted that the time variable in the above definitions, is being treated in exactly the opposite fashion as the spatial variables.

A.2 Properties of Fourier Transforms

There are a few properties of FTs that are of particular interest for the context of this thesis, they are (in no particular order of importance)

Property A.1 (Linearity). If a and b are any two given complex scalars, then

$$\mathcal{F}\{ag(x) + bh(x)\} = a\mathcal{F}\{g(x)\} + b\mathcal{F}\{h(x)\}.$$

Property A.2 (Differentiation). Suppose $f(x)$ is continuously differentiable and both f and its derivative f' are integrable, then

$$\mathcal{F}\left\{\frac{d}{dx}f(x)\right\} = (\iota\xi)\mathcal{F}\{f(x)\},$$

and in general

$$\mathcal{F}\left\{\frac{d^n}{dx^n}f(x)\right\} = (\iota\xi)^n\mathcal{F}\{f(x)\}.$$

where $n \in \mathbb{N}$. In fact, the Fourier transform properties of the Riesz fractional derivatives enables us to generalise this property even to derivatives of non-integral orders:

$$\mathcal{F}\{ {}^R\mathfrak{D}_x^\alpha f(x) \} = -|\xi|^\alpha \mathcal{F}\{f(x)\},$$

where ${}^R\mathfrak{D}_x^\alpha$ denotes the Riesz fractional derivative of order $\alpha \in \mathbb{R}$, in the variable x .

Property A.3 (Convolution theorem). If $f(x)$ and $g(x)$ are integrable functions, then

$$\mathcal{F}\{f(x)\} \cdot \mathcal{F}\{g(x)\} = \mathcal{F}\{(f * g)(x)\},$$

where $*$ denotes convolution $(f * g)(x) = \int_{-\infty}^{\infty} f(y)g(x - y)dy$.

A.3 Discrete Fourier Transforms

For FTs to have any practical viability, there must exist a way of performing the transform (and its inverse), numerically. And since numerics can only be performed on discrete sets, we need a *discrete transform* that converts a list of numbers into another, such that the desired spectral information about the former list is captured in the latter. This can be achieved by defining

Definition A.5 (Discrete Fourier Transform). The **Discrete Fourier Transform (DFT)** v_s of a list u_r of length n is defined to be

$$v_s = \frac{1}{\sqrt{n}} \sum_{r=1}^n u_r e^{2\pi\iota(r-1)(s-1)/n}. \quad (\text{A.3.1})$$

and

Definition A.6 (Discrete Inverse Fourier Transform). The **inverse Discrete Fourier Transform (inverse DFT)** u_r of a list v_s of length n is defined to be

$$u_r = \frac{1}{\sqrt{n}} \sum_{s=1}^n v_s e^{-2\pi i(r-1)(s-1)/n}. \quad (\text{A.3.2})$$

It must be noted that just like FTs and inverse FTs, many definitions of DFT and inverse DFT exist (again often involving different conventions). The definition [A.5](#) here, is the same as in the documentation of Wolfram Mathematica [\[29\]](#). This definition has been chosen here because Wolfram Mathematica was used for all computation aspects of this project.

Appendix B

The Jacobi elliptic trigonometric functions

The Jacobi elliptic functions [30] are a set of special functions which appear as solutions to differential equations of the type

$$\frac{d^2y}{dx^2} = A + By + Cy^3,$$

where all of A , B , and C are real constants. The three basic Jacobi elliptic trig functions are $\text{sn}(x, k)$, $\text{cn}(x, k)$ and $\text{dn}(x, k)$, where k is known as the *elliptic modulus*. These may also be defined using the elliptic integral of the first kind,

$$x = F(\phi, k) = \int_0^\phi \frac{dt}{\sqrt{1 - k^2 \sin^2 t}}.$$

Using this, we define

$$\phi = F^{-1}(x, k) =: \text{am}(x, k),$$

where $\text{am}(x, k)$ is the *Jacobi amplitude*. Now, $\text{sn}(x, k)$, $\text{cn}(x, k)$ and $\text{dn}(x, k)$ may be defined using $\text{am}(x, k)$ in the following fashion

$$\text{sn}(x, k) := \sin \phi = \sin(\text{am}(x, k)),$$

and similarly

$$\text{cn}(x, k) := \cos \phi = \cos(\text{am}(x, k)).$$

Then we have

$$\begin{aligned}\operatorname{dn}(x, k) &:= \sqrt{1 - k^2 \operatorname{sn}^2(x, k)} \\ &= \sqrt{1 - k^2 \sin^2(\operatorname{am}(x, k))} .\end{aligned}$$

From the above definitions, it must be clear that if one defines the complete elliptic integral of the first kind as

$$K(k) = \int_0^{\pi/2} \frac{dt}{\sqrt{1 - k^2 \sin^2 t}},$$

then we have $\operatorname{am}(K, k) = \pi/2$. Hence, the Jacobi elliptic functions $\operatorname{sn}(x, k)$, $\operatorname{cn}(x, k)$ and $\operatorname{dn}(x, k)$ will all be periodic in $K(k)$ w.r.t. their first argument as

$$\begin{aligned}\operatorname{sn}(x + 2mK, k) &= (-1)^m \operatorname{sn}(x, k), \\ \operatorname{cn}(x + 2mK, k) &= (-1)^m \operatorname{cn}(x, k)\end{aligned}$$

and

$$\operatorname{dn}(x + 2mK, k) = \operatorname{dn}(x, k),$$

where m is a positive integer.

Bibliography

1. Bottman, N., Deconinck, B. & Nivala, M. Elliptic solutions of the defocusing NLS equation are stable. *Journal of Physics A: Mathematical and Theoretical* **44**, 285201. doi:[10.1088/1751-8113/44/28/285201](https://doi.org/10.1088/1751-8113/44/28/285201) (June 2011).
2. Iron, D., Ward, M. & Wei, J. The stability of spike solutions to the one-dimensional Gierer–Meinhardt model. *Physica D: Nonlinear Phenomena* **150**, 25–62. doi:[10.1016/S0167-2789\(00\)00206-2](https://doi.org/10.1016/S0167-2789(00)00206-2) (Mar. 2001).
3. Nec, Y. Spike-Type Solutions to One Dimensional Gierer–Meinhardt Model with Lévy Flights. *Studies in Applied Mathematics* **129**, 272–299. doi:[10.1111/j.1467-9590.2012.00550.x](https://doi.org/10.1111/j.1467-9590.2012.00550.x) (2012).
4. Nec, Y. *Pattern formation in systems with anomalous diffusion* PhD thesis (Technion – Israel Institute of Technology, 2009).
5. Malomed, B. *Encyclopedia of Nonlinear Science* (Scott, Alwyn (ed.), New York: Routledge, pp. 639–643, 2005).
6. Hasegawa, A. & Kodama, Y. *Solitons in optical communications Akira Hasegawa and Yuji Kodama* English, xiv, 320 p. : (Clarendon Press ; Oxford University Press Oxford : Oxford ; New York, 1995).
7. Zakharov, V. E. Collapse of Langmuir Waves. *Soviet Journal of Experimental and Theoretical Physics* **35**, 908 (Jan. 1972).
8. Ablowitz, M. J., Prinari, B. & Trubatch, A. D. *Discrete and Continuous Non-linear Schrödinger Systems* doi:[10.1017/CB09780511546709](https://doi.org/10.1017/CB09780511546709) (Cambridge University Press, 2003).
9. Herrmann, R. *Fractional Calculus – An Introduction for Physicists (3rd revised and extended Edition)*, World Scientific Publishing, Singapore, September 2018, 636 pp, ISBN: 978-981-3274-57-0 636 (Sept. 2018).
10. Oldham, K. B. & Spanier, J. *The fractional calculus; theory and applications of differentiation and integration to arbitrary order by Keith B. Oldham and Jerome Spanier* English, xiii, 234 p. (Academic Press New York, 1974).

11. Mandelbrot, B. B. *The fractal geometry of nature* (Freeman, San Francisco, CA, 1982).
12. Mandelbrot, B. B. Self-affine fractals and fractal dimension. *Phys. Scr.* **32**, 257 (1985).
13. Metzler, R. & Klafter, J. The random walk's guide to anomalous diffusion: a fractional dynamics approach. *Physics Reports* **339**, 1–77. doi:[10.1016/S0370-1573\(00\)00070-3](https://doi.org/10.1016/S0370-1573(00)00070-3) (2000).
14. Eliazar, I. & Klafter, J. Anomalous is ubiquitous. *Annals of Physics* **326**, 2517–2531. doi:[10.1016/j.aop.2011.07.006](https://doi.org/10.1016/j.aop.2011.07.006) (2011).
15. Laskin, N. Fractional Schrödinger equation. *Phys. Rev. E* **66**, 056108. doi:[10.1103/PhysRevE.66.056108](https://doi.org/10.1103/PhysRevE.66.056108) (5 Nov. 2002).
16. Goldfain, E. Complexity in quantum field theory and physics beyond the standard model. *Chaos, Solitons and Fractals* **28**. Sir Hermann Bondi 1919–2005, 913–922. doi:[10.1016/j.chaos.2005.09.012](https://doi.org/10.1016/j.chaos.2005.09.012) (2006).
17. Lim, S. Fractional derivative quantum fields at positive temperature. *Physica A: Statistical Mechanics and its Applications* **363**, 269–281. doi:[10.1016/j.physa.2005.08.005](https://doi.org/10.1016/j.physa.2005.08.005) (2006).
18. Bayın, S. Ş. Definition of the Riesz derivative and its application to space fractional quantum mechanics. *Journal of Mathematical Physics* **57**, 123501. doi:[10.1063/1.4968819](https://doi.org/10.1063/1.4968819) (Dec. 2016).
19. Naber, M. Time fractional Schrödinger equation. *Journal of Mathematical Physics* **45**, 3339–3352. doi:[10.1063/1.1769611](https://doi.org/10.1063/1.1769611) (Aug. 2004).
20. Laskin, N. "Fractional quantum mechanics and Lévy path integrals". *Physics Letters A* **268**, 298–305. doi:[10.1016/s0375-9601\(00\)00201-2](https://doi.org/10.1016/s0375-9601(00)00201-2) (Apr. 2000).
21. Some applications of fractional equations. *Communications in Nonlinear Science and Numerical Simulation* **8**. Chaotic transport and complexity in classical and quantum dynamics, 273–281. doi:[10.1016/S1007-5704\(03\)00049-2](https://doi.org/10.1016/S1007-5704(03)00049-2) (2003).
22. Burden, R., Faires, J. & Burden, A. *Numerical Analysis* 10th Edition (Cengage Learning, 2015).
23. Gierer, A. & Meinhardt, H. A theory of biological pattern formation. *Kybernetik* **12**, 30–39. doi:[10.1007/BF00289234](https://doi.org/10.1007/BF00289234) (1972).
24. Meinhardt, H. *Models of Biological Pattern Formation* (Academic Press, London, 1982) (May 1982).

25. Huang, X., Dong, Y. & Zhao, J. HetR homodimer is a DNA-binding protein required for heterocyst differentiation, and the DNA-binding activity is inhibited by PatS. *Proceedings of the National Academy of Sciences* **101**, 4848–4853. doi:[10.1073/pnas.0400429101](https://doi.org/10.1073/pnas.0400429101) (2004).
26. Meinhardt, H. & Klingler, M. A model for pattern formation on the shells of molluscs. *Journal of Theoretical Biology* **126**, 63–89. doi:[10.1016/S0022-5193\(87\)80101-7](https://doi.org/10.1016/S0022-5193(87)80101-7) (1987).
27. WARD, M. J. & WEI, J. Hopf bifurcation of spike solutions for the shadow Gierer–Meinhardt model. *European Journal of Applied Mathematics* **14**, 677–711. doi:[10.1017/S0956792503005278](https://doi.org/10.1017/S0956792503005278) (2003).
28. Boas, M. L. *Mathematical methods in the physical sciences; 3rd ed.* (Wiley, Hoboken, NJ, 2006).
29. *Wolfram language function: “Fourier”*, Wolfram Language and System Documentation Center. Wolfram Research. <https://reference.wolfram.com/language/ref/Fourier.html>.
30. Weisstein, E. W. “*Jacobi Elliptic Functions*” From MathWorld—A Wolfram Web Resource. <https://mathworld.wolfram.com/JacobiEllipticFunctions.html>.