

SOME REACTION DIFFUSION TYPE EQUATIONS IN QUANTUM MECHANICS

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Abstract. Many second order partial differential equations are expressed as a pair of coupled first order partial differential equations. A surprisingly large variety of problems from quantum theory to information sciences can be studied. We examine certain novel features of the solutions of equations arising from these areas of study.

Keywords: Schrödinger equation, Klein Gordon, reaction diffusion equations

1. Introduction

A reaction-diffusion equation comprises of a reaction term and a diffusion term, a typical Reaction Diffusion equation is as follows:

$$\frac{\partial u}{\partial t} = D\Delta u + f(u)$$

$u = u(x, t)$ is a variable which describes concentration of a substance or the population at time t . Δ denotes the Laplace operator. So the first term on the right hand side describes the “diffusion”, including D as diffusion coefficient. The second term, $f(u)$ is a smooth function $f : \mathbb{R} \rightarrow \mathbb{R}$ representing reaction kinetics.

Instead of a scalar equation, one can also introduce systems of reaction diffusion equations, which are of the form

$$(1) \quad \frac{\partial u}{\partial t} = \nabla_x \cdot (\text{diag}(d_1, d_2, \dots, d_m)) \nabla_x u + f(t, x, u, \nabla_x)$$

where $t \geq 0$ denotes time and $x \in \Omega \subset \mathbb{R}^d$ denotes position within a d -dimensional bounded domain Ω with a smooth boundary. The states $u = (u_1, \dots, u_m)$, $i = 1, \dots, m$ describe the concentrations or densities of substances or populations, $u_i = u_i(t, x)$. The functions $d_i(t, x)$ are called diffusion coefficients or diffusivities. On Ω , the bounded domain introduced earlier, boundary conditions need to be specified for equations (1). Typical conditions would include either Dirichlet, which prescribe the value at the boundary $u_i(x, t) = f_D(t, x)$, $x \in \partial\Omega$ or Neumann conditions giving the diffusion flux through the boundary $\partial\Omega$, $d_i(t, x)\nabla_x u_i(t, x) = f_N(t, x)$ or mixed boundary conditions.

One of the fascinating aspects of the natural world is the diversity of shapes that make up the animal and plant kingdoms. How these patterns arise is one of the mysteries of science. The problem that Turing addressed in his seminal paper, "The chemical basis of morphogenesis" [16] was precisely this. He presented a theory in which he proposed that cells actually respond to a chemical pre-pattern. He considered a system of morphogens reacting and diffusing in such a way that, in the absence of diffusion, they exhibited a spatially uniform steady state which would be stable. This phenomenon, termed diffusion-driven instability, has now been shown to occur in chemistry. Experimental results illustrate the formation of striped and spotted patterns, as well as more complicated patterns. This was the first example of what is now called an emergent phenomenon in the sense that the behaviour of the system, in this case a patterning instability, emerges from the components and is not part of the components. In his system, the reaction kinetics are stabilising and we know that diffusion is stabilising in the sense that it homogenises spatial patterns. Therefore, two stabilising systems interacted to produce an instability. In other words, he recognised that it was the integration of components that gave rise to the structures and behaviours we observe, rather than each behaviour being encoded in its own component. Many of these patterns can be exhibited by Turing models and there is now a vast amount of theoretical and experimental literature in this area (see [13], for a review). Turing systems have the form

$$(2) \quad \begin{aligned} \frac{\partial U}{\partial t} &= D_u \nabla^2 U + f(U, V) \\ \frac{\partial V}{\partial t} &= D_v \nabla^2 V + g(U, V). \end{aligned}$$

These equations describe the evolution of the concentrations, $U(\bar{x}, t)$, $V(\bar{x}, t)$ at spatial position \bar{x} and time t , of two chemicals due to diffusion, with constant diffusion coefficients D_u , D_v , respectively, and reaction, modeled by the functions, f and g which are typically non-linear. We now examine solutions of the travelling-wave type for reaction-diffusion equations.

2. The Klein Gordon equation

Many second order partial differential equations are expressed as a pair of coupled first order partial differential equations. A surprisingly large variety of problems

from quantum theory to information sciences can be studied. We examine certain novel features of the solutions. [7]

A single particle can be described by the Klein-Gordon equation for spin 0 and the Dirac equation for spin $1/2\hbar$. It is well-known that the Dirac equation gives (within the correct limits) a relativistic wave-mechanical description of a single electron. It is significant to interpret the definition of a single particle in terms of its wave function. We seek the appropriate generalization of the nonrelativistic equation to obtain the proper relativistic equation describing a particle of a given spin.

For the spin zero particle, the nonrelativistic equation is the Schrödinger equation,

$$(3) \quad \sum_{k=1}^3 \frac{1}{2m} \left[\frac{\hbar}{i} \frac{\partial}{\partial x_k} - \frac{e}{c} A_k \right]^2 \psi = \left(\frac{\hbar}{i} \frac{\partial}{\partial t} - e\phi \right) \psi,$$

where e is charge, m is mass and ψ is the Schrödinger wave function and A_k and ϕ are the vector and scalar potential for the electromagnetic field. The coordinates x_k will as usual be x, y, z as k goes from one to three, $x_4 = ict$, while $x_0 = ct$. We also use the symbol x to represent a vector whose components are x_k . Four vectors generally will be indicated by a Greek subscript, e.g., $x_\mu = (x_k, x_4)$. Similar notation is used for the momentum \mathbf{P} and electromagnetic potentials, $A_k = (A_x, A_y, A_z)$, $A_4 = i\phi$, $A_0 = \phi$, where A_k is the vector potential and ϕ , the scalar. This equation is obtained from the non-relativistic Hamiltonian describing the interaction between a charged particle and the electromagnetic field,

$$(4) \quad H(\mathbf{p}, \mathbf{r}) = 1/2m \sum (p_k - (e/c)A_k)^2 + e\phi$$

by the well-known substitutions derived, for example, by transformation theory from the commutation relations between \mathbf{p} and \mathbf{r} ,

$$(5) \quad p_k \rightarrow (\hbar/i)(\partial/\partial x_k), H \rightarrow \hbar i(\partial/\partial t).$$

To obtain the relativistic generalization of (3) we need only write the relativistic energy-momentum relation and make substitutions (5). We replace (4) by

$$\sum_{\mu=1}^4 (p_\mu - \frac{e}{c} A_\mu)^2 + (mc)^2 = 0,$$

where

$$p_\mu = (p_k, p_4), \quad p_4 = (i/c)H, \\ A_\mu = (A_k, A_4), \quad A_4 = i\phi.$$

For simplicity, we now insert the substitution

$$D_\mu = \partial/\partial x_\mu - (ie/\hbar c)A_\mu \quad \text{and} \quad \kappa = mc/\hbar.$$

Then (3) can be written in the coincide form

$$(6) \quad \sum_{\mu} [D_\mu^2 - \kappa^2] \psi = 0,$$

we seek an approximate wave function ψ . To obtain from the above the equation

$$(7) \quad H\psi = i\hbar(\partial\psi/\partial t).$$

3. A Hamiltonian form of the Klein-Gordon equation

We look for an appropriate ψ such that ψ satisfies the Hamiltonian form for the wave equation (7). To obtain this form it is necessary to resolve ψ into the components representing the two degrees of freedom. The function ψ is then a unicolunar matrix formed from these two components.

The obvious first step in such a development is to introduce $\partial\psi/\partial t$ as an independent component. Let

$$\psi_4 = -\kappa^{-1}D_4\psi.$$

Then the Klein-Gordon equation may be written in a form equivalent as follows:

$$(8) \quad \begin{aligned} D_4\psi + \kappa\psi_4 &= 0, \\ \sum_k D_k^2\psi - \kappa D_4\psi_4 - \kappa^2\psi &= 0. \end{aligned}$$

These equations are already in the Hamiltonian form (7), but the combination ψ and ψ_4 does not prove to be convenient because of the symmetry of (8). Accordingly, we introduce the linear combination,

$$(9) \quad \begin{aligned} \psi &= 1/\sqrt{2}(\varphi + \chi), \\ \psi_4 &= 1/\sqrt{2}(\varphi - \chi). \end{aligned}$$

The equations for φ and χ are

$$\begin{aligned} D_4\varphi &= (1/2\kappa) \sum_k D_k^2(\varphi + \chi) - \kappa\varphi, \\ D_4\chi &= -(1/2\kappa) \sum_k D_k^2(\varphi + \chi) + \kappa\chi, \end{aligned}$$

which may be written more explicitly as

$$(10) \quad \begin{aligned} i\hbar(\partial\varphi/\partial t) &= (1/2m)(\hbar/i\nabla - e\mathbf{A}/c)^2(\varphi + \chi) + (e\phi + mc^2)\varphi, \\ i\hbar(\partial\chi/\partial t) &= -(1/2m)(\hbar/i\nabla - e\mathbf{A}/c)^2(\varphi + \chi) + (e\phi - mc^2)\chi. \end{aligned}$$

For particles with no charge that is taking ($e = 0$), after adjusting constants, equations (10) could be written as

$$(11) \quad \begin{aligned} (\partial\varphi/\partial t) &= \nabla^2(a_1\varphi + a_2\chi) + b_1\varphi \\ (\partial\chi/\partial t) &= \nabla^2(a_3\varphi + a_4\chi) + b_4\chi, \end{aligned}$$

where a_1, b_1, a_2, b_4 are some constants.

Choosing b_2, b_3 to be equal to zero, and setting $\bar{\psi} = \begin{bmatrix} \phi \\ \chi \end{bmatrix}$ this becomes

$$(12) \quad \frac{\partial \bar{\psi}}{\partial t} = \mathcal{A} \nabla^2 \bar{\psi} + \mathcal{B} \bar{\psi}$$

\mathcal{A} and \mathcal{B} are 2×2 matrices, If we choose $\mathcal{A} = \begin{bmatrix} a_1 & a_2 \\ a_3 & a_4 \end{bmatrix}$ and $\mathcal{B} = \begin{bmatrix} b_1 & b_2 \\ b_3 & b_4 \end{bmatrix}$ and $a_1, a_2, a_3, a_4, b_1, b_2, b_3, b_4$ are real numbers, then (12) takes on the form

$$(13) \quad \begin{aligned} \frac{\partial \phi}{\partial t} &= \nabla^2(a_1\phi + a_2\chi) + b_1\phi + b_2\chi \\ \frac{\partial \chi}{\partial t} &= \nabla^2(a_3\phi + a_4\chi) + b_3\phi + b_4\chi \end{aligned}$$

Comparing with equation (2), it is clear that these two equations although representing different physical phenomena have the same structure.

4. Dynamical analysis ([3], [2])

We try to solve equation (12) by the separation of variables [5], [9] and we take a trial solution in the form of

$$(14) \quad \bar{\psi} = \bar{\psi}_q e^{\sigma_q t} e^{iqx} = \begin{bmatrix} \phi_q \\ \chi_q \end{bmatrix} e^{\sigma_q t} e^{iqx}$$

Where $\bar{\psi}_q = \begin{bmatrix} \phi_q \\ \chi_q \end{bmatrix}$ is constant vector. Putting the Equation (14) in (12)

$$\begin{aligned} \sigma_q \bar{\psi}_q e^{\sigma_q t} e^{iqx} &= B \bar{\psi}_q e^{\sigma_q t} e^{iqx} + A(-\bar{\psi}_q) q^2 e^{\sigma_q t} e^{iqx} \\ \sigma_q \bar{\psi}_q &= B \bar{\psi}_q - A \bar{\psi}_q q^2 \end{aligned}$$

To simplify matters, we choose $a_2 = 0 = a_3$. Let us set

$$(15) \quad A_q = B - Aq^2 = \begin{bmatrix} b_1 - a_1q^2 & b_2 \\ b_3 & b_4 - a_4q^2 \end{bmatrix}$$

and we have

$$(16) \quad A_q \bar{\psi}_q = \sigma_q \bar{\psi}_q$$

which is an eigenvalue problem, with σ_q as the eigenvalue and $\bar{\psi}_q$ as the eigenvector of A_q [6]. This problem for a given q has generally two linearly independent eigenvectors that we will denote by $\bar{\psi}_{iq}$ for $i = 1, 2$. If the corresponding eigenvalues are σ_{iq} , the particular solution with wave number q will have the form:

$$(c_1 \bar{\psi}_{1q} e^{\sigma_{1q} t} + c_2 \bar{\psi}_{2q} e^{\sigma_{2q} t}) e^{iqx}$$

where c_1 and c_2 are constant. The solution decays for $Re(\sigma_{iq}) < 0$ for $i = 1, 2$. The characteristic polynomial for the eigenvalue problem Equation (16) can be written as

$$0 = |A_q - \sigma_q I| = \sigma_q^2 - \text{Trace}(A_q)\sigma_q + |A_q|$$

where

$$(17) \quad \begin{aligned} \text{Trace}(A_q) &= b_1 + b_3 - (a_1 + a_4)q^2 \\ |A_q| &= (b_1 - a_1q^2)(b_4 - a_4q^2) - b_2b_3 \end{aligned}$$

and the eigenvalues are:

$$\sigma_q = \frac{1}{2}\text{Trace}(A_q) \pm \frac{1}{2}\sqrt{(\text{Trace}(A_q))^2 - 4|A_q|}$$

The regions of stability (both $Re(\sigma_q)$ negative) and instability (at least one $Re(\sigma_q)$ positive) is given by:

$$\begin{aligned} \text{Trace}(A_q) &< 0 \\ |A_q| &> 0 \end{aligned}$$

Linear stability is guaranteed if

$$(18) \quad \begin{aligned} \text{tr}A_q &= (b_1 - a_1q^2) + (b_4 - a_4q^2) < 0 \\ \det A_q &= (b_1 - a_1q^2)(b_4 - a_4q^2) - b_2b_3 > 0. \end{aligned}$$

5. A nonlinear Schrödinger equation

We now consider the nonlinear Schrödinger equation which appears in several contexts for example [17], [4], [12]. In [4] and [12] it represents semiconductor electronics and in [10] optics in nonlinear media. In [8], photonics and in [15] the foundations of quantum mechanics. The study of these equations has catalyzed the development of mathematical concepts such as Solitons [18]. The nonlinear Schrödinger equation which we refer to here has the form

$$(19) \quad \begin{aligned} i\psi_t &= -\frac{1}{2}\Delta\psi + g(x)|\psi|^2\psi \\ \psi(x, 0) &= \psi_0(x) \end{aligned}$$

with $x \in \mathbb{R}^d$.

Taking a hint from the nonlinear Schrödinger equation (19), we can consider the following system of equations

$$(20) \quad \begin{aligned} \frac{\partial u}{\partial t} &= D_u \frac{\partial^2 u}{\partial x^2} + a_1u(1 - u^2) + b_1v \\ \frac{\partial v}{\partial t} &= D_v \frac{\partial^2 v}{\partial x^2} + a_2u + b_2v \end{aligned}$$

6. Solutions to the reaction-diffusion type nonlinear Schrödinger wave equation

We attempt to solve the equations (20) using a linearization followed by separation of variables as well as a travelling wave method. We first discuss the method of linearization of equation (20).

Linear stability analysis

The aim of this discussion is to derive, and then to understand physically, conditions that are sufficient for the real parts of all growth rates to be negative. We rewrite the system of equations (20) in a more general setting as follows:

$$(21) \quad \begin{aligned} \frac{\partial u}{\partial t} &= D_u \frac{\partial^2 u}{\partial x^2} + f_1(u, v) \\ \frac{\partial v}{\partial t} &= D_v \frac{\partial^2 v}{\partial x^2} + f_2(u, v) \end{aligned}$$

that is, setting $a_1u(1 - u^2) + b_1v = f_1(u, v) = f_1(u, v)$ and $a_2u + b_2v = f_2(u, v)$ and $\mathbf{f}(u, v) = (f_1(u, v), f_2(u, v))$ We begin by assuming that there exists a stationary uniform base solution $\mathbf{u}_b = (\hat{u}, \hat{v})$ and that this satisfies the model after all partial derivatives have been set to zero giving

$$(22) \quad \begin{aligned} f_1(\hat{u}, \hat{v}) &= 0 \\ f_2(\hat{u}, \hat{v}) &= 0 \end{aligned}$$

By linearizing about the base state \mathbf{u}_b , for small perturbations about \mathbf{u}_b , that is if we let $\mathbf{u}_b = \mathbf{u}_0 + \delta\mathbf{u}$, we can show that an arbitrary infinitesimal perturbation $\delta\mathbf{u}_b = (\delta\mathbf{u}, \delta\mathbf{v})$ of the base state will evolve in time according to the following linear constant-coefficient evolution equations:

$$(23) \quad \begin{aligned} \partial_t \delta\mathbf{u} &= a_{11}\delta u + a_{12}\delta v + D_u \partial_x^2 \delta u \\ \partial_t \delta\mathbf{v} &= a_{21}\delta u + a_{22}\delta v + D_v \partial_x^2 \delta v \end{aligned}$$

The constant coefficients a_{ij} come from the 2×2 Jacobian matrix $A = \frac{\partial \mathbf{f}}{\partial \mathbf{u}}$ evaluated at the constant base solution \mathbf{u}_b . The mathematical structure of (23) can be clarified by writing in the vector form

$$(24) \quad \frac{\partial}{\partial t} \delta\mathbf{u} = \mathbf{A} \delta\mathbf{u} = \mathbf{D} \frac{\partial^2}{\partial \mathbf{x}^2} \delta\mathbf{u}$$

Equation (24) or its equivalent form (23) can be solved by the method of separation of variables outlined in Section (). We now approach the problem through another route, viz., The Travelling Wave method.

Travelling wave method

Our aim is to examine solutions of the form [14] $u(x, t) = \phi(x - ct)$ for (20). A travelling wave solution is a solution of the form $u(x, t) = U(z)$, $z = x + ct$, where

c is the wave speed. Assume $c \geq 0$. If a solution $u(x, t)$ represents a travelling wave the shape of the solution remains the same for all t .

$$\frac{\partial u}{\partial t} = c \frac{dU}{dz}, \quad \frac{\partial u}{\partial x} = \frac{dU}{dz}, \quad \frac{\partial^2 u}{\partial x^2} = \frac{d^2U}{dz^2}$$

Using the same transformation on $v(x, t)$, (20) becomes

$$c \frac{dU}{dz} = D_u \frac{d^2U}{dz^2} + a_1 U(1 - U^2) + b_1 V$$

$$c \frac{dV}{dt} = D_v \frac{d^2V}{dz^2} + a_2 U + b_2 V$$

To study a simplified version, take $D_u = 0$ and $D_v = 1$

$$(25) \quad \begin{aligned} cU' &= a_1 U(1 - U^2) + b_1 V \\ cV' &= V'' + a_2 U + b_2 V \end{aligned}$$

Let $V' = W$ Equations (25) can be expressed as

$$\begin{aligned} U' &= \frac{a_1}{c} U(1 - U^2) + \frac{b_1}{c} V \\ V' &= W \\ W' &= cW - a_2 U - b_2 V \end{aligned}$$

The equilibrium points are

$$\begin{aligned} eq_1 &= (0, 0, 0), \\ eq_2 &= \left(\sqrt{\frac{a_1 b_2 - b_1 a_2}{a_1 b_2}}, -\frac{a_2}{b_2} \sqrt{\frac{a_1 b_2 - b_1 a_2}{a_1 b_2}}, 0 \right), \\ eq_3 &= \left(-\sqrt{\frac{a_1 b_2 - b_1 a_2}{a_1 b_2}}, \frac{a_2}{b_2} \sqrt{\frac{a_1 b_2 - b_1 a_2}{a_1 b_2}}, 0 \right) \end{aligned}$$

The Characteristic equation for the equilibrium point eq_1 is

$$-c\lambda^3 + (a_1 + c^2)\lambda^2 - (a_1 c + cb_2)\lambda + (a_1 b_2 - b_1 a_2) = 0.$$

We plot the Characteristic equation to indicate two real and positive Eigenvalues in Figure 1.

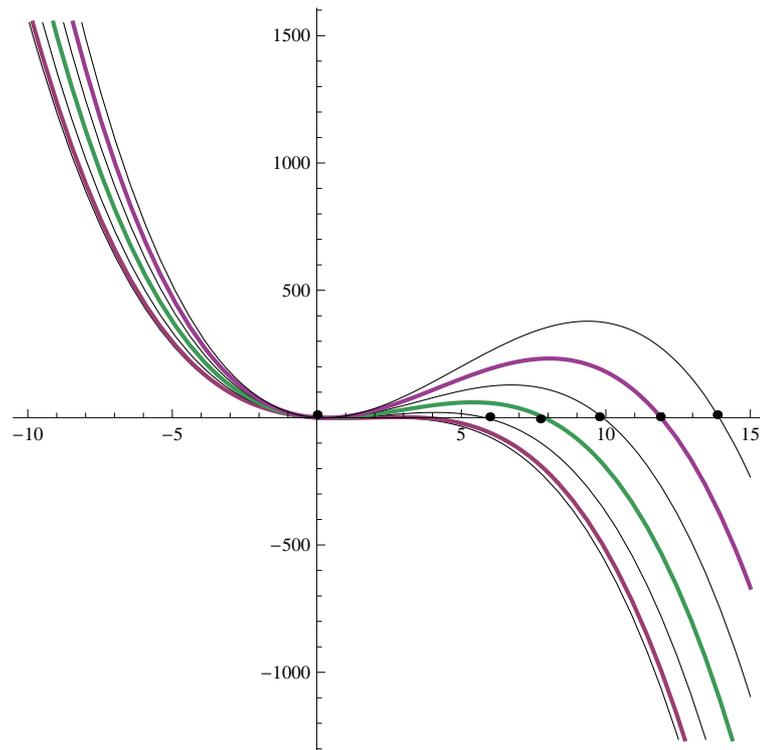


Figure 1: Graphs of the Characteristic Polynomial for $a_1 = b_1 = a_2 = b_2 = 1$, c ranging from 2 to 10, all the different characteristic polynomials showing two positive Eigenvalues, marked as dots on the X-axis

Observing Figure 1, we see that the Eigenvalues are positive, this tells us that the solutions $\rightarrow \infty$ as $t \rightarrow \infty$. Choosing different values for the constants, the Eigenvalues can be complex in which case the solutions would be bounded.

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