Applications of Lie Symmetry Analysis to the Quantum Brownian Motion Model

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ABSTRACT

Lie symmetry group methods provide a useful tool for the analysis of differential equations in a variety of areas in physics and applied mathematics. The nature of symmetry is that it provides information on properties which remain invariant under transformation. In differential equations this invariance provides a route toward complete integrations, reductions, linearisations and analytical solutions which can evade standard techniques of analysis. In this thesis we study two problems in quantum mechanics from a symmetry perspective: We consider for pedagogical purposes the linear time dependent Schrödinger equation in a potential and provide a symmetry analysis of the resulting equations. Thereafter, as an original contribution, we study the group theoretic properties of the density matrix equation for the quantum Brownian motion of a free particle interacting with a bath of harmonic oscillators. We provide a number of canonical reductions of the system to equations of reduced dimensionality as well as several complete integrations.

DECLARATION

I hereby declare that this is my own work, except where due reference has been made and it has not been submitted for any degree to any other institution.

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PUBLICATIONS

The contents of Chapter 4 are my own work and I anticipate that it will be accepted for publication. As of the date below there are no publications from this thesis to report.

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CONTENTS

1. INTRODUCTION

1.1 Summary

The theory of open quantum systems in physics provides a rich source of problems for analysis. These arise in the course of replacing the time evolution equations for closed quantum systems which are assumed to evolve in isolation with equations for open quantum systems which evolve in interaction with their environments. A number of these open systems models are differential equations of various forms [2, 3, 9, 10, 23]. The usual research aim in such cases once the mathematical model has been constructed is to obtain a maximal amount of information from a given equation or system of equations. A useful tool to this end is the application of Lie symmetry groups for differential equations [1, 14, 15, 16, 26]. A differential equation which when subjected to Lie symmetry analysis is found to have corresponding infinitesimal symmetry generators may be integrated or solved on the basis of canonical transformations couched within the symmetry generators.

In this thesis we consider a problem from open quantum systems as a subject of symmetry analysis: The quantum Brownian motion for the behaviour of a free particle immersed in a thermal reservoir - an environment at thermal equilibrium at high temperature. The model is described by the partial differential equation

$$\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m}\left(\frac{\partial^2 \rho}{\partial x^2} - \frac{\partial^2 \rho}{\partial y^2}\right) - \frac{1}{2}a^2(x-y)^2\rho, \tag{1.1}$$

for the density matrix in the position representation $\rho(x, y)$, and has been the subject of a number of studies in the physics literature [3, 9, 10, 29].

Applying symmetry based techniques we subject (1.1) to analysis. The main results are that there are a number of nontrivial integrations for (1.1) which may be arrived at directly using symmetries. Furthermore hidden in the algebraic properties of the equation is the Heisenberg-Weyl group. This leaves it in the local equivalence class of the diffusion equation as well as the Schrödinger equations for the free particle and harmonic oscillator. These are original results of relevance to researchers in open quantum systems and mathematicians working in differential equations and symmetry groups.

The thesis is structured as follows: The remainder of this introduction contains further material on symmetry, quantum mechanics and open quantum systems -

the very basics. Chapter 2 and Chapter 3 are essentially background material for the reader. The theoretical framework and standard algorithms for calculating symmetries are introduced in Chapter 2. We introduce both the tools for calculating and obtaining symmetries and the details of Lie algebras and groups within the context of differential equations. Chapter 3 turns toward the application of symmetry methods for partial differential equations. We use the Schrödinger equation[1] in a potential

$$i\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi \tag{1.2}$$

as an example for illustrating symmetry concepts. Chapter 4 contains the main result of the thesis: the analysis of the quantum Brownian motion model as well as a statement of specific problems where this type of work has potential for future research. A basic idea of quantum mechanics at the level of [23][Ch 2.] and differential equations at the level of [1][Ch.1] has been assumed.

1.2 Lie Symmetries

An important tool in the study of differential equations is the use of Lie symmetry methods which reflect the invariance of the differential equation under infinitesimal transformation. These were introduced by Lie who through his work on continuous groups of geometrical transformations was lead into the study of the symmetries of differential equations [14, 15]. Not long after, Noether studied the Action Integral under infinitesimal transformation proving the eponymous theorem [24].

Although we will deal further with symmetry in Chapter 2 a simple example with all the essentials is to consider the invariance of functions in a two-dimensional space (x, y) where x and y are independent. The infinitesimal symmetries are obtained by taking the transformations

$$\bar{x} = x + \varepsilon\xi(x,y) \quad \bar{y} = y + \varepsilon\eta(x,y), \tag{1.3}$$

where ε is the infinitesimal parameter. The requirement for the invariance of a function $f(x, y)$ is that

$$f(\bar{x},\bar{y}) = f(x,y) \tag{1.4}$$

from which

$$f(\bar{x},\bar{y}) = f(x+\varepsilon\xi, y+\varepsilon\eta). \tag{1.5}$$

The Taylor expansion of this expression in the parameter ε leads to

$$f(\bar{x},\bar{y}) = f(x,y) + \varepsilon\left\{\xi\frac{\partial f}{\partial x} + \eta\frac{\partial f}{\partial y}\right\} \tag{1.6}$$

[1] For the most part we will use units such that $m = \hbar = 1$. This Schrödinger equation is, strictly speaking, missing a factor of one half.

which may be written as the differential operator

$$G = \xi(x, y)\partial_x + \eta(x, y)\partial_y \tag{1.7}$$

acting on f as

$$f(\bar{x}, \bar{y}) = (1 + \varepsilon G)f(x, y). \tag{1.8}$$

G is a symmetry of f if $Gf = 0$, i.e.

$$\xi\frac{\partial f}{\partial x} + \eta\frac{\partial f}{\partial y} = 0\,. \tag{1.9}$$

This can be considered both as an equation for ξ and η given the function f or as an equation for the form of f given a generator G with coefficient functions ξ and η. The former is the statement that an arbitrary function f can have an infinite number of symmetries, i.e. if one simply chooses for an arbitrary k

$$\xi = k(x, y)\frac{\partial f}{\partial y} \quad \text{and} \quad \eta = -k(x, y)\frac{\partial f}{\partial x}\,. \tag{1.10}$$

The latter is that given a generator G a class of functions which admits the generator may be found, eg. consider

$$G = y\partial_x - x\partial_y. \tag{1.11}$$

The constraint (1.9) becomes

$$y\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial y} = 0. \tag{1.12}$$

This has the associated Lagrange's system

$$\frac{dx}{y} = \frac{dy}{-x} \tag{1.13}$$

with the characteristic variable

$$u = x^2 + y^2. \tag{1.14}$$

It may be then be inferred from (1.14) that any function of the form $f(x^2 + y^2)$ possesses G as a symmetry.

This idea is of course generalizable to functions of more independent variables as well as a dependence of one or more of the variables on each other which is the case with ordinary, partial and systems of differential equations. There are various types of symmetries of differential equations studied in the literature [1, 26]. The simplest are point transformations which map the original space of variables into itself. The other types may depend on derivatives of various orders as well as integrals. These are termed generalized and nonlocal symmetries respectively. In this thesis we limit our discussion to symmetry properties under point transformation.

1.3 Closed and Open Quantum Systems

The differential equations (1.1) and (1.2) are both drawn from quantum mechanics. They are examples of open and closed quantum systems respectively. This section gives a brief overview of both, it is not meant to be exhaustive. Details on both quantum mechanics and open system dynamics may be found in [2] and [23] in which the emphasis is more on the various aspects of quantum information and computation.

1.3.1 Closed Quantum Systems

In standard quantum mechanics one works with closed quantum systems which are postulated to evolve unitarily in isolation. They are described by state vectors $|\psi\rangle$ which are the elements of an underlying Hilbert space $\mathcal{H}$ or density matrices ρ formed from the outer product of state vectors[2]

$$\rho = |\psi\rangle\langle\psi|. \tag{1.15}$$

The state vector $|\psi\rangle$ may then be expanded in terms of a basis on $\mathcal{H}$ such as position $|q\rangle$ or momentum $|p\rangle$. We have in the momentum representation, for example,

$$|\psi\rangle = \int dp|p\rangle\langle p|\psi\rangle \tag{1.16}$$

and we denote the momentum space wave functions as

$$\psi(p) = \langle p|\psi\rangle. \tag{1.17}$$

Finally, given the states $|\psi(p)\rangle$ and $|\phi(p')\rangle$ (where the prime is used to distinguish two sets of momentum values) the probability that the states overlap is found according to

$$|\langle\psi|\phi\rangle|^2 = \int dpdp'\psi^*(p)\phi(p')\delta(p'-p), \tag{1.18}$$

where the $*$ denotes the conjugate, and the integration is over the entire range of momentum values. This is assumed to be finite.

The time evolution of a closed quantum system is assumed to be generated by the Hamiltonian, H, to give the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi = H\psi. \tag{1.19}$$

We also have the Liouville-von Neumann equation for the density matrix

$$\frac{\partial\rho}{\partial t} = -i[H,\rho], \tag{1.20}$$

[2] We will only be working with pure states in this thesis see, [2] for details.

where the square brackets denote the commutator. The Schrödinger equation (1.2) is generated by the classical Hamiltonian for a particle in a potential treated as the operator

$$\hat{H} = \hat{p}^2 + V(\hat{x}, t), \tag{1.21}$$

where $\hat{x}$ and $\hat{p} = i\partial/\partial x$ represent the quantisation of classical position and momentum variables such that

$$\hat{x}|x\rangle = x|x\rangle \quad \text{and} \quad \hat{p}|x\rangle = i\frac{\partial}{\partial x}|x\rangle. \tag{1.22}$$

1.3.2 Open Quantum Systems

The difference between closed and open quantum systems is essentially that open quantum systems are assumed to evolve in interaction with their environments while closed quantum systems are assumed to evolve in isolation. To model an open quantum system one considers a larger closed quantum system divided into the open system (which we are interested in) and an environment (which we average over statistically).

The entire system is built on the composite Hilbert space $\mathcal{H} = \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{E}}$ where $\mathcal{H}_{\mathcal{S}}$ is the open system Hilbert space, $\mathcal{H}_{\mathcal{E}}$ is the environment Hilbert space and $\otimes$ denotes the tensor product. For our purposes we will assume that initial states in the entire system are separable[3] whence $|\psi\rangle \in \mathcal{H}$ may be written as $|\psi\rangle_S \otimes |\psi\rangle_E$ where $|\psi\rangle_S \in \mathcal{H}_{\mathcal{S}}$ and $|\psi\rangle_E \in \mathcal{H}_{\mathcal{E}}$.

We have the density matrix for the total system as

$$\rho = \rho_S \otimes \rho_E. \tag{1.23}$$

Since the total system is assumed to be closed the density matrix evolves unitarily according to the Liouville von Neumann equation (1.20). The total system Hamiltonian may be written as

$$H = H_S + H_I + H_E, \tag{1.24}$$

reflecting the environment, the interaction and the system degrees of freedom. In principle, the dynamics of the open system may then be obtained by allowing the unitary evolution of the total system as

$$\rho(t) \to U(t, t_0)\rho(t_0)U^\dagger(t, t_0) \tag{1.25}$$

and then taking the partial trace over the environmental degrees of freedom,

$$\mathrm{tr}_E\{\rho(t)\} = \rho_S(t) = \sum_E {}_E\langle\psi|U\rho(t_0)U^\dagger|\psi\rangle_E, \tag{1.26}$$

[3] These could also, in principle, be entangled states [2].

after a time interval, $t - t_0$, from an initial state for the total system $\rho(t_0)$. However, for systems with many environmental degrees of freedom this is not feasible. The alternative approach is to replace equation (1.20) with an equation for the time evolution of reduced density matrix ρ_S in which the evolution of the environment plays a passive role through dissipative operators and possibly interaction terms in the Hamiltonian valid on the timescale for which the system environment correlations occur. The most common is the Gorini-Kossakowski-Sudharshan-Lindblad equation[4] [8, 17] which describes Markovian, short term, memoryless correlations. This is

$$\frac{d\rho}{dt} = -i[H, \rho] - \frac{1}{2}\sum_{j=1}^{n}\left(\{L_j L_j^\dagger, \rho\} - 2L_j \rho L_j^\dagger\right), \tag{1.27}$$

where H is the Hamiltonian and L are the Lindblad operators. The quantum Brownian motion model equation (1.1) and a number of standard models in open quantum systems are based on this equation [2, 3, 9].

[4] Political correctness.

2. LIE SYMMETRY GROUPS

2.1 Introduction

The idea of a symmetry in its simplest sense relates to regularity in the structure of an object. If an object is regular then it has aspects that persist under types of transformation, eg. in geometry the invariance of the equilateral triangle about reflections about an axis or the invariance of a circle after a rotation about its center. Symmetries are clues about how objects behave under transformations. Lie group theory is the study of symmetry properties of abstract mathematical structures [1, 14, 15, 16, 24, 26].

In the study of the group theoretic properties of differential equations the structure of the symmetry group and the concomitant algebra summarizes the effect of the differential equation on the its space of dependent and independent variables and their derivatives. The symmetry group of an equation, if there is one, determines the structure of the differential equation and the corresponding Lie algebra determines the equivalence class of the differential equation under transformation [1, 26]. The knowledge of the symmetry group can be used to find invariant, mapping, reduction and solution properties of an equation. Isometry between symmetry groups can then be used to identify equivalent differential equations.

2.2 Lie Groups of Transformations

Groups are algebraic structures the ideas of which underly familiar objects such as the integers or matrices. They have diverse applicability and are widely studied. In order to explore the properties of differential equations in a more general and abstract way the notion of continuous groups and groups of transformations are required. This section is an introductory delving into the ideas of group theory. We follow the introduction by Bluman [1] [Ch. 2]. Further details regarding symmetry groups may be found in [1, 26].

Group: A group is a set of elements G with a law of composition between the elements, ϕ, satisfying the following axioms :

(i) **Closure Property:** For any elements x and y of G $\phi(x, y)$ is an element of

G.

(ii) **Associative Property:** For any elements x, y, z of G

$$\phi(x, \phi(y, z)) = \phi(\phi(x, y), z).$$

(iii) **Identity Element:** There exists a unique identity element I of G such that for any element x of G

$$\phi(x, I) = \phi(I, x) = x.$$

(iv) **Inverse Element:** For an element x of G there exists a unique inverse element x^{-1} in G such that

$$\phi(x, x^{-1}) = \phi(x^{-1}, x) = I.$$

Subgroup: A *subgroup* of G is a subset of G which forms a group with the same law of composition ϕ.

Abelian Group: A group G is *abelian* if $\phi(x, y) = \phi(y, x)$ holds for all elements x and y in G.

Groups of Transformations: The set of transformations

$$\bar{x} = X(x; \varepsilon)$$

defined for each x in the space $D \subset \mathbb{R}^n$ depending on the parameter $\varepsilon \in S \subset \mathbb{R}$ with $\phi(\varepsilon, \delta)$ defining a law of composition of parameters ε and δ in S forms a *group of transformations* on D if:

(i) For each ε in S the transformations are one-to-one onto D. In particular $\bar{x} \in D$.

(ii) S with the law of composition ϕ forms a group G, i.e. if $\bar{x} = X(x; \varepsilon)$ and $\bar{y} = X(x; \delta)$, then $\bar{y} = X(x; \phi(\varepsilon, \delta))$, and $\bar{x} = x$ when $\varepsilon = I$.

One-parameter Lie Group of transformations: A *one-parameter Lie group of transformations* is a group of transformations which satisfies the additional conditions[1]:

(i) The parameter ε is continuous, i.e. S is an interval in $\mathbb{R}$, with $0 \in S$, and $\varepsilon = 0$ corresponds to the identity element I.

[1] All statements are for standard forms of transformations.

(ii) X is infinitely differentiable *wrt* x in D and an analytic function of ε in S.

(iii) $\phi(\varepsilon, \delta)$ is an analytic function of ε and δ for $\varepsilon \in S$ and $\delta \in S$.

Lie Algebras:

The *Lie Bracket* $[x, y]_{LB}$ of x and y is

$$[x, y]_{LB} = xy - yx.$$

A *Lie algebra*[2] is a vector space $\mathcal{L}$ equipped with the Lie Bracket that

(i) is *Bilinear*, i.e.

$$[x, ay + bz]_{LB} = a[x, y]_{LB} + b[x, z]_{LB}, \qquad [ay + bz, x]_{LB} = a[y, x]_{LB} + b[z, x]_{LB},$$

(ii) is *Antisymmetric*

$$[x, y]_{LB} = -[y, x]_{LB},$$

(iii) satisfies the *Jacobi Identity*

$$[x, [y, z]]_{LB} + [y, [z, x]]_{LB} + [z, [x, y]]_{LB} = 0$$

for all vectors $x, y, z \in \mathcal{L}$ and $a,\ b \in \mathbb{R}$.

A Lie algebra $\mathcal{L}$ is said to abelian if $[x, y]_{LB} = 0 \ \ \forall\, x,\ y \in \mathcal{L}$.

A Lie algebra $\mathcal{L}$ is called *solvable* if the derived series

$$\mathcal{L} \supseteq \mathcal{L}' = [\mathcal{L}, \mathcal{L}]_{LB} \supseteq \mathcal{L}'' = [\mathcal{L}', \mathcal{L}']_{LB} \supseteq \ldots \supseteq \mathcal{L}^k = [\mathcal{L}^{k-1}, \mathcal{L}^{k-1}]_{LB}$$

is such that $\mathcal{L}^k = 0,$ for some $k \in \mathbb{N}$.

2.3 Symmetries

2.3.1 Infinitesimal Transformations

An infinitesimal transformation in the space of independent variables (x, y) is given by:

$$\bar{x} = x + \epsilon\xi(x, y), \qquad \bar{y} = y + \epsilon\eta(x, y), \tag{2.1}$$

[2] Here, we use an example of a Lie algebra that is relevant to our context. There are a multitude of other examples of Lie Algebras [4].

where ϵ is an infinitesimal parameter. Equivalently we may regard the differential operator

$$G = \xi(x,y)\partial_x + \eta(x,y)\partial_y\,, \tag{2.2}$$

where ∂_x and ∂_y denotes differentiation with regard to the respective variable, as the generator of the transformation (2.1) since

$$\bar{x} = (1+\epsilon G)x, \qquad \bar{y} = (1+\epsilon G)y.$$

Let $y = y(x)$ in the case of a dependence of y on the variable x. Under the restriction that the coefficient functions ξ and η be differentiable functions of x and y the transformation induced in the first derivative dy/dx by an infinitesimal transformation (2.1) is

$$\begin{aligned}
\frac{d\bar{y}}{d\bar{x}} &= \frac{d(y+\epsilon\eta)}{d(x+\epsilon\xi)} \\
&= \frac{dy+\epsilon d\eta}{dx+\epsilon d\xi} \\
&= \left(\frac{dy}{dx}+\epsilon\frac{d\eta}{dx}\right)\left(1+\epsilon\frac{d\xi}{dx}\right)^{-1} \\
&= \frac{dy}{dx}+\epsilon\left(\frac{d\eta}{dx}-\frac{dy}{dx}\frac{d\xi}{dx}\right)+O(\epsilon^2).
\end{aligned}$$

Since ϵ is an infinitesimal,

$$\frac{d\bar{y}}{d\bar{x}} = y' + \epsilon(\eta' - y'\xi') \tag{2.3}$$

and the $(')$ denotes total differentiation *wrt* x. The first extension of the differential operator G is then specified as

$$G^{[1]} = G + (\eta' - y'\xi')\partial_{y'} = \xi\partial_x + \eta\partial_y + (\eta' - y'\xi')\partial_{y'}. \tag{2.4}$$

The generalization for the generator to the nth extension is

$$G^{[n]} = G + \sum_{i=1}^{n}\left\{\eta^{(i)} - \textstyle\sum_{j=1}^{i}\binom{i}{j}y^{(i+1-j)}\xi^{(j)}\right\}\partial_{y^{(i)}} \tag{2.5}$$

and the indices denote total differentiation *wrt* x and $\binom{i}{j}$ are binomial coefficients.

2.3.2 Symmetries of Ordinary Differential Equations

For the nth order ordinary differential equation

$$E\big(x, y, y', y'', \ldots, y^{(n)}\big) = 0$$

if

$$G^{[n]}\Big[E\big(x, y, y', y'', \ldots, y^{(n)}\big)\Big]\Big|_{E=0} = 0 \tag{2.6}$$

the differential equation is invariant under the action of the nth extension of (2.2), admits the one parameter Lie group of point transformations (2.1) and G is a symmetry of the differential equation.

The important feature about the structure of equation (2.6) is that it is a linear first order partial differential equation and the method of characteristics can be used to solve it. It has the associated Lagrange's system

$$\frac{dx}{\xi} = \frac{dy}{\eta} = \frac{dy'}{\eta' - y'\xi'} = \ldots = \frac{dy^n}{\eta^{(n)} - \sum_{j=1}^{n}\binom{n}{j} y^{(n+1-j)}\xi^{(j)}}. \tag{2.7}$$

The new variables obtained on integration may be used to reduce the order of the equation to $n - 1$. In the case of a partial differential equation the number of independent variables can be reduced using the characteristics. The coefficient functions are not necessarily restricted to being point functions of the spatial variables. If ξ and η are functions of x, y and y' and the first extension $G^{[1]}$ is independent of y'' then G is termed a contact symmetry. In the case that ξ and η are functions of x, y, and the derivatives y',..., y^{n-1} a generalized symmetry is obtained. For ξ and η with integrals in their arguments the symmetry G is termed nonlocal.

The imposition that ξ and η be point functions, $\xi = \xi(x, y)$ and $\eta = \eta(x, y)$ and separation by relevant powers of y', $y'^2 \ldots$ etc. leads to a system of over-determined linear partial differential equations from (2.6). The general symmetry generator G obtained on solution is usually written as a number of one parameter symmetries for aesthetic and computational reasons. As an example we give below the symmetry calculations for the ordinary differential equation corresponding to the classical free particle.

Classical Free Particle

The Newton equation for the motion of a free particle in one dimension is given by

$$y'' = 0. \tag{2.8}$$

The infinitesimal symmetries corresponding to (2.8) are obtained from the condition

$$G^{[2]}E\big|_{E=0} = 0, \tag{2.9}$$

where the operator $G^{[2]}$ is the second extension of the infinitesimal generator. We have

$$G = \xi(x,y)\partial_x + \eta(x,y)\partial_y, \tag{2.10}$$

$$G^{[1]} = (\eta' - y'\xi')\partial_{y'} + G \tag{2.11}$$

and

$$G^{[2]} = (\eta'' - 2y''\xi' - y'\xi'')\partial_{y''} + G^{[1]}. \tag{2.12}$$

We may write the differentials η', η''; ξ', ξ'', etc. as,

$$\eta' = \frac{\partial\eta}{\partial x} + y'\frac{\partial\eta}{\partial y}, \tag{2.13}$$

$$\eta'' = \frac{\partial^2\eta}{\partial x^2} + 2y'\frac{\partial^2\eta}{\partial x\partial y} + y'^2\frac{\partial^2\eta}{\partial y^2} + y''\frac{\partial\eta}{\partial y}. \tag{2.14}$$

It follows from condition (2.9) that

$$(\eta'' - 2y''\xi' - y'\xi'') = 0. \tag{2.15}$$

Expanding out the differentials leads to

$$\begin{aligned}\frac{\partial^2\eta}{\partial x^2} + 2y'\frac{\partial^2\eta}{\partial x\partial y} + y'^2\frac{\partial^2\eta}{\partial y^2} + y''\frac{\partial\eta}{\partial y} - 2y''\left(\frac{\partial\xi}{\partial x} + y'\frac{\partial\xi}{\partial y}\right)&\\ -y'\left(\frac{\partial^2\xi}{\partial x^2} + 2y'\frac{\partial^2\xi}{\partial x\partial y} + y'^2\frac{\partial^2\xi}{\partial y^2} + y''\frac{\partial\xi}{\partial y}\right) &= 0\,. \end{aligned}\tag{2.16}$$

The terms involving y'' are set to zero when the differential equation is taken into account. Separating in powers of y' leads to the system of determining equations

$$\frac{\partial^2\eta}{\partial x^2} = 0 \tag{2.17}$$

$$2\frac{\partial^2\eta}{\partial x\partial y} - \frac{\partial^2\xi}{\partial x^2} = 0 \tag{2.18}$$

$$\frac{\partial^2\eta}{\partial y^2} - 2\frac{\partial^2\xi}{\partial x\partial y} = 0 \tag{2.19}$$

$$\frac{\partial^2\xi}{\partial y^2} = 0. \tag{2.20}$$

The system (2.17)-(2.20) has the solution,

$$\eta(x,y) = (A_1y + A_2)x + A_3y^2 + A_4y + A_5 \tag{2.21}$$

$$\xi(x,y) = A_1x^2 + (A_3y + A_6)x + A_7y + A_8\,. \tag{2.22}$$

The symmetry generator (2.10) may now be written in terms of the constants of integration obtained from solving the determining equations as the eight one parameter symmetries

$$\begin{aligned}
G_1 &= \partial_x && (2.23)\\
G_2 &= \partial_y && (2.24)\\
G_3 &= x\partial_x && (2.25)\\
G_4 &= y\partial_y && (2.26)\\
G_5 &= x\partial_y && (2.27)\\
G_6 &= y\partial_x && (2.28)\\
G_7 &= xy\partial_y + x^2\partial_x && (2.29)\\
G_8 &= y^2\partial_y + xy\partial_x, && (2.30)
\end{aligned}$$

where we have set each of the $A_i = \delta_{ij}$ and δ_{ij} is the Kronecker delta function.

2.3.3 Symmetries of Partial Differential Equations

The symmetries of partial differential equations are slightly more involved than the symmetries for ordinary differential equations. The condition for the general partial differential equation

$$E(x_i, y_j, y_{j,i}, \ldots) = 0, \tag{2.31}$$

in which the x_i, $i = 1, m$, are independent variables, the y_j $j = 1, n$, are dependent and $y_{j,\,i}$ denotes a partial derivative with respect to x_i to possess a symmetry

$$G = \xi_i\partial_{x_i} + n_j\partial_{y_j}, \tag{2.32}$$

where summation is implied, is

$$G^{[s]}E|_{E=0} = 0. \tag{2.33}$$

This is exactly the same as the condition for ordinary differential equations generalized to higher dimensions. The restriction that the coefficient functions ξ_i and η_j be constrained to point functions is the usual analysis. As was the case with ordinary differential equations this may be extended to a dependence on derivatives and integrals.

The symmetry properties of partial differential equations and their analysis will be addressed in the next chapters. Note that although the algorithm for obtaining the symmetries of partial differential equations is essentially the same as for ordinary differential equations the number of determining equations increases dramatically with the number of variables. The usual practice is to use a computer package for the calculation of the symmetries. There are a number of these specialized for the calculation of symmetries [11, 25]. In this thesis `PROGRAM LIE` developed by Head [11] is used.

2.4 Lie Algebras

The generators of the infinitesimal transformations or the symmetries

$$G_\alpha = \xi_\alpha \partial_x + \eta_\alpha \partial_y, \qquad \alpha = 1 \dots n \tag{2.34}$$

form a vector space. The dimension of the Lie algebra is the dimension of the vector space of its generating operators and may be finite or infinite. The Lie Bracket can be used to determine the algebraic structure corresponding to the symmetries of a given differential equation, first integral or function. Preservation of the algebraic structure in the symmetries of a differential equation is a sufficient condition for establishment of equivalence classes. The presence of solvable algebras is a useful guideline when examining symmetries for a change of variables to perform a reduction of order [26]. The representations of a Lie Algebra are not unique. Since Lie algebras can be isomorphic to one another a given algebra is usually identified with a standard classification. The classification schemes for standard algebras are discussed in [19, 20] and [21]. We list below the standard classification tables for Lie algebras of dimensions two and three.

Tab. 2.1: Canonical forms of Lie Algebras of Dimension Two

Type	$[G_1, G_2]$	Canonical Forms	Algebra
I	0	$G_1 = \partial_x \, G_2 = \partial_y$	A_1
II	0	$G_1 = \partial_y \, G_2 = x\partial_y$	A_1
III	G_1	$G_1 = \partial_y \, G_2 = x\partial_x + y\partial_y$	A_2
IV	G_1	$G_1 = \partial_y \, , G_2 = y\partial_y$	A_2

Tab. 2.2: Standard Classification of Lie Algebras of Dimension Three

Algebra	Nonzero Commutation Relations		
$3A_1$			
$A_1 \otimes A_2$	$[G_1, G_3] = G_1$		
$A_{3,1}$ (Weyl)	$[G_2, G_3] = G_1$		
$A_{3,2}$	$[G_1, G_3] = G_1,$	$[G_2, G_3] = G_1 + G_2$	
$A_{3,3}\,(D \otimes_s T_2)$	$[G_1, G_3] = G_1,$	$[G_2, G_3] = G_2$	
$A_{3,4}\,(E(1,1))$	$[G_1, G_3] = G_1,$	$[G_2, G_3] = G_2$	
$A^a_{3,5}\,(0 < \lvert a \rvert < 1)$	$[G_1, G_2] = G_1,$	$[G_2, G_3] = aG_2$	
$A_{3,6}\,(E(2))$	$[G_1, G_3] = -G_2,$	$[G_2, G_3] = G_1$	
$A^b_{3,7}\,(b > 0)$	$[G_1, G_3] = bG_1 - G_2,$	$[G_2, G_3] = G_1 + bG_2$	
$A_{3,8}\,(sl(2, \mathbb{R}))$	$[G_1, G_2] = G_1,$	$[G_2, G_3] = G_3,$	$[G_3, G_1] = -2G_2$
$A_{3,9}\,(so(3))$	$[G_1, G_2] = G_3,$	$[G_2, G_3] = G_1,$	$[G_3, G_1] = G_2$

2.5 First Integrals and Noether's Theorem

First integrals in dynamical systems correspond to conserved quantities, such as momenta, charge or energy. The significance of first integrals is that a complete set of first integrals is equivalent to a complete integration i.e. a solution can be deduced in a global functional form albeit a quadrature or implicitly. Note that symmetries may be used directly to find the first integrals corresponding to an ordinary differential equation whereas for calculus of variations problems one applies Noether's theorem.

2.5.1 First Integrals

A function, $I = f(x, y, y', \ldots, y^{n-1})$, is a first integral of an nth ordinary differential equation if

$$G^{[n-1]} I = 0 \tag{2.35}$$

and

$$\left.\frac{dI}{dx}\right|_{E=0} = 0 \tag{2.36}$$

are satisfied and the dependence on y^{n-1} is nontrivial. The first integral is obtained from the n characteristics, u_i, associated with (2.35) and the $n-1$ characteristics, v_i, associated with (2.36). The first integral is then

$$I = h(v_i)\,, \tag{2.37}$$

where h is an arbitrary function of its arguments.

2.5.2 Noether's Theorem

For a first order classical Lagrangian $L(t, x, \dot{x})$, the Action Integral

$$A = \int_{t_1}^{t_2} L(t, x, \dot{x}) dt, \tag{2.38}$$

is invariant under the infinitesimal transformation generated by the differential operator

$$G = T\partial_t + X_i \partial_{x_i}, \tag{2.39}$$

if there exists a function, f, such that

$$\dot{f} = T\frac{\partial L}{\partial t} + X_i \frac{\partial L}{\partial x_i} + \left(\dot{X}_i - \dot{x}_i \dot{T}\right)\frac{\partial L}{\partial \dot{x}_i} + \dot{T}L \tag{2.40}$$

in which the summation over repeated indices is implied. The expression for the first integral,

$$I = f - \left[TL + (X_i - \dot{x}_i T)\frac{\partial L}{\partial \dot{x}_i}\right], \tag{2.41}$$

is obtained when the Euler Lagrange equation [26] is invoked in (2.40).

The differential operator (2.39) is referred to as a Noether symmetry. Every Noether symmetry is a Lie symmetry of the Euler-Lagrange equations [26] related to the Action Integral. The function f is often referred to as a gauge term, a distinction which has its origins in physics. Noether's theorem provides a direct means of calculating first integrals associated to a Lagrangian or Hamiltonian using (2.41). There are obviously extensions to higher order Lagrangians and Lagrangians with more than one independent variable.

The calculation of first integrals and the use of Noether's theorem will not be relevant for this work, we include it for completeness.

3. THE SCHRÖDINGER EQUATION

An old problem in the study of symmetry properties is the study of an equation containing an arbitrary term. This is called the group classification problem and the idea of it is to examine the forms for the term which admit a certain amount of symmetry. This pioneering work was again by Lie [14, 15, 16] who performed the classification of linear equations with two independent complex variables and a potential, implicitly studying the one dimensional time-dependent Schrödinger equation

$$i\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} + V(x,t)u \tag{3.1}$$

for a particle in a potential $V(x,t)$. His results [16] were that (3.1) admits as potentials the harmonic and repulsive oscillator and that these are locally equivalent to the Schrödinger equation for the free particle. Since Lie's original paper was published in 1881, one can guess that there has been much subsequent work on the subject of classification for a variety of Schrödinger equations [1, 26].

The purpose of the present chapter is to introduce the essentials of symmetry analysis using equation (3.1) as our starting point. The group classification of (3.1) leads to forms $V \propto x^2$, $V \propto 1/x^2$ and $V \propto cst$ for the autonomous potential $V = V(x)$ which have respectively 5, 5 and 3 nontrivial symmetries in addition to the infinite number of solution symmetries and the homogeneity symmetries admitted by (3.1) for V arbitrary. These symmetries then provide a route for introducing the analysis. The harmonic oscillator, free particle and Ermakov-Pinney cases ($1/x^2$) are each treated in an application of a symmetry related technique.

The chapter is structured as follows: In the next section we give the proof of the group classification for (3.1). Thereafter we study the properties of the free particle Schrödinger equation and use the infinitesimal symmetry group to construct the finite Lie group of transformations and find the functional forms of the equations group invariant solutions. The harmonic oscillator Schrödinger equation is used to describe mapping and solution properties using symmetry and the Ermakov-Pinney potential equation is used to illustrate the procedure for reduction of order.

3.1 Group Classification

The general form of the symmetry generators of equation (3.1) correspond to the vector field

$$G = \tau(t,x,u)\partial_t + \xi(t,x,u)\partial_x + \eta(t,x,u)\partial_u \tag{3.2}$$

acting on the space of variables (t,x,u). The coefficient functions τ, ξ and η are now found from the determining equations obtained from the condition

$$G^{[2]}E\big|_{E=0} = 0, \tag{3.3}$$

where $G^{[2]}$ is the second prolongation of the vector field (3.2) and E is obtained after rearranging (3.1). Analysis of (3.1) by `PROGRAM LIE` returns the determining equations

$$\begin{aligned}
\tau_{uu} &= 0\\
\tau_u &= 0\\
\tau_x &= 0\\
i\tau_{ux} + \xi_u &= 0\\
2\xi_{ux} - iu\tau_{uu}V - \eta_{uu} &= 0\\
iu\tau_u V + i\tau_{xx} - i\tau_t + 2\xi &= 0\\
-2iu\tau_{ux} + u\xi_u V - 2\eta_{ux} + \xi_{xx} + i\xi_t &= 0\\
-iu\tau_{xx}V - u\eta_u V + u\tau_t V + uV_t\tau + uV_x\xi - iu^2\tau_u V^2 - \eta_{xx} + \eta V - i\eta_t &= 0.
\end{aligned}$$

Once the trivial integrations have been performed the form of the generator G may be written as

$$G = \tau(t)\partial_t + \xi(t,x)\partial_x + \eta(t,x,u)\partial_u. \tag{3.4}$$

This leads to the simplified set of determining equations

$$\eta_{uu} = 0 \tag{3.5}$$

$$\tau_t - 2\xi_x = 0 \tag{3.6}$$

$$2\eta_{xu} - i\xi_t - \xi_{xx} = 0 \tag{3.7}$$

$$uV(\eta_u - \tau_t) - u(V_t\tau + V_x\xi) + i\eta_t - \eta V + \eta_{xx} = 0. \tag{3.8}$$

Equations (3.5)-(3.7) give the following information

$$\eta = a(x,t)u + b(x,t) \tag{3.9}$$

and

$$\xi = \tfrac{1}{2}\tau_t + c(t), \tag{3.10}$$

$$a_x = i\left(\tau_{tt} + c_t\right) \Leftrightarrow a = i\left(\tfrac{1}{8}\tau_{tt}x^2 + \tfrac{1}{2}c_t x\right) + d(t)\,. \tag{3.11}$$

Substitution of (3.9) and (3.10) into equation (3.8) gives

$$uV(a-\tau_t) - uV_t\tau - uV_x(\tfrac{1}{2}\tau_t + c) + i(ua_t + b_t) + (ua_{xx} + b_{xx}) - V(ua+b) = 0. \tag{3.12}$$

Separating this equation in powers of u gives

$$i\frac{\partial a}{\partial t} + \frac{\partial^2 a}{\partial x^2} - \tau_t V - \tau V_t - \xi V_x = 0 \tag{3.13}$$

and

$$i\frac{\partial b}{\partial t} + \frac{\partial^2 b}{\partial x^2} - bV = 0. \tag{3.14}$$

Here, the function $b(x,t)$ satisfies the original differential equation. It generates via (3.9) what is termed a solution symmetry since the solution of the original differential equation is required in order to specify the symmetry. A characteristic property of partial differential equations which are linear, or related to a linear equation is that they possess a generator of this type. Substitution of (3.11) into (3.13) gives the equation for the potential,

$$-\tfrac{1}{8}\tau_{ttt}x^2 - \tfrac{1}{2}c_{tt}x + id + \tfrac{1}{4}i\tau_{tt} - V_t\tau - V_x(\tfrac{1}{2}\tau_t + c_t) = 0. \tag{3.15}$$

For an autonomous potential the following ordinary differential equation is obtained for $V(x)$:

$$(\tfrac{1}{2}\tau_t + c_t)\frac{dV}{dx} = i(d_t + \tfrac{1}{4}\tau_{tt}) - (\tfrac{1}{8}\tau_{ttt}x^2 + \tfrac{1}{2}c_{tt}x) - \tau_t V. \tag{3.16}$$

For $V = V(x)$ arbitrary we have the conditions

$$\begin{array}{rcccccccl}
V: & \tau_t & = & 0 & \Rightarrow & \tau & = & k_0 & \\
V': & \tfrac{1}{2}x\tau_t + c & = & 0 & \Rightarrow & c & = & 0 & \\
-: & \tfrac{1}{8}\tau_{ttt}x^2 + c_{tt}x - i\tfrac{1}{4}\tau_{tt} + id_t & = & 0 & \Rightarrow & \dot{d} & = & 0 & \Rightarrow d = d_0,
\end{array}$$

from (3.16). We have that

$$\eta = d_0 u + b(t,x,u) \tag{3.17}$$
$$\tau = k_0 \tag{3.18}$$
$$\xi = 0. \tag{3.19}$$

This gives the point symmetries

$$\begin{aligned} G_1 &= b(t,x,u)\partial_u & (3.20)\\ G_2 &= u\partial_u & (3.21)\\ G_3 &= \partial_t\,. & (3.22)\end{aligned}$$

The general solution of (3.16) for the potential V is

$$V = \frac{k(t)}{(\frac{1}{2}\tau_t x + c)^2} - \frac{1}{\tau_t}(\tfrac{1}{8}\tau_{ttt}x^2 + c_t x + id_t - i\tfrac{1}{4}\tau_{tt}) + \tfrac{2}{3}\frac{1}{\tau_t^2}(\tfrac{1}{2}\tau_t x + c)(\tfrac{1}{4}\tau_{ttt} + c_{tt}) - \tfrac{1}{6}\frac{\tau_{ttt}}{\tau_t^3}(\tfrac{1}{2}\tau_t x + c)^2. \quad (3.23)$$

The solution for V may then be written as

$$V = \lambda^2(\mu x + \nu)^2 + \frac{\omega^2}{(\mu x + \nu)^2} + \chi^2, \quad (3.24)$$

and λ, ω, χ, μ and ν are constants which depend on the autonomy of V. The following forms for (3.1) may be obtained if the scaling and translation parts of (3.24), μ and ν, are absorbed into the x variable:

$$\begin{aligned} i\frac{\partial u}{\partial t} &= -\frac{\partial^2 u}{\partial x^2} + \chi^2 u, & (3.25)\\ i\frac{\partial u}{\partial t} &= -\frac{\partial^2 u}{\partial x^2} + \lambda^2 x^2 u, & (3.26)\\ i\frac{\partial u}{\partial t} &= -\frac{\partial^2 u}{\partial x^2} + \frac{\omega^2}{x^2}u. & (3.27)\end{aligned}$$

Restrictions on the functional forms of $V(x)$ allow us to integrate (3.16) by separation in powers of x. This enables the admission of a number of new symmetries over and above the solution, homogeneity, and autonomy symmetries, G_1, G_2 and G_3. The symmetry and algebraic properties of equations (3.25), (3.26) and (3.27) are presented below for the values of the parameters $\chi^2 = 0$, $\lambda^2 = 1$ and $\omega^2 = 1$.

3.2 The Free Particle

As one of the oldest problems in quantum mechanics its no surprise the group theoretical properties of the free particle Schrödinger equation

$$i\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2}, \quad (3.28)$$

are well travailed. In addition it is of the equivalence class of a diffusion equation under the point transformation

$$t \to it \tag{3.29}$$

which is a textbook problem in symmetry considered in both Bluman and Kumei [1] as well as Olver [26].

3.2.1 Symmetries and Algebras

The infinitesimal generators returned by `LIE` are:

$$\begin{aligned}
K_1 &= \partial_t && (3.30)\\
K_2 &= \partial_x && (3.31)\\
K_3 &= 2t\partial_t + x\partial_x && (3.32)\\
K_4 &= u\partial_u && (3.33)\\
K_5 &= ux\partial_u + 2it\partial_x && (3.34)\\
K_6 &= \left[\tfrac{1}{2}it + \tfrac{1}{4}x^2\right] u\partial_u + it^2\partial_t + itx\partial_x && (3.35)\\
K_\infty &= k(x,t)\partial_u. && (3.36)
\end{aligned}$$

The function $k(x,t)$ is any solution[1] of

$$i\frac{\partial^2 k}{\partial t} = -\frac{\partial^2 k}{\partial x^2}. \tag{3.37}$$

The equation's algebraic properties follow from the nonzero commutator brackets of the symmetries. The commutator of K_∞ with any of the other symmetries is zero. This follows because it is of the form of the homogeneity symmetry K_4 when $u = k$ is a solution of the equation. The brackets for the nontrivial symmetries $K_1 - K_6$ are:

	K_1	K_2	K_3	K_4	K_5	K_6
K_1	0	0	$2K_1$	0	$2iK_2$	$\frac{1}{2}iK_4 + iK_3$
K_2	0	0	K_2	0	K_4	$\frac{1}{2}K_5$
K_3	$-2K_1$	$-K_2$	0	0	K_5	$2iK_6$
K_4	0	0	0	0	0	0
K_5	$-2iK_2$	$-K_4$	$-K_5$	0	0	0
K_6	$-\frac{1}{2}iK_4 - iK_3$	$-\frac{1}{2}K_5$	$-2iK_6$	0	0	0

[1] Note that while for the equations treated in this thesis the symmetry corresponding to the infinite number of solution symmetries of the partial differential equation satisfies the original equation this is not necessarily the case. In the study of equations which contain nonlinearities in their derivatives the equation may for instance admit a generator which is the solution of a linear partial differential equation. This usually points to a transformation relating the original nonlinear equation to the linear equation found in the symmetries [22].

In order to identify the Lie algebra we look for closed lower dimensional subalgebras contained in K_1-K_6 and use the standard classification tables from Chapter 2. The generators K_2, K_4 and K_5 immediately form a closed subalgebra. These are identified with the Heisenberg-Weyl algebra $A_{3,1}$ which has the commutator brackets

$$[\Sigma_1, \Sigma_2] = 0, \quad [\Sigma_1, \Sigma_3] = 0, \quad [\Sigma_2, \Sigma_3] = \Sigma_1. \tag{3.38}$$

The generators K_1, K_3 and K_6 are not closed directly or in standard form. However, since any linear combination of symmetries is itself a symmetry we may write $\bar{K}_1 = iK_1$, $\bar{K}_3 = \frac{1}{2}(iK_3 + \frac{1}{2}iK_4)$ and $\bar{K}_6 = -iK_6$ obtain

$$[\bar{K}_6, \bar{K}_1] = K_1, \quad [\bar{K}_6, \bar{K}_1] = -2\bar{K}_3, \quad [\bar{K}_3, \bar{K}_6] = \bar{K}_6. \tag{3.39}$$

The algebra is now identified as $sl(2, \mathbb{R})$ or $A_{3,8}$.

The algebra of (3.28) may be written as $\{A_{3,1} \otimes_s A_{3,8} \otimes_s \infty A_1\}$, where the abelian algebra for the commutativity of K_∞ with the other symmetries has been denoted as ∞A_1 and $\otimes_s$ is the semi-direct sum. Further details on the representation theory of Lie algebras may be found in [4].

3.2.2 Lie Groups of Transformations

Another property is that the infinitesimal generators lead directly to the construction of the corresponding finite Lie group of transformations where the sleight of hand used is to solve the associated Lagrange's system for the symmetry as an initial value problem with respect to the group parameter. One finds, for example, from (3.28)

$$\bar{u}(\bar{t}, \bar{x}, \epsilon), \quad \bar{x}(t, x, \epsilon), \quad \bar{t}(t, x, \epsilon), \tag{3.40}$$

where ϵ is the group parameter and the initial condition is

$$u = \bar{u}, \quad t = \bar{t}, \quad x = \bar{x}, \tag{3.41}$$

when $\epsilon = 0$. This gives the functional forms for the group invariant solutions which satisfy

$$i\frac{\partial \bar{u}}{\partial \bar{t}} = -\frac{\partial^2 \bar{u}}{\partial \bar{x}^2}\,. \tag{3.42}$$

The symmetry K_5, for example, has the characteristic system

$$\frac{d\bar{u}}{d\epsilon} = \bar{u}\bar{x}, \quad \frac{d\bar{x}}{d\epsilon} = 2i\bar{t}, \quad \frac{d\bar{t}}{d\epsilon} = 0. \tag{3.43}$$

This may be integrated with the initial value condition (3.41) to give the finite transformations

$$\bar{u} = u \exp(it\epsilon^2 + x\epsilon), \quad \bar{x} = 2it\epsilon + x, \quad \bar{t} = t, \tag{3.44}$$

which enables us to write the functional form for the solution, say $u = f(x, t)$, as

$$u = \exp(-it\epsilon^2 - x\epsilon) \times f(x - 2it\epsilon, t). \tag{3.45}$$

The complete set of integrations is:

	$\bar{u}$	$\bar{t}$	$\bar{x}$
K_1	u	$t+\epsilon$	x
K_2	u	t	$x+\epsilon$
K_3	u	$te^{2\epsilon}$	xe^{ϵ}
K_4	ue^{ϵ}	t	x
K_5	$u\exp(it\epsilon^2+x\epsilon)$	t	$x+2it\epsilon$
K_6	$u\sqrt{(1-i\epsilon t)}\exp\left(\frac{-\epsilon x^2}{4-i\epsilon t}\right)$	$\frac{t}{1-i\epsilon t}$	$\frac{x}{1-i\epsilon t}$

The functional forms for $u(x,t)$ which leave the equation invariant are found by solving for the original variables. We have that

$$
\begin{aligned}
u &= f(x, t-\epsilon) && (3.46)\\
u &= f(x-\epsilon, t) && (3.47)\\
u &= f(e^{-\epsilon}x, e^{-2\epsilon t}) && (3.48)\\
u &= e^{-\epsilon} f(x,t) && (3.49)\\
u &= (1-i\epsilon t)^{-\frac{1}{2}}\exp\left(\frac{-\epsilon x^2}{4-i\epsilon t}\right)\times f\left(\frac{x}{1-i\epsilon t},\frac{t}{1-i\epsilon t}\right). && (3.50)
\end{aligned}
$$

Each of these is a particular type of special solution of (3.28). The form of the solution (3.46) for example reflects invariance under translations in t and (3.47) translations in x while (3.48) provides scaling solutions.

3.3 The Harmonic Oscillator

3.3.1 Symmetries and Algebras

The harmonic oscillator equation

$$i\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} + x^2 u \tag{3.51}$$

arises if the form of the potential is taken to be $V(x) = x^2$. This has the symmetries:

$$\begin{aligned}
H_1 &= i\partial_t && (3.52)\\
H_2 &= u\partial_u && (3.53)\\
H_3 &= e^{-2it}\left(\partial_x + xu\partial_u\right) && (3.54)\\
H_4 &= e^{2it}\left(\partial_x - xu\partial_u\right) && (3.55)\\
H_5 &= e^{4it}\left(\tfrac{1}{2}i\partial_t + x\partial_x + (x^2 - \tfrac{1}{2})u\partial_u\right) && (3.56)\\
H_6 &= e^{-4it}\left(\tfrac{1}{2}i\partial_t - x\partial_x + (x^2 + \tfrac{1}{2})u\partial_u\right) && (3.57)\\
H_\infty &= h(t,x)\partial_u. && (3.58)
\end{aligned}$$

The function $h(t,x)$ here is any solution of

$$i\frac{\partial h}{\partial t} = -\frac{\partial^2 h}{\partial x^2} + x^2 h. \tag{3.59}$$

The table of commutator brackets is given by

	H_1	H_2	H_3	H_4	H_5	H_6
H_1	0	0	$2H_3$	$-2H_4$	$-4H_5$	$4H_6$
H_2	0	0	0	0	0	0
H_3	$-2H_3$	0	0	$-2H_2$	$-4H_4$	0
H_4	$2H_4$	0	$2H_2$	0	0	$4H_3$
H_5	$4H_5$	0	$4H_4$	0	0	$2H_1$
H_6	$-4H_6$	0	0	$-4H_3$	$-2H_1$	0

The Heisenberg-Weyl algebra, $A_{3,1}$, is then formed from H_2, H_3 and H_4 and the $sl(2,\mathbb{R})$ algebra, $A_{3,9}$, from H_1, H_5 and H_6, up to various factors[2].

[2] The author points out that if the standard form of the classical Hamiltonian $H = \frac{1}{2}(\hat{p}^2 + \hat{q}^2)$ for the harmonic oscillator had been used in the calculation instead of $H = \hat{p}^2 + \hat{q}^2$ this would not be necessary.

3.3.2 Solution Surfaces

Another application of symmetry is the construction of invariant solution surfaces and the mapping of solutions to solutions. For example, consider the associated Lagrange's system for H_4

$$\frac{dt}{0} = \frac{dx}{1} = \frac{du}{-xu}. \tag{3.60}$$

The characteristics are found to be

$$v = t \qquad \text{and} \qquad w = ue^{1/2x^2}.$$

Substituting the *ansatz*

$$u = e^{-1/2x^2} f(t) \tag{3.61}$$

into (3.51) gives $f(t) = e^{it}$. Define the solution surface Σ_0 by

$$\begin{aligned}
\Sigma_0 &= u^{-1}e^{-1/2x^2+it} && (3.62)\\
H_4\Sigma_0 &= -2xu^{-1}e^{-1/2x^2+3it} && (3.63)\\
H_4^2\Sigma_0 &= (4x^2-2)u^{-1}e^{1/2x^2+5it} && (3.64)\\
&\vdots
\end{aligned}$$

The solutions

$$\begin{aligned}
u_0 &= e^{-1/2x^2} && (3.65)\\
u_1 &= -2xe^{-1/2x^2+3it} && (3.66)\\
u_2 &= (4x^2-2)e^{-1/2x^2+5it} && (3.67)\\
&\vdots
\end{aligned}$$

illustrate the idea that symmetries map solutions into solutions. H_3 acts as an annihilation operator, whilst H_6 acts as a double annihilation operator. Equally, H_5 is a double ladder operator, mapping by two states at a time, *viz* $u_0 \to u_2 \to u_4$.

3.4 The Ermakov-Pinney Potential

The final form of the Schrödinger equation which was found from the group classification was the Ermakov-Pinney type potential [28]. This gives an equation of the form

$$i\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} + \frac{1}{x^2}u. \tag{3.68}$$

The symmetries of this equation are

$$\begin{aligned}
G_1 &= u\partial_u && (3.69)\\
G_2 &= \partial_t && (3.70)\\
G_3 &= 2t\partial_t + x\partial_x && (3.71)\\
G_4 &= 4itx\partial_x + 4it^2\partial_t - (2it + x^2)u\partial_u && (3.72)\\
G_\infty &= g(x,t)\partial_u, && (3.73)
\end{aligned}$$

where $g(x,t)$ is a solution of the equation

$$i\frac{\partial g}{\partial t} = -\frac{\partial^2 g}{\partial x^2} + \frac{1}{x^2}g. \tag{3.74}$$

The generators G_2, G_3 and G_4 form, up to a closure with an addition of G_1 where appropriate, the $sl(2,\mathbb{R})$ algebra.

As an application we consider the reduction of order of (3.68) using the symmetry generators. The combined symmetry

$$G = G_1 + G_2 + G_3 = (2t+1)\partial_t + u\partial_u + x\partial_x \tag{3.75}$$

has the associated Lagrange's system,

$$\frac{dt}{2(t+1)} = \frac{dx}{x} = \frac{du}{u}. \tag{3.76}$$

This gives the characteristics

$$\zeta = \frac{x}{(t+1)^{\frac{1}{2}}} \qquad \eta = \frac{u}{x} \tag{3.77}$$

for the form of the similarity solution

$$u = xh(\zeta) = xh\left(\frac{x}{(t+1)^{\frac{1}{2}}}\right), \tag{3.78}$$

where h is an arbitrary function of its argument. The substitution of (3.78) into (3.68) and simplification gives the ordinary differential equation

$$\frac{x^2}{(t+1)}h'' + 2\frac{x}{(t+1)^{\frac{1}{2}}}h' - i\frac{1}{2}\frac{x^3}{(t+1)^{\frac{3}{2}}}h' - h = 0. \tag{3.79}$$

This is recognizable as,

$$2\zeta^2 h'' + \zeta(4 - i\zeta^2)h' - 2\nu^2 h = 0, \tag{3.80}$$

which may be solved using the method of Frobenius with the *ansatz*

$$h = \sum_{j=0}^{\infty} a_j \zeta^{j+s} \tag{3.81}$$

and substitution into equation (3.80) to obtain a recurrence relation for the coefficients a_j and the value of s.

3.5 Remarks

We have given a basic outline of the applications of symmetry properties to partial differential equations using a number of standard examples. The group classification problem for the Schrödinger equation was used to illustrate the standard uses of symmetry techniques for the analysis of equations containing arbitrary terms. This provided a number of problems with which to continue the analysis. The free particle Schrödinger equation was used to demonstrate the construction of Lie groups of transformations and group type solutions using symmetry. The harmonic oscillator equation provided a means for demonstrating the mapping properties of solutions and their relation to the corresponding generators. Finally we used the Ermakov-Pinney equation to show how symmetry methods are related to reduction of order. These types of applications will be used in Chapter 4 for the quantum Brownian motion model. In our discussion of Lie algebraic properties we gave the algebras of the corresponding equations in the standard classifications and clarified how these may be obtained using standard tables. A possible omission is that we have not demonstrated the local equivalence of equations using purely algebraic properties. It cannot be emphasized enough that the algebraic properties of its symmetries determine the invariance properties of the differential equation.

4. ANALYSIS OF THE QUANTUM BROWNIAN MOTION MODEL

In open system dynamics the general idea is that one models a reduced quantum subsystem of a larger quantum system which is evolving unitarily and averages over the effects of the remaining environmental degrees of freedom on the subsystem. The fundamental problem is to study the time evolution of the reduced system conditional on environmental dissipation. This may be approached in two ways: One approach is to construct a density operator for the total closed system allow it to evolve unitarily and then use the partial trace to obtain the density operator for the reduced system by statistically averaging over the environmental effects on the open system. This is known as the quantum operations formalism [23]. The alternative is to place a variety of restrictions on the evolution of the system and formulate statistically a quantum dynamical semigroup to reflect the transfer of energy and entropy from the open system to the environment via the build up of system environment correlations [2]. This leads to the formulation of an evolution equation for the density matrix which replaces the Liouville-von Neumann equation for the evolution of a closed quantum system and includes dissipative effects. The most common type is the Lindblad equation [17, 8] which describes the behaviour of open systems for short term, memoryless correlations. The equation for the reduced density matrix ρ has the form

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{2}\sum_{j=1}^{n}\left(\{L_j L_j^\dagger, \rho\} - 2L_j \rho L_j^\dagger\right), \tag{4.1}$$

where H is the Hamiltonian, which may include interaction terms, and L are the dissipative Lindblad operators describing the environmental effects.

A simple open quantum system model both amenable to analysis and ubiquitous in open quantum systems literature is the quantum Brownian motion model [3, 9, 10, 5, 6, 7, 29]. The model consists of a non-relativistic free particle of mass m weakly interacting with a high temperature bath of harmonic oscillators. The master equation for the density operator is

$$\frac{\partial\rho}{\partial t} = \frac{i\hbar}{2m}\left(\frac{\partial^2\rho}{\partial x^2} - \frac{\partial^2\rho}{\partial y^2}\right) - \frac{1}{2}a^2(x-y)^2\rho \tag{4.2}$$

where $a^2 = 4m\gamma kT/\hbar^2$, T is the temperature of the environment, γ is a measure of dissipation, k is Boltzmann's constant and x and y have the meaning of coordinates. This is the Lindblad equation (4.1) with the operators, [10],

$$H = \frac{\hat{p}^2}{2m} \quad \text{and} \quad L = a\hat{x}. \tag{4.3}$$

(Here, $\hat{p}$ and $\hat{x}$ are momentum and position operators.) The appealing physical features of this model are that for both equation (4.2) and its generalizations it has been shown numerically and analytically that the system localizes for certain types of initial conditions i.e. the density operator becomes approximately diagonal and we have, $\rho(x,y) \approx \rho(x,x)$. This is the decoherence phenomenon whereby the quantum fluctuations in the particle dynamics are damped by thermal fluctuations in the environment. An important result is that the particles phase space trajectory becomes approximately equivalent to classical Brownian motion [10].

In this chapter the aim is to study the analytical properties of the quantum Brownian motion equation (4.2) from the perspective of symmetry analysis. A straightforward symmetry analysis by `PROGRAM LIE` reveals that equation (4.2) has sufficient symmetry for it to be interesting. These symmetries suggest a change of variables for the equation into a form which is easier to study. A check of the nonzero commutators of this equation gives the corresponding algebra as $\left\{(A_1 \otimes_s A_{3,1}) \otimes_s A^a_{3,5}\right\}$ where $\otimes_s$ is the semi-direct sum. A curious point is that this contains the Heisenberg-Weyl algebra, $A_{3,1}$, in common with the free particle and harmonic oscillator Schrödinger equations. The symmetries of this equation are then used to reduce the order of the system in terms of either the number of variables, the degree of the derivative or both. Analysis of these reduced equations lead directly to solutions of (4.2) once the variables have been inverted. These are the main part of our results.

4.1 Lie Symmetries and Algebras

We begin by performing the symmetry analysis of equation (4.2). For aesthetic purposes we rewrite the equation as

$$\frac{\partial u}{\partial t} = A\left(\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2}\right) + B(x-y)^2 u, \tag{4.4}$$

where the constants $A = i\hbar/2m$ and $B = -\frac{1}{2}a^2$ have been introduced and we have set $u = \rho$. The analysis by `PROGRAM LIE` returns the symmetries

$$
\begin{aligned}
X_1 &= \partial_x + \partial_y && (4.5)\\
X_2 &= \partial_t && (4.6)\\
X_3 &= u\partial_u && (4.7)\\
X_4 &= -u\partial_u + 2t\partial_t + (x+2y)\partial_x + (2x+y)\partial_y && (4.8)\\
X_5 &= (x-y)u\partial_u - 2At(\partial_x + \partial_y) && (4.9)\\
X_6 &= 2B(x-y)tu\partial_u + \partial_x - 2ABt^2(\partial_x + \partial_y) && (4.10)\\
X_7 &= \left[2A^2B(x-y)t^2 - x\right] u\partial_u + 2At\partial_x - \tfrac{4}{3}(\partial_x + \partial_y) && (4.11)\\
X_\infty &= f(t,x,y)\partial_u\,, && (4.12)
\end{aligned}
$$

where $f(t,x,y)$ is any solution of (4.2).

The symmetries immediately suggest information on the structure of the differential equation. The recurrence of the differential operator $\partial_x + \partial_y$ and the terms $(x-y)$ in the symmetry generators (4.5)-(4.12) suggests the transformation of variables

$$v = x - y \tag{4.13}$$

$$w = x + y. \tag{4.14}$$

Also, it may be observed that (4.4) can be written as

$$\frac{\partial u}{\partial t} = A(\partial_x - \partial_y)(\partial_x + \partial_y)u + B(x-y)^2 u \tag{4.15}$$

from which

$$\frac{\partial u}{\partial t} = A\frac{\partial^2 u}{\partial v \partial w} + Bv^2 u. \tag{4.16}$$

Since it is a straightforward point transformation none of the the essential properties of the solution are altered. The algebraic properties of the equation remain invariant under the transformation. It is this transformed equation which we will concentrate on. The symmetries of this equation are

$$
\begin{aligned}
Y_1 &= \partial_w && (4.17)\\
Y_2 &= \partial_t && (4.18)\\
Y_3 &= 2t\partial_t - v\partial_v + 3w\partial_w && (4.19)\\
Y_4 &= u\partial_u && (4.20)\\
Y_5 &= uv\partial_u - At\partial_w && (4.21)\\
Y_6 &= 2Butv\partial_u - ABt^2\partial_w + \partial_v && (4.22)\\
Y_7 &= (w - ABt^2 v)u\partial_u - At\partial_v + \tfrac{1}{3}A^2Bt^3\partial_w && (4.23)\\
Y_\infty &= g(t,v,w)\partial_u. && (4.24)
\end{aligned}
$$

The function $g(t,v,w)$ is again any solution of (4.16).

The Lie algebra of the symmetries is determined by the commutators of (4.17)-(4.24). These are:

	Y_1	Y_2	Y_3	Y_4	Y_5	Y_6	Y_7
Y_1	0	0	$3Y_1$	0	0	0	$-Y_4$
Y_2	0	0	$2Y_2$	0	$-AY_1$	$-2BY_5$	$-AY_6$
Y_3	$-3Y_1$	$-2Y_2$	0	0	$-Y_5$	Y_6	$3Y_7$
Y_4	0	0	0	0	0	0	0
Y_5	0	AY_1	Y_5	0	0	Y_4	0
Y_6	0	$2BY_5$	$-Y_6$	0	$-Y_4$	0	0
Y_7	Y_4	AY_6	$-3Y_7$	0	0	0	0

In terms of the standard algebraic classification of equation (4.16), the symmetries Y_4, Y_5 and Y_6 constitute a representation of the Weyl algebra $A_{3,1}$ which has the structure

$$[G_1, G_2] = 0, \qquad [G_1, G_3] = 0, \qquad [G_2, G_3] = G_1. \tag{4.25}$$

We may rescale Y_3 as $\bar{Y_3} = \frac{1}{3}Y_3$ to obtain the commutators

$$[Y_1, \bar{Y_3}] = Y_1, \quad \text{and} \quad [Y_2, \bar{Y_3}] = \tfrac{2}{3}Y_2. \tag{4.26}$$

The bracket $[Y_1, Y_2] = 0$, gives that Y_1, Y_2 and $\bar{Y_3}$ are of the form of the algebra $A^a_{3,5}$

$$[G_1, G_3] = G_1, \quad [G_2, G_3] = aG_2 \quad \text{where} \quad (0 < a < 1). \tag{4.27}$$

Since Y_7 commutes with Y_4, Y_5 and Y_6, the algebra may be decomposed as $\{(A_1 \otimes_s A_{3,1}) \otimes_s A^a_{3,5}\}$. This is especially promising since the algebra $A_{3,1}$ is shared with the linear diffusion equation and the Schrödinger equation for the free particle. We will see below that there is a corresponding reduction.

4.2 Reduction by Symmetry

The symmetries of the differential equations (4.4) and (4.16) now give a route into the applications highlighted in the Chapter 3. Each of the non-trivial symmetries (4.5)-(4.11) and (4.17)-(4.23) provides a possible route for reducing either the order of the system or the number of independent variables using the solution of the corresponding associated Lagrange's system [1, 14, 26]. Also note that, in principle, we could also take linear combinations of symmetries and then use those to find characteristics as well provided that the Lagrange's system could be integrated. We find in this section the various reductions to lower dimensional and/or lower order partial differential equations using the symmetry generators. The reduction by Y_1 gives an analytic solution independent of w. The symmetries X_2 (Y_2) and X_3 (Y_4) are used to illustrate the separations of variable solution. The characteristics obtained from Y_4 give a reduction in terms of similarity variables [1] to a second order nonlinear partial differential equation in two-independent variables. Reduction by Y_5 results in a first order nonhomogenous partial differential equation that provides a complete integration of (4.4). The most physically interesting change of variables is that of Y_6 which reduces the quantum Brownian motion model, under transformation, to a type of damped heat equation. The reduced partial differential equation provided by Y_7 has nonlinear and time-dependent coefficients.

Reduction by Y_1

The first reduction is fairly simple. The characteristic system[1] corresponding to $Y_1 = \partial_w$ is

$$\frac{du}{0} = \frac{dw}{1} = \frac{dv}{0} = \frac{dt}{0}. \tag{4.28}$$

The integration of this is

$$u = F(v, t). \tag{4.29}$$

Substitution into equation (4.16) gives the first order differential equation

$$\frac{\partial F}{\partial t} = Bv^2 F. \tag{4.30}$$

The equation has the solution

$$u = \exp[Bv^2 t]\phi(v), \tag{4.31}$$

in terms of x and y, and ρ

$$\rho = \exp\left[-\tfrac{1}{2}a^2(x-y)^2 t\right]\phi(x-y). \tag{4.32}$$

Reduction by Y_2 and Y_4

The symmetries $Y_2 = \partial_t$ and $Y_4 = u\partial_u$ reflect the autonomy and homogeneity of (4.16) (inherited from (4.4)). These allow one to construct the separation of variables solution to the problem [1, 26]. We have trivially that using Y_2 or Y_4 alone that the equation admits the forms

$$u = F(v, w, t) \quad \text{and} \quad u = F(v, w). \tag{4.33}$$

[1] Note that in the following *cst* will denote constants with respect to the characteristics, and we will introduce additional variables as required.

The first is not very helpful and the second is the time-independent solution. However we may also use the linear combination $Y_2 + \chi Y_4$ as a generator for some constant χ. This has the associated Lagrange's system

$$\frac{du}{\chi u} = \frac{dt}{1} = \frac{dv}{0} = \frac{dw}{0} \tag{4.34}$$

from which we may obtain the separation of variables form

$$u = \int d\chi C(\chi) \exp(\chi t) F(v, w), \tag{4.35}$$

where we have introduced the function $C(\chi)$ in the parameter. The form for (4.16) is

$$A \frac{\partial^2 F}{\partial v \partial w} = (\chi - Bv^2) F \tag{4.36}$$

which may be solved directly by applying separation of variables for a second time. If we let $F = V(v)W(w)$ we have,

$$AV'W' = (\chi - Bv^2) VW. \tag{4.37}$$

This may be separated into the ordinary differential equations

$$AV' = \mu(\chi - Bv^2) V \tag{4.38}$$

and

$$\mu W' = W. \tag{4.39}$$

The solution of which is

$$F(v, w) = \int d\mu D(\mu) \exp\left[\frac{\mu}{A}(\chi v - \tfrac{1}{3} B v^3)\right] \exp\left[\frac{w}{\mu}\right], \tag{4.40}$$

where we have integrated over the parameter μ and introduced the function $D(\mu)$. Finally we have

$$u = \int d\chi d\mu C(\chi) D(\mu) \exp\left[\chi t + \frac{\mu}{A}(\chi v - \tfrac{1}{3} B v^3) + \frac{w}{\mu}\right]. \tag{4.41}$$

Reduction by Y_3

The usual idea when searching for similarity transformations is to employ an *ansatz* which reflects invariance under a group of scalings and then substitute into the differential equation to find the correct values of the scaling constants. There is also a close connection to dimensional analysis [1]. The scaling symmetry

$$Y_3 = 2t\partial_t - v\partial_v + 3w\partial_w \tag{4.42}$$

allows us to obtain the correct variables directly. We find the associated Lagrange's system

$$\frac{dt}{2t} = \frac{dv}{-v} = \frac{dw}{3w} = \frac{du}{0}. \tag{4.43}$$

The first and the second equalities give

$$\frac{dt}{2t} + \frac{dv}{v} = 0 \tag{4.44}$$

from which the characteristic

$$t^{1/2}v = k_1. \tag{4.45}$$

The first and the third give

$$\frac{dt}{2t} - \frac{dw}{3w} = 0 \tag{4.46}$$

and

$$t^{1/2}w^{-1/3} = k_2, \tag{4.47}$$

clearly we also have

$$u = cst. \tag{4.48}$$

The solution for u in terms of these characteristics is

$$u = F(t^{1/2}v, t^{1/2}w^{-1/3}) = F(k_1, k_2). \tag{4.49}$$

We now substitute this into (4.16) to obtain the equation

$$\tfrac{1}{2}t^{-1/2}v\frac{\partial F}{\partial k_1} + \tfrac{1}{2}t^{-1/2}w^{-1/3}\frac{\partial F}{\partial k_2} = A\left[-\tfrac{1}{3}tw^{-4/3}\frac{\partial^2 F}{\partial k_1 k_2}\right] + Bv^2F. \tag{4.50}$$

This is identified in the new variables as

$$\tfrac{1}{2}k_1\frac{\partial F}{\partial k_1} + \tfrac{1}{2}k_2\frac{\partial F}{\partial k_2} + \tfrac{1}{3}Ak_2^4\frac{\partial^2 F}{\partial k_1 \partial k_2} - Bk_1^2F = 0. \tag{4.51}$$

Reduction by Y_5

We have that $Y_5 = uv\partial_u - At\partial_t$. The associated Lagrange's system is

$$-\frac{du}{uv} = \frac{dw}{At} = \frac{dv}{0} = \frac{dt}{0}. \tag{4.52}$$

We have

$$v = cst \tag{4.53}$$

and

$$t = cst \tag{4.54}$$

as characteristics. This and the first and second of these equations give the general form for u as

$$u = F(v,t)\exp\left[-\frac{vw}{At}\right]. \tag{4.55}$$

Equation (4.16) is then reduced to a first order nonhomogenous partial differential equation for F

$$\frac{\partial F}{\partial t} + \frac{v}{t}\frac{\partial F}{\partial v} + \left(\frac{1}{t} - Bv^2\right)F = 0. \tag{4.56}$$

This can be solved from the associated Lagrange's system

$$\frac{dt}{1} = \frac{tdv}{v} = \frac{dF}{F\left(Bv^2 - \frac{1}{t}\right)}. \tag{4.57}$$

This gives the solution for F

$$F(v,t) = \frac{1}{t}\exp[-\tfrac{1}{3}Bv^2 t]\Pi\left(\frac{v}{t}\right). \tag{4.58}$$

And, finally for ρ

$$\rho = \frac{1}{t}\exp\left[-\frac{1}{6}a^2(x-y)^2 t + i\frac{2m}{\hbar}\left(\frac{x^2-y^2}{t}\right)\right]\Pi\left(\frac{x-y}{t}\right), \tag{4.59}$$

where Π is an arbitrary function of its argument.

Reduction by Y_6

The symmetry $Y_6 = 2Butv\partial_u - ABt^2\partial_w + \partial_v$ gives the system

$$\frac{du}{-2Butv} = \frac{dw}{ABt^2} = \frac{dv}{-1} = \frac{dt}{0}. \tag{4.60}$$

The second and third characteristics give

$$ABt^2 + w = cst = g_1 \tag{4.61}$$

and from the last we have

$$t = cst = g_2. \tag{4.62}$$

The form for u is

$$u = \exp(Bg_2 v^2)F(g_1, g_2). \tag{4.63}$$

Substitution into (4.16) leads to

$$\frac{\partial F}{\partial g_2} - A^2 B g_2^2 \frac{\partial F}{\partial g_1^2} = 0. \tag{4.64}$$

This is identifiable as the backwards heat equation

$$\frac{\partial F}{\partial s} + \frac{\hbar^2 a^2}{8m}\frac{\partial^2 F}{\partial r^2} = 0 \tag{4.65}$$

in the time variable $s = 1/t = 1/g_2$ and $r = g_1$. This is clearly the most interesting case. The solution for ρ can then be written in terms of these as

$$\rho = \exp\left[-\tfrac{1}{2}a^2 t(x-y)^2\right] F(r,s), \tag{4.66}$$

where F is any solution of (4.77) and where the variables r and s are now defined by

$$r = -\frac{i\hbar}{2m} \times \tfrac{1}{2}a^2t^2 + (x+y) \quad \text{and} \quad s = \frac{1}{t}. \tag{4.67}$$

The properties of this solution will be discussed further in the next section.

Reduction by Y_7

The final symmetry gives the characteristic system,

$$\frac{du}{(w - ABt^2 v)u} = -\frac{dv}{At} = \frac{3dw}{A^2Bt^3} = \frac{dt}{0}. \tag{4.68}$$

The second and the third of these give the characteristic

$$\tfrac{1}{3}ABt^2 v + w = cst = h_1. \tag{4.69}$$

We also have

$$t = cst = h_2. \tag{4.70}$$

Integration for u gives

$$u = \exp\left[\frac{3w^2}{2A^2Bh_2^3} + \tfrac{1}{2}Bh_2v^2\right] F(h_1,h_2). \tag{4.71}$$

This leads to the following equation in the characteristic variables

$$\frac{\partial F}{\partial h_2} + \frac{h_1}{h_2}\frac{\partial F}{\partial h_1} + \tfrac{1}{3}A^2Bh_2^2\frac{\partial^2 F}{\partial h_1^2} - \frac{9h_1^2}{2A^2Bh_2^4}F = 0. \tag{4.72}$$

4.3 Analytical Solutions

We found in the previous section that there were several possible reductions of the quantum Brownian motion equation to equations of lower dimensionality as well as degree. We found that Y_1, Y_5, and Y_6 allow for reductions to equations which may be solved exactly and the Y_2 and Y_4 can be used to construct the separation of variables solution to the problem. These give solutions for the distribution $\rho(x, y, t)$ of the density matrix in the position representation

$$\rho = \int dxdy \rho(x, y, t)|x\rangle\langle y|, \tag{4.73}$$

once the variables have been inverted. The solutions which we obtained were

$$\rho(x, y, t) = \exp\left[-\tfrac{1}{2}a^2(x-y)^2 t\right] \Phi\left(x-y\right), \tag{4.74}$$

$$\rho(x, y, t) = \frac{1}{t}\exp\left[-\frac{1}{6}a^2(x-y)^2 t + i\frac{2m}{\hbar}\left(\frac{x^2-y^2}{t}\right)\right] \Pi\left(\frac{x-y}{t}\right), \tag{4.75}$$

where Φ and Π are arbitrary functions of their arguments, and

$$\rho(x, y, t) = \exp\left[-\tfrac{1}{2}a^2(x-y)^2 t\right] F(r, s) \tag{4.76}$$

where $F(r, s)$ is the solution to the backwards heat equation

$$\frac{\partial F}{\partial s} + \frac{\hbar^2 a^2}{8m}\frac{\partial^2 F}{\partial r^2} = 0 \tag{4.77}$$

with the variables r and s defined by

$$r = -i\frac{i\hbar}{4m} \times a^2 t^2 + (x+y) \quad \text{and} \quad s = \frac{1}{t}. \tag{4.78}$$

Since the backwards heat equation (4.77) is a well known problem the various forms of the solution may be obtained directly [26, 27]. The following solutions are well known for α, β, μ arbitrary constants and $k = -\hbar^2 a^2/8m$,

$$\begin{aligned}
F(r,s) &= r^{2n} + \sum_{j=1}^{n} \frac{(2n)(2n-1)\ldots(2n-2j-1)}{j!}(ks)^j r^{2n-2j} \\
F(r,s) &= r^{2n+1} + \sum_{j=1}^{n} \frac{(2n+1)(2n)\ldots(2n-2j+1)}{j!}(ks)^j r^{2n-2j+1}, \\
F(r,s) &= \alpha \frac{r}{s^{3/2}} \exp\left(\frac{-r^2}{4ks}\right) + \beta, \\
F(r,s) &= \alpha \frac{r}{s^{1/2}} \exp\left(\frac{-r^2}{4ks}\right) + \beta, \\
F(r,s) &= \alpha \exp(-k\mu^2 s)\cos(\mu r) + \beta, \\
F(r,s) &= \alpha \exp(-k\mu^2 s)\sin(\mu r) + \beta, \\
F(r,s) &= \alpha \exp(-\mu r)\sin(\mu r - 2k\mu^2 s) + \beta, \\
F(r,s) &= \alpha \exp(-\mu r)\cos(\mu r - 2k\mu^2 s) + \beta, \\
F(r,s) &= \alpha \mathrm{erf}\left(\frac{r}{2\sqrt{ks}}\right) + \beta, \\
F(r,s) &= \alpha \mathrm{erfc}\left(\frac{r}{2\sqrt{ks}}\right) + \beta \\
F(r,s) &= \alpha \left[\sqrt{\frac{s}{\pi}} \exp\left(-\frac{r^2}{4ks}\right) - \frac{s}{2\sqrt{k}} \mathrm{erfc}\left(\frac{r}{2\sqrt{ks}}\right)\right].
\end{aligned}$$

Here, n is a positive integer, erf is the error function and erfc is the complementary error function. These are probability distributions defined by

$$\mathrm{erf} z \equiv \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\xi^2) d\xi, \tag{4.79}$$

and $\mathrm{erfc} z = 1 - \mathrm{erf} z$.

Note that for the construction of solutions to (4.77) we may also use symmetry analysis as a starting point. The symmetries of (4.77) are:

$$\begin{aligned}
Z_1 &= \partial_s &(4.80)\\
Z_2 &= \partial_r &(4.81)\\
Z_3 &= 2s\partial_s + r\partial_r &(4.82)\\
Z_4 &= F\partial_F &(4.83)\\
Z_5 &= \frac{\hbar^2 a^2}{4m} s\partial_r + Fr\partial_F &(4.84)\\
Z_6 &= \left(r^2 - \frac{\hbar^2 a^2}{4m} s\right) F\partial_F + \frac{\hbar^2 a^2}{2m} sr\partial_r + \frac{\hbar^2 a^2}{2m} s^2\partial_s &(4.85)\\
Z_\infty &= f(r,s)\partial_F, &(4.86)
\end{aligned}$$

where $f(r,s)$ is any solution of (4.77).

These may be used to construct various types of solution for the heat equation. For example, the symmetry Z_5 gives

$$F(r,s) = C_1 s^{1/2} \exp\left[\frac{r^2}{4ks}\right], \tag{4.87}$$

where C_1 is a constant of integration. Also, by repeated action of the symmetry generators on the solutions we may also construct an infinite hierarchy of polynomial solutions above in a similar vein as for the harmonic oscillator equation in Chapter 3. The surface defined by

$$\Sigma_0 = C_1 = us^{1/2} \exp\left(\frac{-r^2}{4ks}\right) \tag{4.88}$$

acted on by Z_5 provides the hierarchy

$$u_0 = \Sigma_0 s^{-1/2} \exp\left(\frac{r^2}{4ks}\right), \tag{4.89}$$

$$u_1 = \Sigma_1 s^{-1/2} \exp\left(\frac{r^2}{4ks}\right) \times \left(r - \frac{r}{2s}\right) \ldots \tag{4.90}$$

and so forth using $Z_5^n \Sigma_n$. Further details on the symmetry approach to construction of solutions to the heat equation may be found in [26].

The results above are a fairly decent beginning for constructing analytic solutions for the quantum Brownian motion model. Many of these results are original. Of course, these solutions are provided independent of initial, boundary and terminal conditions. One could use symmetry to include these in the construction by arguing that the symmetry be consistent with the boundary conditions [22].

Clearly the imposition of terminal conditions at $t = \infty$ and at $t = 0$ will place restrictions on the nature of the arbitrary functions Π, Φ and the form of the solution for F. A further constraint is that the solution be normalizable which is required since ρ is a probability distribution. This is the condition from quantum mechanics that

$$\mathrm{tr}\,\rho = 1, \tag{4.91}$$

or

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy\rho(x,y,t)\delta(x-y) = 1, \tag{4.92}$$

where δ is the Dirac delta function. If all these conditions are met it would be interesting to explore whether the decoherence behaviour and the tendency for the solution to localize i.e. the important physical aspects of the model mentioned in the introduction to this Chapter are valid for our solutions and their possible extensions. This is a question for future research.

4.4 Extensions

We also point out that the version of the quantum Brownian motion model which we have studied can be generalized to include both potential and dissipative terms [2]. This is merely modifying the standard Lindblad equation with the Hamiltonian and Lindblad operators

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}), \tag{4.93}$$

and

$$L = a\hat{x} + ib\hat{p}. \tag{4.94}$$

Here the constants a, b again relate to specific thermal properties of the bath. The term involving b is the dissipator while $V(x)$ is the potential. The constants have the meaning

$$a = \left(\frac{\hbar^2}{4m\gamma kT}\right)^{1/2} \qquad b = \left(\frac{\hbar^2}{4m\gamma kT}\right)^{1/2}\frac{\gamma}{\hbar}, \tag{4.95}$$

where k is Boltzmann's constant, the parameter γ is a measure of the dissipation and T is the temperature of the bath. The master equation (4.1) takes the form

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H,\rho] - \frac{i}{\hbar}\gamma\,[\hat{x},\{\rho,\hat{p}\}] - \frac{2M\gamma kT}{\hbar^2}[\hat{x},[\hat{x},\rho]] \tag{4.96}$$

which is written in the position representation as

$$\frac{\partial\rho}{\partial t} = \frac{i\hbar}{2m}\left(\frac{\partial^2\rho}{\partial x^2} - \frac{\partial^2\rho}{\partial y^2}\right) - \gamma(x-y)\left(\frac{\partial\rho}{\partial x} - \frac{\partial\rho}{\partial y}\right) - \frac{2m\gamma kT}{\hbar^2}(x-y)^2\rho - \frac{i}{\hbar}(V(x)-V(y))\rho. \tag{4.97}$$

A useful exercise would be an analysis of this problem especially with regard to group classification. Another would be to modify the potential, for example, to include a situation such as one encounters with the nonlinear Schrödinger equation with the aim of finding analytical solutions. The clue is that the algebraic structure of the modified equation (4.16) corresponds to the free particle equation and it is to be expected that similar algebraic properties hold for related problems including the dissipative harmonic oscillator and possibly the time dependent harmonic oscillator. The latter of which is known to be integrable by quadrature for the Schrödinger equation [12, 28].

4.5 Discussion

In this chapter we have studied the model equation for the quantum Brownian motion equation from a symmetry perspective. The symmetries of the model equation point out a simplified form of the problem as a route for the analysis. The algebraic properties and reduction of this equation to a series of other partial differential equations were also found. Among these was a mapping of the quantum Brownian model to the diffusion equation. This was used to construct a variety of analytical solutions to the model. We also discussed possible extensions of this work to more general forms of the quantum Brownian motion model including quantum Brownian motion with potentials. The analysis is expected to be of use to practitioners in open quantum systems and quantum mechanics.

5. SUMMARY

The main work of this thesis has been the application of Lie symmetry group based techniques [1, 14, 15, 16, 26] to the partial differential equation for the quantum Brownian motion model from open quantum systems [2, 9, 10]. Chapters 1-3 contains the background material for the analysis. The main results are contained in Chapter 4.

Chapter 1 introduces the problem and the basic ideas from quantum mechanics and open quantum systems.

Chapter 2 contains an introduction to the theory of Lie symmetry groups for differential equations. In this chapter the basic algorithm for calculating the symmetries of a differential equation and the rudiments of symmetry analysis are explained. The theoretical background concerning Lie groups, and Lie algebras are included. The properties of Lie algebras necessary for the development of later text are explained and tables of low dimensional Lie algebras are for reference.

Chapter 3 gives a survey of the applications of Lie symmetry groups to the one dimensional time dependent Schrödinger equation in an autonomous potential as an example of the application of symmetry groups to partial differential equations. This chapter acts as an introduction to the techniques available when applying symmetry groups to partial differential equations within the context of a standard problem. The various techniques of Lie analysis for partial differential equations were applied to the Free Particle, Harmonic Oscillator and Ermakov-Pinney partial Schrödinger equations.

Chapter 4 contains the main results of the thesis - the symmetry analysis of equation (4.2). A symmetry analysis of this equation is performed and the symmetries are used to study the transformation and algebraic properties of the model. The main results are that a number of new analytical solutions for the model may be obtained by mapping the problem to the $1 + 1$ diffusion equation using the symmetries. The results are discussed in §4.3 and mark a valuable contribution to the subject in that the quantum Brownian motion model is well known the literature [2, 10] and this research indicates that the model contains further, previously unknown, analytical properties. Possible extensions of this line of research aimed at further symmetry analysis for related models would in this case also be valuable. This is discussed in §4.4.

Overall, I have introduced the theory of Lie symmetry groups [1, 26] and discussed various applications to problems in quantum mechanics and specifically presented an analysis of the quantum Brownian motion model [9, 10] from the theory of open quantum systems [2].

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