



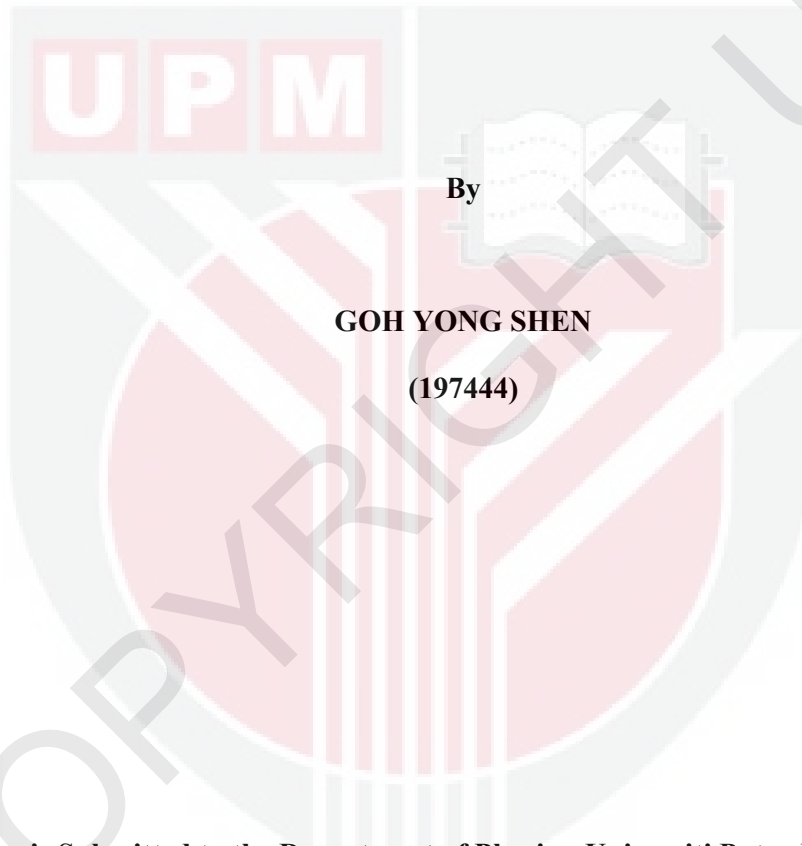
UNIVERSITI PUTRA MALAYSIA

DIRAC QUANTISATION OF MOTION ON A HELICOID

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DIRAC QUANTISATION OF MOTION ON A HELICOID



By

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**Thesis Submitted to the Department of Physics, Universiti Putra Malaysia, in
Partial Fulfilment of the Requirements for the Degree of Bachelor of Science in
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DEDICATION

To the pursuit and pursuers of knowledge



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ABSTRACT

DIRAC QUANTISATION OF MOTION ON A HELICOID

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FEBRUARY 2022

SUPERVISOR : ASSOC. PROF. DR. HISHAMUDDIN ZAINUDDIN

FACULTY : FACULTY OF SCIENCE

The quantisation of motion on curved manifolds through canonical quantisation has always been a tricky issue. It is well-established in the literature that Dirac's quantisation procedure requires the use of the Cartesian coordinate system, which is problematic for curved manifolds as there is no global Cartesian coordinate system for these surfaces. In order to overcome this problem, the canonical quantisation scheme is enhanced to include additional requirements. This thesis aims to determine the best geometric approach to take in the canonical quantisation for curved manifolds and identify the geometric potential and geometric momentum from the best approach with the help of the enhanced canonical quantisation (ECQ) scheme.

To achieve the objective of this thesis, the motion of a particle on a helicoid is quantised using Dirac's canonical quantisation procedure for constrained systems and the ECQ scheme. The problem will be approached through the intrinsic geometry approach via the system's local coordinates and the submanifold approach via the Cartesian coordinate system. The system will first undergo a classical mechanical treatment to determine its Dirac brackets, which will be followed up with

the quantum mechanical treatment to determine its commutators through canonical quantisation.

The results have shown that the quantisation of motion on a helicoid cannot be achieved through the intrinsic geometry approach due to a breakdown in algebraic structures. However, it can be achieved through the submanifold approach, and a self-consistent description of the problem is obtained. These results have validated the importance of the Cartesian coordinate system in canonical quantisation and have shown the importance of using the enhanced canonical quantisation scheme for the quantisation of motion on curved manifolds.

ABSTRAK

PENKUARTUMAN GERAKAN PADA PERMUKAAN HELIKOID MELALUI PENKUARTUMAN DIRAC

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FEBRUARI 2022

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Pengkuantuman gerakan pada manifold lengkung melalui pengkuantuman berkanun merupakan sesuatu isu yang susah diselesaikan. Hal ini disebabkan oleh pengkuantuman berkanun yang diasaskan oleh Dirac memerlukan penggunaan koordinat Cartesian dalam sesebuah sistem. Namun, pengkuantuman gerakan pada manifold lengkung telah merumitkan situasi tersebut atas kekurangan sistem koordinat Cartesian yang sejagat dalamnya. Untuk mengatasi kekangan ini, pengkuantuman berkanun telah dipertingkatkan melalui penambahan syarat. Tesis ini bertujuan untuk menentukan kaedah geometri yang paling sesuai digunakan dalam pengkuantuman berkanun untuk manifold lengkung yang dikaji dan menentukan potensi geometrik serta momentum geometrik dari kaedah tersebut melalui pengkuantuman berkanun yang dipertingkatkan.

Untuk mencapai objektif tesis ini, gerakan zarah pada permukaan helikoid telah dikuantumkan melalui pengkuantuman berkanun Dirac dan pengkuantuman

berkanun yang dipertingkatkan. Masalah ini akan dikaji melalui dua kaedah, iaitu melalui kaedah geometri intrinsik yang menggunakan koordinat lokal sistem, dan melalui kaedah submanifold yang menggunakan koordinat Cartesian. Untuk kedua-dua kaedah, kurungan Poisson untuk sistem zarah akan ditentukan dahulu. Seterusnya, komutator-komutatornya akan ditentukan melalui pengkuantuman berkanun.

Hasil kajian ini telah menunjukkan pengkuantum gerakan pada permukaan helikoid tidak boleh dilaksanakan melalui kaedah geometri intrinsik akibat penguraian struktur algebra. Namun begitu, pengkuantum gerakan pada permukaan helikoid boleh dilaksanakan melalui kaedah submanifold dan sesuatu penggambaran sistem yang konsisten boleh ditentukan. Hasil kajian ini telah mengesahkan kepentingan penggunaan koordinat Cartesian dalam pengkuantuman berkanun. Hasil kajian ini juga menunjuk betapa pentingnya pengkuantuman berkanun yang dipertingkatkan dalam pengkuantuman gerakan pada manifold lengkung.

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I would like to thank my Final Year Project supervisor, Associate Professor Dr. Hishamuddin Zainuddin for his guidance and help throughout this thesis. This thesis would never have been completed to this extent without the times when we huddled and discussed quantisation and the finer points in this work.

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Many thanks to all my supportive friends, lecturers in Universiti Putra Malaysia, and my parents. As much as this thesis is my own work, a part of it will forever belong to those who supported me throughout its progress.

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CHAPTER 1

INTRODUCTION

1.1 Brief Introduction and History of Quantum Mechanics

Quantum mechanics is the hallmark of modern physics. From the earliest founding experiment of Thomas Young's double-slit experiment to the development of full-fledged mathematical tools that help in the ongoing investigation of quantum phenomena, quantum mechanics continues to play a big role in Physics academia.

Oftentimes, people tend to misconstrue the history of quantum mechanics into a short period where quantum mechanical development was rapid. However, the truth is that quantum mechanics developed, and is still developing, over a century from the first discovery of a quantum phenomenon by Thomas Young up till the formulation of quantum mechanics by Schrödinger, Heisenberg and Born.

Quantum mechanics is a theory aimed at studying the behaviour of matter and light on an atomic scale. Feynman (1997) succinctly opined that "things on a very small scale behave like nothing that you have any direct experience about." Its main tenet of the uncertainty principle and new subtleties for causality caused scepticism among those who helped launch this new era of physics, such as Hendrik Lorentz, Max Planck, and Albert Einstein. Regardless of what they thought at that time, quantum mechanics has become the de facto method of studying matter at an atomic scale.

1.2 Canonical Quantisation

At the beginning of the field, there was an effort to find a linkage between classical mechanics and quantum mechanics. A quantum model is developed from a classical model of a particular system that is well-established, with the requirement that the

system will go back to the classical model when the classical limit of $\hbar \rightarrow 0$ is reached. This is known as quantisation.

Quantisation can generally be seen as the transition from a classical system to a quantum mechanical system. Regarding this field of physics, the mathematical physicist Edward Nelson once remarked that "quantisation is a mystery." Numerous schemes to achieve quantisation are available, such as canonical quantisation, geometric quantisation, and Wigner-Weyl quantisation. However, quantisation is seen as an "art" as there are no fixed guidelines on which of these schemes to use in any given circumstances.

The quantisation scheme considered in this thesis is known as canonical quantisation. Generally, canonical quantisation aims to quantise a classic system while maintaining its formal structure, such as its symmetry, as much as possible. Dirac noted that quantisation can be achieved by multiplying $i\hbar$ with the Poisson brackets of a system (Dirac, 1930, 1931). However, for constrained systems, Dirac (1931) theorised that the Poisson brackets need to be replaced with the more generalised Dirac bracket.

A major disadvantage to Dirac's canonical quantisation is that the dynamical coordinates and momenta of the system must be in terms of the Cartesian coordinate system, and not a curvilinear coordinate system (Dirac, 1930). With this constraint, it is difficult to achieve quantisation of motion on curved manifolds using Dirac's canonical quantisation scheme.

In the existing literature, many methods are explored to pacify the requirement for the Cartesian coordinate system in Dirac's canonical quantisation

scheme, among which are Abelian conversion (Hagen Kleinert & Shabanov, 1997) and other conversion methods (Diță, 1997).

A recent breakthrough in this line of inquiry comes from the quantisation of the geometric momentum from the confining potential approach and the enlarged canonical quantisation scheme (Liu et al., 2007). By expanding Dirac's quantisation scheme to include secondary commutation relations, the quantisation of motion on curved manifolds can be done with Dirac's quantisation procedure. These two breakthroughs have shown the importance of the Cartesian coordinate system in Dirac's canonical quantisation.

1.3 Project Scope

This thesis focuses on the quantisation of motion on curved manifolds, namely on a helicoid. This thesis uses Dirac's method of quantisation for constrained systems and the enhanced canonical quantisation (ECQ) scheme. The problem of quantising motion on a helicoid will be approached in two distinctive manners, namely the intrinsic geometry approach and the submanifold approach. The intrinsic geometry approach makes use of the system's local coordinates whereas the submanifold approach makes use of Cartesian coordinates. In both approaches, a classical mechanical treatment is first done to determine the Dirac brackets of the system. This is followed by a quantum mechanical treatment where the commutators are obtained via canonical quantisation. The commutators obtained are then analysed to determine if the momentum operators and the potential of the system are aligned with the geometric momentum and geometric potential found in the Schrödinger formalism.

1.4 Problem Statement

The quantisation of classical systems in curved spaces has always been a contentious issue. In canonical quantisation, the original formulation by Dirac only considers

systems in flat space, which makes use of the Cartesian coordinate system (Dirac, 1930, 1931). Furthermore, obtaining the geometric momentum through canonical quantisation for a particle constrained on a helicoid has not been explored fully. It is also not well-known if the geometric momentum and geometric potential of the aforementioned system can be obtained solely by quantisation with the intrinsic geometry approach. Not only that, the lack of a known proper momentum operator expression for a system constrained on a helicoid is also an issue as this prevents the ease of description for the system and it will be a setback for potential application, such as its application in the helicoidal motion of particles in a magnetic field. Finally, the effects of geometries on curved surfaces cannot be ignored and must be studied to have a better understanding of the behaviour of electrons in various materials, such as carbon nanostructures.

1.5 Objectives

The goal of this thesis is to study the quantisation of the motion of a particle constrained on a helicoid by using both the intrinsic geometry approach and the submanifold approach. The main objectives are as follows:

1. To verify the validity of solely approaching the quantisation of motion of a system constrained on a helicoid through the intrinsic geometry approach and the submanifold approach.
2. To compare the quantisation of motion for a system constrained on a helicoid using the intrinsic geometry approach to the submanifold approach.
3. To determine the geometric potential and geometric momentum of the system constrained on a helicoid.

4. To identify the quantisation approach that leads to the geometric momenta and geometric potential formulated through the Schrödinger formalism.

1.6 Thesis Structure

This thesis composes of five main chapters. Chapter 1 offers an introduction to the quantisation of constrained systems, the project scope, the problem statement, and the objectives of this thesis. In Chapter 2, a brief literature review is done on Dirac's method of quantisation for constrained systems, quantisation through intrinsic geometry, the confining potential approach, the enlarged canonical quantisation scheme, and recent advances with the enlarged canonical quantisation scheme. Chapter 3 expounds on the theories and methodologies that will be used in this thesis in detail. As this chapter aims to be self-contained, necessary concepts in classical mechanics and quantum mechanics are included. Chapter 3 also introduces Dirac's method of quantisation for constrained systems and the ECQ scheme before stating the methodology used in this thesis. Chapter 4 presents the results and discussion for the quantisation of motion of a particle constrained on a helicoid through the intrinsic geometry approach and the submanifold approach. Lastly, Chapter 5 concludes this thesis and offers suggestions for future research.

CHAPTER 2

LITERATURE REVIEW

2.1 Dirac's Method of Quantisation for Constrained Systems

Dirac (1931) stated that a classical system can be quantised by supplanting its Poisson brackets with commutators.

$$[\hat{A}, \hat{B}] = i\hbar\{A, B\} \quad (2.1)$$

The Poisson bracket in Equation (2.1) makes use of the Hamiltonian formalism in classical mechanics. However, for constrained systems, the Hamiltonian formalism is too restrictive as not all velocities of the dynamical variables can be expressed as canonical momenta, thereby making it impossible for the Hamiltonian of the system to be independent of velocity.

To quantise constrained systems, Dirac (1930) generalised the Hamiltonian formalism and Poisson brackets. From the Lagrangian of the constrained system, primary and secondary constraints of the system are found, and these constraints are further classified into first-class constraints and second-class constraints. For a system constrained on a curved manifold, all constraints are second-class constraints. In this case, the Poisson bracket is generalised and supplanted by Dirac brackets (Dirac, 1931).

However, Dirac (1930, 1931) stated that this quantisation procedure for second-class constraints can only be used in a system with the Cartesian coordinate system. This presents a challenge for the quantisation of motion on curved manifolds as a global Cartesian coordinate system is not available and curvilinear local coordinates are used in such a system. Any attempts to use Dirac's quantisation

procedure in non-Cartesian systems result in an operator-ordering problem for the position operator \hat{q} and the momentum operator \hat{p} .

2.2 Quantisation through Intrinsic Geometry

In the literature, one method to achieve quantisation of motion on curved manifolds relies on intrinsic geometry, which quantises the system by making use of its local coordinates. One way to overcome the operator ordering problem in the intrinsic geometry approach is to entirely forego the quantisation of momentum. Instead, the angular momentum \hat{L} is quantised instead. Podolsky (1928) achieved this by postulating that the Laplacian operator in the Hamiltonian operator should be replaced by the Laplace-Beltrami operator ∇_{LB} , such that the Hamiltonian operator is given by $\hat{H} = -\frac{\hbar^2}{2}\nabla_{LB}$ and the kinetic energy of the system is $T = -\frac{\hbar^2}{2m}\nabla_{LB}$. Hence, the operator-ordering problem is avoided by quantising \widehat{L}_a^2 instead of \hat{p} .

Doubts towards Podolsky's formulation began to arise when DeWitt's approach of quantifying the system through a generalised Feynman's time-sliced path integral yields a different expression of the Hamiltonian. The Hamiltonian obtained by DeWitt (1957) contains an additional term with a proportionality constant α and the Riemannian scalar curvature \bar{R} . The Hamiltonian operator is found to be

$$\hat{H} = -\frac{\hbar^2}{2}\nabla_{LB} + \alpha\hbar^2\bar{R} \quad (2.2)$$

where the proportionality constant α is given as $\alpha = \frac{1}{24}$. By changing and improving upon DeWitt's methods, other values of the constant α were reached, such as $\alpha = \frac{1}{12}$ (Cheng, 1972) and $\alpha = \frac{1}{8}$ (Dekker, 1980). Subsequent research by Kleinert (1990)

showed that the absence of the \bar{R} term is a necessary requirement, thus validating Podolsky's original findings.

Even though the expression of the Hamiltonian and the kinetic energy of the system is agreed upon, the literature does not agree with each other on the correct method and general procedure for the quantization of motion on a curved manifold through canonical quantisation with the intrinsic geometry approach (Diță, 1997; Hagen Kleinert & Shabanov, 1997).

2.3 Confining Potential Approach

Another approach found in the literature is the confining potential approach initiated by Jensen and Koppe (1971) and developed fully by Da Costa (1981). In this approach, a $(N - 1)$ -dimensional curved surface is formed by limiting an N -dimensional system on a flat space \mathbb{R}^N , where $N \geq 2$. For this to be done, a limiting case of a curved shell of equal thickness z_0 is considered, and the limit of $z_0 \rightarrow 0$ is taken. The effective Schrödinger equation is then formulated.

This approach leads to the geometric potential $V_g = \frac{\hbar^2}{2m}(M^2 - K)$ that is dependent on the mean curvature M of the curved surface and the Gaussian curvature K . Experimentally, the geometric potential is featured prominently in recent studies (Kartashov et al., 2011; Onoe et al., 2012; Szameit et al., 2010).

As for the Cartesian quantum momentum operator $\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ and the geometric kinetic energy T for an embedded surface in \mathbb{R}^3 , Liu *et al.* (2007) proved that $\hat{\mathbf{p}}$ and T have the general forms of

$$\hat{\mathbf{p}} = -i\hbar(\mathbf{r}^\mu \partial_\mu + M\mathbf{n}) \quad (2.3)$$

$$T = -\frac{\hbar^2}{2m}\nabla^2 + V_g, \quad V_g = -\frac{\hbar^2}{2m}(M^2 - K) \quad (2.4)$$

where V_g is the geometric potential, $\mathbf{r} = [x(x^\mu, x^\nu), y(x^\mu, x^\nu), z(x^\mu, x^\nu)]$ is the position vector on the surface and $\mathbf{r}^\mu = g^{\mu\nu}\mathbf{r}_\nu$. At any point on \mathbf{r} , $\mathbf{n} = (n_x, n_y, n_z)$ denotes the normal and $M\mathbf{n}$ is the mean curvature vector field. It is important to note that Einstein summation notation is used in Equation (2.3). This quantum momentum operator $\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ is referred to as the geometric momentum.

2.4 Enlarged Canonical Quantisation Scheme

In the existing literature, there are five forms of geometric momenta for a particle confined on a spherical surface, where each is characterised by two real parameters, α and β (Falck & Hirshfeld, 1983; Hong et al., 2000; Ikegami et al., 1992; Ishikawa et al., 1996; Schnitzer, 1985). In general, the components of these geometric momenta are denoted as $p_{(\alpha,\beta)x}, p_{(\alpha,\beta)y}, p_{(\alpha,\beta)z}$. These different forms of the geometric momenta arose due to different formalisms and geometric points used. Out of all the five geometric momenta in literature, only one of them is acceptable as it fulfils the fundamental commutator relations and it is a self-adjoint operator (Liu et al., 2011).

By making use of the equation of motion,

$$\dot{f} = [f, H]_D \quad (2.5)$$

where f is either the position x_i or the momentum p_i , Liu *et al.* (2011) realised that a proper momentum description for a free particle on a two-dimensional sphere can be achieved by enforcing secondary fundamental commutation relations, which are determined through the quantisation of Equation (2.5).

Through these secondary fundamental commutator relations, Liu *et al.* (2011) showed that the canonical momenta p_φ is not a proper momentum for a free particle on a two-dimensional sphere as its commutator $[\widehat{p}_\varphi, \widehat{H}]$ violates Dirac's quantisation rule, such that $[\widehat{p}_\varphi, \widehat{H}] \neq i\hbar[p_\varphi, H]_D$.

This expansion of the canonical quantisation scheme to include $[\widehat{f}, \widehat{H}] = i\hbar[f, H]_D$, where f is either the position x_i or the momentum p_i , is referred to as the enlarged canonical quantisation scheme.

With this scheme, the concept of geometric momentum can be incorporated into Dirac's canonical quantisation scheme (Liu *et al.*, 2011). Hence, Dirac's method of quantisation for constrained systems can now be used for the quantisation of motion on curved manifolds.

2.5 Advances with the Enlarged Canonical Quantisation Scheme

The inclusion of the geometric momenta into Dirac's method of quantisation for constrained systems has begun a lot of research in this field. The quantisation of motion on confined systems with other geometries, such as the torus (Xun *et al.*, 2013) and the catenoid (Xun & Liu, 2013), have shown that quantum theory built up from only intrinsic geometry is inconsistent with Dirac's quantisation rule of $[\widehat{A}, \widehat{B}] = i\hbar[A, B]_D$, but a quantum theory built up by assuming the geometry is embedded as a submanifold is consistent.

Apart from the direct usage of the enlarged scheme, many recent studies indirectly support the usage of the enlarged scheme. A discriminant developed by Zhang *et al.* (2015) shows that quantisation through intrinsic geometry is improper for a free particle embedded on a two-dimensional sphere. Panahi and Jahangiri (2016) also showed that their representation for momentum operators of a

constrained particle on an ellipsoid has the same form as the geometric momenta given in Equation (2.3).



CHAPTER 3

THEORY AND METHODOLOGY

3.1 A Forage into Classical Mechanics

Classical mechanics aims to describe the motion of point particles, or objects that can be idealised as point particles, through dynamical equations of motion. One of the earliest treatments in classical mechanics involves solving second-order differential equations, such as the dynamical equations that arise from Newton's second law of motion. Newtonian mechanics takes a more localised manner in its approach by concerning itself with the physical quantities of particles in the next infinitesimal time interval. However, subsequent formalisms in classical mechanics, such as the Lagrangian formalism and the Hamiltonian formalism, take on a more global approach by considering the entire trajectory of the body (Shankar, 1994).

As these two formulations are fundamental to Dirac's canonical quantisation, this section aims to introduce the Lagrangian formalism and the Hamiltonian formalism of classical mechanics. These two formalisms will serve as a jumping point from classical mechanics to quantum mechanics.

3.1.1 The Lagrangian Formalism

Through calculus of variation, the equations of motion of a classical dynamical system can be formulated from the action integral

$$I = \int_{t_1}^{t_2} L(\dot{x}(t), x(t), t) dt \quad (3.1)$$

where the function L is known as the Lagrangian. To generalise the case, there is an explicit-time dependence in the Lagrangian to consider the possibility that the system is affected by an external time-dependent field.

Now, the action of the neighbouring path $x(t) + \delta x(t)$ is considered. However, the constraint $\delta x(t_1) = \delta x(t_2) = 0$ is applied on the neighbouring path. Physically, this means that all paths coincide and meet at the same points at the beginning and at the end of the trajectory. The action of this neighbouring path is given by

$$I + \delta I = \int_{t_1}^{t_2} L(\dot{x}(t) + \delta \dot{x}(t), x(t) + \delta x(t), t) dt \quad (3.2)$$

The path required is the path in which the variation vanishes to the first order. As an analogy, recall that for a function $f(x)$, the first-order change $\delta f^{(1)}$ in f vanishes if there is a slight change δx in value at the minimum x^0 .

Hence, the path required is given by

$$0 = \delta I = \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial \dot{x}(t)} \delta \dot{x}(t) + \frac{\partial L}{\partial x(t)} \delta x(t) \right] dt$$

By integrating the first term by parts,

$$\begin{aligned} \int_{t_1}^{t_2} \frac{\partial L}{\partial \dot{x}(t)} \delta \dot{x}(t) &= \frac{\partial L}{\partial \dot{x}(t)} \delta x(t) \Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \delta x(t) \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}(t)} \right) \right] dt \\ &= - \int_{t_1}^{t_2} \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}(t)} \right) \delta x(t) dt \end{aligned}$$

where the first term vanishes due to the constraint of $\delta x(t_1) = \delta x(t_2) = 0$.

Hence,

$$\begin{aligned} 0 = \delta I &= \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial \dot{x}(t)} \delta \dot{x}(t) + \frac{\partial L}{\partial x(t)} \delta x(t) \right] dt \\ &= \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial x(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}(t)} \right] \delta x(t) dt \end{aligned}$$

As δx is arbitrary, the equation $\delta I = 0$ can be fulfilled if and only if

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}(t)} \right) - \frac{\partial L}{\partial x(t)} = 0 \quad \text{for } t_1 \leq t \leq t_2 \quad (3.3)$$

where Equation (3.3) is the classical equation of motion, known as the Euler-Lagrange equation.

In the discussion above, the Lagrangian formulation is described and defined with only one degree of freedom. However, the formulation above can be generalised to finitely many degrees of freedom.

For N degrees of freedom, N equations of motions are given by the form

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}_i(t)} \right) - \frac{\partial L}{\partial x_i(t)} = 0 \quad 1 \leq i \leq N \quad (3.4)$$

One of the main appeals of the Lagrangian formalism is that Equation (3.4) is form-invariant under an arbitrary change in coordinates. This means that the Euler-Lagrange equation is not solely defined for n Cartesian coordinates (x_1, \dots, x_n) only, but for any set of canonical coordinates (q_1, \dots, q_n) . Hence, Equation (3.4) can be written as

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i(t)} \right) - \frac{\partial L}{\partial q_i(t)} = 0 \quad 1 \leq i \leq N \quad (3.5)$$

As an analogy to Newton's second law of motion, Equation (3.5) can be made to have the same form by defining

$$p_i(t) = \frac{\partial L}{\partial \dot{q}_i(t)} \quad (3.6)$$

as the canonical momentum conjugate to q_i while the quantity

$$F_i(t) = \frac{\partial L}{\partial q_i(t)} \quad (3.7)$$

is defined as the generalised force conjugate to q_i .

3.1.2 The Hamiltonian Formalism

The other formalism fundamental to Dirac's method of quantisation is the Hamiltonian formalism. To ease the discussion from here onwards, the Lagrangian L is assumed to have no explicit time-dependence.

In the preceding discussion, the canonical momentum is defined from the Euler-Lagrange equation as Equation (3.6). In principle, it is assumed that $\dot{q}(t)$ can be solved in terms of $q(t)$ and $p(t)$, such that $\dot{q} = \dot{q}(q, p)$. Essentially, the configuration space (q_i, \dot{q}_i) is assumed to be able to transition to the phase space (q_i, p_i) . However, as will be discussed in Section 3.2.2, a specific requirement needs to be met for this transition to occur.

The fundamental Hamiltonian function $H(p, q)$ is given through the Legendre transformation as

$$H(q, p) \equiv \sum_N q_N(q, p) p_N - L(\dot{q}(q, p), q) \quad (3.8)$$

Then,

$$\frac{\partial H}{\partial q_N} = \sum_M \frac{\partial q_M}{\partial q_N} p_M - \frac{\partial L}{\partial q_N} - \sum_M \frac{\partial L}{\partial \dot{q}_M} \frac{\partial \dot{q}_M}{\partial q_N}$$

Using the relation given in Equation (3.6), the first and third term cancels out. The remaining term is defined as

$$p_N = - \frac{\partial H}{\partial q_N} \quad (3.9)$$

The partial derivative of the Hamiltonian H with respect to p_N is then taken.

$$\frac{\partial H}{\partial p_N} = \dot{q}_N + \sum_M p_M \frac{\partial \dot{q}_M}{\partial p_N} - \sum_M \frac{\partial L}{\partial \dot{q}_M} \frac{\partial \dot{q}_M}{\partial p_N}$$

With the same relation, the second and third term cancels out, leaving the following relation

$$\dot{q}_N = \frac{\partial H}{\partial p_N} \quad (3.10)$$

Equations (3.9) and (3.10) are the general equations of motion given by the Hamiltonian formalism.

3.1.3 Poisson Brackets

An important operation in Hamiltonian formalism is the Poisson bracket. It is often useful to express the Hamiltonian equations of motion using Poisson brackets.

Given two functions $A(q_i, p_i)$ and $B(q_i, p_i)$ on a phase space, the Poisson bracket is defined as

$$\{A, B\} \equiv \sum_{i=1}^N \left[\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right] \quad (3.11)$$

The Poisson bracket has the following properties:

Anticommutativity

$$\{A, B\} = -\{B, A\}$$

Bi-linearity

$$\{fA + gB, C\} = f\{A, C\} + g\{B, C\} = \{C, fA + gB\} \quad f, g \in \mathbb{R}$$

Leibniz rule

$$\{AB, C\} = \{A, C\}B + A\{B, C\}$$

Jacobi identity

$$\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$$

where $C = C(q_i, p_i)$ is a function of q_i and p_i .

From the definition of Poisson brackets in Equation (3.11), it follows that the following relations must be obeyed for canonical coordinates (q_i, p_j)

$$\{q_i, q_j\} = 0 \quad (3.12)$$

$$\{p_i, p_j\} = 0 \quad (3.13)$$

$$\{q_i, p_j\} = \delta_{ij} \quad (3.14)$$

where δ_{ij} is the Kronecker delta.

For the canonical coordinates (q_i, p_j) and the Hamiltonian H , the following relations express the Hamiltonian equation of motion with Poisson brackets.

$$\{q_i, H\} = \frac{\partial H}{\partial p_i} = \dot{q}_i \quad (3.15)$$

$$\{p_j, H\} = \frac{\partial H}{\partial q_j} = \dot{p}_j \quad (3.16)$$

In general, for any dynamical variable $f(q, p)$

$$\dot{f}(q, p) = \sum \left[\frac{\partial f}{\partial p_j} \dot{p}_j + \frac{\partial f}{\partial q_j} \dot{q}_j \right] = \{f, H\} \quad (3.17)$$

Equations (3.15)-(3.17) show that dynamical equations of motion can be written with Poisson brackets.

3.2 Bridging the Classical-Quantum Gap

3.2.1 Correspondence between Poisson Brackets and Commutators

Bilinear brackets play a vital role in both classical mechanics and quantum mechanics. As mentioned in Section 3.1.2, Poisson brackets complement the Hamiltonian formalism and are used to describe the time-dependence of classical variables. In quantum mechanics, for any linear operators \hat{A} and \hat{B} in a Hilbert space, the commutator is defined as

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \quad (3.18)$$

Both types of brackets have similar algebraic properties. Similar to Poisson brackets, the commutator obeys linearity, anti-symmetry, Leibniz rule and the Jacobi identity.

Dirac recognised the formal correspondence between the Poisson bracket in classical mechanics and the commutator in quantum mechanics and devised a quantisation method to bridge the Hamiltonian formalism with quantum mechanics. This quantisation method is known as canonical quantisation, and it maps the Poisson brackets to commutators with the following rule

$$[\hat{A}, \hat{B}] = i\hbar\{A, B\} \quad (3.19)$$

where \hat{A} is a quantum operator and A is a classical variable.

Hence, with the canonical relations between the dynamical variables q and p given by Equation (3.12) to (3.14), the corresponding quantum operators \hat{q} and \hat{p} must obey the following canonical commutation relations

$$[\hat{q}_i, \hat{q}_j] = 0 \quad (3.20)$$

$$[\hat{p}_i, \hat{p}_j] = 0 \quad (3.21)$$

$$[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij} \quad (3.22)$$

where δ_{ij} is the Kronecker delta.

3.2.2 Constrained Systems

As stated in Section 3.1.2, it is assumed that the $\dot{q}(t)$ can be solved in terms of $q(t)$ and $p(t)$ through Equation (3.9), and that the Hamiltonian of the system is given by Equation (3.8). However, these relations can only be applicable if the transformation from a configuration space (q_i, \dot{q}_i) to a phase space (q_i, p_i) is invertible.

The invertibility of this transformation can be determined through the determinant of a Hessian matrix

$$\det \frac{\partial p_i}{\partial \dot{q}_j} = \det \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} = \det W_{ij} \quad (3.23)$$

where W_{ij} is a Hessian matrix.

The Lagrangian is said to be regular if the condition $\det W_{ij} \neq 0$ is fulfilled. If so, the transformation from a configuration space to a phase space is invertible. Hence, the Hamiltonian can be determined via Equation (3.8).

However, if $\det W_{ij} = 0$, the Lagrangian is said to be singular. This condition implies that not all conjugate momenta in the system are independent variables due to the existence of constraints between the dynamical variables. Hence, not all N independent velocities can be expressed in terms of these independent momenta. This breaks the requirement that the Hamiltonian $H(p, q, t)$ must be independent of velocity. With that, the aforementioned conversion from a Lagrangian to a Hamiltonian cannot be used. Since the previous definition of a Hamiltonian requires independence from velocities, this definition is no longer applicable for systems with

singular Lagrangians. The Poisson bracket will also not truly describe a system with constraints completely as the canonical Poisson brackets in Equations (3.12) to (3.14) might not be satisfied. Systems with these restrictions are known as constrained systems.

To quantise constrained systems, Dirac generalised the Hamiltonian formalism and Poisson brackets (Dirac, 1931). The following sections will explore Dirac's generalisation of the Hamiltonian formalism and Poisson brackets to quantise constrained systems.

3.2.3 The Canonical Hamiltonian and the Primary Hamiltonian

As mentioned in Section 3.2.2, the inability to invert the configuration space to phase space stems from the condition

$$\det \frac{\partial p_i}{\partial q_j} \neq 0$$

The relations that inhibit invertibility are known as primary constraints because they are directly obtained from the Lagrangian of the constrained system. These constraints are denoted by

$$\phi_m(q_i, p_j) \approx 0 \quad m = 1, 2, \dots, M \quad (3.24)$$

where M = total number of primary constraints.

The \approx symbol in Equation (3.24) denotes a weak equality. To transform the weak equality into a strong equality, the corresponding Poisson bracket must first be evaluated.

As usual, the Hamiltonian for a constrained system can be found through the Legendre transformation, as given by Equation (3.8). This Hamiltonian is known as the canonical Hamiltonian in Dirac's generalisation and it is denoted by H_{can} .

$$H_{can}(q, p) \equiv \sum_N \dot{q}_N(q, p) p_N - L(\dot{q}(q, p), q) \quad (3.25)$$

However, due to the existence of primary constraints ϕ_m , the canonical Hamiltonian is no longer unique as the primary constraints can be included into the canonical Hamiltonian to form the primary Hamiltonian H_p . The primary Hamiltonian is given by

$$H_p = H_{can} + \lambda_m \phi_m \quad (3.26)$$

where λ_m are the undetermined Lagrangian multipliers. It must be noted that Einstein summation notation is used. It follows that

$$H_p \approx H_{can} \quad (3.27)$$

as $\phi_m \approx 0$, as stated in Equation (3.24).

As a result of Equation (3.27), all relations for the Hamiltonian of an unconstrained system as discussed in Section 3.1.2 can be adapted to the primary Hamiltonian. The following Hamiltonian equations can be written with Poisson brackets as

$$\dot{q}_i \approx \{q_i, H_p\} = \frac{\partial H_p}{\partial p_i} = \frac{\partial(H_{can} + \lambda_m \phi_m)}{\partial p_i} \quad (3.28)$$

$$\dot{p}_i \approx \{p_i, H_p\} = \frac{\partial H_p}{\partial q_i} = \frac{\partial(H_{can} + \lambda_m \phi_m)}{\partial q_i} \quad (3.29)$$

In general, for any dynamical variable $f(q, p)$, the time evolution is given by

$$\dot{f}(q, p) \approx \{f, H_p\} = \{f, H_{can} + \lambda_m \phi_m\} \quad (3.30)$$

An important requirement imposed by Dirac's method is that the constraints must be invariant under time evolution. With that requirement, the time evolutions of the primary constraints are given as

$$\begin{aligned} \dot{\phi}_\alpha &\approx \{\phi_\alpha, H_{can} + \lambda_\beta \phi_\beta\} \\ &= \{\phi_\alpha, H_{can}\} + \lambda_\beta \{\phi_\alpha, \phi_\beta\} + \{\phi_\alpha, \lambda_\beta\} \phi_\beta \\ &\approx \{\phi_\alpha, H_{can}\} + \lambda_\beta \{\phi_\alpha, \phi_\beta\} \approx 0 \end{aligned} \quad (3.31)$$

where ϕ_α and ϕ_β are primary constraints, and the strong equality in Equation (3.24) is used to eliminate $\{\phi_\alpha, \lambda_\beta\}$.

The process of determining the time evolution of the primary constraint may either lead to more constraints, known as secondary constraints, or lead to the expressions for some of the Lagrange multipliers λ . The secondary constraints are denoted by

$$\phi_k \approx 0 \quad k = M + 1, M + 2, \dots, M + K \quad (3.32)$$

where M = total number of primary constraints and K = total number of secondary constraints.

This process continues with the newly determined secondary constraints until all the constraints have been determined to be independent of time evolution.

To facilitate further discussions, all constraints are collectively denoted by

$$\phi_j \approx 0 \quad j = 1, \dots, M + K \quad (3.33)$$

Dirac further classified the system's primary and secondary constraints into:

First-Class Constraints

First-class constraints are a set of constraints that have weakly vanishing Poisson brackets with all constraints in the system. First-class constraints are denoted by

$$\{\phi_{\bar{\alpha}}, \phi_{\bar{\beta}}\} \approx 0 \quad (3.34)$$

Second-Class Constraints

Second-class constraints are the set of constraints that has at least one non-vanishing Poisson bracket with the other constraints. Second-class constraints are denoted by

$$\{\phi_{\bar{\alpha}}, \phi_{\bar{\beta}}\} \neq 0 \quad (3.35)$$

As all constraints on a curved manifold are second-class constraints, the former will not be relevant to our discussion.

With all the constraints determined, the next step is to incorporate both primary and secondary constraints into the newly determined Hamiltonian theory. However, the incorporation of these constraints is not clear-cut as there is a possibility that the Poisson brackets are not compatible with the constraints. In general, even though a constraint is weakly equal to zero, the Poisson bracket of the constraint with any dynamical variable f may not vanish.

$$\phi_A \approx 0 \Rightarrow \{f, \phi_A\} \neq 0 \quad (3.36)$$

To address this incompatibility, the Poisson bracket is generalised by Dirac.

3.2.4 Dirac Brackets

Firstly, a matrix consisting of the Poisson brackets of all constraints can be constructed as

$$C_{AB}(q, p) \equiv \{\phi_A(q, p), \phi_B(q, p)\} \quad (3.37)$$

Each element in the matrix can be simplified by transforming the weak equality into a strong one after the Poisson brackets have been evaluated.

Dirac has shown that if the matrix consists of second-class constraints in the Poisson brackets, the matrix C_{AB} must be non-singular, such that its inverse $(C_{AB})^{-1}$ exists and

$$\det C \neq 0 \quad (3.38)$$

With the existence of the inverse matrix C^{-1} , it is important to note that

$$C_{AD}(C^{-1})_{DB} = (C^{-1})_{BD}C_{DA} = \delta_{AB} \quad (3.39)$$

The generalised Poisson bracket between any two dynamical variables f and g can be defined with the inverse matrix C^{-1} as

$$[f(q, p), g(q, p)]_D = \{f(q, p), g(q, p)\} - \{f(q, p), \phi_A\}C_{AB}^{-1}\{\phi_B, g(q, p)\} \quad (3.40)$$

where $[,]_D$ is the Dirac bracket and the Einstein summation convention is used above.

To digress slightly, the Dirac bracket in Equation (3.40) satisfies the necessary conditions on Poisson brackets and commutators. Given two functions $A(q_i, p_i)$ and $B(q_i, p_i)$, Dirac brackets follow anticommutativity, linearity, Leibniz rule and the Jacobi identity.

Anticommutativity

$$[A, B]_D = -[B, A]_D$$

Bi-linearity

$$[fA + gB, C]_D = f[A, C]_D + g[B, C]_D = [C, fA + gB]_D \quad f, g \in \mathbb{R}$$

Leibniz rule

$$[AB, C]_D = [A, C]_D B + A[B, C]_D$$

Jacobi identity

$$[A, [B, C]_D]_D + [B, [C, A]_D]_D + [C, [A, B]_D]_D = 0$$

Recall from Section 3.2.3 that the main motivating factor to generalise Poisson brackets into Dirac brackets is the incompatibility between the constraints and the Poisson bracket. The Dirac bracket is compatible with the constraints, where

$$\begin{aligned} [F, \phi_A]_D &= \{F, \phi_A\} - \{F, \phi_B\}(C^{-1})_{BD}\{\phi_D, \phi_A\} \\ &= \{F, \phi_A\} - \{F, \phi_B\}(C^{-1})_{BD}C_{DA} \\ &= \{F, \phi_A\} - \{F, \phi_B\}\delta_{BA} \\ &= \{F, \phi_A\} - \{F, \phi_A\} = 0 \end{aligned} \tag{3.41}$$

such that the Dirac bracket of the constraint with any dynamical variable vanishes.

With the Dirac bracket, in a theory with only second-class constraints, the canonical quantisation scheme for constrained Hamiltonian systems is given by

$$[\hat{A}, \hat{B}] = i\hbar[A, B]_D \tag{3.42}$$

where \hat{A} is a quantum operator and A is a classical variable.

With Equation (3.42) and Dirac brackets, the canonical commutation relations are supplanted by the following commutation relations (Weinberg, 2015).

$$[q_i, p_j] = i\hbar \left[\delta_{ij} - \frac{\partial \phi_A}{\partial p_i} (C_{AB}^{-1}) \frac{\partial \phi_B}{\partial q_j} \right] \quad (3.43)$$

$$[q_i, q_j] = i\hbar \frac{\partial \phi_A}{\partial p_i} (C_{AB}^{-1}) \frac{\partial \phi_B}{\partial p_j} \quad (3.44)$$

$$[p_i, p_j] = i\hbar \frac{\partial \phi_A}{\partial q_i} (C_{AB}^{-1}) \frac{\partial \phi_B}{\partial q_j} \quad (3.45)$$

Hence, for a system with only second-class constraints, the commutation relations in Equations (3.43) to (3.45) must be satisfied. Dirac's canonical quantisation scheme for constrained systems with second-class constraints given in Equation (3.42) yields the same equation of motion as the classical Lagrangian method (Das, 2021; Weinberg, 2015).

3.3 A Problem Arises – Quantisation on Curved Surfaces

The previous discussions on classical mechanics and canonical quantisation aim to serve as an introduction to the main problem explored in this thesis, namely the quantum motion on curved manifolds. The curved manifold explored in this thesis is the helicoid.

Dirac stated that the canonical quantisation scheme is only valid in a Cartesian coordinate system (Dirac, 1930, 1931). The problem arises when the scheme is used on a system constrained to a curved manifold as a global Cartesian coordinate system does not exist in such a system. However, local coordinates can be used approximately.

Even after solving the lack of a global Cartesian coordinate system on a curved manifold, another point of discussion arises. While conventional quantum

mechanics is established within the framework of intrinsic geometry, recent studies have shown that canonical quantisation cannot be done solely through the framework of intrinsic geometry (Liu et al., 2011; Xun et al., 2013). Instead, the quantisation of motion on various curved manifolds supports the usage of the Cartesian coordinate system, as stated by Dirac, by embedding the surface into a submanifold. However, Dirac's original proposal for canonical quantisation did not include this possibility of embedding the surface into a submanifold, hence the quantisation of a curved manifold was ruled out by Dirac (Dirac, 1931).

To further explore this problem, this section aims to introduce the enlarged canonical quantisation (ECQ) scheme.

3.3.1 Mathematical Preliminaries

In this section, elementary differential geometry will be discussed.

For a two-dimensional curved surface Σ^2 embedded in a three-dimensional Cartesian space \mathbb{R}^3 , the surface Σ^2 is parameterised by

$$q^\mu \equiv (u, v) \quad \mu = 1, 2 \quad (3.46)$$

where the range of u and v are dependent on the curved surface. In the case of a helicoid, the range is given by $u, v \in (-\infty, +\infty)$.

In the three-dimensional Cartesian space \mathbb{R}^3 , the position \mathbf{r} is given by

$$\mathbf{r} \equiv (x(u, v), y(u, v), z(u, v)) \quad (3.47)$$

while the normal vector \mathbf{n} is given by

$$\mathbf{n} = (n_x, n_y, n_z) \equiv \frac{\mathbf{r}_u \times \mathbf{r}_v}{|\mathbf{r}_u \times \mathbf{r}_v|} \quad (3.48)$$

where $\mathbf{r}_\mu \equiv \frac{\partial \mathbf{r}}{\partial x^\mu}$.

The contravariant and covariant components of \mathbf{r} are related with one another through

$$\mathbf{r}^\mu = g^{\mu\nu} \mathbf{r}_\nu = g^{\mu\nu} \frac{\partial \mathbf{r}}{\partial x^\nu} \quad (3.49)$$

where the coefficients $g^{\mu\nu}$ are elements of the inverse matrix $g_{\mu\nu}$

$$g_{\mu\nu} = \mathbf{e}_\mu \cdot \mathbf{e}_\nu \quad (3.50)$$

where $g_{\mu\nu}$ is the metric of the coordinate system.

At each point in \mathbf{r} , the extrinsic curvature and the intrinsic curvature can be characterised by the mean curvature vector $M\mathbf{n}$ and the Gaussian curvature K respectively. The mean curvature vector $M\mathbf{n}$ locally describes the curvature of an embedded surface whereas the Gaussian curvature K describes curvature based on the distances measured on the surface. In other words, the mean curvature is an extrinsic measure of curvature whereas the Gaussian curvature is an intrinsic measure of curvature.

3.3.2 Methods of Quantisation

There are two unique formalisms for quantisation on a curved surface, namely the Schrödinger formalism and the Dirac formalism.

Schrödinger Formalism

The Schrödinger formalism makes use of the confining potential approach pioneered by Jensen and Koppe (1971) and developed fully by Da Costa (1981). This approach introduces a confining potential that limits the motion of a particle to the surface

being considered by exerting an infinite force as the particle tends to leave the system. In this formalism, the Schrödinger equation is first formulated in \mathbb{R}^3 in a curved shell of an equal and finite thickness δ . A squeezing limit of $\delta \rightarrow 0$ is then applied to the curved shell to confine the particle in Σ^2 to obtain an expression of the effective Schrödinger equation. This formalism leads to a unique geometric potential V_g , which is given by

$$V_g = -\frac{\hbar^2}{2m}(M^2 - K) \quad (3.51)$$

where M is the mean curvature and K is the Gaussian curvature.

Liu *et al.* (2007) determined that the Cartesian quantum momentum operator $\hat{\mathbf{p}}$ for an embedded surface in \mathbb{R}^3 has the general form of

$$\hat{\mathbf{p}} = -i\hbar(\mathbf{r}^\mu \partial_\mu + M\mathbf{n}) \quad (3.52)$$

where $\mathbf{r}^\mu \partial_\mu$ is the gradient operator on a two-dimensional surface.

The geometric kinetic energy T is also determined to contain the geometric potential V_g (Liu et al., 2007) and it is given by

$$T = -\frac{\hbar^2}{2m}\nabla^2 + V_g \quad (3.53)$$

where $\nabla^2 = \sum \frac{\partial^2}{\partial x_i^2}$ is the Laplacian operator.

Dirac Formalism

Another formalism used for the quantisation of motion on curved manifolds is Dirac's general procedure on treating constrained systems. This procedure relies on

Dirac brackets. This formalism leads to a curvature driven potential V_D (Homma et al., 1990; Ikegami et al., 1992), which is given by

$$V_D = -\frac{\hbar^2}{2m}(\alpha M^2 - \beta K) \quad (3.54)$$

where α and β are real parameters.

Even though Equations (3.51) and (3.54) look similar, the ambiguity of Equation (3.54) due to α and β is undesirable. This ambiguity leads to various formulations of the geometric potential, among which are $p_\mu = -i\hbar\left(\partial_\mu + \frac{r_\mu}{2}\right)$ (Shimizu et al., 1992) and even the geometric momentum $\hat{\mathbf{p}}$ mentioned in Equation (3.51).

Since the geometric momentum and geometric potential are determined to have the forms given in Equations (3.52) and (3.53), it is argued that the values of α and β in the Equation (3.54) from Dirac formalism must be made compatible with Schrödinger formalism (Liu et al., 2011). To close the gap between both formalism, a generalised canonical quantisation procedure, known as the enlarged canonical quantisation (ECQ) scheme, is proposed (Liu et al., 2011).

3.3.3 Enlarged Canonical Quantisation (ECQ) Scheme

All quantum systems must obey the fundamental canonical commutation relations set out in Equations (3.20) to (3.22). As these relations are obtained via Dirac's mapping of Poisson brackets to commutators, there is a possibility of generalising this mapping further by introducing $[\hat{A}, \hat{B}]/(i\hbar) = [A, B]_D$ for any pairs of two quantities A and B in a system constrained to a curved manifold. This proposal includes the possibility that $[A, B]_D$ will be reduced to a Poisson bracket for a constraint-free system. However, Xun and Liu (2013) noted that this is a dangerous proposal as

some commutators obtained might be superfluous or incompatible with existing theories.

As a result, a generalised version of Dirac's canonical quantisation procedure must be developed for systems with second-class constraints on a curved manifold. The generalisation explored in this thesis is the enlarged canonical quantisation (ECQ) scheme by Liu *et. al* (2011). This scheme proposes that if quantisation is to be done on a system with second-class constraints, then the set of operators $\{\hat{x}, \hat{p}, \hat{H}\}$ needs to be quantised simultaneously.

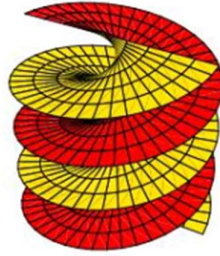
The enlarged canonical quantisation scheme requires a new commutation relation $[\hat{f}, \hat{H}]$, where \hat{H} is the Hamiltonian operator and $\hat{f} = \hat{x}_\mu$ and \hat{p}_μ in the case of local coordinates, or $\hat{f} = \hat{x}_i$ and \hat{p}_i for Cartesian coordinates. This additional commutation relation must obey

$$[\hat{f}, \hat{H}] = i\hbar[f, H]_D \quad (3.55)$$

As Equation (3.55) does not apply to systems with no second-class constraints, it is aptly termed the secondary fundamental commutation relations, whereas the relations in Equations (3.20) to (3.22) are termed the primary fundamental commutation relations.

3.4 Geometric Considerations

This thesis aims to examine the quantum motion on the helicoid within canonical quantisation through the intrinsic geometry approach and the submanifold approach. The helicoid is a minimal surface with a helix as its boundary, as shown in Figure 1 (Weisstein, n.d.). It can be described as a surface made up of lines that rotated around its axis with a constant angular rate while being displaced at a constant rate (*Helicoid*,



n.d.). Visually, the helicoid has the shape of a screw thread and has been likened to Archimedes screw.

Figure 1: A helicoid (Weisstein, n.d.)

The helicoid can be expressed in parametric form by

$$x = u \cos v \quad (3.56)$$

$$y = u \sin v \quad (3.57)$$

$$z = rv \quad (3.58)$$

where $u \in (-\infty, +\infty)$, $v \in (-\infty, +\infty)$ and $r \in (-\infty, +\infty)$

The helicoid can also be described by its surface equation in Cartesian coordinates by

$$f(x) \equiv z - a \arctan\left(\frac{y}{x}\right) = 0 \quad (3.59)$$

The constraint equation on the surface of the helicoid is given by

$$g(x) \equiv r - a = 0 \quad (3.60)$$

where $a \neq 0$ determines the slant.

Since the helicoid is a minimum surface, the mean curvature M of a helicoid is zero. The Gaussian curvature K is given by $K = -\frac{a^2}{(a^2+u^2)^2}$.

Helicoids play an ever-increasing role in many multidisciplinary fields. In the field of material science, new types of topological semimetals with surface states of double- and quad-helicoid surfaces are predicted to exist (Fang et al., 2016). Through studying the quantum dynamics of an electron confined to a helicoid, Atanasov *et al.* (2009) were able to draw parallels between the helicoidal surface and the Hall effect. In the field of biophysics, helicoids can be used to model β -sheet proteins so that energy storage and catalysis, nanomedicine and drug delivery can be studied more efficiently (Gupta & Saxena, 2012).

3.5 Methodology

In this thesis, the intrinsic geometry approach and the submanifold approach in canonical quantisation are differentiated through their mathematical description of the helicoid. In the intrinsic geometry approach, the helicoid is described mathematically using local coordinates (u, v) through the parametric equations given in Equations (3.56) to (3.58). However, the submanifold approach relies on the surface equation given in the Cartesian coordinate system in Equation (3.59), given in Cartesian coordinates.

This thesis aims to verify which of the approaches above can successfully quantise the motion of a particle constrained on a helicoid. This is done by comparing the momentum operators of each approach with the general form of the geometric momentum given in Equation (3.52). The compatibility between the secondary fundamental commutation relations obtained and Dirac's canonical quantisation is also determined.

For each approach, a classical mechanical treatment and a quantum mechanical treatment are done. In the classical mechanical treatment, the Lagrangian is determined through its respective mathematical description of the system. The

canonical momenta p_i in Equation (3.6) and the primary constraint of the system are determined. With the Legendre transformation and the canonical momenta, the primary Hamiltonian in Equation (3.26) can be found. The secondary constraints are then determined, leading to the formulation of primary fundamental Dirac brackets in Equation (3.43) to (3.45), and the secondary Dirac brackets given in Equation (3.55).

After the classical mechanical treatment, a quantum mechanical treatment must be done with a quantum Hamiltonian. The Dirac brackets obtained in the classical mechanical treatment are mapped to commutators using Dirac's treatment of $[\hat{A}, \hat{B}] = i\hbar[A, B]_D$. However, for commutators $[\hat{p}_i, \hat{H}]$, the forms of \hat{p}_i must be determined directly using the found commutators. This is done so that the validity of the momentum operators can be determined with respect to the general form of the geometric momentum given in Equation (2.3). The commutators $[\hat{p}_i, \hat{H}]$ can then be directly evaluated with the quantum Hamiltonian H . The results will be evaluated to determine if it is consistent with Dirac's canonical quantisation and compatible with the geometric potential found through the Schrödinger formalism, which is given in Equation (3.53).

To ease the calculation of Poisson brackets, Dirac brackets and the Dirac matrix, Wolfram Mathematica (Version 12.1) was used throughout this thesis. The scripts used in this thesis are made available in Appendix A.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Dirac's Canonical Quantisation for a Helicoid within Intrinsic Geometry

As mentioned in Section 3.5, the intrinsic geometry approach in Dirac's canonical quantisation for systems with second-class constraints makes use of the local coordinates (u, v) of the helicoid. The helicoid is mathematically defined to be

$$\mathbf{r} = (u \cos v, u \sin v, rv) \quad (4.1)$$

where $u \in (-\infty, +\infty)$, $v \in (-\infty, +\infty)$ and $r \in (-\infty, +\infty)$ are dynamic variables.

In this section, the classical mechanical motion on the helicoid is obtained through Dirac's theory for constrained systems. After that, the quantum mechanics of such a motion is derived.

4.1.1 Classical Mechanical Treatment

The Lagrangian L in the local coordinate system must first be determined.

The time derivatives of each component of \mathbf{r} and their squares can be easily determined.

$$x = u \cos v \quad \Rightarrow \dot{x}^2 = \dot{u}^2 \cos^2 v + u^2 \dot{v}^2 \sin^2 v - 2u\dot{u}\dot{v} \sin v \cos v \quad (4.2)$$

$$y = u \sin v \quad \Rightarrow \dot{y}^2 = u^2 \dot{v}^2 \cos^2 v + 2u\dot{u}\dot{v} \sin v \cos v + \dot{u}^2 \sin^2 v \quad (4.3)$$

$$z = rv \quad \Rightarrow \dot{z}^2 = r^2 \dot{v}^2 + v^2 \dot{r}^2 + 2r\dot{r}\dot{v} \quad (4.4)$$

With Equation (4.2) to (4.4), the kinetic energy of a point particle of mass m on a helicoid is given by

$$K = \frac{1}{2} m (\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$$

$$= \frac{1}{2}m[\dot{v}^2(u^2 + r^2) + 2r\dot{r}v\dot{v} + \dot{r}^2v^2 + \dot{u}^2] \quad (4.5)$$

With the assumption that the potential energy U is zero, and by introducing a Lagrange multiplier λ that is enforcing the equation of constraint $g(x) = (r - a)$, the Lagrangian L of the system is then found to be

$$\begin{aligned} L &= K + U - \lambda g(x) \\ &= \frac{1}{2}m[\dot{v}^2(u^2 + r^2) + 2r\dot{r}v\dot{v} + \dot{r}^2v^2 + \dot{u}^2] - \lambda(r - a) \end{aligned} \quad (4.6)$$

where a determines the pitch of the helicoid and λ is treated as a dynamical variable.

Due to the absence of $\dot{\lambda}$ in Equation (4.6), the determinant of the Hessian matrix W is $\det W = \det \frac{\partial p_i}{\partial \dot{q}_j} = 0$. The condition for invertibility outlined in Equation (3.23) cannot be satisfied, so the Lagrangian is singular. Hence, Dirac's canonical quantisation scheme for a constrained system must be used.

The canonical momenta conjugate to the dynamic variables r, u, v and λ are found through Equation (3.6) to be

$$p_r = \frac{\partial L}{\partial \dot{r}} = mv(r\dot{v} + \dot{r}v) \quad (4.7)$$

$$p_u = \frac{\partial L}{\partial \dot{u}} = m\dot{u} \quad (4.8)$$

$$p_v = \frac{\partial L}{\partial \dot{v}} = m(r^2\dot{v} + u^2\dot{v} + r\dot{r}v) \quad (4.9)$$

$$p_\lambda = 0 \quad (4.10)$$

From Equation (3.24), p_λ is the primary constraint. The primary constraint is denoted as

$$\varphi_1 \equiv p_\lambda \approx 0 \quad (4.11)$$

where \approx signifies a weak equality.

The exact expression for \dot{r} , \dot{u} and \dot{v} are determined by solving the system of equations in Equations (4.7) to (4.9). The time derivatives of the dynamical coordinates u , v and r are found to be

$$\dot{u} = \frac{p_u}{m} \quad (4.12)$$

$$\dot{v} = \frac{vp_v - p_r r}{mu^2 v} \quad (4.13)$$

$$\dot{r} = \frac{1}{mu^2 v^2} [(u^2 + r^2)p_r - vrp_v] \quad (4.14)$$

The canonical Hamiltonian H_{can} can be found using the Legendre transform given in Equation (3.8). However, since the Lagrangian in Equation (4.6) is not independent of the velocities of the dynamical coordinates, the Lagrangian must first be expressed in terms of the canonical momenta to remove its velocity dependence. This can be done by substituting Equations (4.12) to (4.14) into the Lagrangian. The Lagrangian independent of velocity is determined to be

$$L = \frac{(r^2 + u^2)p_r^2 - 2rvp_r p_v + v^2(p_v^2 + u^2 p_u^2)}{mu^2 v^2} - \lambda(r - a) \quad (4.15)$$

Hence, the canonical Hamiltonian H_{can} is

$$\begin{aligned} H_{can} &= p_n \dot{q}_n - L \\ &= p_r \dot{r} + p_u \dot{u} + p_v \dot{v} + p_\lambda \dot{\lambda} - L \\ &= \frac{1}{2} [(r^2 + u^2)p_r^2 - 2rvp_r p_v + v^2(p_v^2 + u^2 p_u^2)] + \lambda(r - a) + \dot{\lambda} p_\lambda \end{aligned} \quad (4.16)$$

By including the primary constraint φ_1 and an arbitrary function of time η , the primary Hamiltonian H_p is given as

$$H_p = \frac{(r^2 + u^2)p_r^2 - 2rvp_r p_v + v^2(u^2 p_u^2 + p_v^2)}{2mu^2 v^2} + \lambda(r - a) + \eta p_\lambda \quad (4.17)$$

where the $\dot{\lambda}$ in Equation (4.16) has been absorbed by the arbitrary function η .

With that, the secondary constraints can then be determined by taking the Poisson brackets between the previous constraints and the primary Hamiltonian H_p .

Hence, the second constraint is

$$\varphi_2 \equiv \dot{\varphi}_1 = \{\varphi_1, H_p\} = \{p_\lambda, H_p\} = \frac{\partial p_\lambda}{\partial \lambda} \frac{\partial H_p}{\partial p_\lambda} - \frac{\partial p_\lambda}{\partial p_\lambda} \frac{\partial H_p}{\partial \lambda} = a - r \approx 0 \quad (4.18)$$

The third constraint is

$$\varphi_3 \equiv \dot{\varphi}_2 = \{\varphi_2, H_p\} = \{a - r, H_p\} = \frac{rvp_v - p_r(r^2 + u^2)}{mu^2 v^2} \approx 0 \quad (4.19)$$

The fourth constraint is

$$\varphi_4 \equiv \dot{\varphi}_3 = \{\varphi_3, H_p\} = f \approx 0 \quad (4.20)$$

where

$$f \equiv \frac{(r^2 + u^2)\lambda}{mu^2 v^2} + \frac{2(p_v v - p_r r)(p_r(r^2 + u^2) - p_u r u v^2 - p_v r v)}{m^2 u^4 v^4}$$

After the Poisson brackets were evaluated, the weak equalities become strong equalities. From the constraints given above, the following expressions can be obtained by transforming the weak equalities into strong equalities.

$$\varphi_1 = p_\lambda = 0 \quad (4.21)$$

$$\varphi_2 = a - r = 0 \Rightarrow r = a \quad (4.22)$$

$$\varphi_3 = 0 \Rightarrow p_r = \frac{p_v r v}{r^2 + u^2} \quad (4.24)$$

$$\varphi_4 = 0 \Rightarrow \lambda = \frac{2(p_v v - p_r r)[p_r(r^2 + u^2) - p_u r u v^2 - p_v r v]}{m u^2 v^2 (r^2 + u^2)} \quad (4.25)$$

With the expression of p_r in Equation (4.24), the Lagrange multiplier λ in Equation (4.25) is simplified to

$$\lambda = \frac{2 r u v}{m (r^2 + u^2)^2} p_u p_v \quad (4.26)$$

With the strong equalities evaluated, Equations (4.21) to (4.25) can be used on the primary Hamiltonian to obtain a simplified version of the canonical Hamiltonian, denoted as H .

$$H = \frac{1}{2m} [p_v^2 + (a^2 + u^2)p_u^2] \quad (4.27)$$

A matrix consisting of Poisson brackets C and its inverse C^{-1} can be determined with Equation (3.37).

The matrix C is determined through Mathematica to be

$$C = \begin{bmatrix} 0 & 0 & 0 & C_{14} \\ 0 & 0 & -C_{14} & C_{24} \\ 0 & C_{14} & 0 & C_{34} \\ -C_{14} & -C_{24} & -C_{34} & 0 \end{bmatrix} \quad (4.28)$$

where

$$C_{14} = -\frac{a^2 + u^2}{m u^2 v^2} \quad (4.29)$$

$$C_{24} = \frac{4a^2 p_v v - 2v[a^2 p_u u v + p_v(2a^2 + u^2)]}{m^2 u^4 v^4} \quad (4.30)$$

$$C_{34} = \frac{f(u, v)}{m^3 u^6 v^6} \quad (4.31)$$

with

$$f(u, v) = \frac{a^2 v^2 p_v^2 [(a^2 + u^2)^2 + 2a^4 v^2]}{(a^2 + u^2)^2} - \frac{2a^2 v^2 p_v^2 (a^2 (2v^2 + 1) + u^2)}{a^2 + u^2} + v^2 \left[\frac{4a^2 u^3 v p_u p_v}{a^2 + u^2} + a^2 (2v^2 + 1) p_v^2 - u^3 v p_u p_v \right].$$

By making use of the constraints obtained in Equations (4.21) to (4.25), the elements C_{24} and C_{34} can be simplified to

$$C_{24} = -\frac{2(a^2 v p_u + u p_v)}{m^2 u^3 v^3} \quad (4.32)$$

$$C_{34} = -\frac{2p_v [2a^2 u (u p_u + v p_v) + 3a^4 p_u - u^4 p_u]}{m^3 u^3 v^3 (a^2 + u^2)^2} \quad (4.33)$$

The inverse of the Dirac matrix C^{-1} is determined via Mathematica to be

$$C^{-1} = \begin{bmatrix} 0 & C_{12}^{-1} & C_{13}^{-1} & C_{14}^{-1} \\ -C_{12}^{-1} & 0 & C_{23}^{-1} & 0 \\ -C_{13}^{-1} & -C_{22}^{-1} & 0 & 0 \\ -C_{14}^{-1} & 0 & 0 & 0 \end{bmatrix} \quad (4.34)$$

where

$$C_{12}^{-1} = \frac{2uv p_v [2a^2 u (u p_u + v p_v) + 3a^4 p_u - u^4 p_u]}{m(a^2 + u^2)^4} \quad (4.35)$$

$$C_{13}^{-1} = \frac{2uv(a^2 v p_u + u p_v)}{(a^2 + u^2)^2} \quad (4.36)$$

$$C_{14}^{-1} = -C_{23}^{-1} = \frac{m u^2 v^2}{a^2 + u^2} \quad (4.37)$$

With the inverse matrix C^{-1} obtained, Dirac brackets can be evaluated. Dirac brackets are defined in Equation (3.40) as

$$[f(q, p), g(q, p)]_D = \{f(q, p), g(q, p)\} - \{f(q, p), \phi_A\} C_{AB}^{-1} \{\phi_B, g(q, p)\}$$

Hence, the Dirac brackets of the generalised positions $q_\mu (= u, v)$ and momenta p_ν are

$$[q_\mu, q_\nu]_D = 0 \quad (4.38)$$

$$[p_\mu, p_\nu]_D = 0 \quad (4.39)$$

$$[q_\mu, p_\nu]_D = \delta_{\mu\nu} \quad (4.40)$$

The equations of motion for position u, v and momenta p_u, p_v are

$$\dot{u} \equiv [u, H]_D = \frac{p_u}{m} \quad (4.41)$$

$$\dot{v} \equiv [v, H]_D = \frac{p_v}{m(a^2 + u^2)} \quad (4.42)$$

$$\dot{p}_u \equiv [p_u, H]_D = \frac{up_v^2}{m(a^2 + u^2)^2} \quad (4.43)$$

$$\dot{p}_v \equiv [p_v, H]_D = 0 \quad (4.44)$$

With the equations of motion determined, the classical treatment for Dirac's canonical quantisation for a helicoid within intrinsic geometry is completed. However, it is interesting to note that Equations (4.41) to (4.44) can also be obtained directly using Lagrangian and Hamiltonian formalism.

It can be seen that Equations (4.41) and (4.42) have been found directly through the Lagrangian in Equations (4.12) and (4.13).

\dot{p}_u and \dot{p}_v can be obtained directly through Hamiltonian formalism by using Equation (3.9) with the simplified canonical Hamiltonian H .

$$\dot{p}_u = -\frac{\partial H}{\partial u} = \frac{up_v^2}{(a^2 + u^2)^2} \quad (4.45)$$

$$\dot{p}_v = \frac{\partial H}{\partial v} = 0 \quad (4.46)$$

Since the equations of motions $\dot{u}, \dot{v}, \dot{p}_u$ and \dot{p}_v can be obtained via Lagrangian and Hamiltonian formalism, Dirac's theory of the classical motion on a helicoid is complete and coherent.

4.1.2 Quantum Mechanical Treatment

From this point onwards, the hat notation on operators will be removed as no confusion will arise.

In quantum mechanics, the general form of the Hamiltonian H of the helicoidal system (Bracken, 2021; Xun & Liu, 2013) is given as

$$\begin{aligned} H &= -\frac{\hbar^2}{2m} [\nabla^2 + (\alpha M^2 - \beta K)] \\ &= -\frac{\hbar^2}{2m} \left(\frac{1}{a^2 + u^2} \frac{\partial^2}{\partial v^2} + \frac{u}{(a^2 + u^2)} \frac{\partial}{\partial u} + \frac{\partial^2}{\partial u^2} + \beta \frac{a^2}{(a^2 + u^2)^2} \right) \end{aligned} \quad (4.47)$$

where α and β are real parameters, $M = 0$ and $K = -\frac{a^2}{(a^2 + u^2)^2}$.

Dirac's method of quantisation for constrained systems states that the commutator $[A, B]$ is related to its corresponding Dirac brackets $[A, B]_D$ through the relation $[A, B] = i\hbar[A, B]_D$. Hence, the following commutators can be found from Equations (4.38) to (4.40) and Equations (4.41) to (4.44).

$$[q_\mu, q_\nu] = 0, \quad [p_\mu, p_\nu] = 0 \quad [q_\mu, p_\nu] = i\hbar\delta_{\mu\nu} \quad (4.48)$$

and

$$[u, H] = \frac{i\hbar}{m} p_u \quad (4.49)$$

$$[v, H] = i\hbar \frac{p_v}{m(a^2 + u^2)} \quad (4.50)$$

As for the commutators $[p_u, H]$ and $[p_v, H]$, care must be taken to ensure that momentum obtained through the intrinsic geometry method is compatible with canonical quantisation. Hence, the momentum operators p_u and p_v must first be determined.

By introducing a dummy function $f(u, v)$, the commutators of $[u, H]$ in Equation (4.48) and $[v, H]$ in Equation (4.49) can be evaluated to obtain p_u and p_v .

To obtain the operator p_u , the commutator $[u, H]$ is used.

$$[u, H]f = (uH - Hu)f$$

where

$$uHf = -\frac{\hbar^2}{2m} \left[\frac{u}{a^2 + u^2} \frac{\partial^2 f}{\partial v^2} + \frac{u^2}{a^2 + u^2} \frac{\partial f}{\partial u} + u \frac{\partial^2 f}{\partial u^2} + \frac{\beta a^2 u f}{(a^2 + u^2)^2} \right]$$

$$Huf = -\frac{\hbar^2}{2m} \left[\frac{1}{a^2 + u^2} \left(\frac{\partial^2}{\partial v^2} (uf) + u \frac{\partial}{\partial u} (uf) \right) + \frac{\partial^2}{\partial u^2} (uf) + \frac{\beta a^2 u f}{(a^2 + u^2)^2} \right]$$

Hence,

$$[u, H] = -\frac{\hbar^2}{m} \left[\frac{u}{2(a^2 + u^2)} + \frac{\partial}{\partial u} \right] = \frac{i\hbar}{m} p_u$$

$$\Rightarrow p_u = -i\hbar \left[\frac{\partial}{\partial u} + \frac{u}{2(a^2 + u^2)} \right] \quad (4.51)$$

To obtain the operator p_v , the commutator $[v, H]$ is used.

$$[v, H]f = (vH - Hv)f$$

where

$$vHf = -\frac{\hbar^2}{2m} \left[\frac{v}{a^2 + u^2} \frac{\partial^2 f}{\partial v^2} + \frac{uv}{a^2 + u^2} \frac{\partial f}{\partial u} + v \frac{\partial^2 f}{\partial u^2} + \frac{va^2 \beta f}{(a^2 + u^2)^2} \right]$$

$$Hvf = -\frac{\hbar^2}{2m} \left[\frac{1}{a^2 + u^2} \left(\frac{\partial^2}{\partial v^2} (vf) + u \frac{\partial}{\partial u} (vf) \right) + \frac{\partial^2}{\partial u^2} (vf) + \frac{\beta a^2 vf}{(a^2 + u^2)^2} \right]$$

Hence,

$$vHf - Hvf = -\frac{\hbar^2}{2m} \left[\frac{1}{(a^2 + u^2)} \frac{\partial f}{\partial v} \right]$$

$$[v, H] = -\frac{\hbar^2}{2m} \left[\frac{1}{(a^2 + u^2)} \frac{\partial f}{\partial v} \right] = i\hbar \frac{p_v}{m(a^2 + u^2)}$$

$$\Rightarrow p_v = -i\hbar \frac{\partial}{\partial v} \quad (4.52)$$

Using Mathematica, the commutator $[p_u, H]$ is determined.

$$[p_u, H] = p_u H - H p_u$$

$$= (-i\hbar^3) \frac{u}{m(a^2 + u^2)^2} \frac{\partial^2}{\partial v^2} - iu\hbar^3 \left[\frac{u^2 + a^2(-5 + 8\beta)}{4m(a^2 + u^2)^3} \right]$$

with $p_v^2 = -\hbar^2 \frac{\partial^2}{\partial v^2}$, the first term of $[p_u, H]$ can be simplified as

$$(-i\hbar^3) \frac{u}{m(a^2 + u^2)^2} \frac{\partial^2}{\partial v^2} = i\hbar \frac{up_v^2}{m(a^2 + u^2)^2} = i\hbar [p_u, H]_D$$

where the last equality makes use of Equation (4.43).

Hence, the commutator $[p_u, H]$ is determined.

$$[p_u, H] = i\hbar [p_u, H]_D - \frac{i\hbar^3 u}{4m(a^2 + u^2)^3} [a^2(-5 + 8\beta) + u^2] \quad (4.53)$$

The commutator $[p_v, H]$ is also evaluated by introducing a dummy function $f(u, v)$.

$$[p_v, H]f = p_v Hf - H p_v f$$

where

$$p_v H f - H p_v f = \frac{i\hbar^3}{2m} \left[\left(\frac{u}{a^2 + u^2} \right) \left(\frac{\partial^2 f}{\partial v \partial u} - \frac{\partial^2 f}{\partial u \partial v} \right) + \frac{\partial}{\partial v} \left(\frac{\partial^2 f}{\partial u^2} \right) - \frac{\partial^2}{\partial u^2} \left(\frac{\partial f}{\partial u} \right) \right]$$

Since u and v are independent variables and f is a continuous dummy function, the partial derivatives are commutable.

Hence,

$$[p_v, H] = 0 \quad (4.54)$$

Through the quantisation of the Dirac brackets in Equations (4.43) and (4.44), it can be seen that Equation (4.54) is satisfactory. However, there is a discrepancy between Equation (4.44) and Equation (4.53) as both equations cannot reconcile with one another regardless of the value of β chosen.

Hence, it can be concluded that the intrinsic geometry approach towards quantisation on a helicoid cannot be achieved as there is a breakdown in algebraic structure between the commutator $[p_u, H]$ and its corresponding Dirac bracket $[p_u, H]_D$.

4.2 Dirac's Canonical Quantisation for a Helicoid as a Submanifold

In using Dirac's canonical quantisation for a helicoid as a submanifold, the surface equation of the helicoid in Cartesian coordinates (x, y, z) is used instead of its parametric equations. The surface equation of the helicoid is given by

$$f(x) \equiv z - \arctan \frac{y}{x} = 0 \quad (4.55)$$

As with the previous section, a classical mechanical treatment is first done with Dirac's theory for constrained systems. After that, the quantum mechanics for this constrained system is derived and analysed.

4.2.1 Classical Mechanical Treatment

The Lagrangian L of the system with a Lagrangian constraint λ is given by

$$L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - \lambda f(x) \quad (4.56)$$

where the Lagrangian multiplier λ is treated as a dynamical variable.

The canonical momenta conjugate to the dynamical variables x, y, z and λ are found through Equation (3.6) to be

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i \quad (4.57)$$

$$p_\lambda = \frac{\partial L}{\partial \dot{\lambda}} = 0 \quad (4.58)$$

where $i = 1, 2, 3$ and $x_1 = x, x_2 = y$ and $x_3 = z$.

From the condition given in Equation (3.24), p_λ is the primary condition. The primary condition is denoted as

$$\phi_1 \equiv p_\lambda \equiv 0 \quad (4.59)$$

The canonical Hamiltonian H_{can} is determined using the Legendre transform.

$$\begin{aligned} H_{can} &= p_n \dot{q}_n - L \\ &= \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \dot{y}^2 + \frac{1}{2} m \dot{z}^2 + \lambda f(x) + \dot{\lambda} p_\lambda \\ &= \frac{1}{2m} p_i^2 + \lambda f(x) + \dot{\lambda} p_\lambda \end{aligned} \quad (4.60)$$

The primary Hamiltonian H_p can be found by including the primary constraint ϕ_1 and an arbitrary function of time η .

$$H_p = \frac{1}{2m} p_i^2 + \lambda f(x) + \eta p_\lambda \quad (4.61)$$

where the λ in Equation (4.59) has been absorbed by the arbitrary function η

The secondary constraints of the system can now be determined.

$$\varphi_2 \equiv \dot{\varphi}_1 = \{p_\lambda, H_p\} = -\left(z - a \arctan \frac{y}{x}\right) \approx 0 \quad (4.62)$$

$$\varphi_3 \equiv \dot{\varphi}_2 = \{\varphi_2, H_p\} = \frac{a(p_y x - p_x y) - p_z(x^2 + y^2)}{m(x^2 + y^2)} \approx 0 \quad (4.63)$$

$$\varphi_4 \equiv \dot{\varphi}_3 = \frac{\lambda(a^2 + x^2 + y^2)}{m(x^2 + y^2)} + \frac{2a(-p_y x + p_x y)(p_x x + p_y y)}{m^2(x^2 + y^2)^2} \approx 0 \quad (4.64)$$

Since all Poisson brackets associated with their respective constraint have been evaluated, the weak equalities can be switched to strong equalities. With that, the following relations are found.

$$p_\lambda = 0 \quad (4.65)$$

$$z = a \arctan \frac{y}{x} \quad (4.66)$$

$$p_z = \frac{a(p_y x - p_x y)}{x^2 + y^2} \quad (4.67)$$

$$\lambda = \frac{-2a(p_x y - p_y x)(p_x x + p_y y)}{m(x^2 + y^2)(a^2 + x^2 + y^2)} \quad (4.68)$$

Using Wolfram Mathematica and the constraints of the system found, a matrix consisting of Poisson brackets D and its inverse D^{-1} can be determined.

The matrix D is determined to be

$$D = \begin{bmatrix} 0 & 0 & 0 & D_{14} \\ 0 & 0 & -D_{23} & D_{24} \\ 0 & D_{14} & 0 & D_{34} \\ -D_{14} & -D_{24} & -D_{34} & 0 \end{bmatrix} \quad (4.69)$$

where

$$D_{14} = -\frac{a^2 + x^2 + y^2}{m(x^2 + y^2)} \quad (4.70)$$

$$D_{24} = -\frac{2a^2(p_x x + p_y y)}{m^2(x^2 + y^2)^2} \quad (4.71)$$

$$D_{34} = \frac{4a^2(p_y x - p_x y)^2}{m^3(x^2 + y^2)^3} \quad (4.72)$$

Its inverse D^{-1} is determined to be

$$D^{-1} = \begin{bmatrix} 0 & D_{12}^{-1} & D_{13}^{-1} & D_{14}^{-1} \\ -D_{12}^{-1} & 0 & -D_{14}^{-1} & 0 \\ -D_{13}^{-1} & D_{14}^{-1} & 0 & 0 \\ D_{14}^{-1} & 0 & 0 & 0 \end{bmatrix} \quad (4.73)$$

where

$$D_{12}^{-1} = \frac{4a^2(p_y x - p_x y)^2}{m(x^2 + y^2)(a^2 + x^2 + y^2)^2} \quad (4.74)$$

$$D_{13}^{-1} = \frac{2a^2(p_x x + p_y y)}{(a^2 + x^2 + y^2)^2} \quad (4.75)$$

$$D_{14}^{-1} = \frac{m(x^2 + y^2)}{a^2 + x^2 + y^2} \quad (4.76)$$

The fundamental Dirac brackets are found using Equation (3.40).

$$[x_i, x_j]_D = 0 \quad (4.77)$$

$$[x_i, p_j]_D = \delta_{ij} - \frac{a^2}{(x^2 + y^2)(a^2 + x^2 + y^2)} \chi_i \chi_j \quad (4.78)$$

$$[p_i, p_j]_D = -\frac{a^2}{(x^2 + y^2)(a^2 + x^2 + y^2)} [\chi_i \Omega_j - \chi_j \Omega_i] \quad (4.79)$$

where

$$\chi_i = \delta_{1i} y - \delta_{2i} x + \delta_{3i} \left(\frac{x^2 + y^2}{a} \right)$$

$$\Omega_j = \delta_{1j}p_y - \delta_{2j}p_x + \delta_{3j} \frac{2(xp_x + yp_y)}{a}$$

The equations of motion for the generalised position x_i and generalised momentum p_i are

$$\dot{x}_i \equiv [x_i, H]_D = \frac{p_i}{m} \quad (4.80)$$

$$\dot{p}_i \equiv [p_i, H]_D = -\frac{2a(p_x x + p_y y)}{(x^2 + y^2)(a^2 + x^2 + y^2)} p_z \chi_i \quad (4.81)$$

Since the equations of motion are determined, the classical treatment for Dirac's canonical quantisation for a helicoid as a submanifold is completed.

4.2.2 Quantum Mechanical Treatment

The fundamental Dirac brackets in Equations (4.77) to (4.79) are transformed to commutators with Dirac's quantisation procedure. The fundamental commutation relations are given by

$$[x_i, x_j] = 0 \quad (4.82)$$

$$[x_i, p_j] = i\hbar \left(\delta_{ij} - \frac{a^2}{(x^2 + y^2)(a^2 + x^2 + y^2)} \chi_i \chi_j \right) \quad (4.83)$$

$$[p_i, p_j] = i\hbar [p_i, p_j]_D \quad (4.84)$$

As mentioned by Homma *et al.* (1990) and Ikegami *et al.* (1992), the main problem with Dirac's formalism of quantisation on curved surfaces is that many momenta can satisfy the fundamental commutation relations above. Hence, as in Section 4.1, the momentum operators p_i must be determined first.

From Equation (4.80), the commutator between the position x_i and the Hamiltonian is

$$[x_i, H] = i\hbar \frac{p_i}{m} \quad (4.85)$$

To determine the momenta p_i , the commutator must be evaluated individually between the position x_i and the quantum Hamiltonian H given in Equation (4.46). The method of evaluating the commutator is similar to the method shown in Section 4.1. A dummy function $f = f(u, v)$ is introduced, and the commutators are evaluated based on the definition of a commutator.

To obtain the operator p_x , the commutator $[x, H]$ is used.

$$[x, H]f = (xH - Hx)f \quad (4.86)$$

where

$$xHf = -\frac{\hbar^2}{2m} \left[\frac{x}{a^2 + u^2} \frac{\partial^2 f}{\partial v^2} + \frac{u}{a^2 + u^2} x \frac{\partial f}{\partial u} + x \frac{\partial^2 f}{\partial u^2} + \frac{\beta a^2 x f}{(a^2 + u^2)^2} \right]$$

$$Hxf = -\frac{\hbar^2}{2m} \left[\frac{1}{a^2 + u^2} \frac{\partial^2}{\partial v^2} (xf) + \frac{u}{a^2 + u^2} \frac{\partial}{\partial u} (xf) + \frac{\partial^2}{\partial u^2} (xf) + \frac{\beta a^2 x f}{(a^2 + u^2)^2} \right]$$

By taking the difference between both expressions,

$$xHf - Hxf = -\frac{\hbar^2}{2m} \left[-\frac{1}{a^2 + u^2} \left(2 \frac{\partial x}{\partial v} \frac{\partial f}{\partial v} + \frac{\partial^2 x}{\partial v^2} f \right) - \frac{u}{a^2 + u^2} \frac{\partial x}{\partial u} f - \left(\frac{\partial^2 x}{\partial u^2} f + 2 \frac{\partial x}{\partial u} \frac{\partial f}{\partial u} \right) \right]$$

Since $x = u \cos v$, after differentiation,

$$xHf - Hxf = \frac{\hbar^2}{m} \left[-\frac{1}{a^2 + u^2} u \sin v \frac{\partial}{\partial v} + \cos v \frac{\partial}{\partial u} \right] = i\hbar \frac{p_x}{m}$$

$$\Rightarrow p_x = -i\hbar \left[\cos v \frac{\partial}{\partial u} - \frac{1}{a^2 + u^2} (u \sin v) \frac{\partial}{\partial v} \right] \quad (4.87)$$

A similar process is repeated for $[y, H]$ and $[z, H]$ to obtain the operators p_y and p_z .

$$p_y = -i\hbar \left[\frac{u \cos v}{a^2 + u^2} \frac{\partial f}{\partial v} + \sin v \frac{\partial f}{\partial u} \right] \quad (4.88)$$

$$p_z = -i\hbar \frac{a}{a^2 + u^2} \frac{\partial}{\partial v} \quad (4.89)$$

The momentum operators in Equations (4.87) to (4.89) are the Cartesian components of the geometric momentum given in Equation (2.3). The full proof of this is provided in Appendix B.

To express Equation (4.83), a property of commutators needs to be considered. If both operators \hat{A} and \hat{B} in a commutator is Hermitian, the commutator $[\hat{A}, \hat{B}]$ must be anti-Hermitian. However, this is not the case with Equation (4.83) as

$$\begin{aligned} [p_i, H]^\dagger &= \left[i\hbar \frac{-2a(p_x x + p_y y)}{(x^2 + y^2)(a^2 + x^2 + y^2)} p_z \chi_i \right]^\dagger \\ &= \chi_i p_z \left[\frac{2\hbar a(x p_x + y p_y)}{(a^2 + x^2 + y^2)(x^2 + y^2)} \right] \\ &\neq -[p_i, H] \end{aligned}$$

To achieve the condition of anti-Hermiticity, the commutator $[p_i, H]$ can be written by considering the symmetry

$$[p_i, H] = i\hbar \left(\frac{F_i + F_i^\dagger}{2} \right) \quad (4.90)$$

where

$$F_i = \frac{-2a(p_x x + p_y y)}{(x^2 + y^2)(a^2 + x^2 + y^2)} p_z \chi_i, \quad \chi_i = \delta_{1i} y - \delta_{2i} x + \delta_{3i} \frac{(x^2 + y^2)}{a} \quad (4.91)$$

To determine the validity of Dirac's canonical quantisation of a helicoid as a submanifold, the secondary commutation relation $[p, H]$ must be evaluated and analysed. By evaluating $[p_i, H]$ with the momentum operators given in Equations (4.87) to (4.89) through Mathematica, the following expressions for the commutator are obtained.

$$\begin{aligned}
 [p_1, H] &\equiv [p_x, H] \\
 &= \frac{i\hbar^3 a^2}{m(a^2 + u^2)^3} \left[-2u\beta \cos v - 3u \sin v \frac{\partial}{\partial v} \right. \\
 &\quad \left. + (a^2 + u^2) \left(\cos v \frac{\partial}{\partial u} + 2 \sin v \frac{\partial}{\partial u} \frac{\partial}{\partial v} \right) \right]
 \end{aligned} \tag{4.92}$$

$$\begin{aligned}
 [p_2, H] &\equiv [p_y, H] \\
 &= \frac{i\hbar^3 a^2}{m(a^2 + u^2)^3} \left[-2u\beta \sin v + 3u \cos v \frac{\partial}{\partial v} \right. \\
 &\quad \left. + (a^2 + u^2) \left(\sin v \frac{\partial}{\partial u} - 2 \cos v \frac{\partial}{\partial u} \frac{\partial}{\partial v} \right) \right]
 \end{aligned} \tag{4.93}$$

$$[p_3, H] \equiv [p_z, H] = \frac{i\hbar^3 a}{m(a^2 + u^2)^3} \left[(a^2 - 2u^2) \frac{\partial}{\partial v} + 2u(a^2 + u^2) \frac{\partial}{\partial u} \frac{\partial}{\partial v} \right] \tag{4.94}$$

By making use of the expression on the right-hand side of Equation (4.90), the operator-ordering problem due to Dirac's canonical quantisation scheme on the operator can be explored. The operator-ordering problem exists due to the ambiguity of the positioning of the position operators and momentum operators. There are three possible permutations between the operators in conflict.

$$\begin{aligned}
[p_i, H] = & -i\hbar \left\{ \alpha_1 \left[x g_i \frac{1}{2} (p_x p_z + p_z p_x) + y g_i \frac{1}{2} (p_y p_z + p_z p_y) \right] \right. \\
& + \alpha_2 \left[\frac{1}{2} (p_x p_z + p_z p_x) x g_i + \frac{1}{2} (p_y p_z + p_z p_y) y g_i \right] \\
& \left. + \alpha_3 \left[\frac{1}{2} (p_x x g_i p_z + p_z x g_i p_x) + \frac{1}{2} (p_y y g_i p_z + p_z y g_i p_y) \right] \right\}
\end{aligned} \tag{4.95}$$

where α_k , ($k = 1,2,3$) are three real parameters that satisfy $\sum \alpha_k = 1$ and

$$g_i = \frac{2\alpha_i}{m(x^2 + y^2)(a^2 + x^2 + y^2)} \tag{4.96}$$

If a specific permutation in (4.95) is incorrect, $\alpha_i = 0$ will eliminate it from $[p_i, H]$.

By evaluating Equation (4.95) for each i using Mathematica, the following expressions are obtained.

$$\begin{aligned}
[p_x, H] = & \frac{i\hbar^3 a^2}{m(a^2 + u^2)^3} \left[-3u\alpha_2 \cos v - 3u(\alpha_1 + \alpha_2) \sin v \frac{\partial}{\partial v} \right. \\
& \left. + (a^2 + u^2) \left((2\alpha_2 + \alpha_3) \cos v \frac{\partial}{\partial u} + 2(\alpha_1 + \alpha_2) \sin v \frac{\partial}{\partial u} \frac{\partial}{\partial v} \right) \right]
\end{aligned} \tag{4.97}$$

$$\begin{aligned}
[p_y, H] = & \frac{i\hbar^3 a^2}{m(a^2 + u^2)^3} \left[-3u\alpha_2 \cos v + 3u(\alpha_1 + \alpha_2) \cos v \frac{\partial}{\partial v} \right. \\
& \left. + (a^2 + u^2) \left((2\alpha_2 + \alpha_3) \sin v \frac{\partial}{\partial u} - 2(\alpha_1 + \alpha_2) \cos v \frac{\partial}{\partial u} \frac{\partial}{\partial v} \right) \right]
\end{aligned} \tag{4.98}$$

$$\begin{aligned}
[p_z, H] = & \frac{i\hbar^3 a}{m(a^2 + u^2)^3} [u^2(-3\alpha_1 - \alpha_2 + \alpha_3) + a^2(2\alpha_2 + \alpha_3)] \frac{\partial}{\partial v} \\
& + 2u(a^2 + u^2)(\alpha_1 + \alpha_2) \frac{\partial}{\partial u} \frac{\partial}{\partial v}
\end{aligned} \tag{4.99}$$

By comparing Equations (4.92) - (4.94) to Equations (4.97) to (4.99), the following relations are obtained.

$$\alpha_1 = \alpha_2 = \frac{1}{2} - \frac{\alpha_3}{2} \tag{4.100}$$

$$\beta = \frac{3}{4}(1 - \alpha_3) \tag{4.101}$$

By allowing the value of α_3 to be $\alpha_3 = -\frac{1}{3}$, the value of $\beta = 1$ is found.

With that, the geometric potential for a helicoid is given as $V = \frac{\hbar^2}{2m}K$, which agrees with the geometric potential found by the confining potential approach in Equation (2.4).

Hence, the submanifold approach does not offer a problematic description after quantisation, unlike the intrinsic geometry approach. The submanifold approach through the enlarged canonical quantisation (ECQ) scheme is also compatible with the confining potential approach, which requires that $\beta = 1$.

CHAPTER 5

CONCLUSION

5.1 Conclusion

In this work, the quantisation of motion on a helicoid is explored with Dirac's canonical quantisation. By taking the geometry of the problem into account, an intrinsic geometry approach and a submanifold approach are used. In both approaches, the quantisation of motion on a helicoid is first explored with a classical mechanical treatment where the Dirac brackets for all commutation relations are found. After that, a quantum mechanical treatment is done whereby the Dirac brackets are transformed into commutators via Dirac's canonical quantisation.

In general, there are two conditions that each approach mentioned above need to fulfil. The first condition is that the commutator obtained must be a product of $i\hbar$ and Dirac brackets. Apart from that, the geometric momentum obtained from canonical quantisation must be in the same form as the geometric momentum obtained by Liu *et al.* (2007). The classical mechanical treatment and quantum mechanical treatment are done on both approaches to determine if the conditions above are fulfilled.

This thesis has shown that the intrinsic approach, which makes use of the local coordinates of the system, results in an algebraic breakdown between the Dirac bracket and the commutator. However, with the submanifold approach, the description of the system is self-consistent. Not only that, the momentum operators of $\hat{p}_x, \hat{p}_y, \hat{p}_z$ obtained from the submanifold approach are in line with Equation (2.3). With the help of the enhanced canonical quantisation (ECQ) scheme, the expression of the geometric potential V is found to be similar to the form determined through the confining potential approach. This shows that the ECQ scheme is a necessary

generalisation for canonical quantisation to be used on a system constrained on a helicoid.

It is interesting to note the impact of the ECQ scheme on the quantisation process studied in this thesis. Previous attempts to quantise a particle constrained on a curved manifold without the ECQ scheme, such as by Kleinert and Shabanov (1997) and Diță (1997), were hindered by the operator-ordering problem. The operator-ordering problem was resolved by considering Abelian transformation or the implementation of Lie algebra. However, in this thesis, with the ECQ scheme, the operator-ordering problem is resolved without such methods. Instead, the problem is resolved by directly determining the momentum operator and the commutator, as shown in Equations (4.97) to (4.99). This process allows the operator-ordering problem to be solved by determining the values of α_i in Equation (4.95).

5.2 Future Works and Projects

With the results in this study, the Schrödinger equation for this system can be written. It is hoped that the equation can be solved so that the wave function of the particle constrained on the helicoid can be determined.

Moreover, due to the inherently vague nature of quantisation, it will be interesting to explore the quantisation of motion on a helicoid with a different quantisation method and compare the results obtained. There is a possibility that the momentum operators obtained will differ between each quantisation method.

This thesis also aims to determine the validity and usefulness of the enhanced canonical quantisation scheme. Hence, it would be interesting for future research on canonical quantisation on other curved manifolds to include the ECQ scheme.

Further research needs to be done on a variety of curved manifolds to determine the boundaries of the ECQ scheme.

Another future work that can be done regarding the ECQ scheme is to develop a quantum mechanical determinant to show that the intrinsic geometry approach cannot be used to quantise the motion of a particle on a helicoid. In the literature, Zhang *et al.* (2015) has derived a quantum mechanical discriminant to show that the quantisation of a free particle on a two-dimensional sphere cannot be done within intrinsic geometry. It is worth looking into a determinant for a helicoid and then generalising the determinant for any curved manifolds.

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APPENDIX A

WOLFRAM MATHEMATICA SCRIPTS

Wolfram Mathematica (Version 12.1) is used in this thesis to ease the calculation of Poisson brackets, Dirac brackets and commutators. This appendix details the Mathematica scripts used in this thesis.

A.1 Poisson Brackets

The script for Poisson brackets is adapted from Gerd Baumann's Mathematica for Theoretical Physics, Volume 1 (Baumann, 2005).

```
PoissonBracket[a_, b_, q_List, p_List] := Block[{pk, n}, n = Length[q];  
If[n == Length[p],  
pk = FullSimplify[  
Sum[D[a, q[[j]]] D[b, p[[j]]] - D[b, q[[j]]] D[a, p[[j]]], {j, 1,  
n}], Print["Incompatible lengths"]]]
```

Figure 2: Code to determine Poisson brackets

A.2 Dirac Brackets

Since Dirac brackets are the sum of multiple Poisson brackets and their corresponding matrix elements, the script for Dirac brackets is reliant on the script for Poisson brackets. A sample script to determine the Dirac bracket $[x, p_x]_D$ is shown.



```

XPX = FullSimplify[(PoissonBracket[x,
  p1, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}]*
  MatDI[[1, 2]]*
  PoissonBracket[p2,
  px, {x, y, z, \[Lambda]}, {px, py, pz,
  p\[Lambda]}]) + (PoissonBracket[x,
  p1, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}]*
  MatDI[[1, 3]]*
  PoissonBracket[p3,
  px, {x, y, z, \[Lambda]}, {px, py, pz,
  p\[Lambda]}]) + (PoissonBracket[x,
  p1, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}]*
  MatDI[[1, 4]]*
  PoissonBracket[p4,
  px, {x, y, z, \[Lambda]}, {px, py, pz,
  p\[Lambda]}]) + (PoissonBracket[x,
  p2, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}]*
  MatDI[[2, 1]]*
  PoissonBracket[p1,
  px, {x, y, z, \[Lambda]}, {px, py, pz,
  p\[Lambda]}]) + (PoissonBracket[x,
  p2, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}]*
  MatDI[[2, 3]]*
  PoissonBracket[p3,
  px, {x, y, z, \[Lambda]}, {px, py, pz,
  p\[Lambda]}]) + (PoissonBracket[x,
  p3, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}]*
  MatDI[[3, 1]]*
  PoissonBracket[p1,
  px, {x, y, z, \[Lambda]}, {px, py, pz,
  p\[Lambda]}]) + (PoissonBracket[x,
  p3, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}]*
  MatDI[[3, 2]]*
  PoissonBracket[p2,
  px, {x, y, z, \[Lambda]}, {px, py, pz,
  p\[Lambda]}]) + (PoissonBracket[x,
  p4, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}]*
  MatDI[[4, 1]]*
  PoissonBracket[p1,
  px, {x, y, z, \[Lambda]}, {px, py, pz, p\[Lambda]}])])

```

Figure 3: Code to determine the Dirac bracket of $[x, p_x]_D$

A.3 Differential Operator Paclet

As most operators in this thesis have "open-ended" differential operators, the differential operator paclet developed by Woll (2018) is used.

The differential operator packet can be installed with the following code.

```
PacletInstall["https://github.com/carlwooll/DifferentialOperator/  
releases/download/0.1/ DifferentialOperator-0.0.1.paclet"]
```

Figure 4: Code to install DifferentialOperator paclet by Woll (2018)



APPENDIX B
CARTESIAN COMPONENTS OF GEOMETRIC MOMENTUM

The general form of geometric momentum proposed by Liu *et al.* (2007) is

$$\mathbf{p} = -i\hbar(\mathbf{r}^\mu \partial_\mu + M\mathbf{n}) \quad (\text{B.1})$$

where \mathbf{r} is the position vector on the surface and $\mathbf{r}^\mu = g^{\mu\nu} \mathbf{r}_\nu = g^{\mu\nu} \partial \mathbf{r} / \partial x^\nu$, for $\mu = 1, 2$.

The metric of the helicoid must first be determined. From Equation (4.1) and the equation of constraint, the Cartesian coordinates (x, y, z) in terms of the local coordinates (u, v) are given as

$$x = u \cos v \quad y = u \sin v \quad z = rv = av \quad (\text{B.2})$$

Hence, the position vector R can be written as

$$\mathbf{R} = (u \cos v)\hat{i} + (u \sin v)\hat{j} + (av)\hat{k} \quad (\text{B.3})$$

The bases are given by

$$\hat{e}_1 = \frac{\partial \mathbf{R}}{\partial u} = (\cos v)\hat{i} + (\sin v)\hat{j} \quad (\text{B.4})$$

$$\hat{e}_2 = \frac{\partial \mathbf{R}}{\partial v} = (-u \sin v)\hat{i} + (u \cos v)\hat{j} + a\hat{k} \quad (\text{B.5})$$

The metric g_{ij} is given by

$$\begin{aligned} g_{ij} &= \begin{bmatrix} \hat{e}_1 \cdot \hat{e}_1 & \hat{e}_1 \cdot \hat{e}_2 \\ \hat{e}_2 \cdot \hat{e}_1 & \hat{e}_2 \cdot \hat{e}_2 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & u^2 + a^2 \end{bmatrix} \end{aligned} \quad (\text{B.6})$$

The inverse of g_{ij} is given by

$$g^{ij} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{u^2 + a^2} \end{bmatrix} \quad (\text{B. 7})$$

The geometric momentum p_1 is first considered. From the general form proposed,

$$p_1 = -i\hbar(r_x^1 \partial_1 + r_x^2 \partial_2) \quad (\text{B. 8})$$

where, from the definition of r^μ ,

$$\begin{aligned} r_x^1 &= g^{1\nu} \frac{\partial \mathbf{R}}{\partial x^\nu} \\ &= g^{11} \left(\frac{\partial \mathbf{R}}{\partial x^1} \right)_x + g^{12} \left(\frac{\partial \mathbf{R}}{\partial x^2} \right)_x \\ &= g^{11} \left(\frac{\partial \mathbf{R}}{\partial u} \right)_x \\ &= \cos v \end{aligned} \quad (\text{B. 9})$$

$$\begin{aligned} r_x^2 &= g^{2\nu} \frac{\partial \mathbf{R}}{\partial x^\nu} \\ &= g^{21} \left(\frac{\partial \mathbf{R}}{\partial x^1} \right)_x + g^{22} \left(\frac{\partial \mathbf{R}}{\partial x^2} \right)_x \\ &= -\frac{u \sin v}{a^2 + u^2} \end{aligned} \quad (\text{B. 10})$$

Hence,

$$p_1 = -i\hbar(r_x^1 \partial_1 + r_x^2 \partial_2) = -i\hbar \left(\cos v \frac{\partial}{\partial u} - \frac{u \sin v}{a^2 + u^2} \frac{\partial}{\partial v} \right) \quad (\text{B. 11})$$

The geometric momentum p_2 is now considered. From the general form,

$$p_2 = -i\hbar(r_y^1 \partial_1 + r_y^2 \partial_2) \quad (\text{B. 12})$$

where

$$\begin{aligned}
 r_y^1 &= g^{1\nu} \frac{\partial \mathbf{R}}{\partial x^\nu} \\
 &= g^{11} \left(\frac{\partial \mathbf{R}}{\partial x^1} \right)_y + g^{12} \left(\frac{\partial \mathbf{R}}{\partial x^2} \right)_y \\
 &= g^{11} \left(\frac{\partial \mathbf{R}}{\partial u} \right)_y \\
 &= \sin v
 \end{aligned} \tag{B.13}$$

$$\begin{aligned}
 r_y^2 &= g^{2\nu} \frac{\partial \mathbf{R}}{\partial x^\nu} \\
 &= g^{21} \left(\frac{\partial \mathbf{R}}{\partial x^1} \right)_y + g^{22} \left(\frac{\partial \mathbf{R}}{\partial x^2} \right)_y \\
 &= \frac{u \cos v}{a^2 + u^2}
 \end{aligned} \tag{B.14}$$

Hence,

$$p_2 = -i\hbar(r_y^1 \partial_1 + r_y^2 \partial_2) = -i\hbar \left(\sin v \frac{\partial}{\partial u} - \frac{u \cos v}{a^2 + u^2} \frac{\partial}{\partial v} \right) \tag{B.15}$$

Lastly, the geometric momentum p_3 is considered. From the general form,

$$p_3 = -i\hbar(r_z^1 \partial_1 + r_z^2 \partial_2) \tag{B.16}$$

where

$$\begin{aligned}
 r_z^1 &= g^{1\nu} \frac{\partial \mathbf{R}}{\partial x^\nu} \\
 &= g^{11} \left(\frac{\partial \mathbf{R}}{\partial x^1} \right)_z + g^{12} \left(\frac{\partial \mathbf{R}}{\partial x^2} \right)_z \\
 &= 0
 \end{aligned} \tag{B.17}$$

$$\begin{aligned}
r_z^2 &= g^{2\nu} \frac{\partial \mathbf{R}}{\partial x^\nu} \\
&= g^{21} \left(\frac{\partial \mathbf{R}}{\partial x^1} \right)_z + g^{22} \left(\frac{\partial \mathbf{R}}{\partial x^2} \right)_z \\
&= \frac{a}{a^2 + u^2}
\end{aligned} \tag{B.18}$$

Hence,

$$p_3 = -i\hbar(r_z^1 \partial_1 + r_z^2 \partial_2) = -i\hbar \frac{a}{a^2 + u^2} \frac{\partial}{\partial v} \tag{B.19}$$

All three momenta obtained in Equations (4.86) to (4.88) are shown to be Cartesian components of the geometric momentum proposed by Liu *et al.* (2007).