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Geometry and Semiclassics of Tetrahedral Grain of Space

Santanu B. Antu

Bard College, aa3296@bard.edu

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Geometry and Semiclassics of a Tetrahedral Grain of Space

A Senior Project submitted to
The Division of Science, Mathematics, and Computing
of
Bard College

by
Santanu Bosu Antu

Annandale-on-Hudson, New York
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Abstract

The quantum theory of gravity has eluded physicists for many decades. The apparent contradiction between the physics describing the microscopic and the macroscopic regimes has given rise to some beautiful theories and mathematics. In this paper, we discuss some aspects of one of those theories, namely *loop quantum gravity* (LQG). Specifically, we discuss the discreteness of spacetime, a feature that distinguishes LQG from some of the other contending theories. After a general discussion in the introduction, we discuss the dynamics and quantization of the simplices (tetrahedra) that make up the spacetime. The discrete geometry of these tetrahedral grains of spacetime has some beautiful physical and mathematical properties. We use semiclassical physics and some classical results in algebraic geometry and topology to investigate many of these properties.

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Dedication

To my beloved parents,

This paper is dedicated to you with deep gratitude and love. Your endless support, encouragement, and sacrifices have been instrumental in my academic achievements. Despite the distance, you have always been a source of inspiration and strength, and I feel blessed to have you in my life. Your unwavering support has been the cornerstone of my success, and I cannot thank you enough for all that you have done for me.

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Introduction

1.1 Motivation

The physics of the early and mid-twentieth century has been extremely successful in producing a more complete description of nature in comparison to the classical Newtonian physics. The theories that were central to this rapid evolution were the quantum theory and general relativity. Many attempts, even to these days, have been made to find experiments that disprove these theories in their respective regimes, but most of them further solidified their validity [12, 23]. Despite the success of these theories, there remains many open problems in physics that demand new theories and experiments—the baryon asymmetry problem, singularity of black holes, the black hole information paradox, early universe cosmology, dark matter, unification of force and a theory of quantum gravity to name a few. These problems are not necessarily related, but some of them might not be mutually exclusive. For instance, a theory of quantum gravity can be

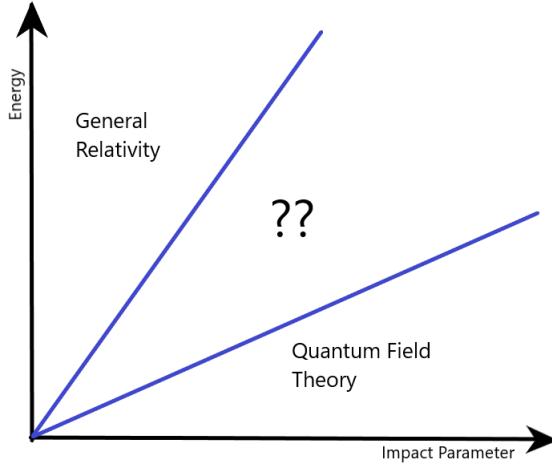


Figure 1.1.1: A plot of Energy vs impact parameter where different theories are applicable.

productive in solving some of the questions about the center of a black hole and early universe cosmology [2, 5, 8, 18]. Besides, the apparent philosophical contradiction between quantum field theory (QFT) and general relativity (GR) beg the question of a unified theory. Consider, for example, the scattering problem in the quantum realm. In the case of large impact parameter between two particles, the scattering problem is very precisely solved using QFT ¹. However, this is only true when the distance is large enough to ignore the gravitational interaction between the particles. To get a fundamental understanding of the structure of spacetime and matter, we can not ignore the weak but important gravitational interaction. Since GR treats gravitational field as a metric in spacetime, we actually need to consider spacetime itself to have a quantum nature.

For a more convincing argument, suppose we want to measure some field at a point x . Say, we do this by having a particle at point x with uncertainty Δx . By the uncertainty principle, we know that the momentum of this particle p is such that $p^2 > (\hbar/\Delta x)^2$. Now, in the relativistic limit, we have $p \sim E/c$. But in GR, any kind of energy has a gravitational mass $m \sim E/c^2$. Combining this all together, we have $m \sim \hbar/(c\Delta x)$. Now if we want to make the measurement

¹Impact parameter is defined as the perpendicular distance from the center of a potential to the straight line a particle takes far away from the potential.

more and more precise (decreasing the uncertainty in x), the gravitational mass is concentrated in smaller and smaller region. However, this cannot be done arbitrarily, since for $\Delta x \sim Gm/c^2$, a black hole of mass $m \sim \Delta x c^2/G$ is formed. Combining this expression for mass with the previous approximate equality, we can say that the minimum size where we can localize the particle is $\Delta x = L_p = \sqrt{\frac{\hbar G}{c^3}} \sim 10^{-35}$ m. We can think of this as the smallest length scale possible. We will refer to this as the Planck length. This is the intuitive idea of space itself having a smallest quanta ². The smooth geometry that we use to do QFT is not complete in this sense. Quantum theory itself poses a limit on the smoothness of the geometry of space.

In this paper, we will discuss the quantization of the simplest grains of space—a tetrahedron. An analogous system that will motivate many of the results is the algebra of angular momentum from elementary quantum mechanics. For the purpose of completeness, we review the key results here. Let $\mathbf{L} = L^i \hat{e}_i$, where $i = 1, 2, 3$, be the angular momentum of some quantum system ³. In classical mechanics, \mathbf{L} acts as the generator of infinitesimal rotation in the sense that it is an element of the Lie algebra that generate the Lie group of proper rotations, namely $SO(3)$. In the Poisson bracket formulation of Hamiltonian mechanics, it can also be shown, using the defining equation of angular momentum ($\mathbf{L} = \mathbf{r} \times \mathbf{p}$), that the components of the angular momentum vector has the following bracket structure:

$$\{L^i, L^j\} = \epsilon^{ij}_k L^k. \quad (1.1.1)$$

Here, for two arbitrary smooth functions $f(q, p, t)$ and $g(q, p, t)$ depending on the generalized coordinate (q), generalized momentum (p) and time (t), the Poisson bracket is defined as $\{f, g\} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}$. Following Dirac ⁴, we obtain the quantum mechanical relations by replacing the

²For a more thorough argument, see [9].

³From here on, the Einstein summation convention is always used unless stated otherwise. Occasionally, we will write out the entire sum for the sake of clarity.

⁴See Chapter IV of *The Principles of Quantum Mechanics*. by P.A.M Dirac

Poisson bracket relation with the following commutator relation [14].

$$\{\cdot, \cdot\} \rightarrow \frac{1}{i\hbar}[\cdot, \cdot]. \quad (1.1.2)$$

Using Dirac's prescription, our 1.1.1 gives rise to the algebra of angular momentum in quantum mechanics:

$$[\hat{L}^i, \hat{L}^j] = i\hbar\epsilon^{ij}{}_k \hat{L}^k \quad (1.1.3)$$

Notice that in turning to the quantum mechanical world, we replaced the dynamical variables L^i with the corresponding quantum mechanical operators \hat{L}^i . It follows from elementary treatment of quantum mechanics and $SU(2)$ representation theory that $\hat{\mathbf{L}}^2 = \hat{L}^i \hat{L}^i$ commutes with each of the components of $\hat{\mathbf{L}}$, and if the components follow the algebra 1.1.3, then the eigenvalues of $|\hat{\mathbf{L}}|$ are given by:

$$L_j = \sqrt{j(j+1)}\hbar, \quad \text{where } j \in \left\{ \frac{1}{2}, 1, \frac{3}{2}, 2, \dots \right\}. \quad (1.1.4)$$

Note that the eigenvalues of this operator are discrete. This is a key theme in many quantum mechanical system, and will be important for our case as well. It can be shown that for a compact phase space, the spectra is always discrete [31]. This is the reason why we have discrete energy spectra for infinite square well and simple harmonic oscillator. In the case of angular momenta, the phase space is just the space of directions, which is certainly compact, and so it gives rise to a discrete spectrum.

1.2 Triangulation of Space and Geometry of Tetrahedra

We now switch to a discussion of the simplest grains of space—the object of our main discussion in this paper. It is intuitively obvious that we can fill out a page of paper or a torus (or any visualizable 2D manifold⁵) with triangular pieces (possibly curved). There is a general theorem in the study of differentiable manifolds that we can always triangulate a smooth manifold regardless of its dimension [11,36]. For our three dimensional Euclidean space, the “triangles” are tetrahedra. According to GR, the geometry of spacetime is the same as gravitational field. Following this line of logic, quantizing the geometry of spacetime amounts to quantizing gravity.

In this paper, we will take area as a fundamental variable in discretizing space. There are several reasons for this choice. Firstly, a closed two dimensional area can partition space, and so it allows us to concretely talk about what we mean by a discrete grain of space. Besides, the quantum geometry that we are going to study is relevant only at Planck scale. In the natural unit system, the unit of area is $\frac{\hbar G}{c^3}$, and unlike a length variable, it does not involve an operation of square root. Hence, area is an interesting variable both from the point of view of geometry and the from an unit-argument. With areas as a starting point, we state some essential properties of a tetrahedron, which will be the central object of interest for us, in terms of its face areas and area vectors.

Consider a tetrahedron with the normal vectors \vec{A}_i , where $i = 1, 2, 3, 4$. Following [33], we list some nice properties of this set of vectors that we will use repeatedly in this paper.

- Take a vertex of the tetrahedron at the origin, and label the three edges emanating from the vertex as \vec{l}^i for $i = 1, 2, 3$. Let M be a 3x3 matrix where the three columns are the

⁵For a discussion on manifolds, see [25].

three edge-length vectors. If F is the matrix with the three face-area vectors adjacent to the chosen vertex as its columns, then we have

$$F^T = -\frac{1}{2}(\det M)M^{-1}. \quad (1.2.1)$$

- They satisfy the following closure relation:

$$\sum_{i=1}^4 \vec{A}_i = 0. \quad (1.2.2)$$

- In fact, if we take any four vectors satisfying the closure condition (1.2.2), then the geometry (areas, edge lengths, volume etc.) are determined up to an $SO(3)$ rotation and translation [30].
- Using some fundamental identities of vector calculus, it can be shown that the squared volume V^2 of the tetrahedron is given by:

$$V^2 = \frac{2}{9}\epsilon_{ijk}A_1^i A_2^j A_3^k = \frac{2}{9}\det F. \quad (1.2.3)$$

Here, we have chosen an appropriate right-handed orientation for \vec{A}_1, \vec{A}_2 and \vec{A}_3 so that the squared volume is positive.

1.3 Quantizing Geometry

Following Dirac's prescription for quantizing a system, we can start with the Hamiltonian dynamics of GR, and promote the Poisson brackets of dynamical variables to commutators

of operators to arrive at some canonical quantization relations. However, the leap of going from Poisson bracket to commutators is ultimately a postulate. Here, motivated by (1.1.3), we postulate [3] the following fundamental commutation relation.

$$[A_\alpha^i, A_\beta^j] = i\delta_{\alpha,\beta}l_0^2\epsilon^{ij}_k A_\alpha^k, \quad (1.3.1)$$

where l_0^2 is proportional to \hbar and has a dimension of squared area. Using dimensional analysis, it can be shown that $l_0^2 = \gamma \frac{\hbar G}{c^3}$, where γ is a unitless number that fixes the scale of quantization. One immediate consequence the commutation relation (1.3.1) is that the areas have discrete values given by

$$A = l_0^2\sqrt{j(j+1)}, \quad j = \frac{1}{2}, 1, \frac{3}{2}, 2, \dots \quad (1.3.2)$$

Now, suppose we have a tetrahedron with face area eigenvalues labeled by j_1, \dots, j_4 . We associate to each of the four faces A_i of the tetrahedron a unitary representation of $SU(2)$ that act on a Hilbert space \mathcal{H}_{j_i} . The total Hilbert space without any restrictions on the area is then $\mathcal{H} = \mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} \otimes \mathcal{H}_{j_3} \otimes \mathcal{H}_{j_4}$. If we take into account the closure relation of the area vectors, then the space should be invariant under global $SU(2)$ action. Then the quantum states live in the space

$$\mathcal{K} = \text{Inv}_{SU(2)}[\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} \otimes \mathcal{H}_{j_3} \otimes \mathcal{H}_{j_4}]. \quad (1.3.3)$$

Now, clearly the volume of the tetrahedron given by 1.2.3 is invariant under rotation, and hence we have an eigenvalue problem for the Hermitian operator of the volume. It can be shown that the spectrum of this volume operator is discrete [1], [32]. In this paper, we will mostly focus

on the discreteness of a single simplex, namely a tetrahedron. This is not an imposed condition by us. As stated by Carlo Rovelli in [33], “Geometry is not discrete because we focused on a tetrahedron: geometry is discrete because area and volume of any tetrahedron (in fact, any polyhedron) take only quantized values.”

Similar to any quantum mechanical system, the quantum mechanics of a tetrahedron is determined by a set of commuting observables. In our case the complete set of commuting observables are the areas of the faces and the volume. Notice that a classical tetrahedron is determined by the six edge-lengths of the sides. However, in the quantum tetrahedron, we have the typical quantum “fuzziness.” This is analogous to angular momentum in quantum mechanics, where we can simultaneously diagonalize only the total angular momentum and a component of it in one direction [33]. So, we have a fundamental uncertainty in the shape of the tetrahedron. Here, we will focus on the semiclassics of the tetrahedron in an effort to understand the quantum behavior motivated from the classical ground. In the next few chapters, we will develop some of the tools to study the semiclassics, derive the Bohr-Sommerfeld quantization condition and WKB wavefunctions, and some of the deep relation of these tetrahedra with the study of elliptic curves.

Semiclassical Physics

Quantum theory describes the physics at the atomic and subatomic level, and its algebra is fundamentally different from that in the classical regime. For instance, unlike the classical variables, many of the quantum variables (e.g., position and momentum) don't commute. While classical and quantum phenomena can seem very disparate from each-other, semiclassical mechanics can serve as a bridge between the more intuitive classical world and the bewildering quantum world. Semiclassical mechanics is an effective theory in many phenomena where the classical theory can be recovered by taking the limit $\hbar \rightarrow 0$, while the quantum behavior is observed for positive finite \hbar ¹. Historically, many of the results of quantum mechanics were motivated by extending ideas from classical mechanics. For instance, Bohr's quantization of angular momentum of electron in an atom was a strange mixture of Newtonian mechanics and

¹Even though \hbar is a fundamental constant of nature, we can treat it as a parameter in any problem. Setting $\hbar = 0$ amounts to zooming out of the quantum world to the classical world.

quantum ideas [7]. In this chapter, a summary of semiclassical mechanics is presented, and the theory is applied to an example to illustrate how it works.

2.1 The Variational Formulation of Mechanics

An understanding of the variational formulation is necessary to connect classical mechanics with quantum theory. The central object in the variational formulation of mechanics is called an *action functional*. A substantial part of classical mechanics can be derived by studying the stationary points of this object. First, we formally define a *functional*.

Definition 2.1.1. (Functional) Let \mathcal{F} be a function-space over some number field K . A functional F is a map from the function-space \mathcal{F} to the number field K .

$$F : \mathcal{F} \rightarrow K. \quad (2.1.1)$$

If $f \in \mathcal{F}$, a functional F taking f as an input is denoted $F[f(x)]$, where $x \in K$, or briefly by $F[f]$.

Intuitively, a functional is a “function of functions.” In classical mechanics, we are interested in the action functional S of the form $S[\mathbf{q}(t)] = \int_{t_i}^{t_f} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) dt$, where L is a function called the *Lagrangian*, and $\mathbf{q}(t)$ is a trajectory (with fixed end-points) as a function of time t . More precisely, the arguments of the Lagrangian function L are $\mathbf{q} \in \mathbb{Q}$, $\dot{\mathbf{q}} \in T_{\mathbf{q}}\mathbb{Q}$ and $t \in \mathbb{R}$, where \mathbb{Q} is the configuration manifold of the system, and $T_{\mathbf{q}}\mathbb{Q}$ is the tangent space at \mathbf{q} . On physical grounds, we require \mathbb{Q} to be a differentiable manifold.² Formally, we consider $(\mathbf{q}, \dot{\mathbf{q}})$ as an element of a larger space called the *tangent bundle*.

²For a brief discussion of differentiable manifolds, see Appendix ??.

Definition 2.1.2. (Tangent Bundle) Let \mathbb{Q} be a differentiable manifold. Then the tangent bundle of \mathbb{Q} , denoted as $T\mathbb{Q}$, is defined as $T\mathbb{Q} = \{(x, y) : x \in \mathbb{Q} \text{ and } y \in T_x\mathbb{Q}\}$, where $T_x\mathbb{Q}$ is the tangent space of \mathbb{Q} at a point $x \in \mathbb{Q}$.

So, formally a Lagrangian is a differentiable function $L : T\mathbb{Q} \times \mathbb{R} \rightarrow \mathbb{R}$. We assume that this function is sufficiently differentiable, since we want to discard the pathological situations that are not physically reasonable. The usefulness of the action functional and the Lagrangian is due to *Hamilton's principle*, which states that the physical trajectories of a set of particles are the ones that extremize the action functional. In other words, for the physical trajectories $\mathbf{q}(t)$, we have $\delta S = 0$.³

Then it can be shown that the action functional S of the given form is stationary ($\delta S = 0$) when L satisfies the Euler-Lagrange equations (see [21], chapter 3.1.1):

$$\frac{\partial L}{\partial q^\alpha} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^\alpha} = 0, \quad (2.1.2)$$

where q^α is a component of \mathbf{q} . This is a general result in variational calculus, and holds for any (sufficiently nice) Lagrangian L . The Lagrangian that gives rise to a physical trajectory for a set of particles interacting with conservative forces is $L = T - V$, where T is the kinetic energy, and V is the potential energy of the system (see [21], chapter 2.2.1). Euler-Lagrange equation is a system of n second order differential equations on \mathbb{Q} , where n is the number of independent generalized coordinates. Together with the $2n$ initial conditions, the trajectories of the particles are completely determined. However, the formal definition of the Lagrangian as a function from the tangent bundle of a configuration manifold to the real line suggests we look at the problem in a more elegant way. On $T\mathbb{Q}$, the Euler-Lagrange equations can be written as a system of $2n$

³Intuitively, this is similar to finding the extreme values of a function in calculus. However, since S is a functional as opposed to a function, the derivative is defined as $\frac{\delta S}{\delta q} = \lim_{h \rightarrow 0} \frac{S[q+h\phi] - S[q]}{h}$ for arbitrary function ϕ in the function space.

first order differential equations:

$$\frac{dq^\alpha}{dt} = \dot{q}^\alpha, \quad \frac{d\dot{q}^\alpha}{dt} = W^\alpha(\mathbf{q}, \dot{\mathbf{q}}, t), \quad (2.1.3)$$

where $W^\alpha(\mathbf{q}, \dot{\mathbf{q}}, t)$ can be obtained from the Euler-Lagrange equation. This gives an explicit expression for the evolution of q^α , but the evolution of \dot{q}^α is more complicated, and is not directly available from the Euler-Lagrange equation. This problem is circumvented by using a different mathematical structure than the tangent bundle. Instead of adjoining the tangent space $T_p\mathbb{Q}$ to each point p of \mathbb{Q} , we adjoin the cotangent space $T_p^*\mathbb{Q}$ to each point. Recall that the cotangent space $T_p^*\mathbb{Q}$ is the dual space of the tangent space $T_p\mathbb{Q}$, i.e., the set of linear functionals from $T_p\mathbb{Q}$ to \mathbb{R} . The resulting space is called a *cotangent bundle*.

Definition 2.1.3. (Cotangent bundle) Let \mathbb{Q} be a differentiable manifold. Let $T_x\mathbb{Q}$ denote the tangent space of \mathbb{Q} at a point $x \in \mathbb{Q}$, and let $T_x^*\mathbb{Q}$ denote the dual space of $T_x\mathbb{Q}$. Then the cotangent bundle of \mathbb{Q} is defined as $T^*\mathbb{Q} = \{(x, y) : x \in \mathbb{Q} \text{ and } y \in T_x^*\mathbb{Q}\}$. In the context of classical mechanics, the space $T^*\mathbb{Q}$ is referred to as the *phase space*.

If we define the canonical momentum corresponding to q^α as $p_\alpha = \frac{\partial L}{\partial \dot{q}^\alpha}$, then as discussed in the Appendix ??, p_α is an element of $T_q^*\mathbb{Q}$. From the Euler-Lagrange equation, we then recover a rather nice form of the evolution of q^α and p_α :

$$\frac{dq^\alpha}{dt} = \dot{q}^\alpha, \quad \frac{dp_\alpha}{dt} = \frac{\partial L}{\partial q^\alpha}(\mathbf{q}, \dot{\mathbf{q}}, t). \quad (2.1.4)$$

This is not quite in the desired form, since we want all our equations to depend on the generalized coordinates and generalized momenta ⁴. Notice that we can do this by inverting the relation $p_\alpha = \frac{\partial L}{\partial \dot{q}^\alpha}$ to get $\dot{q}^\alpha(\mathbf{q}, \mathbf{p}, t)$ and substituting it in the right hand side of equations (2.1.4).

⁴In this context, we will use the word “generalized” and “canonical” interchangeably.

This substitution essentially removes the asymmetry between our treatment of the generalized coordinates and momenta. Although this is not exactly seen in (2.1.4), it can be explicitly presented using the Hamiltonian function.

We want to write the right hand side of the equations (2.1.4) explicitly as a function of $(\mathbf{q}, \mathbf{p}, t)$.

Suppose $L(\mathbf{q}, \dot{\mathbf{q}}, t) \equiv \tilde{L}(\mathbf{q}, \dot{\mathbf{q}}(\mathbf{q}, \mathbf{p}, t), t)$. Then we have $\frac{\partial \tilde{L}}{\partial q^\alpha} = \frac{\partial L}{\partial q^\alpha} + \frac{\partial L}{\partial \dot{q}^\beta} \frac{\partial \dot{q}^\beta}{\partial q^\alpha} = \frac{\partial L}{\partial q^\alpha} + p_\beta \frac{\partial \dot{q}^\beta}{\partial q^\alpha}$. Taking all the functions of $(\mathbf{q}, \mathbf{p}, t)$ on one side, we get:

$$\frac{\partial L}{\partial q^\alpha} = -\frac{\partial}{\partial q^\alpha} \left[p_\beta \dot{q}^\beta(\mathbf{q}, \mathbf{p}, t) - \tilde{L}(\mathbf{q}, \mathbf{p}, t) \right]. \quad (2.1.5)$$

Similarly, we can take the partial derivative of \tilde{L} with respect to p_α and get $\frac{\partial \tilde{L}}{\partial p_\alpha} = \frac{\partial L}{\partial p_\alpha} \frac{\partial \dot{q}^\beta}{\partial p_\alpha} = p_\beta \frac{\partial \dot{q}^\beta}{\partial p_\alpha}$. Using the fact that $\frac{\partial}{\partial p_\alpha} (p_\beta \dot{q}^\beta) = \dot{q}^\alpha + p_\beta \frac{\partial \dot{q}^\beta}{\partial p_\alpha}$, we can write \dot{q}^α as

$$\dot{q}^\alpha = \frac{\partial}{\partial p_\alpha} \left[p_\beta \dot{q}^\beta(\mathbf{q}, \mathbf{p}, t) - \tilde{L}(\mathbf{q}, \mathbf{p}, t) \right]. \quad (2.1.6)$$

Now, let $H(\mathbf{q}, \mathbf{p}, t) = p_\beta \dot{q}^\beta(\mathbf{q}, \mathbf{p}, t) - \tilde{L}(\mathbf{q}, \mathbf{p}, t)$. Then the pair of equations (2.1.4) becomes:

$$\dot{q}^\alpha = \frac{\partial H}{\partial p_\alpha}, \quad \dot{p}_\alpha = -\frac{\partial H}{\partial q^\alpha} \quad (2.1.7)$$

These are *Hamilton's canonical equations*, and the function $H(\mathbf{q}, \mathbf{p}, t)$ is called the *Hamiltonian* of the system. Hamilton's equations describe the dynamics of the system on the phase space. This can be cast in a way that is closer to quantum mechanics using the *Poisson bracket* formulation.

Definition 2.1.4. (Poisson Bracket) Let $T^*\mathbb{Q}$ be the cotangent bundle of a differentiable manifold \mathbb{Q} . Let f and g be two functions on $T^*\mathbb{Q}$. Then the Poisson bracket of f with g is defined

as⁵

$$\{f, g\} = \frac{\partial f}{\partial q^\alpha} \frac{\partial g}{\partial p_\alpha} - \frac{\partial f}{\partial p_\alpha} \frac{\partial g}{\partial q^\alpha}. \quad (2.1.8)$$

Using the Poisson bracket, we can rewrite Hamilton's equations as

$$\dot{q}^\alpha = \{q^\alpha, H\} \quad \dot{p}_\alpha = \{p_\alpha, H\}. \quad (2.1.9)$$

In general, the time evolution of a dynamical function f (namely, a function on $T^*\mathbb{Q}$) can be written as

$$\frac{df(q, p, t)}{dt} = \frac{\partial f}{\partial q^\alpha} \frac{dq^\alpha}{dt} + \frac{\partial f}{\partial p_\alpha} \frac{dp_\alpha}{dt} + \frac{\partial f}{\partial t} = \{f, H\} + \frac{\partial f}{\partial t}. \quad (2.1.10)$$

The last equality is obtained using (2.1.7) and (2.1.8). We can also compute the “fundamental Poisson brackets,” which are the Poisson brackets between the generalized coordinates and momenta:

$$\{q^\alpha, q^\beta\} = 0, \quad \{p_\alpha, p_\beta\} = 0, \quad \{q^\alpha, p_\beta\} = \delta_\beta^\alpha. \quad (2.1.11)$$

It can be proved from the definition that the Poisson bracket satisfies bilinearity, anti-commutativity and the Jacobi identity. These properties define an algebraic structure called a *Lie algebra*. In fact the function space $\mathcal{F}(T^*\mathbb{Q})$ is a Lie algebra where the Lie bracket is defined as the Poisson bracket. A reader familiar with quantum mechanics has already seen another form of Lie bracket, namely the *commutator* of linear operators in *Hilbert space*. This is where the boundary between classical mechanics and quantum mechanics becomes very thin. As described in [14] by Paul Dirac, in quantum mechanics we simply make the following replacement

⁵In the mathematical literature, a Poisson bracket is more generally defined in terms of anticommutativity, bilinearity, Leibniz's rule and the Jacobi identity. This definition is equivalent in the case of canonical coordinates and momenta in phase space.

of a classical Poisson bracket with the quantum mechanical commutator:

$$\{\cdot, \cdot\} \rightarrow \frac{1}{i\hbar}[\cdot, \cdot]. \quad (2.1.12)$$

Classical mechanics as a limit of quantum theory is more obviously seen in the *Hamilton-Jacobi* formulation. First, we present a simple derivation of the Hamilton-Jacobi equation, and then we relate it to the Schrödinger equation, establishing the connection between the classical and quantum realm. Consider the action integral $S = \int_{t_0}^t dt L(\mathbf{q}, \dot{\mathbf{q}}, t)$. Using the definition of Hamiltonian, we can rewrite this as:

$$S = \int_{t_0}^t dt (p_\alpha \dot{q}^\alpha - H) = \int_{q_0=q(t_0)}^q p_\alpha dq^\alpha - \int_{t_0}^t H dt. \quad (2.1.13)$$

This is a line integral in the q - t plane, and so we have:⁶

$$\frac{\partial S}{\partial q^\alpha} = p_\alpha, \quad (2.1.14)$$

$$\frac{\partial S}{\partial t} = -H(q, p, t) = -H\left(q, \frac{\partial S}{\partial q}, t\right). \quad (2.1.15)$$

Here, (2.1.14) and (2.1.15) give us a momentum (vector) field and an energy field on the configuration space. Equation (2.1.15) is called the Hamilton-Jacobi equation. It is a first order partial differential equation, whose solution (with proper initial conditions) determines the trajectory of the particles. These trajectories are the integral curves of the momentum field. Equation (2.1.14) also gives us a very useful insight about the wave-particle duality. Consider a single particle in Cartesian coordinates. Then (2.1.14) tells us that the momentum $\mathbf{p} = \nabla S$. Hence, the momentum of the particle is perpendicular to the surfaces with constant action S .

⁶Here $\frac{\partial S}{\partial q} := (\frac{\partial S}{\partial q^1}, \dots, \frac{\partial S}{\partial q^n})$, where n is the number of degrees of freedom.

This is very similar to geometric optics, where the momentum of a photon is perpendicular to the wavefront (surfaces with constant phase). This, of course, is an analogy. However, we shall see in the next section how this is related to single-particle quantum mechanics.

Before relating the classical and quantum picture, we point out a subtlety in the definition of action in classical mechanics. There are usually two different definitions of action—one is the integral of the Lagrangian ($S = \int_{t_i}^{t_f} L dt$), which is referred to as the action, and the other is the integral of momentum ($S_0 = \int_{\mathbf{q}_i}^{\mathbf{q}_f} \mathbf{p} \cdot d\mathbf{q}$), which is referred to as the *abbreviated action*. In the action integral, the fixed quantities are the initial and final times and the end points of a trajectory. On the other hand, in the abbreviated action integral, we fix the endpoints and the total energy of the system.⁷ Despite the difference, the variational principles arising from extremizing S and S_0 coincide for a conservative system. In our study of semiclassical mechanics, we will always use the abbreviated action S_0 since we are interested in conservative systems. We will follow the convention of referring to the abbreviated action as the action.

2.2 From Schrödinger to Hamilton-Jacobi

In this section, we establish a precise connection between the Hamilton-Jacobi equation and Schrödinger equation. We will assume the case of only one particle moving in three-dimensions. Generalization to multi-particle (non-interacting) systems is not difficult. Even in their usual appearance, the two equations look very similar:

$$\text{Hamilton-Jacobi: } \frac{\partial S}{\partial t} = -H\left(q, \frac{\partial S}{\partial q}, t\right) \quad (2.2.1)$$

$$\text{Schrödinger: } i\hbar \frac{\partial \Psi}{\partial t} = H(\hat{q}, \hat{p}, t)\Psi. \quad (2.2.2)$$

⁷See Chapter 8.6 of [17] for details.

We assume that the Hamiltonian is of the form $H(q, p) = \frac{p^2}{2m} + V(q)$. Then, using (2.1.14), the Hamilton-Jacobi equation (2.2.1) becomes:

$$\frac{\partial S}{\partial t} = -\frac{||\nabla S||^2}{2m} - V(q) \quad (2.2.3)$$

For the Schrödinger's equation, a natural ansatz for the solution is $\Psi(q, t) = A(q, t)e^{\frac{i}{\hbar}\varphi(q, t)}$.

Plugging this into (2.2.2) and cancelling the exponentials, we get:

$$-A\frac{\partial\varphi}{\partial t} + i\hbar\frac{\partial A}{\partial t} = \left(\frac{1}{2m}(A\nabla\varphi \cdot \nabla\varphi) + VA\right) - \hbar\left(\frac{i}{2m}A\nabla^2\varphi + \frac{i}{m}\nabla A \cdot \nabla\varphi\right) - \frac{\hbar^2}{2m}\nabla^2 A. \quad (2.2.4)$$

At this point, we treat \hbar as a parameter in the problem, and hence we can equate the coefficients of the different powers of \hbar from the left and right side. After some simplification, we get:

$$\text{Zeroth Order in } \hbar: \frac{\partial\varphi}{\partial t} = -\frac{1}{2m}||\nabla\varphi||^2 - V, \quad (2.2.5)$$

$$\text{First Order in } \hbar: \frac{\partial A}{\partial t} + \frac{1}{2m}(2\nabla\varphi \cdot \nabla A + A\nabla^2\varphi) = 0 \quad (2.2.6)$$

The zeroth order term in the Schrödinger equation is a Hamilton-Jacobi equation of the form (2.2.3). To make it clear, we make the identification $\varphi \leftrightarrow S$. With this identification, the Hamilton-Jacobi equation comes directly from the Schrödinger equation as a first approximation. The first order approximation in \hbar is called the *amplitude transport equation*. Since A in our ansatz is of the form of an (real) amplitude of a wave function, it is natural to interpret $\rho(q, t) \equiv A(q, t)^2$ as the probability density of the particle at a location q and time t . Also, (2.1.14) motivates us to define a velocity field $\mathbf{v} \equiv \frac{1}{m}\nabla S$. With these two definitions, the first order

amplitude transport equation becomes

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (2.2.7)$$

This is a continuity equation that is analogous to the conservation of probability in quantum mechanics. Hence, the ansatz that we started with is a very sensible one, and produces some of the essential features of the quantum theory. This ansatz, namely,

$$\Psi(q, t) = A(q, t) e^{\frac{i}{\hbar} S(q, t)} \quad (2.2.8)$$

is called the WKB wavefunction.⁸ The WKB method is a general technique to find the asymptotic solutions of certain differential equations. In this particular instance, we applied it to the Schrödinger equation. A properly normalized WKB wavefunction requires three ingredients—the action in the exponent, the amplitude factor and a correction factor due to certain singularities. As discussed in the previous section, the action as a function of the generalized coordinate q with energy E as a parameter is given by⁹

$$S(q, E) = \int_{q_0}^q p(q', E) dq', \quad (2.2.9)$$

where q_0 is some conventional point on the constant energy manifold. This is, however, not the most general form of the action integral that appears in the WKB wavefunction. For the purpose of applying the theory to compute the wavefunctions of a tetrahedral grain of space, we need a small generalization of (2.2.9). An action integral for a WKB eigenfunction requires

⁸This is named after Gregor Wentzel, Hendrik Anthony Kramers, Léon Brillouin and Harold Jeffreys. In fact this is a special case of the asymptotic series in the exponent of the form $\exp[\frac{i}{\hbar}(S_0 + (\hbar/i)S_1 + (\hbar/i)^2 S_2 + \dots)]$. Here, we have $S_0 = S$ and $S_1 = \ln A$. In what follows, we will often use this notation.

⁹We will only consider time independent Schrödinger equation, so time as an argument of the action and other functions will often be dropped.

both an integral along a constant E -manifold as well as along a constant q -manifold. Suppose

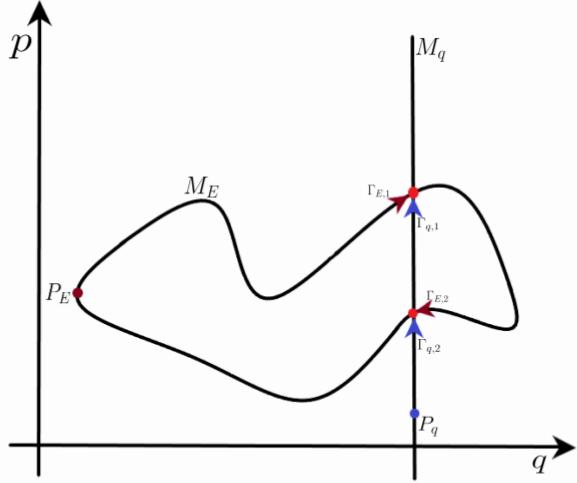


Figure 2.2.1: Contours of action integral in one-dimension.

M_E and M_q are respectively manifolds with fixed energy and fixed generalized coordinate on the phase space. Let P_E and P_q be two conventional initial points of integration on the two manifolds respectively. Also, suppose that the two manifolds M_E and M_q intersect at points $\{C_1, C_2, \dots, C_n\}$ for $n \in \mathbb{N}$. Denote the path from the conventional point P_E to C_i as $\Gamma_{E,i}$ and the path from the conventional point P_q to C_i as $\Gamma_{q,i}$. Then the exponential part of the WKB formula (2.2.8) for each $i \in \{1, 2, \dots, n\}$ is given by [19]:

$$\exp \left[i \left(S_{E,i} - S_{q,i} - \mu_i \frac{\pi}{2} \right) \right], \quad (2.2.10)$$

where μ_i is a Maslov index (see next section), and

$$S_{E,i} = \int_{\Gamma_{E,i}} p(q', E) dq' \quad \text{and} \quad S_{q,i} = \int_{\Gamma_{q,i}} p(q', E) dq'. \quad (2.2.11)$$

Since we are interested in the energy eigenfunctions of the Schrödinger equation, following [27], the amplitude factor is given by

$$A(q) = \frac{1}{(2\pi i)^{1/2}} \left| \det \frac{\partial^2 S}{\partial q \partial E} \right|^{\frac{1}{2}}, \quad (2.2.12)$$

where E is the energy of the system. As an example, suppose that we have a single particle in a potential well $V(q)$. The classical Hamiltonian for this problem is $H = \frac{p^2}{2m} + V(q)$, where p is the momentum of the particle. We know that $\frac{\partial S}{\partial q} = p$, and on a constant energy curve (specified by $H = E$) in the phase space, $p = \pm \sqrt{2m(E - V(q))}$. So, $\left| \frac{\partial^2 S}{\partial q \partial E} \right| = \left| \frac{\partial p}{\partial E} \right| = \frac{m}{p}$. Therefore, the amplitude for the WKB wavefunction (2.2.8) is given by

$$A(q) = \sqrt{\frac{m}{2\pi i p}} \sim \sqrt{\frac{m}{2\pi p}}. \quad (2.2.13)$$

The final ingredient for the WKB wavefunction is the Maslov index, which is necessary when we have branching points on our manifold of constant energy. This is our topic of the next section. Before that, we will briefly examine the regime of validity of the WKB approximation. We consider the stationary (time-independent) part of $\varphi = S = S_0$ and $S_1 = \ln A$ in equation (2.2.4). Notice that for a time-independent Schrödinger equation, the left hand side of (2.2.4) vanishes. Then the right hand side implies that the coefficient in each order of \hbar vanishes. For the first order term, this means (using the fact that $\nabla S_0 = p$) that

$$\|\nabla S_1\| = \frac{\|\nabla^2 S_0\|}{\|\nabla S_0\|} = \frac{\|\nabla p\|}{\|p\|}. \quad (2.2.14)$$

It is also necessary that a first order term is much smaller compared to the zeroth order term. For a rough necessary estimate, we will compare the term $A\nabla^2 S$ in the first order with the

term $\frac{1}{2m}A||\nabla S||^2$ in the zeroth order. It is necessary that $\frac{1}{2m}||\nabla S_0||^2 \gg \frac{\hbar}{m}||(\nabla A/A) \cdot \nabla S_0|| = \frac{\hbar}{m}||\nabla \ln A \cdot \nabla S_0||$. We then have, using (2.2.14), that

$$||p|| \gg \hbar||\nabla S_1|| = \hbar \frac{||\nabla p||}{||p||}. \quad (2.2.15)$$

Using the relation $p^2 = 2m(E - V)$, we can deduce that $||\nabla V|| = \frac{1}{m}||p|| \cdot ||\nabla p||$. Multiplying by the local De Broglie wavelength $\lambda \approx \frac{\hbar}{||p||}$ and using (2.2.15), we get

$$\lambda||\nabla V|| \ll \frac{||p||^2}{2m}. \quad (2.2.16)$$

This is a necessary condition for the WKB approximation to be valid. Physically, this means that the potential energy can not vary too rapidly over the distance of the particle's De Broglie wavelength compared to the kinetic energy. This condition is certainly violated at the classical turning points of the potential, where $||p|| = 0$. Hence, the WKB method can be valid at the classically allowed and forbidden regions away from the classical turning points. However, we need a connection formula to join the two separate pieces of the solution together.

This fact along with the form of the momenta and energy (Hamiltonian) fields being related to each other by the derivatives of the action as in (2.1.14) and (2.1.15) leads us to look at the problem from a more general mathematical point of view. In the next section, we will introduce *Lagrangian manifolds* and *singular points* on them, which will be productive in understanding the peculiar behavior of WKB wavefunctions near classical turning points.¹⁰

¹⁰This next section is motivated by Robert Littlejohn's unpublished lectures on classical dynamics.

2.3 Lagrangian Manifolds and Caustics

The momentum in the Hamilton-Jacobi theory is not arbitrary, but rather of a very special form. It is the gradient of a function (as in (2.1.14)). Hence, the momentum field is irrotational. In a $2n$ dimensional phase space, where $n \in \mathbb{N}$, the condition (2.1.14) poses n independent constraints. So, we generally get an n dimensional surface in the $2n$ dimensional phase space. A mathematical treatment of such momentum fields requires a small generalization of this idea. For this purpose, we define a Lagrangian manifold on the phase space.

Definition 2.3.1. (Lagrangian Manifold) Consider a classical system described by n generalized coordinates (q^1, q^2, \dots, q^n) , where $n \in \mathbb{N}$. Then the phase space \mathcal{M}^{2n} of the system is $2n$ dimensional. A Lagrangian manifold \mathcal{L}^n is an n -dimensional submanifold of \mathcal{M}^{2n} such that if $dz_1 = (d\mathbf{q}, d\mathbf{p})$ and $dz_2 = (d\mathbf{q}', d\mathbf{p}')$ are tangent vectors to \mathcal{L}^n , then we have¹¹

$$\omega(dz_1, dz_2) := d\mathbf{p} \cdot d\mathbf{q}' - d\mathbf{q} \cdot d\mathbf{p}' = 0. \quad (2.3.1)$$

Here the dot products in (2.3.1) are the standard Euclidean dot products.

One special (and obvious) case is that all smooth curves in a two dimensional phase space are Lagrangian manifolds. This is so because at any point of the curve, the tangent vectors are linearly dependent.

Now, suppose that our generalized coordinates and momenta live on some Lagrangian manifold in the phase space. Also, assume that the momenta can be expressed as a function of the generalized coordinates, that is $p_i = p_i(q^i)$. Then we have $dp_i = \frac{\partial p_i}{\partial q^j} dq^j$ and $dp'_i = \frac{\partial p_i}{\partial q'^j} dq'^j$.

¹¹The d refers to infinitesimal displacement vector, not a differential form.

Then using (2.3.1), we have

$$d\mathbf{p} \cdot d\mathbf{q}' - d\mathbf{p}' \cdot d\mathbf{q} = \frac{\partial p_i}{\partial q^j} dq^j dq'^i - \frac{\partial p_i}{\partial q'^j} dq'^j dq^i = \left(\frac{\partial p_i}{\partial q^j} - \frac{\partial p_i}{\partial q'^j} \right) dq^i dq'^j = 0. \quad (2.3.2)$$

As dq^i and dq'^j are arbitrary, we have $\frac{\partial p_i}{\partial q^j} = \frac{\partial p_i}{\partial q'^j}$. This relation guarantees that the canonical momentum can be expressed as a gradient. In other words, $p_i = \frac{\partial S}{\partial q^i}$ for some function S . Here, S is indeed the action integral as can be seen by comparing this with (2.1.13). In a 2-dimensional phase space, this relation is trivially satisfied, and so every smooth curve in 2D is a Lagrangian manifold.¹²

Since a Lagrangian manifolds \mathcal{L}^n is an n dimensional hypersurface in a $2n$ dimensional phase space, we can locally parameterize \mathcal{L}^n using n coordinates. Let $\mathbf{u} = (u^1, u^2, \dots, u^n)$ be local coordinates on the Lagrangian manifold \mathcal{L}^n . Then the generalized coordinates and canonical momenta can be expressed (locally) as a function of $u = (u^1, u^2, \dots, u^n)$ i.e. $\mathbf{q} = \mathbf{q}(\mathbf{u})$ and $\mathbf{p} = \mathbf{p}(\mathbf{u})$. Now, if the Jacobian matrix $\frac{\partial \mathbf{q}}{\partial \mathbf{u}}$ is not singular, then we can invert $\mathbf{q} = \mathbf{q}(\mathbf{u})$, and get $\mathbf{u} = \mathbf{u}(\mathbf{q})$. In that case, we can write the momentum as a function of the coordinates, that is $\mathbf{p} = \mathbf{p}(\mathbf{q}(\mathbf{u}))$. Using the multivariable chain rule, we can write

$$\frac{\partial p_i}{\partial q^j} = \frac{\partial p_i}{\partial u^k} \frac{\partial u^k}{\partial q^j}. \quad (2.3.3)$$

Notice that when the Jacobian matrix $\frac{\partial \mathbf{q}}{\partial \mathbf{u}}$ is singular, (2.3.3) is not well-defined. The set of points where this Jacobian matrix is singular are called the *singular points* of \mathcal{L}^n , and the projections of these points on the configuration space are called *caustics*.¹³ A simple visualizable instance of the occurrence of caustics of a Lagrangian manifold happens in one di-

¹²Notice that, this derivation is very much dependent on the fact that we can write \mathbf{p} as a function of \mathbf{q} .

¹³We will often conflate the two terms, but this doesn't cause any confusion.

dimension. Consider the Lagrangian manifold given in Figure 2.3.1. At the indicated brown points on the manifold, it is clear that $\frac{dp}{dq}$ diverges, and hence those are singular points.

Geometrically, it is clear that the points of singularity occur when a tangent vector on the manifold projects down to a point in one of the coordinates of the configuration space. This can also be seen analytically.

Consider a small tangent vector $\delta z = (d\mathbf{q}, d\mathbf{p})$ on a Lagrangian manifold. Using the chain rule, we get $d\mathbf{q} = \frac{\partial \mathbf{q}}{\partial \mathbf{u}} d\mathbf{u}$ and $d\mathbf{p} = \frac{\partial \mathbf{p}}{\partial \mathbf{u}} d\mathbf{u}$. If the matrix $\frac{\partial \mathbf{q}}{\partial \mathbf{u}}$ is singular, then there is some non-zero $d\mathbf{u}$ for which $d\mathbf{q}$ is constantly zero. Hence, we get the projection of a tangent vector of the manifold to be a point on some coordinate in the configuration space. This is also a classical turning point in the configuration space.

The locations of caustics very much depend on the coordinatization of the Lagrangian manifold. Hence, we can change representations at certain regions on the manifold to avoid the caustics. In one dimension, we can certainly see that the caustics never occur at the same place in position and momentum representation. It was shown by Maslov that there is always some patch-work of position and momentum representation such that we can avoid the caustics [29].

In general, we will need to consider both position and momentum representations of the action integral to calculate the action in the WKB ansatz properly. We now focus on the Hamilton-Jacobi equation (2.2.1), since this is the equation we need to solve to find the action. If our Lagrangian manifold doesn't have a caustic, we consider the action $S(q, p)$ as the generator

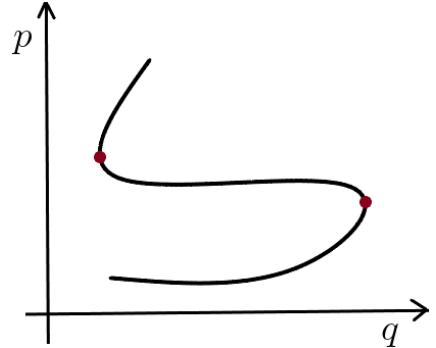


Figure 2.3.1: The brown points are the singularities on the 1-D Lagrangian manifold depicted here on a 2-D phase space.

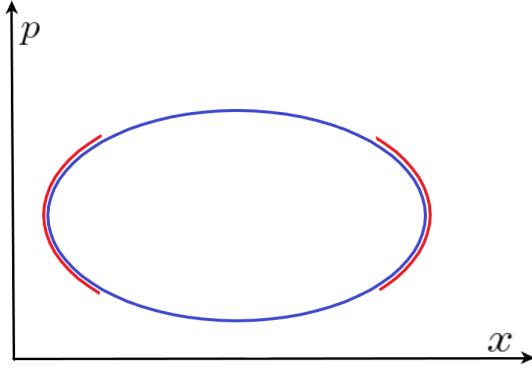


Figure 2.3.2: Here is a cover of a one-dimensional Lagrangian manifold where we avoid the caustics by changing representations. We work in the position basis over the whole manifold except the red region, where we switch to the momentum basis.

of the manifold. In the case of manifolds with caustics, we need to consider a patch-work of generating functions.

Consider a one-dimensional Lagrangian manifold \mathcal{L}' in a two-dimensional phase space at $t = 0$. Then \mathcal{L}' has some generating function $S(q', t')$. It turns out that under time evolution, the final manifold \mathcal{L}'' is also Lagrangian.¹⁴ Hence, \mathcal{L}'' also has some generating function. This generating function should satisfy the Hamilton-Jacobi equation and the initial condition. As shown in [28], the generating function $S(q'', t'')$ for the manifold \mathcal{L}'' is given by

$$S(q'', t'') = S(q', t') + R(q'', t''; q', t'), \quad (2.3.4)$$

where $R(q'', t''; q', t')$ is Hamilton's principal function, which is the line integral of $pdq - Hdt$ from (q', t') to (q'', t'') along a physical orbit. By applying the chain rule, we have $\frac{\partial S(q'', t'')}{\partial q''} = p''$ and $\frac{\partial S(q'', t'')}{\partial t''} = -H(q'', p'', t'')$.¹⁵ If we let $q'' \mapsto q'$ and $t'' \mapsto t'$, then we also recover the initial conditions, since the Hamilton's principal function vanishes. Hence $S(q'', t'')$ indeed satisfy the Hamilton-Jacobi equation along with the required initial condition.

¹⁴It is not very hard to prove this using the Liouville's theorem from classical mechanics.

¹⁵Notice that t' , t'' and q'' are the independent parameters/variables here. Once we know these three, we can write $q' = q'(q'', t', t'')$.

At the level of amplitude transport equation (2.2.7), we know that the probability density of particles is the square of the WKB amplitude. In other words, $\rho = A^2$. By conservation of probability, we know that $\rho(q', t')dq' = \rho(q'', t'')dq''$. Generalizing this in higher dimensions, we get

$$A(\mathbf{q}'', t'') = A(\mathbf{q}', t') \left| \det \frac{\partial \mathbf{q}'}{\partial \mathbf{q}''} \right|^{1/2}. \quad (2.3.5)$$

Then, using (2.3.4) and (2.3.5), we get the solution of the initial value problem to be

$$\psi(\mathbf{q}'', t'') = A(\mathbf{q}', t') \left| \det \frac{\partial \mathbf{q}'}{\partial \mathbf{q}''} \right|^{1/2} \exp \frac{i}{\hbar} [S(\mathbf{q}', t') + R(\mathbf{q}'', t''; \mathbf{q}', t')]. \quad (2.3.6)$$

We can see that the wavefunction diverges when \mathbf{q}'' is a caustic. As discussed previously, we switch to a momentum representation near these points. For now, consider a one dimensional case. The momentum wavefunction has a similar WKB approximation, which is given by $\phi(p) \sim e^{iT(p)}$, where $T(p) = - \int^p q dp'$ is the action in the momentum space. Here, $q = q(p)$ determined by $T(p)$, is a position field in the momentum space. Now, given the momentum space wavefunction $\phi(p)$, we want to perform an inverse Fourier transform on it to analyze how it changes around the caustic (c in Figure 2.3.3).

Note that the derivatives of the momentum space action integrals are

$$T'(p) = -q_L(p), \quad T''(p) = \left(\frac{\partial q}{\partial p} \right) \Big|_L. \quad (2.3.7)$$

Here, the fact that the derivative is taken on the Lagrangian manifold is emphasized by the subscript. We will take the inverse Fourier transform of the WKB wavefunction in the momentum space at point 1 and 2 in Figure 2.3.3 to understand how the position wavefunction change

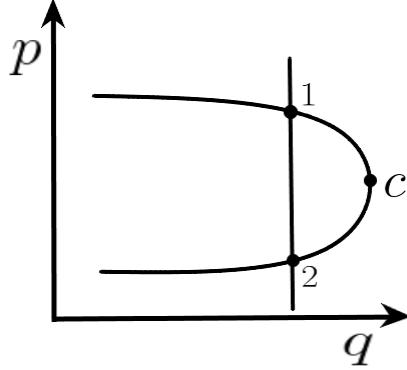


Figure 2.3.3: A Lagrangian manifold in the phase space. The two branches about the caustic are labeled by 1 and 2. Near the caustic c , we switch to a momentum representation.

across the caustic. It turns out that the amplitude is continuous across the caustic, so we will only calculate the phase contribution:

$$\psi(q) \sim \int e^{i(pq+T(p))} dp. \quad (2.3.8)$$

We will use stationary phase approximation to evaluate the integral. Note that the exponent is stationary when $q + T'(p) = 0$, or $q = q_L$. Then we have

$$\psi(q) \sim \int e^{i(pq+T(p))} dp \sim \int e^{\frac{i}{2}T''(p-p_L)^2} dp \sim \begin{cases} e^{i\pi/4} & \text{if } T'' > 0, \\ e^{-i\pi/4} & \text{if } T'' < 0. \end{cases} \quad (2.3.9)$$

Here, we have used the symbol \sim to denote that the rest of the integral is the same for both branches. The two cases in Equation (2.3.9) give rise to the Maslov index. It is clear from Figure 2.3.3 that $T''(p_c) = 0$, where p_c is the momentum coordinate of the caustic. Depending on whether T'' goes from positive to negative or negative to positive, we have different changes in Maslov index ($\Delta\mu$). Since $\text{sgn}(T'') = -\text{sgn}(dp/dq)$ away from the caustic, and the change in

phase in (2.3.9) is $\frac{\pi}{2}$, we have the following rule for the change in Maslov index:

$$\frac{dp}{dq} \text{ goes } - \rightarrow + \implies \Delta\mu = +1, \quad \text{and} \quad \frac{dp}{dq} \text{ goes } + \rightarrow - \implies \Delta\mu = -1. \quad (2.3.10)$$

With the conceptual understanding of the origin of Maslov index in one dimension, we now focus on its calculation. As before, we will only consider a one-dimensional Lagrangian manifold on phase space given by a fixed energy $H = E$, where H is the Hamiltonian. Since we are switching representations from a position basis to a momentum basis near the caustic, this is obtained by the canonical transformation $q \rightarrow p$ and $p \rightarrow -q$.¹⁶ Hence, working on a basis (say, q) involves a change in sign near the caustic. Let γ be a shorthand for $T'' = \left(\frac{\partial q}{\partial p}\right) \Big|_L$. Suppose t is the flow parameter along constant energy.¹⁷ Then we have

$$\gamma = \left(\frac{\partial q}{\partial p}\right) \Big|_L = \left(\frac{\partial q}{\partial t}\right) \Big|_E \left(\frac{\partial t}{\partial p}\right) \Big|_E = \frac{\dot{q}}{\dot{p}} = \frac{\{q, H\}}{\{p, H\}}. \quad (2.3.11)$$

The change of sign at the caustic in Equation (2.3.9) is characterized by the flow of γ . Taking the t -derivative of γ , we get

$$\dot{\gamma} = \frac{\ddot{q}}{\dot{p}} - \frac{\dot{q}\ddot{p}}{\dot{p}^2}. \quad (2.3.12)$$

We know that the caustic is a turning point in our classical phase space. So $\dot{q} = 0$. Also, at the caustic, we have $\nabla_{(q,p)} H \propto \dot{q}$.¹⁸ This is clear geometrically from Figure 2.3.3, but can also be seen as a vanishing of symplectic form at the caustic (See [19], Chapter 2). Hence, we have $dE_c = edq_c$, where e is a proportionality constant. The subscript c is used to emphasize that we

¹⁶A canonical transformation is defined as a transformation that leaves the form of Hamilton's equation invariant. For details, see [17].

¹⁷In this case, t is time. However, for a general Hamiltonian system, it could be some other parameter.

¹⁸Here, the gradient is just $\hat{q}\frac{\partial}{\partial q} + \hat{p}\frac{\partial}{\partial p}$.

are evaluating everything at the caustic. So at the caustic, we have

$$\dot{p} = \{p, H\} = \frac{\partial H}{\partial q} = e. \quad (2.3.13)$$

Then $\dot{\gamma} = -\Delta\mu$ at the caustic is given by:

$$\dot{\gamma}_c = \frac{\ddot{q}_c}{\dot{p}_c} = \frac{1}{e} \{\{q, H\}, H\}. \quad (2.3.14)$$

The calculation of the Maslov index completes our general discussion of semiclassical mechanics.

Now, we will apply the WKB method to a quantum harmonic oscillator to illustrate an example.

2.4 WKB Wavefunctions of a Simple Harmonic Oscillator

The application of semiclassics to a quantum tetrahedron in the next chapter is rife with subtleties and long calculations. To get a clear understanding of the methods, having a simple example in our mind is very helpful. Here, we illustrate the applications of the methods discussed in the previous sections to a harmonic oscillator. This example is simple, but captures the essential subtlties of the theory. One can refer back to this example when a confusion arises in a more complicated problem. Consider a one-dimensional simple harmonic oscillator with mass $m = 1$ and angular frequency $\omega = 1$. Then, the Hamiltonian of this system is given by:

$$H(q, p) = \frac{1}{2}(q^2 + p^2). \quad (2.4.1)$$

We know from quantum mechanics that the exact eigenfunctions of this oscillator are obtained by solving the time-independent Schrödinger equation. Set $\hbar = 1$. Then the n -th eigenfunction

is given by:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \pi^{1/2}}} e^{-\frac{x^2}{2}} \tilde{H}_n(x), \quad (2.4.2)$$

where $\tilde{H}(x)$ is the n -th Hermite polynomial. As described in the previous sections, to calculate the WKB eigenfunctions for this problem, we need three ingredients—the action, the amplitude and the maslov indices at the caustics. First, we calculate the action integral starting from the

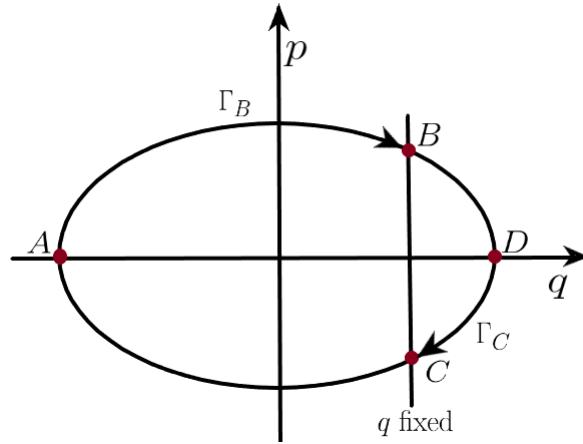


Figure 2.4.1: Orbit of a harmonic oscillator in the phase space. The point A is a conventional initial point for the action integral. The vertical line corresponds to a fixed but arbitrary q . Due to the two branches, we have to consider the integral from A to both the intersection points B and C . The point D is a caustic on our Lagrangian manifold that the orbit crosses.

conventional point A to a point with fixed but arbitrary q along the orbit in the phase space. Let E be the energy of the oscillator. Then, the coordinate of the point A is $(-\sqrt{2E}, 0)$. There are two branches as shown in the Figure 2.4.1. Denote the two paths as Γ_B and Γ_C respectively. Then the two action integrals are:

$$S_{AB} = \int_{\Gamma_B} p(q) dq = \int_{-\sqrt{2E}}^q \sqrt{2E - q^2} dq = \frac{\pi E}{2} + E \arcsin\left(\frac{q}{\sqrt{2E}}\right) + \frac{q}{2} \sqrt{2E - q^2}, \quad (2.4.3)$$

$$\begin{aligned} S_{AC} &= \int_{\Gamma_C} p(q) dq = \int_{-\sqrt{2E}}^{\sqrt{2E}} \sqrt{2E - q^2} dq + \int_{\sqrt{2E}}^q -\sqrt{2E - q^2} dq \\ &= \frac{3\pi E}{2} - E \arcsin\left(\frac{q}{\sqrt{2E}}\right) - \frac{q}{2} \sqrt{2E - q^2}. \end{aligned} \quad (2.4.4)$$

The amplitudes for both of the branches are the same due to symmetry, and it is obtained using (2.2.13) and ignoring the overall phase factor:

$$A(q) = \frac{1}{\sqrt{2\pi}(2E - q^2)^{1/4}}. \quad (2.4.5)$$

Also notice that at the caustic D , the slope of $p(q)$ changes from negative to positive. Hence, we have an extra phase of $+\frac{\pi}{2}$ on the second branch by (2.3.10). Putting this all together, we get the following wavefunction:

$$\psi(x) = \frac{1}{\sqrt{2\pi}(2E - q^2)^{1/4}} \left(e^{i\left(\frac{\pi E}{2} + E \arcsin\left(\frac{q}{\sqrt{2E}}\right) + \frac{q}{2}\sqrt{2E - q^2}\right)} + e^{i\left(\frac{3\pi E}{2} - E \arcsin\left(\frac{q}{\sqrt{2E}}\right) - \frac{q}{2}\sqrt{2E - q^2} + \frac{\pi}{2}\right)} \right). \quad (2.4.6)$$

Factoring the common phase $e^{i\pi E}$ from the exponentials (and ignoring it), and using the fact that the energy of the n -th eigenstate of the harmonic oscillator is $E_n = (n + \frac{1}{2})$, we get the n -th WKB eigenfunction for $|q| < \sqrt{2E}$:

$$\psi_n(y) = \frac{2}{\sqrt{2\pi}[(2n+1)(1-y^2)]^{1/4}} \cos\left(\left(n + \frac{1}{2}\right) \left(\arcsin(y) + y(1-y^2)^{1/2}\right) - \frac{n\pi}{2}\right), \quad (2.4.7)$$

where $y = \frac{q}{\sqrt{2n+1}}$. This is only valid in the classically allowed region away from the caustic. We can extend this formula to the classically forbidden region by an analytic continuation using the following expression for the arcsin function in the complex plane:

$$\arcsin(z) = -i \ln\left(iz + |1 - z^2|^{1/2} e^{\frac{i}{2} \arg(1-z^2)}\right). \quad (2.4.8)$$

This gives us the WKB wavefunctions in the classically forbidden region $|q| > \sqrt{2E}$:

$$\psi_n(y) = \frac{(y + (y^2 - 1)^{1/2})^{(n+1/2)}}{[(2n+1)(y^2 - 1))]^{1/4}} \exp\left(-\left(n + \frac{1}{2}\right)y(y^2 - 1)^{1/2}\right); \quad y > 1, \quad (2.4.9)$$

$$\psi_n(y) = \frac{(-y + (y^2 - 1)^{1/2})^{(n+1/2)}}{[(2n+1)(y^2 - 1))]^{1/4}} \exp\left(\left(n + \frac{1}{2}\right)y(y^2 - 1)^{1/2}\right); \quad y < -1, \quad (2.4.10)$$

where $y = \frac{q}{\sqrt{2n+1}}$, and the condition $|q| > \sqrt{2E}$ is equivalent to the two cases above.

As we can see in Figure 2.4.2, the exact and the WKB wavefunctions agree to an excellent degree away from the caustic. The general method of calculating the action, the amplitude and the Maslov indices works in other semiclassical systems as well. In the next chapter, we will study such a system where the Hamiltonian does not take the form of the sum of a potential and kinetic energy. We will see that the semiclassical techniques discussed in this chapter work equally nicely in a completely different problem.

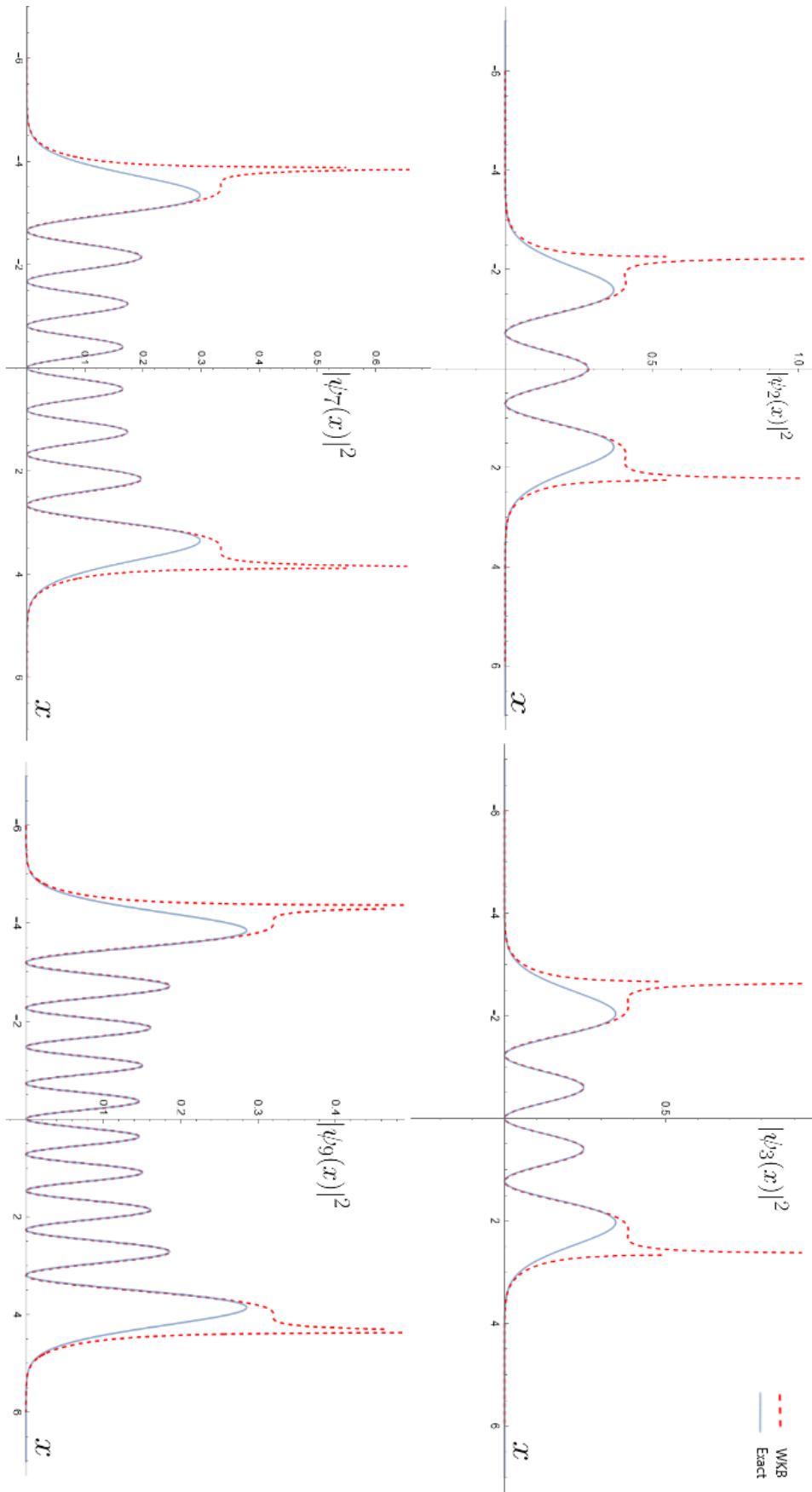


Figure 2.4.2: Comparison of the exact and the WKB eigenfunctions of a simple harmonic oscillator for energy eigenstates $n = 2, 3, 7, 9$. The WKB wavefunctions diverge at the caustics.

Semiclassics of Quantum Tetrahedra

In this chapter, we will apply the ideas discussed in the previous chapter to the case of the quantum tetrahedron described in the introduction. It was shown by Kapovich and Milson in a different context that the space of a polyhedron with fixed face areas has a symplectic structure.[22] Hence, we can study the dynamics of polyhedra in a systematic way using the Hamiltonian formalism. Here, we will do exactly that and consider some quantum properties. This will give rise to a semiclassical model of a tetrahedral grain of space. In particular, we will study the classical Hamiltonian of this problem, and calculate the Bohr-Sommerfeld quantization and the WKB wavefunctions of the shapes of tetrahedra.

3.1 Setup of the Problem

As described in the first chapter, the Hilbert space for our tetrahedron is the global $SU(2)$ invariant subspace of the tensor product of the Hilbert space associated with each face of the tetrahedron (see equation 1.3.3). This generalizes to the Hilbert space of any arbitrary convex polyhedron with n faces:

$$\mathcal{K}_n = \text{Inv}_{SU(2)} \bigotimes_{i=1}^n \mathcal{H}_{j_i}. \quad (3.1.1)$$

This subspace is called the space of *intertwiners*. As described in [19], a finite dimensional intertwiner space is related to the quantization of a classical phase space. We start by developing the classical phase space here. The starting point is a theorem due to Minkowski [30].

Theorem 3.1.1 (Minkowski's Theorem). *Given n vectors $\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_n \in \mathbb{R}^3$, where $n \in \mathbb{N}$, such that $\mathbf{A}_1 + \dots + \mathbf{A}_n = 0$, there is a unique n -faced polyhedron (up to rotation and translation) with $\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_n$ as its normal area vectors.*

Following [22], we can associate a classical phase space to the space of these polyhedra. We can interpret the partial sum

$$\mu_k = \left| \sum_{i=1}^{k+1} \mathbf{A}_i \right|; \quad (i = 1, \dots, n-3) \quad (3.1.2)$$

as the generator of rotation about the $\mu_k = \sum_{i=1}^{k+1} \mathbf{A}_i$ axis once we choose a suitable Poisson bracket structure. As suggested by Schwinger, we can associate the following Poisson bracket structure to this space [35]. Suppose f and g are functions of the area vectors. Then we define

the Poisson bracket:

$$\{f, g\} = \sum_{i=1}^n \mathbf{A}_i \cdot \left(\frac{\partial f}{\partial \mathbf{A}_i} \times \frac{\partial g}{\partial \mathbf{A}_i} \right), \quad (3.1.3)$$

where the notation $\frac{\partial F}{\partial \mathbf{A}_i}$ is a shorthand for the vector $\frac{\partial F}{\partial A_i^x} \hat{\mathbf{x}} + \frac{\partial F}{\partial A_i^y} \hat{\mathbf{y}} + \frac{\partial F}{\partial A_i^z} \hat{\mathbf{z}}$. Conjugate to μ_k , the generator of rotations about the μ_k axis, we have some kind of generalized coordinate. Since our μ_k is interpreted as an angular momentum, it turns out that the conjugate coordinate is an angle. Let ϕ_k be the angle between

$$\mathbf{v}_k = \left(\sum_{i=1}^k \mathbf{A}_i \right) \times \mathbf{A}_{k+1} \quad \text{and} \quad \mathbf{w}_k = \left(\sum_{i=1}^{k+1} \mathbf{A}_i \right) \times \mathbf{A}_{k+2}. \quad (3.1.4)$$

It can be shown that under the Poisson bracket relation (3.1.3), we have:

$$\{\mu_k, \phi_l\} = \delta_{kl}. \quad (3.1.5)$$

The space of $\{\mu_k\}_{k=1}^{n-3}$ and $\{\phi_l\}_{l=1}^{n-3}$ is a classical phase space where the fundamental Poisson brackets are given by (3.1.5). As we saw in the previous chapter, dynamical problems on a phase space is most naturally solved by the Hamiltonian formulation. For our quantum tetrahedron, an interesting Hamiltonian operator is given by the volume operator in loop quantum gravity, which is the quantum analogue of the volume expression in ordinary Riemannian space. Due to what is known as a regularization scheme, there are different volume operators in loop quantum gravity, for example, the Rovelli-Smolin operator [32] and the Ashtekar-Lewandowski operator [1]. However, in the case of a tetrahedron, these volume operators coincide. The Hilbert space

in this case is

$$\mathcal{K}_4 = \text{Inv}_{SU(2)}[\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2} \otimes \mathcal{H}_{j_3} \otimes \mathcal{H}_{j_4}]. \quad (3.1.6)$$

The dimension d of this Hilbert space is obtained by the symmetric coupling of three angular momenta as described by Lévy-Leblond and Lévy-Nahas in [26]:

$$d = k_{\max} - k_{\min} + 1, \quad (3.1.7)$$

where k_{\min} is the maximum of the difference of two j_i 's and k_{\max} is the minimum of the sum of two j_i 's. This is due to the triangle inequality of the coupling of angular momenta. Suppose, we sort the j_i 's in ascending order. Then $k_{\min} = \max\{|j_1 - j_2|, |j_3 - j_4|\}$ and $k_{\max} = \min\{j_1 + j_2, j_3 + j_4\}$. The matrix elements of the squared volume operator, due to Lévy-Leblond and Lévy-Nahas in [26], is given by

$$\hat{Q} = (8\pi\gamma l_p^2)^3 \sum_{k=k_{\min}+1}^{k_{\max}} 2i \frac{\Delta(k, A_1 \cdot A_2) \Delta(k, A_3, A_4)}{\sqrt{k^2 - 1/4}} (|k\rangle\langle k-1| - |k-1\rangle\langle k|), \quad (3.1.8)$$

where l_p is the Planck length, $|k\rangle$ is a basis element in \mathcal{K}_4 using $\mathcal{H}_{j_1} \otimes \mathcal{H}_{j_2}$ as intermediate coupling space, $A_i = j_i + \frac{1}{2}$, and

$$\Delta(a, b, c) = \frac{1}{4} \sqrt{(a+b+c)(-a+b+c)(a-b+c)(a+b-c)} \quad (3.1.9)$$

is the area of a triangle with sides a, b and c . The operator itself is given by Barbieri [3]:

$$\hat{Q} = \frac{2}{9} \hat{\mathbf{A}}_1 \cdot (\hat{\mathbf{A}}_2 \times \hat{\mathbf{A}}_3). \quad (3.1.10)$$

We will study the spectrum and eigenfunctions of this operator. In our semiclassical study of the quantum tetrahedron, Q will be the classical Hamiltonian, where $\mathbf{A}_1, \mathbf{A}_2$ and \mathbf{A}_3 are three area vectors of the tetrahedron.¹

3.2 Phase Space and Classical Hamiltonian of Quantum Tetrahedra

The study of Hamiltonian dynamics in the Kapovich-Milson phase space simplifies immensely in the case of a tetrahedron. In this case, Minkowski's Theorem (3.1.1) gives us a unique tetrahedron (up to rotation and translation) with face area vectors $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$ and \mathbf{A}_4 if we have $\sum_{i=1}^4 \mathbf{A}_i = 0$. Denote the magnitude of the area vector \mathbf{A}_i as A_i for all $i \in \{1, 2, 3, 4\}$.

Notice that if we fix the magnitudes of the four area vectors, we still have two degrees of freedom that determine the shape of the tetrahedron. A tetrahedron is determined completely by its six edge-lengths. Thus, if the four area vectors are fixed, the shape can still be varied in a two dimensional space. We will denote this space as \mathcal{P}_4 .

Using the Kapovich-Milson phase space construction from the previous section, we find that our canonical momentum is $A = |\mathbf{A}_1 + \mathbf{A}_2|$, and the conjugate coordinate of A is ϕ —the angle between $\mathbf{v} = \mathbf{A}_1 \times \mathbf{A}_2$ and $\mathbf{w} = \mathbf{A} \times \mathbf{A}_3$, where $\mathbf{A} = \mathbf{A}_1 + \mathbf{A}_2$. The specialization of Poisson bracket relation (3.1.5) in this case is

$$\{A, \phi\} = 1. \quad (3.2.1)$$

¹It is a simple exercise in vector algebra to show that the squared volume is actually given by (3.1.10).

This can be interpreted as A generating a rotation by angle ϕ about the \mathbf{A} axis, and is analogous to the angular momentum operator \hat{J}_z generating rotation about the z -axis.

The topology of the phase space with A and ϕ as conjugate variables is unlike the one in introductory classical mechanics. This is because there are limitations in the allowed values of A in our problem due to the geometry of the tetrahedron.² To see this, suppose, without loss of generality, that we label the areas of the faces with ascending order in magnitude. In other words, we have

$$A_1 \leq A_2 \leq A_3 \leq A_4, \text{ where } A_i \text{ is the magnitude}$$

of \mathbf{A}_i for all $i \in \{1, 2, 3, 4\}$. Notice that due to the triangle inequality, A is restricted between $A_{\min} \equiv \max\{A_2 - A_1, A_4 - A_3\}$ and $A_{\max} \equiv \min\{A_1 + A_2, A_3 + A_4\}$. These are the magnitudes of A when two of the area vectors become colinear. For each A such that $A_{\min} < A < A_{\max}$, the angle ϕ goes from 0 to 2π . For $A = A_{\min}$ and $A = A_{\max}$, the conjugate angle ϕ becomes degenerate, and we only get a single point for each. This is topologically the same as a 2-sphere. Following Figure 3.2.2, we can embed this sphere of radius $r = (A_{\max} - A_{\min})/2$ in \mathbb{R}^3 with its center at $(A_{\min} + A_{\max})/2$.

A nice way to see this is due to the closure relation in the Minkowski's theorem. Since the area vectors add up to zero, we can associate with a tetrahedron an abstract area-tetrahedron, where four adjacent “edges” are formed by the area vectors. Then the angle ϕ is simply the dihedral angle between the two triangles formed by vectors \mathbf{A}_1 and \mathbf{A}_2 , and \mathbf{A}_3 and \mathbf{A}_4 . This lines up with (3.1.4) using the closure relation of the area vectors. As suggested before, we will

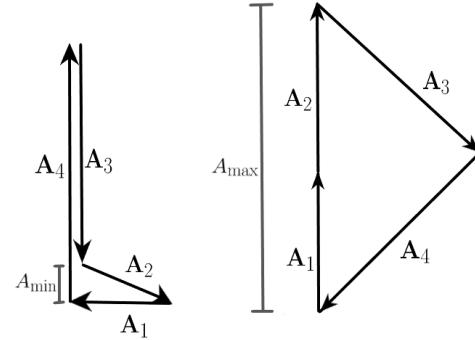


Figure 3.2.1: The minimum and maximum absolute value of A for Euclidean tetrahedron.

²We will only consider Euclidean tetrahedron in flat space here.

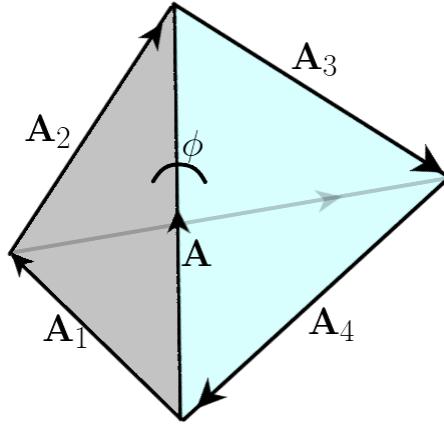


Figure 3.2.2: Abstract tetrahedron formed by the area vectors of an Euclidean tetrahedron.

study the spectrum of the squared volume operator, whose classical analogue is given by:

$$Q = \frac{2}{9} \mathbf{A}_1 \cdot (\mathbf{A}_2 \times \mathbf{A}_3). \quad (3.2.2)$$

Due to the rotational invariance of Q , we can reduce it to a function of A and ϕ . To see this, notice that by the argument given in the previous paragraph, ϕ is the angle between vectors $\mathbf{v} = \mathbf{A}_1 \times \mathbf{A}_2$ and $\mathbf{w} = \mathbf{A}_3 \times \mathbf{A}_4$. Taking the cross product, we get

$$\begin{aligned} \mathbf{v} \times \mathbf{w} &= (\mathbf{A}_1 \times \mathbf{A}_2) \times (\mathbf{A}_3 \times \mathbf{A}_4) \\ \implies |\mathbf{v}||\mathbf{w}| \sin \phi &= (\mathbf{A}_1 \cdot (\mathbf{A}_2 \times \mathbf{A}_4)) \mathbf{A}_3 - (\mathbf{A}_1 \cdot (\mathbf{A}_2 \times \mathbf{A}_3)) \mathbf{A}_4 \\ \implies 4\Delta\bar{\Delta} \sin \phi &= (\mathbf{A}_1 \cdot (\mathbf{A}_2 \times \mathbf{A}_3))(-\mathbf{A}_3 - \mathbf{A}_4) \\ \implies 4\Delta\bar{\Delta} \sin \phi &= \frac{9}{2} Q \mathbf{A} \\ \therefore Q &= \frac{8\Delta\bar{\Delta}}{9A} \sin \phi. \end{aligned} \quad (3.2.3)$$

Notice that here we have used the fact that $|\mathbf{v}|$ and $|\mathbf{w}|$ are twice the areas of the triangle formed by \mathbf{A}_1 and \mathbf{A}_2 (call it Δ) and the triangle formed by \mathbf{A}_3 and \mathbf{A}_4 (call it $\bar{\Delta}$). Here, we

can calculate the areas Δ and $\bar{\Delta}$ using Heron's formula:

$$\Delta = \frac{1}{4} \sqrt{[(A_1 + A_2)^2 - A^2][A^2 - (A_1 - A_2)^2]}, \quad (3.2.4)$$

$$\bar{\Delta} = \frac{1}{4} \sqrt{[(A_3 + A_4)^2 - A^2][A^2 - (A_3 - A_4)^2]}. \quad (3.2.5)$$

Hence, we have found the form of a classical Hamiltonian Q as a function of canonical momentum A and coordinate ϕ . The form of this Hamiltonian is quite different from the kinetic-plus-potential form of a Hamiltonian in classical mechanics. This makes the calculations of the action integral tedious even though the machinery to compute the WKB wavefunctions is similar to the kinetic-plus-potential Hamiltonian. However, as we will see, Now, we will focus on a closed action integral along an arbitrary orbit of constant volume in the phase space, which will give us a quantization condition similar to the Bohr-Sommerfeld quantization of energy levels.

3.3 Bohr-Sommerfeld Quantization of a Tetrahedron

The spectra of the volume operator³ (3.1.10) is approximated accurately using the Bohr-Sommerfeld quantization rule. Roughly speaking, this quantization rule restricts the allowed values of the symplectic area enclosed by an orbit in the phase space. For a classical Hamiltonian of the form $H = \frac{p^2}{2m} + V(q)$, the Bohr-Sommerfeld quantization rule requires the action $I(E) = \oint p(q, E) dq$ to be an integer multiple of the Planck's constant, where E is the energy level of the orbit. The allowed energy levels are then obtained by inverting this relation.

By an analogy to this condition, we define our action integral in the phase space as $I(q) = \oint A(\phi, q) d\phi$, where q is a level value of the Hamiltonian Q . Then, the Bohr-Sommerfeld

³We will refer to \hat{Q} as the volume operator for brevity even though it is the squared volume operator.

quantization condition for our problem is:

$$I(q) = \oint A d\phi = 2\pi n, \quad (3.3.1)$$

where we have set $\hbar = 1$. To evaluate this integral directly, we need A as a function of ϕ .

However, it is not easy to invert the relation (3.2.3) to obtain $A(\phi)$. We circumvent this problem

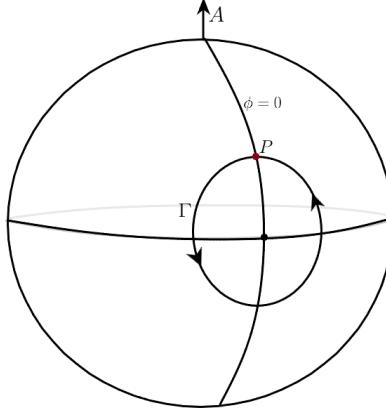


Figure 3.3.1: Contour of integration Γ of constant volume in the phase space sphere. As a convention, we take P as our initial point. The closed action integral along the curve Γ gives rise to the Bohr-Sommerfeld quantization condition for our problem.

by converting the ϕ -integral (3.3.1) to a λ -integral $\oint A \frac{d\phi}{d\lambda} d\lambda$, where λ is the variable conjugate to Q .⁴ This is most conveniently done using a Poisson bracket. Since Q is the Hamiltonian of this problem, we get $\frac{d\phi}{d\lambda}$ by the Poisson bracket of ϕ with Q :

$$\frac{d\phi}{d\lambda} = \{\phi, Q\} = \frac{\partial \phi}{\partial A} \frac{\partial Q}{\partial \phi} - \frac{\partial \phi}{\partial \phi} \frac{\partial Q}{\partial A} = -\frac{\partial Q}{\partial A}. \quad (3.3.2)$$

Using the expression of $Q(A, \phi)$ in (3.2.3), we get

$$\frac{d\phi}{d\lambda} = \frac{Q}{A} - \frac{QA}{16\Delta^2}[(A_1 + A_2)^2 + (A_1 - A_2)^2 - 2A^2] - \frac{QA}{16\bar{\Delta}^2}[(A_3 + A_4)^2 + (A_3 - A_4)^2 - 2A^2]. \quad (3.3.3)$$

⁴This is analogous to parameterizing x as a function of time t and changing the integration as $\int dx \rightarrow \int \frac{dx}{dt} dt$.

Then, after the change of variable, the closed action integral (3.3.1) becomes:

$$I = Q \oint \left(1 - \sum_{i=1}^4 \frac{A^2}{A^2 - \bar{r}_i} \right) d\lambda, \quad (3.3.4)$$

where $\bar{r}_i \in \{(A_1 - A_2)^2, (A_1 + A_2)^2, (A_4 - A_3)^2, (A_3 + A_4)^2\}$ and $\bar{r}_1 \leq \bar{r}_2 \leq \bar{r}_3 \leq \bar{r}_4$. We have taken Q out of the integral since it is fixed along an orbit. To complete the integral, we need to compute $A^2(\lambda)$. We again use a Poisson bracket:

$$\frac{dA^2}{d\lambda} = \{A^2, Q\} = 2A\{A, Q\} = \frac{1}{9} \sqrt{(4\Delta)^2(4\bar{\Delta})^2 - 324Q^2A^2}. \quad (3.3.5)$$

The expression under the square-root is a quartic, and we write it as:

$$P_4(A^2, Q^2) = P_0(A^2) - (2A)^2(9Q)^2. \quad (3.3.6)$$

Notice that $P_0(A^2) \equiv (4\Delta)^2(4\bar{\Delta})^2$ is a quartic polynomial in $x \equiv A^2$ with roots \bar{r}_i introduced in (3.3.4). Let r_1, r_2, r_3 and r_4 be the roots of the quartic polynomial $P_4(x)$. Then we can solve for $\lambda(x)$ by integrating (3.3.5):

$$\lambda(x) = 9 \int_{r_2}^x \frac{d\tilde{x}}{\sqrt{(\tilde{x} - r_1)(\tilde{x} - r_2)(-\tilde{x} + r_3)(-\tilde{x} + r_4)}}. \quad (3.3.7)$$

Here, we have assumed that the roots of the quartic in the denominator are distinct and we order them as $r_1 < r_2 < r_3 < r_4$. This is an elliptic integral. We will express it in terms of the standard Jacobi form of elliptic functions. Using [10], we get the following expression for $\lambda(x)$:

$$\lambda(x) = 9g \operatorname{sn}^{-1} \left(\sqrt{\frac{(r_3 - r_1)(x - r_2)}{(r_3 - r_2)(x - r_1)}}, m \right), \quad (3.3.8)$$

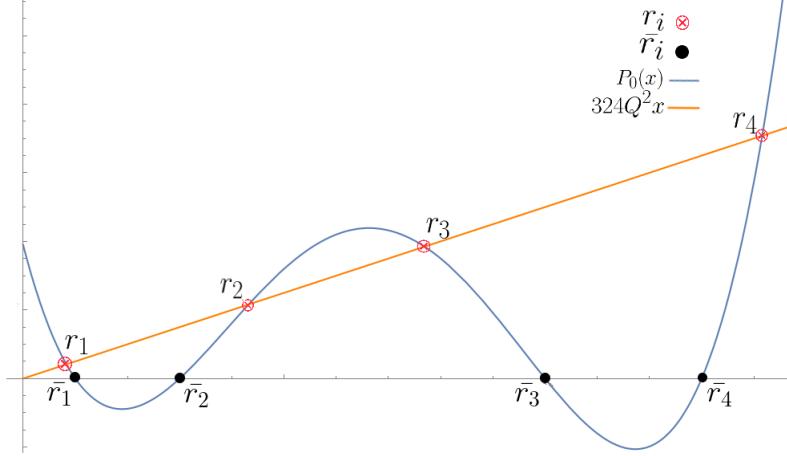


Figure 3.3.2: A quartic polynomial $P_0(x)$ with a linear perturbation term $324Q^2x$. In the figure, \bar{r}_i are the roots of $P_0(x)$, and r_i are the roots of $P_4(x)$. In our problem, the classically allowed region is the region between r_2 and r_3 .

where

$$g = \frac{2}{\sqrt{(r_4 - r_2)(r_3 - r_1)}} \quad \text{and} \quad m = \frac{(r_3 - r_2)(r_4 - r_1)}{(r_4 - r_2)(r_3 - r_1)}. \quad (3.3.9)$$

The quantity m is the square of the elliptic modulus parameter. The relation (3.3.8) can be inverted to get $x(\lambda)$:

$$x(\lambda) = A^2(\lambda) = \frac{r_2(r_3 - r_1) - r_1(r_3 - r_2)\text{sn}^2\left(\frac{\lambda}{9g}, m\right)}{(r_3 - r_1) - (r_3 - r_2)\text{sn}^2\left(\frac{\lambda}{9g}, m\right)}. \quad (3.3.10)$$

This is the volume evolution of the intermediate coupling A^2 . With this, we have all the necessary pieces to calculate the integrals of the five terms in (3.3.4). The first integral is:

$$Q \oint d\lambda = 9g \times 2K(m), \quad (3.3.11)$$

where K is the complete elliptic integral of the first kind. The closed integral is $2K(m)$ instead of $4K(m)$ ⁵ since the Jacobi sn function appear as a square in the expression (3.3.10), and so the

⁵The period of an elliptic integral is $4K(m)$.

period is halved. The other four integrals in (3.3.4) are of the form

$$\oint \frac{A^2}{A^2 - \bar{r}_i} d\lambda = \oint \frac{r_2(r_3 - r_1) - r_1(r_3 - r_2) \operatorname{sn}^2(\frac{\lambda}{9g}, m)}{(r_3 - r_1)(r_2 - \bar{r}_i) - (r_1 - \bar{r}_i)(r_3 - r_2) \operatorname{sn}^2(\frac{\lambda}{9g}, m)} d\lambda \quad (3.3.12)$$

for $i \in \{1, 2, 3, 4\}$. This integral can be reduced to the form $\oint adu + \oint \frac{bdu}{1 - \alpha_i^2 \operatorname{sn}^2(u)}$, where a, b and α_i are constants, and we have introduced $u \equiv \frac{\lambda}{9g}$. The integral $\oint adu$ is similar to (3.3.11), and the integral $\oint \frac{bdu}{1 - \alpha_i^2 \operatorname{sn}^2(u)}$ gives rise to a complete elliptic integral of the third kind, and is denoted by $\Pi(\alpha_i^2, m)$. Collecting all these terms together, we get the following expression for the closed action integral:

$$I(Q) = \left(aK(m) + \sum_{i=1}^4 b_i \Pi(\alpha_i^2, m) \right), \quad (3.3.13)$$

where

$$a \equiv 18gQ \left(1 - \sum_{i=1}^4 \frac{r_1}{r_1 - r_i} \right) \quad \text{and} \quad b_i \equiv \frac{18gQ\bar{r}_i(r_2 - r_1)}{(r_2 - \bar{r}_i)(r_1 - \bar{r}_i)}. \quad (3.3.14)$$

Although the closed action integral has been written in a concise way, notice that each of the roots of $P_4(x)$ implicitly depends on Q . To find the allowed volume levels, we need to perform a numerical inversion. This was done for different sets of values in [6], and the allowed volumes were compared with the ones that we get from the eigenvalues of the exact volume operator (3.1.8). Now that we have derived the Bohr-Sommerfeld quantization of a quantum tetrahedron, we will shift our focus to its WKB eigenfunctions.

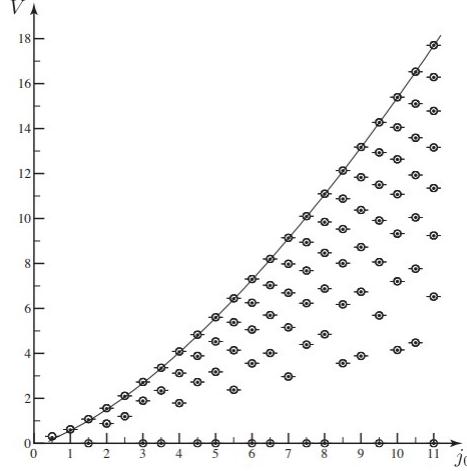


Figure 3.3.3: A comparison between the Bohr-Sommerfeld spectrum and the spectrum of the volume operator (3.1.8) in loop quantum gravity for spins $(j, j, j, j + 1)$. Remember that the area A_r and the corresponding spin j_r are related by $A_r = j_r + \frac{1}{2}$. This figure is collected from [6].

3.4 WKB Eigenfunctions of a Tetrahedron

As described in the previous chapter, the calculation of the WKB eigenfunctions requires three necessary pieces: the amplitude, the action integral starting from conventional initial points to a set of points on the orbit and the Maslov indices at the caustics. We will write down the wavefunctions in the A -basis.

Using a formula analogous to (2.2.12), the amplitude of the wavefunction is⁶

$$R(A) = \frac{1}{\sqrt{18gK}} \frac{1}{\sqrt{\{A, Q\}}} = \frac{1}{\sqrt{18gK} \sqrt{\frac{8\Delta\bar{\Delta}}{9A} \cos \phi}} = \frac{1}{\sqrt{gK}} \frac{\sqrt{A}}{((16\Delta\bar{\Delta})^2 - (18AQ)^2)^{1/4}} \quad (3.4.1)$$

for all allowed intermediate coupling A . The calculation of the action integral is similar to the closed action integral in the previous section. The only difference is that for the WKB wavefunctions, we calculate the action integral not on a closed loop of constant Q , but from some conventional initial point to the intersection points of the constant A -manifold M_A and

⁶This is a generalization of (2.2.12). The factor $\sqrt{2\pi}$ is replaced by the square root of our period $\sqrt{18gK}$. For a complete discussion, see [19].

the constant Q -manifold M_Q . In our problem, there are two intersection points C_1 and C_2 (see Figure 3.4.1). Suppose that the conventional initial points of integrations are P_A and P_Q for M_A and M_Q respectively. Let $\Gamma_{A,1}$ and $\Gamma_{A,2}$ be the contours from P_A to C_1 and C_2 respectively along the manifold M_A , and let $\Gamma_{Q,1}$ and $\Gamma_{Q,2}$ be the contours from P_Q to C_1 and C_2 respectively along the manifold M_Q .⁷ Notice that due to symmetry about the $\phi = \frac{\pi}{2}$ circle on the sphere, the amplitudes for both of the branches of the WKB approximation are the same. Suppose that the action integrals along the contours $\Gamma_{Q,1}, \Gamma_{Q,2}, \Gamma_{A,1}$ and $\Gamma_{A,2}$ are $S_{Q_1}, S_{Q_2}, S_{A_1}$ and S_{A_2} respectively. Since the amplitude factor is the same for both of the branches, the WKB

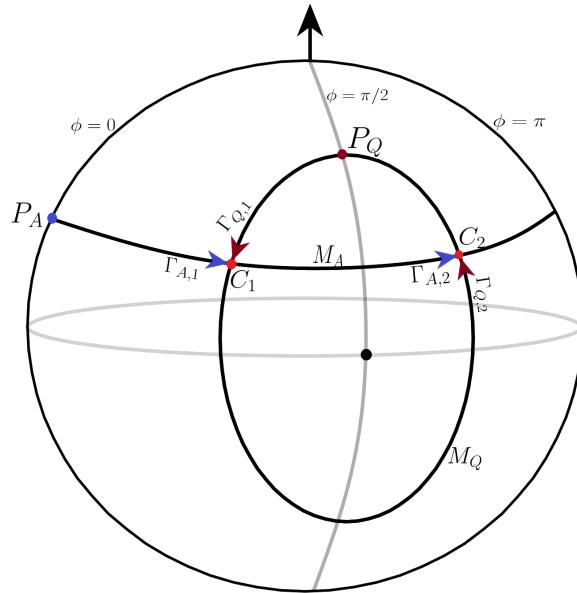


Figure 3.4.1: The points P_A and P_Q are our conventional initial points of integrations on the constant A manifold M_A and constant Q manifold M_Q respectively. The two manifolds intersect at points C_1 and C_2 . The contours $\Gamma_{A,1}$ and $\Gamma_{A,2}$ are integration paths from P_A to C_1 and C_2 respectively along the manifold M_A . Similarly, the contours $\Gamma_{Q,1}$ and $\Gamma_{Q,2}$ are integration paths from P_Q to C_1 and C_2 respectively along the manifold M_Q .

wavefunction is proportional to the sum of the exponential factors (2.2.10) in the WKB formula:

$$\psi(A) \propto \left(\exp \left[i \left(S_{Q_2} - S_{A_2} - \mu_2 \frac{\pi}{2} \right) \right] + \exp \left[i \left(S_{Q_1} - S_{A_1} - \mu_1 \frac{\pi}{2} \right) \right] \right). \quad (3.4.2)$$

⁷We fix some convenient orientation on the manifolds as shown in Figure 3.4.1. The wavefunctions due to different choices of orientations differ by a common phase factor as long as we are consistent with the orientation.

We can factor out $\exp\left(\frac{i}{2}\left((S_{Q_2} + S_{Q_1}) - (S_{A_2} + S_{A_1}) - (\mu_1 + \mu_2)\frac{\pi}{2}\right)\right)$ from the sum, and ignore it as an overall phase. Then the wavefunction is proportional to the cosine of the difference of the different action integrals along the contours:

$$\begin{aligned}\psi(A) &\propto \exp\left[\frac{i}{2}\left((S_{Q_2} - S_{Q_1}) - (S_{A_2} - S_{A_1}) - (\mu_2 - \mu_1)\frac{\pi}{2}\right)\right] \\ &\quad + \exp\left[\frac{-i}{2}\left((S_{Q_2} - S_{Q_1}) - (S_{A_2} - S_{A_1}) - (\mu_2 - \mu_1)\frac{\pi}{2}\right)\right] \\ &= 2 \cos\left(\frac{\delta S_Q - \delta S_A - \delta\mu\frac{\pi}{2}}{2}\right),\end{aligned}\tag{3.4.3}$$

where $\delta\mu = (\mu_2 - \mu_1)$ is the difference in Maslov indices on the two branches, δS_Q is the action integral from C_1 to C_2 along M_Q , and δS_A is the action integral from C_1 to C_2 along M_A . Notice that due to the exponential expression of cosine, we have to include a factor of 2 with the amplitude. The calculation of δS_Q is similar to the calculation of the closed action integral I in the previous section, and is given by the following expression:

$$\delta S_Q = Q \left[9gu - \sum_{i=1}^4 \left(\frac{9gr_1}{r_1 - \bar{r}_i} u + 9g\Pi(\alpha_i^2, \operatorname{am}(u, m), m) \left(\frac{r_2}{r_2 - \bar{r}_i} - \frac{r_1}{r_1 - \bar{r}_i} \right) \right) \right],\tag{3.4.4}$$

where $u = \frac{\lambda}{9g}$. This is a function of A using (3.3.8). The calculation of δS_A is simple since A is constant along Γ_A . Let $\phi_0 = \arcsin\left(\frac{9QA}{8\Delta\bar{\Delta}}\right)$. The lower and upper limits of the integral for δS_A are ϕ_0 and $\pi - \phi_0$. So we have

$$\delta S_A = \int_{\phi_0}^{\pi - \phi_0} Ad\phi = A \int_{\phi_0}^{\pi - \phi_0} d\phi = A \left(\pi - 2 \arcsin\left(\frac{9QA}{8\Delta\bar{\Delta}}\right) \right).\tag{3.4.5}$$

The last piece of our WKB wavefunction is the difference in Maslov indices $\delta\mu$. The Maslov indices only appear in the wavefunction when an integration contour passes through a caustic of the Lagrangian manifold on which it lives in. More specifically, this occurs when (3.4.1) diverges;

along our paths of integration, there is one caustic at $\phi = \frac{\pi}{2}$. Therefore, we have a Maslov index for the second branch of integration. Following the calculation procedure discussed in Section 2.3, we need to assemble a few pieces first. We calculate the parameter $\dot{\gamma}$ defined by:

$$\dot{\gamma} = \frac{1}{e} \{\{A, Q\}, Q\}, \quad (3.4.6)$$

where e is defined by the equation: $dQ|_c = e \cdot dA|_c$ (the subscript c denotes the evaluation of the differential at the caustic). If the parameter $\dot{\gamma}$ is negative, then the change in the Maslov index $\delta\mu$ is $+1$ and if it is positive, then $\delta\mu$ is -1 .

Our first step is to compute e . For this purpose, we take the differential of Q in (3.2.3) at the caustic:

$$dQ|_c = \frac{8}{9} d \left(\frac{\Delta \bar{\Delta}}{A} \sin \phi \right) \Big|_c. \quad (3.4.7)$$

Since $d \sin \phi = \cos \phi d\phi$, and $\cos \phi$ is zero at the caustic $\phi = \frac{\pi}{2}$, this becomes:

$$dQ|_c = Q|_c \left[-\frac{1}{A} + \sum_{i=1}^4 \frac{A}{A^2 - r_i} \right] \Big|_c dA. \quad (3.4.8)$$

So, our e is given by:

$$e = Q|_c \left[-\frac{1}{A} + \sum_{i=1}^4 \frac{A}{A^2 - r_i} \right] \Big|_c. \quad (3.4.9)$$

The other piece to compute the Maslov index is the following Poisson bracket:

$$\{\{A, Q\}, Q\} = Q^2|_c \left[-\frac{1}{A} + \sum_{i=1}^4 \frac{A}{A^2 - r_i} \right] \Big|_c. \quad (3.4.10)$$

Then, (3.4.6) becomes

$$\dot{\gamma} = Q_c. \quad (3.4.11)$$

For a Euclidean tetrahedron, Q_c is always positive, so we have $\delta\mu = -1$. Therefore, the wavefunction for a tetrahedral grain of space in the classically allowed region $r_2 < A^2 < r_3$ is:

$$\psi(A) = \frac{2}{\sqrt{gK}} \frac{\sqrt{A}}{((16\Delta\bar{\Delta})^2 - (18AQ)^2)^{1/4}} \cos\left(\frac{\delta S_Q - \delta S_A - \delta\mu\frac{\pi}{2}}{2}\right), \quad (3.4.12)$$

where δS_Q is given by (3.4.4) and δS_A is given by (3.4.5). The wavefunction in the classically forbidden region can be obtained similarly. The only difference in that case is that we perform the action integrals in the region where A^2 is between r_1 and r_2 or between r_3 and r_4 in Figure 3.3.2. Aside from that, we have an exponentially growing or an exponentially decaying factor from the exponential piece of the WKB wavefunction. This is in contrast to the oscillatory behavior of the wavefunction that we get in the classically allowed region.

Similar to the calculation of the wavefunctions of the simple harmonic oscillator in the classically forbidden regions, here we also need to perform an analytic continuation of the arcsin function. We do that using (2.4.8), and the wavefunction we get for A^2 between r_3 and r_4 is:

$$\psi(A) = \frac{1}{\sqrt{gK'}} \frac{\sqrt{A}}{((16\Delta\bar{\Delta})^2 - (18AQ)^2)^{1/4}} \exp(\delta S_{Qf} - \delta S_{Af}), \quad (3.4.13)$$

where $K' = K(1 - m)$ is the complement of the complete elliptic integral of the first kind $K(m)$ that appears in (3.4.12), and

$$\delta S_{Qf} = Q \left[9gu - \sum_{i=1}^4 \left(\frac{9gr_2}{r_2 - \bar{r}_i} u + 9g\Pi(\alpha_{if}^2, \text{am}(u, m_f), m_f) \left(\frac{r_3}{r_3 - \bar{r}_i} - \frac{r_2}{r_2 - \bar{r}_i} \right) \right) \right], \quad (3.4.14)$$

where $m_f = \frac{(r_4-r_3)(r_2-r_1)}{(r_4-r_2)(r_3-r_1)}$ and $\alpha_{if}^2 = \frac{(r_4-r_3)(r_2-\bar{r}_i)}{(r_4-r_2)(r_3-\bar{r}_i)}$. Similarly, the wavefunction for A^2 such that $r_1 < A^2 < r_2$ is given by

$$\psi(A) = \frac{1}{\sqrt{gK'}} \frac{\sqrt{A}}{((16\Delta\bar{\Delta})^2 - (18AQ)^2)^{1/4}} \exp(\delta S_Q - \delta S_A), \quad (3.4.15)$$

where $K' = K(1-m)$, and

$$\delta S_{QF} = Q \left[9gu - \sum_{i=1}^4 \left(\frac{9gr_3}{r_3 - \bar{r}_i} u + 9g\Pi(\alpha_{iF}^2, \text{am}(u, m_F), m_F) \left(\frac{r_2}{r_2 - \bar{r}_i} - \frac{r_3}{r_3 - \bar{r}_i} \right) \right) \right], \quad (3.4.16)$$

where $m_F = m_f = \frac{(r_4-r_3)(r_2-r_1)}{(r_4-r_2)(r_3-r_1)}$ and $\alpha_{iF}^2 = \frac{(r_2-r_1)(r_3-\bar{r}_i)}{(r_3-r_1)(r_2-\bar{r}_i)}$. This completes the discussion of the calculation of the WKB eigenfunctions of a tetrahedral grain of space. To demonstrate the accuracy of the WKB method applied to this problem, we include some plots in the end of this chapter for comparison with the exact wavefunctions found by diagonalizing (3.1.8).

Notice that the moduli of the complete elliptic integrals in (3.4.13) and (3.4.15) are the same. This is not a coincidence, and it is because if we consider closed action integrals in the two classically forbidden regions, they turn out to be the same. The closed action integral in the intervals $[r_2, r_3]$, $[r_3, r_4]$ and $[r_1, r_2]$ are given respectively by:

$$I_1 = 18gQ \left(\left[1 - \sum_{i=1}^4 \frac{r_1}{r_1 - \bar{r}_i} \right] K(m) - \sum_{i=1}^4 \left[\frac{r_2}{r_2 - \bar{r}_i} - \frac{r_1}{r_1 - \bar{r}_i} \right] \Pi(\alpha_i^2, m) \right), \quad (3.4.17)$$

$$I_2 = \frac{18gQ}{i} \left(\left[1 - \sum_{i=1}^4 \frac{r_2}{r_2 - \bar{r}_i} \right] K(m_f) - \sum_{i=1}^4 \left[\frac{r_3}{r_3 - \bar{r}_i} - \frac{r_2}{r_2 - \bar{r}_i} \right] \Pi(\alpha_{if}^2, m_f) \right), \quad (3.4.18)$$

$$I_3 = \frac{18gQ}{i} \left(\left[1 - \sum_{i=1}^4 \frac{r_3}{r_3 - \bar{r}_i} \right] K(m_f) - \sum_{i=1}^4 \left[\frac{r_2}{r_2 - \bar{r}_i} - \frac{r_3}{r_3 - \bar{r}_i} \right] \Pi(\alpha_{iF}^2, m_f) \right), \quad (3.4.19)$$

where α_{if}^2 , α_{iF}^2 and m_f are the same as in (3.4.15) and (3.4.16). Noticing the fact that $\alpha_{if}^2 \alpha_{iF}^2 = m_f$, and using the identity

$$\Pi(\alpha^2, m) = K(m) - \Pi(m/\alpha^2, m), \quad (3.4.20)$$

we can show that $I_2 = I_3$. So, we actually have two independent closed cycles on the phase space. This aspect of the problem will be discussed in the next chapter.

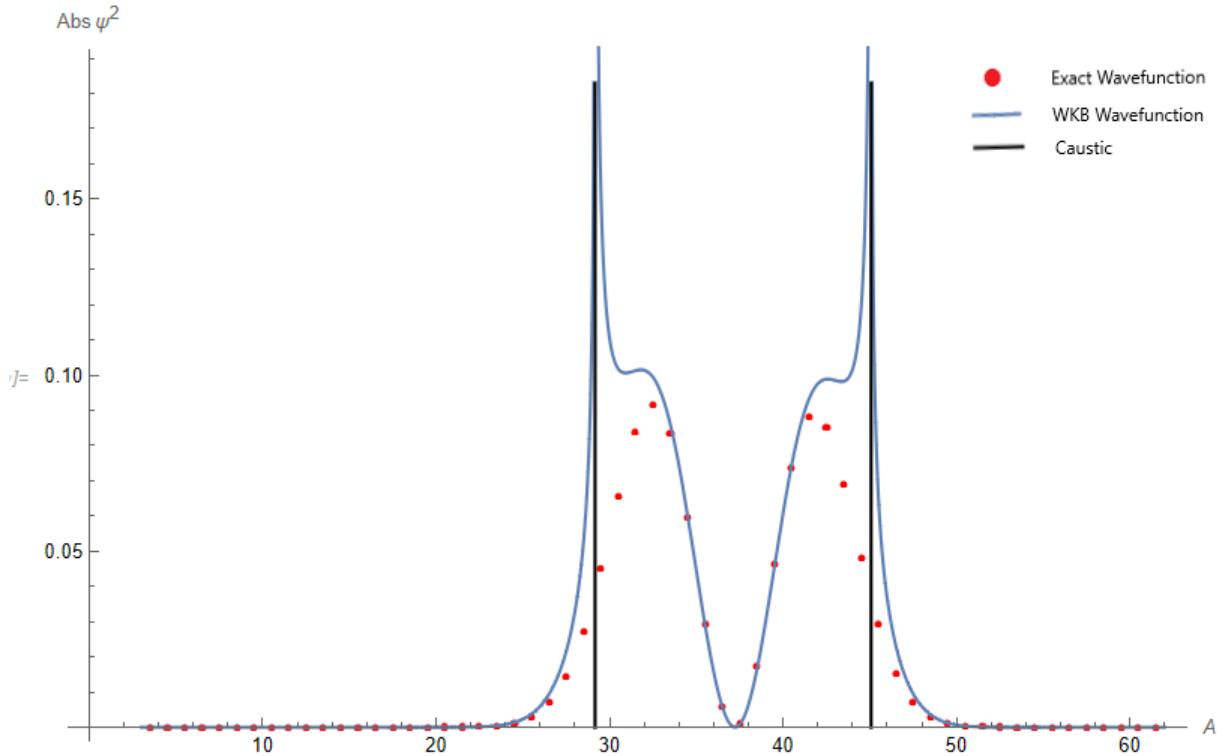


Figure 3.4.2: First squared eigenfunction for $A_1 = 30$, $A_2 = 31$, $A_3 = 32$ and $A_4 = 35$.

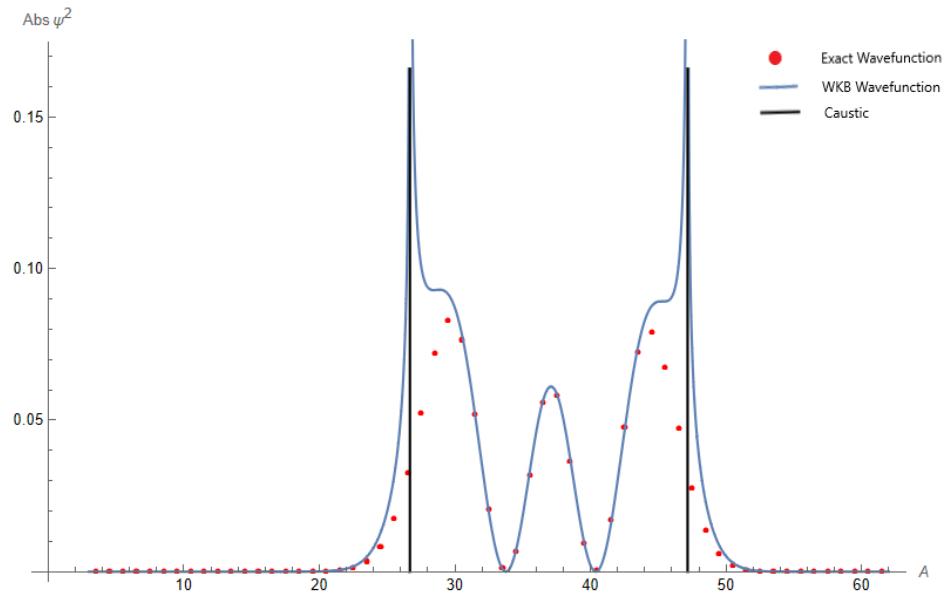


Figure 3.4.3: Second squared eigenfunction for $A_1 = 30, A_2 = 31, A_3 = 32$ and $A_4 = 35$.

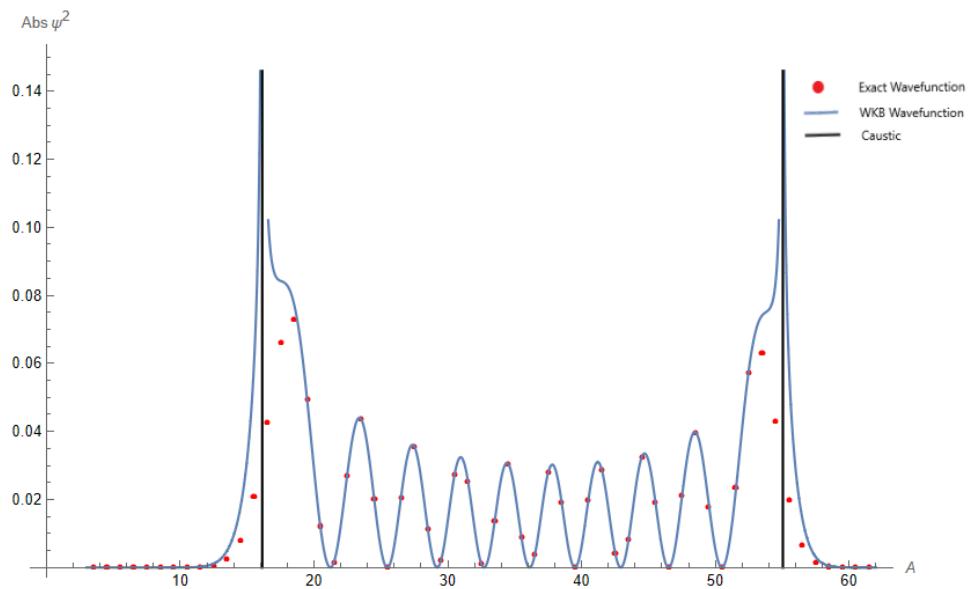


Figure 3.4.4: Ninth squared eigenfunction for $A_1 = 30, A_2 = 31, A_3 = 32$ and $A_4 = 35$.

Quantum Geometry and Picard-Fuchs Equation

In the previous chapter, we noticed that the closed action integrals on both of the classically forbidden regions of a quantum tetrahedron are the same. This is not a coincidence, and the root of this interesting fact lies in the topological structure of the phase space and the algebraic geometry of the problem. In this chapter, we will briefly discuss these mathematical aspects that are well-studied in the mathematical literature, but have only recently been applied to semiclassics and quantum geometry.

4.1 Complexification of Phase Space

To have a better understanding of the underlying structure, we revert our focus to a standard kinetic-plus-potential Hamiltonian in classical mechanics: $H(q, p) = \frac{p^2}{2m} + V(q)$. Let E be a level value of the Hamiltonian $H(q, p)$. Then the closed action integral along an orbit is given by $\oint p(q, E) dq$. Since the expression for $p(q, E)$ involves taking a square root, we have two different choices of signs in the integration. This sign ambiguity is most efficiently understood in terms of a complex configuration space.

Suppose that q_1 and q_2 are two classical turning points on the real line of the complexified q -space. By definition, $p(q, E)$ vanishes at these points, and so these are the branch points on the complex configuration space. Suppose that we choose our branch cut along the real line from q_1 to q_2 . Then the closed action integral $S_{12}(E) = \oint_{C_{12}} p(q, E) dq$ enclosing q_1 and q_2 on the complex plane is nonzero. Other action integrals enclosing two other branch points are also calculated similarly. However, there are only finitely many independent closed action integrals on the complexified configuration space. This is determined by the topological properties of the Riemann surface defined by the momentum $p(q, E)$. Since $p(q, E)$ is a double valued function on the complex plane, the Riemann surface defined by it is constructed from two copies of the complex plane. The number of branch cuts on the complex plane is determined by the number of roots of $2m(E - V(q))$. If there are n roots of $2m(E - V(q))$, then the number of branch cuts is $\frac{n}{2}$ if n is even, and it is $\frac{n+1}{2}$ if n is odd. Gluing the extended complex plane along the branch cuts, we get a Riemann surface of genus g , where $g \in \mathbb{N}$ and is one less than the number of branch cuts. On a genus g surface, there are $2g$ independent integration cycles. Aside from that, $p(q, E)$ can have additional poles, which give rise to punctures on the Riemann surface. Integrations around the poles are non-trivial, and if there are s poles on the complex plane from $p(q, E)$,

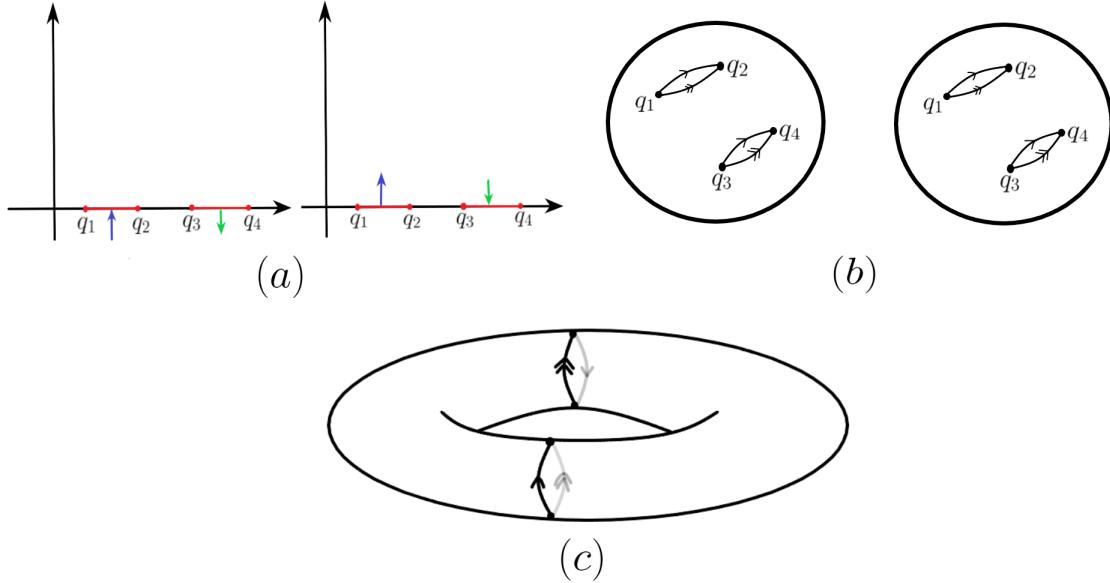


Figure 4.1.1: Construction of a genus $g=1$ Riemann surface from a complexified configuration space. In (a), we have two copies of a complex plane, where each copy has two branch cuts. The two copies of complex plane are equivalent to two Riemann surfaces with two cuts in each as shown in (b). We glue the two Riemann surfaces along the two branch cuts to obtain a genus $g = 1$ surface in (c).

then there are $2s$ punctures on the Riemann surface (since it is constructed from two copies of a complex plane). However, a cycle around a puncture can be deformed into a sum of other cycles on the Riemann surface. So, in total there are $2g + 2s - 1$ independent cycles on the surface when there is a singularity. In the absence of singularities, there are $2g$ independent cycles.¹ It is a well-known fact in the study of complex manifolds that on a one-dimensional complex manifold, the number of independent cycles is equal to the number of linearly independent one-forms. Take the one-form $\Lambda(E) = p(q, E)dq$ on our Riemann surface. The derivatives of $\Lambda(E)$ give us new one forms on the manifold. Suppose that after N derivatives of $\Lambda(E)$ with respect to E , where $N \in \mathbb{N}$, we get a linearly dependent one-form. The linear dependence in the context of one-forms is slightly different from the one discussed in the context of vectors. If a number of one-forms are linearly dependent, then there is a linear combination of them which is a total

¹This argument is inspired by [24].

differential of some function on the manifold. Then we have

$$\sum_{i=0}^N \alpha_i \frac{\partial^i \Lambda(E)}{\partial E^i} = df, \quad (4.1.1)$$

where $N \in \mathbb{N}$ and f is a smooth function. Upon integrating around a closed cycle, we obtain

$$\sum_{i=0}^N \alpha_i \frac{\partial^i S}{\partial E^i} = 0, \quad (4.1.2)$$

where S is an action integral. This is a Picard-Fuchs equation. Here we have expressed the equation in terms of the action function.² The solutions of the Picard-Fuchs equation are the different classical actions on the independent cycles.

4.2 Picard-Fuchs Equation of Quantum Tetrahedron

The starting point for computing the Picard-Fuchs equation for a classical Hamiltonian is the expression of momentum as a function of coordinate q and energy E . Depending on the potential function $V(q)$ in a classical Hamiltonian, we get different forms of Picard-Fuchs equation (see [4], [24] for example). Our problem of quantum tetrahedron is not derived from a classical Hamiltonian. Nonetheless, the quartic expression (3.3.6) gives us a direct route to study a Picard-Fuchs equation for our problem.

²In the mathematical literature, the Picard-Fuchs equation is often studied in terms of period rather than action. The period along a cycle is the first derivative of the action on that cycle. From a physical point of view, action is a more interesting variable since it determines the first order quantization.

The evolution of A^2 along an orbit of fixed Q is given by (3.3.5), which we rewrite here for its relevance:

$$\frac{dx}{d\lambda} = \pm \frac{1}{9} \sqrt{(x - \bar{r}_1)(x - \bar{r}_2)(x - \bar{r}_3)(x - \bar{r}_4) - 324Q^2x}, \quad (4.2.1)$$

where we have introduced the short hand x for A^2 . Let us $P_4(x) = P_0(x) - 324Q^2x$ denote the quartic under the square root in (4.2.1), where $P_0(x) = (x - \bar{r}_1)(x - \bar{r}_2)(x - \bar{r}_3)(x - \bar{r}_4)$ is independent of Q . Let r_1, r_2, r_3 and r_4 be the roots of $P_4(x)$. For a generic quartic, the roots r_1, r_2, r_3 and r_4 are all distinct. We will assume this throughout our discussion.³ Then, following the discussion of the previous section, we have two copies of a complex x -plane with two branch cuts on each copy. Hence, the Riemann surface is topologically equivalent to a torus ($g = 1$). It can be shown from (3.3.4) that there are four poles on our complex plane, and the integrals around the poles are independent of Q and are all equal.⁴ Therefore, we only have two independent non-trivial cycles. This aligns with our discussion following (3.4.19) that we only have two independent non-trivial action integrals on our phase space manifold.

Therefore, it is apparent that we have a Picard-Fuchs equation that is second order in period or third order in action. Now, we focus on the computation of the Picard-Fuchs equation. The form of our quartic curve in (4.2.1) is very convenient in this regard. The quartic $P_4(x)$ can be written in terms of the elementary symmetric polynomials in r_1, r_2, r_3, r_4 :

$$P_4(x) = x^4 + 4b_3x^3 + 6b_2x^2 + 4b_1x + b_0, \quad (4.2.2)$$

³Although the coalescence of roots has interesting properties in algebraic geometry. See [15] for example.

⁴This can be done using the residue theorem.

where

$$\begin{aligned}
 b_0 &= r_1 r_2 r_3 r_4, \\
 b_1 &= -\frac{(r_1 r_2 r_3 + \cdots + r_2 r_3 r_4)}{4}, \\
 b_2 &= \frac{(r_1 r_2 + r_1 r_3 + \cdots + r_3 r_4)}{6}, \\
 b_3 &= -\frac{(r_1 + r_2 + r_3 + r_4)}{4}.
 \end{aligned} \tag{4.2.3}$$

Notice that the coefficients in (4.2.2) depend on Q through their dependencies on r_i . They also have the magnitudes of the area vectors A_1, A_2, A_3 and A_4 as moduli parameters. Now the quartic polynomial $P_4(x)$ can be converted to the Weierstrass form

$$\tilde{P}_4(x) = 4x^3 - g_2(Q)x - g_3(Q) \tag{4.2.4}$$

using the uniformization process of a quartic described in [4], where

$$g_2(Q) = b_4 b_0 - 4b_3 b_1 + 3b_2^2, \tag{4.2.5}$$

$$g_3(Q) = b_4 b_2 b_0 + 2b_3 b_2 b_1 - b_4 b_1^2 - b_3^2 b_0 - b_2^3. \tag{4.2.6}$$

We also introduce the discriminant Δ and the J -invariant of an elliptic curve:

$$\Delta \equiv g_2^3 - 27g_3^2, \tag{4.2.7}$$

$$J \equiv \frac{g_2^3}{g_2^3 - 27g_3^2}. \tag{4.2.8}$$

After converting our quartic polynomial to the Weierstrass normal form, we can use the Griffiths-Dwork technique discussed in [13] to compute the Picard-Fuchs equation of a quantum tetra-

hedron. It is convenient to write down the Picard-Fuchs equation using $W = 324Q^2$ as our deformation parameter:

$$\frac{d^3S}{dW^3} + B_1(W) \frac{d^2S}{dW^2} + B_0 \frac{dS}{dW} = 0, \quad (4.2.9)$$

where

$$B_1 = \frac{g'_3}{g_3} - \frac{g'_2}{g_2} + \frac{J'}{J} - \frac{J''}{J'}, \quad (4.2.10)$$

$$B_0 = \frac{(J')^2}{144J(J-1)} + \frac{\Delta'}{12\Delta} \left(B_1 + \frac{\Delta''}{\Delta'} - \frac{13\Delta'}{12\Delta} \right). \quad (4.2.11)$$

Here the prime symbol denotes a derivative with respect to W . We computed these coefficients using [20], and these are presented in Appendix A.

4.3 An Application of Picard-Fuchs Equation

It was discovered by Dunham in 1932 that from a Schrödinger equation, we can find an asymptotic series for action in the WKB ansatz to get an all order WKB approximation [16]:

$$a(E, \hbar) = \sqrt{2} \oint_{\alpha} \left(\sqrt{E - V} - \frac{\hbar^2}{2^6} \frac{(V')^2}{(E - V)^{5/2}} - \frac{\hbar^4}{2^{13}} \left(\frac{49(V')^4}{(E - V)^{11/2}} - \frac{16V'V'''}{(E - V)^{7/2}} \right) - \dots \right) dq, \quad (4.3.1)$$

where the subscript α of the integral denotes that we are integrating over one of the cycles on a complexified configuration space. For a genus-1 system, there is also another cycle β on the complex torus. It turns out that the functional forms of all the higher order terms in the action integral along the β cycle are the same as they are in the α -cycle in (4.3.1) [4]. Denote the

asymptotic expansion of the action integral on the two cycles as:

$$a(E, \hbar) = \sum_{n=0}^{\infty} \hbar^{2n} a_n(E), \quad \text{and} \quad a^D(E, \hbar) = \sum_{n=0}^{\infty} \hbar^{2n} a_n^D(E), \quad (4.3.2)$$

where $a(E, \hbar)$ is the action on the α -cycle and $a^D(E, \hbar)$ is the action on the β -cycle (also known as the *dual action*). The relation between these two actions is that they are two of the independent solutions of a third order Picard-Fuchs equation. For a genus-1 system, the other independent solution of the third order Picard-Fuchs equation is a constant.⁵ Furthermore, all the terms in this expansion can be reduced to integrals involving the elliptic integrals of the first, second and third kind for a genus-1 system. In this case, as described in [4], a higher order term $a_n(E)$ in the expansion of $a(E, \hbar)$ in (4.3.2) can be written as a differential operator D_E^n acting on a_0 , and similarly for a_0^D :

$$a_n(E) = D_E^n a_0(E) \quad (4.3.3)$$

$$a_0^D(E) = D_E^n a_0^D(E) \quad (4.3.4)$$

for all $n \in \mathbb{N}$. Notice that the differential operator D_E^n is the same for both the action and the dual action. Moreover, due to the fact that $a_0(E)$ and $a_0^D(E)$ satisfy the same third order Picard-Fuchs equation, we can reduce the differential operator D_E^n to a second order differential operator. After the reduction, (4.3.3) and (4.3.4) can be written as:

$$a_n(E) = f_n^{(0)}(E) a_0(E) + f_n^{(1)}(E) \frac{da_0(E)}{dE} + f_n^{(2)}(E) \frac{d^2 a_0(E)}{dE^2}, \quad (4.3.5)$$

$$a_0^D(E) = f_n^{(0)}(E) a_0^D(E) + f_n^{(1)}(E) \frac{da_0^D(E)}{dE} + f_n^{(2)}(E) \frac{d^2 a_0^D(E)}{dE^2}. \quad (4.3.6)$$

⁵For a discussion on higher genus systems, see [24].

We emphasize that the coefficients $f_n^{(0)}$, $f_n^{(1)}$ and $f_n^{(2)}$ are the same for (4.3.5) and (4.3.6). This makes Picard-Fuchs equation a very powerful tool for studying the higher order behavior of quantization and the WKB wavefunctions. This is so because the perturbative data of a quantum mechanical problem is encoded in the action $a(E, \hbar)$, while the non-perturbative data is encoded in the dual action $a^D(E, \hbar)$, and both of them are related by the Wronskian of a Picard-Fuchs differential equation. Understanding the relation between this two difference action can provide an easy route to the higher order corrections of the WKB wavefunctions [4],[24].

The relevance of the Picard Fuchs equation in our problem is due to our interest in the higher order behavior of the WKB wavefunctions and the Bohr-Sommerfeld quantization presented in the previous chapter. The way Dunham derived the asymptotic expansion in [16] was by using the Schrödinger equation to get a recursion relation among different powers of \hbar . However, for our problem, we don't have a Schrödinger-like differential equation to start with. Using the exact volume operator derived by Lévy-Leblond and Lévy-Nahas in [26], which is given by

$$\hat{Q} = (8\pi\gamma l_p^2)^3 \sum_{k=k_{\min}+1}^{k_{\max}} 2i \frac{\Delta(k, A_1 \cdot A_2) \Delta(k, A_3, A_4)}{\sqrt{k^2 - 1/4}} (|k\rangle\langle k-1| - |k-1\rangle\langle k|), \quad (4.3.7)$$

can shed some light in the recursion relation required for higher order action correction. Some work has been done in this side by Schulten and Gordon in [34], although it has not been applied in the context of our problem. For future work related to this project, deriving a Schrödinger-like differential equation can be a productive staring point, which will give us better approximation than what we derived using first order WKB wavefunctions and Bohr-Sommerfeld quantization.

Appendix A

Picard-Fuchs Coefficients

We present the coefficients (4.2.10) and (4.2.11) for our Picard-Fuchs equation (4.2.9). In the following expressions for B_1 and B_0 , we have introduced $s_0 = b_0$, $s_1 = \frac{b_1}{4}$, $s_2 = \frac{b_2}{6}$ and $s_3 = \frac{b_3}{4}$:

$$\begin{aligned}
B1 = & (12288 s0^4 - 16 s0^3 (320 s2^2 + 96 s1 s3 - 32 s2 s3^2 - 27 s3^4 - 96 s3 W) + \\
& s0^2 (256 s2^4 - 2048 s2^3 s3^2 - 864 s1^2 (8 s2 - s3^2) + 54 s3^2 W (-5 s3^3 + 16 W) + 12 s2^2 (87 s3^4 - 832 s3 W) + \\
& 6 s1 (1664 s2^2 s3 - 640 s2 s3^3 + 45 s3^5 + 2304 s2 W - 288 s3^2 W) - 3 s2 (45 s3^6 - 1280 s3^3 W + 2304 W^2)) - \\
& (s1 - W)^2 (-16 s2^5 + 162 s1^3 s3 + 8 s2^4 s3^2 + 4 s2^2 (17 s3^3 - 81 W) W + 6 s3 (2 s3^3 - 27 W) W^2 + \\
& s2 s3^2 W (-8 s3^3 + 27 W) - s2^3 (s3^4 + 144 s3 W) - 3 s1^2 (108 s2^2 - 9 s2 s3^2 - 4 s3^4 + 162 s3 W) + \\
& 2 s1 (72 s2^3 s3 + 3 s3 W (-4 s3^3 + 81 W) + s2^2 (-34 s3^3 + 324 W) + s2 (4 s3^5 - 27 s3^2 W))) + \\
& 2 s0 (1944 s1^4 + 32 s2^6 - 16 s2^5 s3^2 - 16 s2^3 W (5 s3^3 + 12 W) + 9 s2^2 s3^2 W (s3^3 + 116 W) + \\
& 3 s2 s3 W^2 (-155 s3^3 + 864 W) - 6 s1^3 (432 s2 s3 - 113 s3^3 + 1296 W) + 2 s2^4 (s3^4 + 88 s3 W) - \\
& 3 s1^2 (64 s2^3 - 348 s2^2 s3^2 + 155 s2 s3^4 - 18 s3^6 - 2592 s2 s3 W + 678 s3^3 W - 3888 W^2) + \\
& 6 W^2 (9 s3^6 - 113 s3^3 W + 324 W^2) - \\
& s1 (176 s2^4 s3 - 16 s2^3 (5 s3^3 + 24 W) + 9 s2^2 (s3^5 + 232 s3^2 W) + 18 W (6 s3^6 - 113 s3^3 W + 432 W^2) + \\
& s2 (-930 s3^4 W + 7776 s3 W^2))) / \\
& ((-3 s1^2 s3 + s0 (48 s1 - 32 s2 s3 + 9 s3^3 - 48 W) + W (-4 s2^2 + s2 s3^2 - 3 s3 W) + s1 (4 s2^2 - s2 s3^2 + 6 s3 W)) \\
& (256 s0^3 + s0^2 (-128 s2^2 + 144 s2 s3^2 - 3 s3 (64 s1 + 9 s3^3 - 64 W)) - \\
& (s1 - W)^2 (27 s1^2 + 4 s2^3 - s2^2 s3^2 + 18 s2 s3 W + W (-4 s3^3 + 27 W) - 2 s1 (9 s2 s3 - 2 s3^3 + 27 W)) + \\
& 2 s0 (8 s2^4 - 2 s2^3 s3^2 + s1^2 (72 s2 - 3 s3^2) + 40 s2^2 s3 W - 9 s2 (s3^3 - 8 W) W - 3 s3^2 W^2 + \\
& s1 (-40 s2^2 s3 + 9 s2 (s3^3 - 16 W) + 6 s3^2 W))))
\end{aligned}$$

```

B0 =
(3 (1024 s0^3 s3 - 8 s0^2 s3 (64 s2^2 - 32 s2 s3^2 + 3 s3 (8 s1 + s3^3 - 8 W) ) +
(s1 - W)^2 (24 s1^2 s3 + s2 s3 (-4 s2 + s3^2)^2 + (80 s2^2 - 24 s2 s3^2 + s3^4) W + 24 s3 W^2 -
s1 (80 s2^2 - 24 s2 s3^2 + s3^4 + 48 s3 W) ) +
s0 (-960 s1^3 + 4 s2^2 s3 (-4 s2 + s3^2)^2 + s3^2 (-4 s2 + s3^2) (-100 s2 + 21 s3^2) W -
336 s3 (-4 s2 + s3^2) W^2 + 960 W^3 + 48 s1^2 (28 s2 s3 - 7 s3^3 + 60 W) -
s1 (400 s2^2 s3^2 - 184 s2 s3^4 + 21 s3^6 + 2688 s2 s3 W - 672 s3^3 W + 2880 W^2) )) /
(4 (s0 (48 s1 - 32 s2 s3 + 9 s3^3 - 48 W) + (s1 - W) (4 s2^2 - s2 s3^2 + 3 s3 (-s1 + W))) +
(256 s0^3 + s0^2 (-128 s2^2 + 144 s2 s3^2 - 3 s3 (64 s1 + 9 s3^3 - 64 W)) -
(s1 - W)^2 (27 s1^2 + 4 s2^3 - s2^2 s3^2 + 18 s2 s3 W + W (-4 s3^3 + 27 W) - 2 s1 (9 s2 s3 - 2 s3^3 + 27 W)) +
2 s0 (8 s2^4 - 2 s2^3 s3^2 + s1^2 (72 s2 - 3 s3^2) + 40 s2^2 s3 W - 3 s3^2 W^2 + 9 s2 W (-s3^3 + 8 W) +
s1 (-40 s2^2 s3 + 9 s2 (s3^3 - 16 W) + 6 s3^2 W))) )

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