ON THE QUANTIZATION PROBLEM IN CURVED SPACE

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science

by

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ABSTRACT

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The nonrelativistic quantum mechanics of particles constrained to curved surfaces is studied. There is open debate as to which of several approaches is the correct one. After a review of existing literature and the required mathematics, three approaches are studied and applied to a sphere, spheroid, and triaxial ellipsoid.

The first approach uses differential geometry to reduce the problem from a three-dimensional problem to a two-dimensional problem. The second approach uses three dimensions and holds one of the separated wavefunctions and its associated coordinate constant. A third approach constrains the particle in a three-dimensional space between two parallel surfaces and takes the limit as the distance between the surfaces goes to zero.

Analytic methods, finite element methods, and perturbation theory are applied to the approaches to determine which are in agreement. It is found that the differential geometric approach has the most agreement.

Constrained quantum mechanics has application in materials science, where topological surface states are studied. It also has application as a simplified model of Carbon-60, graphene, and silicene structures. It also has application as in semiclassical quantum gravity, where spacetime is a pseudo-Riemannian manifold, to which the particles are constrained.
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PREFACE

This document is the product of two years of research into quantum mechanics and differential geometry. Many other related topics were investigated, such as the Dirac equation, geometric quantization, symplectic geometry, Fourier methods, infinite dimensional differential geometry, and fractional dimensional space. The cylinder and Möbius strips were also solved during the course of the research.

During these studies it was found that there is still disagreement between the various methods used. This was the genesis of the thesis you now read. It was decided to compare and contrast the various formulations and find which one was the correct one.

Ben Bernard

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For my wife and child, for their patience and understanding during two long years of study.
LIST OF ABBREVIATIONS

DG  differential geometric
FEM  finite element method
FFT  fast Fourier transform
nm  nanometers
QM  quantum mechanics
ODE  ordinary differential equation
PDE  partial differential equation
CHAPTER I

Introduction

This thesis studies the quantum mechanics of particles constrained to curved surfaces using differential geometric methods. This has application in materials science, where molecules can form two-dimensional topological objects, such as fullerenes, graphene, and silicene.

It is a somewhat different problem than the three-dimensional quantum dot problem, as the dimensionality is lowered, thereby changing the three-dimensional Laplace operator to a two-dimensional Laplace-Beltrami operator, and the curvature of the surface produces a potential energy term.

The quantum mechanics of particles constrained to a surface was first researched in 1971 by Jensen and Koppe [1]. In 1981 da Costa et al [2] explored such a system in more detail. Other papers include Ley-Koo and Castillo-Animas [4], who studied the prolate spheroid by holding the $\xi$ coordinate in the spheroidal wave equation constant, Encinosa and Etemadi [3], who studied Monge patches with cylindrical symmetry, and Kleinert [6], who studied Dirac quantization on a sphere.

There exist multiple methods for deriving and solving the Schrödinger equation for a particle constrained to surfaces. One approach (Refs. [1; 2; 3]) uses differential geometry to reduce the dimensionality of the three-dimensional partial differential equation (PDE) to a two-dimensional one. Another method (Ref. [4]) is to solve
the three-dimensional PDE and hold the surface normal coordinate constant. A third method (Refs. [7; 6]) involves incorporating the constraints into the classical Hamiltonian and quantizing its Dirac bracket. There are other methods as well (Refs. [8; 9; 10]) which are beyond the scope of this thesis.

Finally, one may treat one or more terms in the equation as a perturbation; however this only holds as long as those terms are small compared with standard solutions. This is a standard method taught in most quantum mechanics courses, and is generally easy to implement if one knows the unperturbed state well. However, this method breaks down as the shape deviates from the unperturbed state. For example, a highly eccentric spheroid will have significant error if a sphere is used for its unperturbed state. A nearly spherical triaxial ellipsoid, on the other hand, will likely have fairly accurate results.

This plethora of techniques presents a problem: while each technique produces results consistent with itself, the techniques produces results that do not agree with other techniques. This was noted by Ref. [11], which compared the method of da Costa (Ref. [2]) with the method of Dirac (Ref. [7]) in the hope of resolving this issue. It was found there that the da Costa equation agrees with Dirac’s formalism when two ordering parameters are used in conjunction with a conserved constraint in the latter approach, and physical ordering is adopted for those parameters. The divergent surface-normal term does not appear under the Dirac formalism because it disappears under the Dirac bracket. This consolidates the Dirac and da Costa methods, as they are equivalent.

The aim of this thesis is to analyze each of the methods and determine which is the best method to use for a given problem. It is likely to depend on the surface in question; for example some simple surfaces such as the sphere and cylinder have easily derived analytical solutions. Other surfaces may have a metric tensor that is sufficiently simple to allow the curvature term to be neglected. Still other surfaces are
separated into ordinary differential equation (ODE)s that can be more readily solved by numerical methods. Then there is the class of surfaces that is not easily solved by any method.

In this thesis, the general procedure is outlined, and then finite element analysis is used to study the sphere, spheroid, and triaxial ellipsoid. The sphere has no curvature term using the differential geometric approach. The spheroid has a separable curvature term, and the curvature term for the triaxial ellipsoid is not separable. The triaxial ellipsoid has never been studied. It is hoped that studying these surfaces will shed light on which is the proper method.
CHAPTER II

Mathematical Review

2.1 Differential Geometry of Two-Dimensional Riemannian Manifolds Embedded in $\mathbb{R}^3$

2.1.1 Introduction

Throughout this text, unless stated otherwise, like indices will be summed over. Partial derivatives will be denoted variously by the following notations as makes the most sense for the context:

$$\frac{\partial f^i}{\partial q^j} = \partial_j f^i = f^i_{,j}. \quad (2.1)$$

To begin the study of constrained quantum mechanics, several differential geometric tools will be needed. We begin with a parametrization (also known as a coordinate chart) $r(q^i)$ from Cartesian coordinates to generalized coordinates $q^i$ that are tangent to the surface at all points on the surface:

$$r = \begin{bmatrix} x(q) \\ y(q) \\ z(q) \end{bmatrix}. \quad (2.2)$$

The first and second partial derivatives of the components of the parametriza-
tion make up the Jacobian and Hessian matrices, respectively. The elements of the Jacobian matrix are given by
\[ J_j^i = \frac{\partial r^i}{\partial q^j}, \] (2.3)
and each element of the parametrization has its own Hessian matrix, which collectively can form a rank-three tensor:
\[ H^i_{jk} = \frac{\partial^2 r^i}{\partial q^j \partial q^k}. \] (2.4)

From the parametrization we can construct the metric tensor, or first fundamental form. This describes how the distances between points change under coordinate transformations. For a surface, it is given by [12]
\[ g_{ij} = \frac{\partial r}{\partial q^i} \cdot \frac{\partial r}{\partial q^j}. \] (2.5)

If \( g_{ij} = 0, i \neq j \), then the coordinate system is orthogonal and the components of the metric are often referred to as scale factors \( h_i \), with \((h_i)^2 = g_{ii}\) [13].

Also from the parametrization, we can derive the unit normal vector. This vector field has unit norm and is orthogonal to the surface at all points passing through the surface. It is given by [14]
\[ \mathbf{n} = \frac{\frac{\partial \mathbf{r}}{\partial q^i} \times \frac{\partial \mathbf{r}}{\partial q^j}}{\left\| \frac{\partial \mathbf{r}}{\partial q^i} \times \frac{\partial \mathbf{r}}{\partial q^j} \right\|}. \] (2.6)

Once we have the normal vector, we can now compute the second fundamental form, given by [8]
\[ h_{ij} = \mathbf{n} \cdot \frac{\partial^2 \mathbf{r}}{\partial q^i \partial q^j}. \] (2.7)

The second fundamental form is closely related to the shape operator (also known as
the Weingarten map). It is given by the matrix [2]

\[
\alpha = \frac{1}{g} \begin{bmatrix}
g_{12}h_{21} - g_{22}h_{11} & h_{11}g_{21} - h_{21}g_{11} \\
h_{22}g_{12} - h_{12}g_{22} & h_{21}g_{12} - h_{22}g_{11}
\end{bmatrix}
\]  

(2.8)

We will now take a slight detour to show, using linear algebra, that the shape operator provides a linear map between the first and second fundamental forms, and that its determinant and trace are related to the mean and Gaussian curvatures. Begin with the Weingarten equations in matrix form.

\[
\alpha = \frac{1}{g} \begin{bmatrix}
g_{12}h_{21} - g_{22}h_{11} & h_{11}g_{21} - h_{21}g_{11} \\
h_{22}g_{12} - h_{12}g_{22} & h_{21}g_{12} - h_{22}g_{11}
\end{bmatrix}
\]  

\[
= \frac{1}{g} \begin{bmatrix}
-g_{22}h_{11} + g_{12}h_{21} & -h_{21}g_{11} + h_{11}g_{21} \\
-g_{22}h_{12} + g_{12}h_{22} & -h_{22}g_{11} + h_{21}g_{12}
\end{bmatrix}
\]  

\[
= \frac{1}{g} \begin{bmatrix}
h_{11} & h_{21} \\
h_{12} & h_{22}
\end{bmatrix} \begin{bmatrix}
-g_{22} & g_{12} \\
g_{12} & -g_{22}
\end{bmatrix} \begin{bmatrix}
h_{11} & h_{21} \\
h_{21} & h_{22}
\end{bmatrix} \begin{bmatrix}
g_{12} & g_{11} \\
g_{12} & -g_{11}
\end{bmatrix}
\]  

(2.9)

The first and second fundamental forms are symmetric matrices, so

\[
\alpha = \frac{1}{g} \begin{bmatrix}
h_{11} & h_{12} \\
h_{21} & h_{22}
\end{bmatrix} \begin{bmatrix}
g_{22} & -g_{12} \\
-g_{21} & g_{11}
\end{bmatrix}
\]  

(2.10)
and we have the simple relation

$$\alpha = -\mathbf{h}\mathbf{g}^{-1},$$

(2.11)

which is more elegantly written as

$$\mathbf{h} = -\alpha\mathbf{g}.$$  

(2.12)

Once these components can be found, we can calculate the Gaussian curvature using the formula

$$K = \frac{h}{g} = -\det\alpha,$$

(2.13)

where \( h = \det\mathbf{h} \) and \( g = \det\mathbf{g} \). The Gaussian curvature is an intrinsic curvature and an invariant of the surface.

The next quantity is the mean curvature, which is an extrinsic curvature that can be calculated in several ways. Among them is (Ref. [2])

$$M = \frac{1}{2g} (g_{11}h_{22} + g_{22}h_{11} - 2g_{12}h_{12}) = -\text{Tr}\alpha.$$  

(2.14)

Because it is an extrinsic property, it is not invariant but instead depends on its embedding.

Finally, following the postulate of Podolsky in 1928 [15], we will need to replace the Laplace operator in the Schrödinger equation with the Laplace-Beltrami operator. The Laplace-Beltrami operator is [2]

$$\mathcal{D} \left[ \chi_t (q^1, q^2) \right] = \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^1} \left( \frac{\sqrt{g}}{g_{11}} \frac{\partial \chi_t}{\partial q^1} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^2} \left( \frac{\sqrt{g}}{g_{22}} \frac{\partial \chi_t}{\partial q^2} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^2} \left( \frac{\sqrt{g}}{g_{21}} \frac{\partial \chi_t}{\partial q^1} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^1} \left( \frac{\sqrt{g}}{g_{12}} \frac{\partial \chi_t}{\partial q^2} \right).$$

(2.15)
The operator \( \mathcal{D} \) will often be notated as \( \nabla^2 \) or \( \nabla^2_{LB} \) using an abuse of notation.

Note that when the coordinate system is orthogonal, the metric is diagonal, and the curvature term becomes

\[
M^2 - K = \frac{(g_{11}h_{22} + g_{22}h_{11})^2 - 4g_{11}g_{22}h_{11}h_{22}}{4(g_{11})^2(g_{22})^2},
\]

\[
= \frac{(g_{11})^2(h_{22})^2 + 2g_{11}g_{22}h_{11}h_{22} + (g_{22})^2(h_{11})^2 - 4g_{11}g_{22}h_{11}h_{22}}{4(g_{11})^2(g_{22})^2},
\]

\[
= \frac{(g_{11}h_{22} - g_{22}h_{11})^2}{4(g_{11})^2(g_{22})^2},
\]

\[
= \frac{1}{4} \left( \frac{g_{11}h_{22} - g_{22}h_{11}}{g_{11}g_{22}} \right)^2,
\]

\[
= \frac{1}{4} \left[ \frac{h_{11}}{g_{22}} - \frac{h_{22}}{g_{11}} \right]^2, \tag{2.16}
\]

which simplifies calculations considerably.

### 2.1.2 The Gauss-Bonnet theorem

We close this section on classical differential geometry with an important result. But first we will need two more definitions.

The Euler characteristic of a surface is a topological invariant related to the genus of the surface (the number of holes in the surface). For a surface with genus \( g \), it is

\[
\chi = 2 - 2g. \tag{2.17}
\]

A surface with no holes has genus zero, hence \( \chi = 2 \).

The geodesic curvature is a measure of curvature relative to the curvature of the shortest paths on a curved surface in such a way that the geodesic curvature along such paths is zero. Full details of geodesic curvature are not needed for this project and are therefore beyond the scope of this thesis.

The Gauss-Bonnet theorem, which states that the geometry of a surface \( \mathcal{M} \) with
Gaussian curvature $K$, geodesic curvature $k_g$ and Euler characteristic $\chi(M)$ is related to its topology by
\[
\int_M K\, da + \int_{\partial M} k_g\, ds = 2\pi \chi(M). \tag{2.18}
\]

For a closed surface without boundary, such as an ellipsoid, there are no boundaries to integrate and the central term can be omitted. Thus we are left with the integral curvature
\[
\int_M K\, da = 4\pi, \tag{2.19}
\]
which is a topological invariant.

## 2.2 Differential Forms

### 2.2.1 Introduction to differential forms

Differential forms are the integrands of integrals including the suffix $dx$, where $x$ is the variable of integration. The line, surface, or volume being integrated over is called a chain. A $p$-dimensional integral involves a $p$-form with a $p$-chain. The forms and chains must have the same dimensionality. For example, a function $f$ is a zero-form, $dx$ is a one-form, $dA = dx \wedge dy$ is a two-form, and $dV = d^3x = dx \wedge dy \wedge dz$ is a three-form.

The $\wedge$ in the two-form is a generalization of the cross product called the wedge, or exterior, product. The wedge product is associative and distributive. It also has the property that $a \wedge a = 0$. The wedge product of an $n$-form with an $m$-form is an $(n + m)$-form. The wedge product of a $p$-form $a$ and a $q$-form $b$ obeys the relation [16; 17]
\[
a \wedge b = (-1)^{pq} b \wedge a. \tag{2.20}
\]

A zero-form $f$ is just a function. Integrals of zero-forms are ordinary integrals.
A one-form $F$ may be written as

$$ F = F_x dx + F_y dy + F_z dz. \quad (2.21) $$

This is often shown in vector calculus texts (such as Ref. [14]) as $\mathbf{F} \cdot d\mathbf{r}$. Therefore integrals of one-forms are line integrals.

A two-form is the wedge product of two one-forms. The wedge product of two one-forms in three dimensions is the cross product of them. A two-form exists in two-dimensions. Thus a two-form can be written

$$ F = F_x dx \wedge dy + F_y dy \wedge dz + F_z dz \wedge dx. \quad (2.22) $$

A three-form is the wedge product of a one-form and a two-form, or the triple wedge product of three one-forms. The space of three-forms in three-dimensional space is one-dimensional because there is only one combination of $dx$, $dy$, and $dz$, $dx \wedge dy \wedge dz$. Integrals of three-forms are volume integrals.

### 2.2.2 The exterior derivative and its relation to divergence, gradient, and curl

The exterior derivative of $f$ with respect to a $p$-form in $\mathbb{R}^n$ with basis $\left\{ e_1, e_2, ... e_{(n)} \right\}$ is a $(p + 1)$-form given by the relation[18]

$$ df = \sum_{i=1}^{(n)} \sum_{k=1}^{n} \frac{\partial f}{\partial x^i} dx^i. \quad (2.23) $$

We now look at the exterior derivatives of various types of forms in $\mathbb{R}^3$. We begin with a zero-form $f$. Its exterior derivative is the one-form

$$ df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy + \frac{\partial f}{\partial z} dz = \nabla f. \quad (2.24) $$
For a one-form $F = F_x dx + F_y dy + F_z dz$ we have the two-form
\[ dF = \left( \frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) dy \wedge dz + \left( \frac{\partial F_y}{\partial z} - \frac{\partial F_z}{\partial x} \right) dz \wedge dx + \left( \frac{\partial F_z}{\partial x} - \frac{\partial F_x}{\partial y} \right) dx \wedge dy = \nabla \times F. \] (2.25)

For a two-form we have the three-form
\[ dF = \left( \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \right) dx dy dz = \nabla \cdot F. \] (2.26)

The exterior derivative of a three-form $fdx \wedge dy \wedge dz$ is always zero by Poincaré’s Lemma [19],
\[ d(fdx \wedge dy \wedge dz) = \frac{\partial f}{\partial x} dx \wedge dx \wedge dy \wedge dz + \frac{\partial f}{\partial y} dy \wedge dx \wedge dy \wedge dz \\
+ \frac{\partial f}{\partial z} dz \wedge dx \wedge dy \wedge dz, \]
\[ = 0. \] (2.27)

This is often written as $d^2 = 0$.

Thus we see that the gradient, curl, and divergence correspond to the exterior derivatives of zero-, one-, and two-forms respectively.

### 2.2.3 The Hodge dual operator

We are now in a position to discuss the Hodge star operator, $\ast$. Its motivation is to find the dual of an $n$-form in $q$-dimensional space. The Hodge operator gives the dual of a form. Given a $p$-form in $\mathbb{R}^n$, the Hodge operator $\ast$ returns an $(n - p)$-form
\[ \ast \left( \prod_{k=1}^{p} df^i_{1k} \right) = \frac{1}{(n - p)!} \epsilon_{i_1 i_2 \ldots i_p i_{p+1} i_{n}} \prod_{k=p+1}^{n} dx^i_{1k}. \] (2.28)
This rather terse definition is due to the requirement that Stokes’s theorem,

\[ \int_{\partial \Omega} f = \int_{\Omega} df \]  \hspace{1cm} (2.29)

is satisfied, where \( \Omega \) is a chain and \( \partial \Omega \) is its boundary. For one-forms in three-dimensional space,

\[ \ast dx = dy \wedge dz, \quad \ast dy = dz \wedge dx, \quad \text{and} \quad \ast dz = dx \wedge dy. \]  \hspace{1cm} (2.30)

The Hodge dual of a two-form in three-dimensional space is a one-form, given by

\[ \ast(dy \wedge dz) = dx, \quad \ast(dz \wedge dx) = dy, \quad \text{and} \quad \ast(dx \wedge dy) = dz. \]  \hspace{1cm} (2.31)

Finally, the Hodge dual of a three-form is a zero-form in three-dimensional space.
2.2.4 The Laplace operator

Applying the exterior derivative and Hodge dual of a zero form twice in an orthogonal basis is the Laplacian. Explicitly,

\[ *d * df = *d \left( \frac{\partial f}{\partial q^1} dq^1 + \frac{\partial f}{\partial q^2} dq^2 + \frac{\partial f}{\partial q^3} dq^3 \right), \]

\[ = *d \left[ \frac{\hat{e}_1}{\sqrt{g_{11}}} \frac{\partial f}{\partial q^1} + \frac{\hat{e}_2}{\sqrt{g_{22}}} \frac{\partial f}{\partial q^2} + \frac{\hat{e}_3}{\sqrt{g_{33}}} \frac{\partial f}{\partial q^3} \right], \]

\[ = *d \left[ \frac{\hat{e}_2 \wedge \hat{e}_3}{\sqrt{g_{11}}} \frac{\partial f}{\partial q^1} + \frac{\hat{e}_3 \wedge \hat{e}_1}{\sqrt{g_{22}}} \frac{\partial f}{\partial q^2} + \frac{\hat{e}_1 \wedge \hat{e}_2}{\sqrt{g_{33}}} \frac{\partial f}{\partial q^3} \right], \]

\[ = *d \left[ \sqrt{g_{22}g_{33}} \frac{\partial f}{\partial q^1} dq^2 \wedge dq^3 + \sqrt{g_{11}g_{33}} \frac{\partial f}{\partial q^2} dq^3 \wedge dq^1 + \sqrt{g_{11}g_{22}} \frac{\partial f}{\partial q^3} dq^1 \wedge dq^2 \right], \]

\[ = * \left[ \frac{\partial}{\partial q^1} \left( \sqrt{g_{22}g_{33}} \frac{\partial f}{\partial q^1} \right) + \frac{\partial}{\partial q^2} \left( \sqrt{g_{11}g_{33}} \frac{\partial f}{\partial q^2} \right) \right. \]

\[ + \left. \frac{\partial}{\partial q^3} \left( \sqrt{g_{11}g_{22}} \frac{\partial f}{\partial q^3} \right) \right] (dq^1 \wedge dq^2 \wedge dq^3), \]

\[ = \frac{1}{\sqrt{g}} \left[ \frac{\partial}{\partial q^1} \left( \sqrt{gg_{11}} \frac{\partial f}{\partial q^1} \right) + \frac{\partial}{\partial q^2} \left( \sqrt{gg_{22}} \frac{\partial f}{\partial q^2} \right) + \frac{\partial}{\partial q^3} \left( \sqrt{gg_{33}} \frac{\partial f}{\partial q^3} \right) \right], \]

\[ *d * df = \nabla^2 f. \quad (2.32) \]

Therefore the Laplacian maps a zero-form to a zero-form.

In summary, the exterior derivative and the Hodge dual provide the tools necessary to derive the gradient, curl, divergence, and Laplacian in any three-dimensional orthogonal coordinate system.

2.3 The Finite Element Method

The purpose of this section is to summarize the theory behind the finite element method. This consists of two parts: putting the equation into a weak form using the Galerkin method, and then performing numerical analysis of this weak form. This section draws heavily from [20] and the reader is encouraged to read that treatise on the subject.
2.3.1 Weak formulation

We begin with a given linear second order differential equation, which can be put into the form

\[ f[y'', y', y, x] = 0, \]  

(2.33)

where \( f \) is a functional of differential operators operating on \( y(x) \). We first slice the continuum into a discrete lattice with \( n + 1 \) nodes connecting \( n \) segments. We then approximate \( y(x) \) as a linear combination of shape functions \( \phi_i(x) \) over these segments [20]:

\[ y(x) \equiv \sum_{i=1}^{n+1} a_i \phi_i(x). \]  

(2.34)

This is not an identity but an approximation. Therefore there is a residual error intrinsic to the formulation. This residual is defined as [20]:

\[ R(y, x) \equiv f[y'', y', y, x]. \]  

(2.35)

We seek to minimize this residual function by assuming that the weighted integral over its domain is zero [20]:

\[ \int_0^L W(x) R(y, x) dx = 0. \]  

(2.36)

where \( W(x) \) is a weighting function. In the Galerkin method, the weighting functions are taken to be the shape functions. This produces [20]

\[ \int_0^L \phi(x) R(y, x) dx = 0. \]  

(2.37)

Equation (2.37) is not sufficient because the first order derivatives are not continuous at the nodes, which means that the second order derivatives do not exist at
those points. Integration by parts provides the required form [20]

\[
\int_0^L \phi(x) R(y'', y', y, x) dx = \phi(x) \int R(y'', y', y, x) dx - \int_0^L \left[ \frac{d\phi}{dx} \int R(y'', y', y, x) dx \right] dx.
\]

(2.38)

In the case of a linear differential equation,

\[
f[y'', y', y, x] = Ay'' + By' + Cy + D,
\]

(2.39)

this integral is

\[
\phi(x) \int R(y'', y', y, x) dx - \int_0^L \left[ \frac{d\phi}{dx} \int R(y'', y', y, x) dx \right] dx = \\
\phi(x) \left( A \frac{dy}{dx} + By + C \right)_0^L - \int_0^L \left[ \frac{d\phi}{dx} \left( A \frac{dy}{dx} + By + C \right) \right] dx,
\]

leaving the weak form as the integral equation

\[
\phi(x) \left( A \frac{dy}{dx} + By + C \right)_0^L - \int_0^L \left[ \frac{d\phi}{dx} \left( A \frac{dy}{dx} + By + C \right) \right] dx = 0.
\]

(2.41)

This form has the advantage of not requiring the second derivative be a continuous

function and is therefore better suited to our purpose.

### 2.3.2 Numerical analysis

The next step is to implement numerical analysis over the weak form given in

equation (2.41). We begin by focusing on a single segment with nodes \(x_i\) and \(x_{i+1}\),

with values \(y(x_i)\) at the node \(x_i\) and \(y(x_{i+1})\) at the node \(x_{i+1}\). We set up our shape

functions such that \(\phi_{i+1}(x_i) = 0\) and \(\phi_i(x_i) = 1\) [20]. We then have shape functions

that only affect the neighboring nodes. We can then write this section of the overall
system as [20]

\[ y(x) = \frac{d\phi_i}{dx}a_i + \frac{d\phi_{i+1}}{dx}a_{i+1} = \begin{bmatrix} \frac{d\phi_i}{dx} & \frac{d\phi_{i+1}}{dx} \end{bmatrix} \begin{bmatrix} a_i \\ a_{i+1} \end{bmatrix}, \] (2.42)

where the \( a_i \) terms are coefficients from the linear combination in equation (2.34). This form is then plugged into the weak form given by equation (2.41) and written in matrix form, ultimately producing a linear algebra equation allowing for the solution of the \( a_i \) terms. These terms are then back-substituted into equation (2.34) and the numeric value of \( y(x) \) is determined.

Reference [20] uses a heat diffusion problem as an example. Given the boundary value problem

\[
\begin{aligned}
-\frac{d^2T}{dx^2} &= Q, \quad x = 0, \\
-\frac{dT}{dx} &= q, \quad T = T_L, x = L,
\end{aligned}
\] (2.43)

we arrive at the weak form [20]

\[
\int_0^L K \frac{d\phi}{dx} \frac{dT}{dx} dx - \int_0^L \phi Q dx - K \phi \left. \frac{dT}{dx} \right|_0^L = 0.
\] (2.44)

Using equation (2.34) gives [20]

\[
\sum_{j=1}^{n+1} \left\{ K \left( \int_0^L \frac{d\phi_i}{dx} \frac{d\phi_j}{dx} dx \right) a_j \right\} - \int_0^L \phi_i Q dx + \phi_i \left( -K \frac{dT}{dx} \right)_0^L = 0, \quad i = 1, 2, \ldots n + 1.
\] (2.45)

We then choose the shape functions [20]

\[
\phi_i(x) = \frac{x_{i+1} - x}{x_{i+1} - x_i}, \quad (2.46)
\]

\[
\phi_{i+1}(x) = \frac{x - x_i}{x_{i+1} - x_i}, \quad (2.47)
\]
such that each node only depends on its neighboring nodes.

Using these, we arrive at the system [20]

\[
K \left( \int_0^{L/2} \frac{d\phi^T}{dx} \frac{d\phi}{dx} dx \right) a - Q \int_0^L \phi dx - \begin{bmatrix} q \\ 0 \end{bmatrix} = 0,
\]

(2.48)

where \( \phi = \begin{bmatrix} \phi_i & \phi_{i+1} \end{bmatrix} \) (note that it is a row vector) and \( a = \begin{bmatrix} a_i \\ a_{i+1} \end{bmatrix} \). Evaluating \( \phi \) at our values of \( x \) results in [20]

\[
\phi = \begin{bmatrix} 1 - \frac{2x}{L} & \frac{2x}{L} \end{bmatrix}
\]

(2.49)

\[
\frac{d\phi}{dx} = \begin{bmatrix} -\frac{2}{L} & \frac{2}{L} \end{bmatrix}.
\]

(2.50)

Using this in equation (2.48) and integrating gives for the first element [20]

\[
\frac{2K}{L} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} - \frac{QL}{4} \begin{bmatrix} 1 \\ 1 \end{bmatrix} - \begin{bmatrix} q \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.
\]

(2.51)

This process is then repeated for each element, giving similar results, and the system is then assembled with the form

\[
\frac{2K}{L} \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & 1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} q \\ 0 \\ 0 \end{bmatrix} + \frac{QL}{4} \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.
\]

(2.52)

Assembly is done such that the matrix is nearly block diagonal, except that each block is superimposed along the upper left and lower right element and added together. The vector with the \( \frac{QL}{4} \) term is similarly superimposed and added, although
it is not diagonal; rather it is stacked. All elements of the \[
\begin{bmatrix}
q \\
0 \\
0 \\
\end{bmatrix}
\] vector beyond the first element are zero because if no flux is specified, we assume that it is zero [20].

Once assembled, this system is solved using linear algebraic methods for the vector \( \mathbf{a} \). This solution is then fed back into equation 2.34 to find the numerical approximation of the original boundary value problem.
CHAPTER III

Review of Constrained Quantum Mechanics

3.1 Review of Existing Literature

There are several methods for analyzing particles constrained to curved surfaces. We will review them in this chapter.

3.1.1 Jensen and Koppe (Ref. [1]) and da Costa (Ref. [2])

Ref. [1], published in 1971, derives the fundamentals of the theory and may be considered the first paper on the subject. Ref. [2], published ten years later, clarifies and more firmly derives the results of Ref. [1]. A summary of these papers is now given. Both references give essentially the same derivation and so the two sources will be combined.

The method Ref. [1] suggests is studying a particle confined between two parallel surfaces and reducing the distance between them until the surface-tangential portion is the only term that remains. The program is as follows: set up a system of parallel surfaces distance \( d \) apart with infinite potential outside the surfaces and no potential between them. Then solve the eigenvalue problem for several different values of \( d \). Fit the slope of each eigenvalue to the form \( E = A/d^2 - \epsilon \). The value of \( \epsilon \) is the energy eigenvalue of the particle as the distance between the surfaces goes to zero. Ref. [1] uses a ring as an example.
The method of Ref. [2] reduces the three-dimensional system to a two-dimensional PDE; unfortunately even when separable these can be quite unwieldy. First, an appropriate coordinate system is selected. Such a coordinate system will have two orthogonal coordinates tangential to the surface and one orthogonal to the surface. The metric tensor is derived, and from it the Weingarten equations, second fundamental form, mean and Gaussian curvatures, and the Laplace-Beltrami operator are derived for the coordinate system. These are used to form a surface tangential Schrödinger equation, which might be separable. Ref. [2] uses a bookbinder surface as an example. Ref. [5] uses this method to solve the problem of a particle constrained to the surface of a spheroid.

The process for calculation of a particle constrained to a curved surface as described in Ref. [2] is illustrated in Figure 3.1. The ultimate goal is to convert the three-dimensional problem into a two-dimensional problem by using coordinates tangential and normal to the surface.

3.1.1.1 Geometric construction

Begin with a parameterized two-dimensional surface \( \mathbf{r} \). Create a coordinate system using tangential coordinates \((q^1, q^2)\) and a coordinate \( q^3 \) that is normal to the surface everywhere. This gives us the mapping

\[
\mathbf{r}(q^1, q^2) = \begin{bmatrix} x(q^1, q^2) \\ y(q^1, q^2) \\ z(q^1, q^2) \end{bmatrix},
\]

which produces the metric tensor

\[
g_{ij} = \mathbf{r}_i \cdot \mathbf{r}_j.
\]
The normal vector is therefore

$$\hat{N} = \frac{\mathbf{r}_1 \times \mathbf{r}_2}{|\mathbf{r}_1 \times \mathbf{r}_2|}$$

(3.3)

The surrounding space can likewise be parameterized as

$$\mathbf{R}(q^1, q^2, q^3) = \mathbf{r}(q^1, q^2) + q^3\hat{N}(q^1, q^2)$$

(3.4)

We now introduce a potential barrier to constrain the particle to the surface,

$$V_{\lambda}(q^3) = \begin{cases} 
0, & |q^3| < \frac{d}{2} \\
V_0, & q^3 > \frac{d}{2}
\end{cases}$$

(3.5)

where \(d\) is the width of the well and \(V_0\) is the energy value.
Taking the determinant of the shape operator gives

$$\det \alpha = -\det h \det (g^{-1}) = -\frac{h}{g} = -K,$$

and its trace gives

$$\text{Tr} \alpha = -\frac{1}{g} (g_{11} h_{22} + g_{22} h_{11} - 2 g_{12} h_{21}) = -2M.$$

Continuing with the derivation of the Laplace-Beltrami operator, we find the gradients of the embedding. The derivatives of the normal vector are given by

$$\hat{N}_i = \alpha_{ij} r_j,$$

which leads to the second fundamental form,

$$h_{ij} = r_{ij} \cdot \hat{N}.$$

The derivative of the parameterization of the surrounding space is

$$R_i = r_i + \left\{ q^3 \hat{N} \right\}_i = r_i + q^3 \alpha_{ij},$$

while the derivative of the surface coordinates are

$$r_{ij} = (\delta_{ij} + q^3 \alpha_{ij}) r_j.$$

The derivative of the parameterization of the surrounding space with respect to $q^3$ is the normal vector:

$$R_{i3} = \hat{N}.$$
3.1.1.2 Formulation of the three-dimensional metric and Laplacian

The next goal is to define a metric in the three-dimensional space. The derivation goes as follows:

\[ G_{ij} = \mathbf{R}_i \cdot \mathbf{R}_j \]

\[ = (\delta_{ik} + q^3 \alpha_{ik})\mathbf{r}_k \cdot (\delta_{jm} + q^3 \alpha_{jm})\mathbf{r}_m \]

\[ = (\delta_{ik} + q^3 \alpha_{ik})(\delta_{jm} + q^3 \alpha_{jm})(\mathbf{r}_k \cdot \mathbf{r}_m) \]

\[ = (\delta_{ik} \delta_{jm} + \delta_{ik} q^3 \alpha_{jm} + q^3 \alpha_{ik} \delta_{jm} + q^3 \alpha_{ik} q^3 \alpha_{jm})(\mathbf{r}_k \cdot \mathbf{r}_m) \]

\[ = (\mathbf{r}_i \cdot \mathbf{r}_j) + q^3(\alpha_{jm} \mathbf{r}_i \cdot \mathbf{r}_m) + \alpha_{ik}(\mathbf{r}_k \cdot \mathbf{r}_j) + (q^3)^2 \alpha_{ik} \alpha_{jm}(\mathbf{r}_k \cdot \mathbf{r}_m) \]

\[ = g_{ij} + q^3(\alpha_{jm} g_{im} + \alpha_{ik} g_{kj}) + (q^3)^2 \alpha_{ik} \alpha_{jm} \]

\[ = g_{ij} + [\alpha g + (\alpha g)^T] q^3 + (\alpha g \alpha^T) q^3 \]

(3.13)

Switching to full matrix notation,

\[ G = g + [\alpha g + (\alpha g)^T] q^3 + (\alpha g \alpha^T) q^3, \]

\[ = g + [-h g^{-1} g + (-h g^{-1} g)^T] q^3 + [\alpha g^{-1} g (-h g^{-1})^T] q^3, \]

\[ = g + [-h + (-h)^T] q^3 + [-h (-h g^{-1})^T] q^3, \]

\[ = g - 2hq^3 + h(-h g^{-1})^T q^3, \]

\[ = g - 2hq^3 + h g^{-1} h (q^3)^2 \]

(3.14)

\[ G g^{-1} = g^{-1} - 2h g^{-1} q^3 + h g^{-1} h^{-1} (q^3)^2, \]

\[ = I + 2\alpha q^3 + \alpha^2 (q^3)^2, \]

\[ = (I + \alpha q^3)^2. \]

(3.15)
This leaves the equation

\[ \mathbf{G} = (\mathbf{I} + \alpha \mathbf{q}^3)^2 \mathbf{g} \]  

(3.16)

The volume element plays a role in the separation of the Schrödinger equation. The determinant is given by

\[ \det \mathbf{G} = [\det (\mathbf{I} + \alpha \mathbf{q}^3)]^2 \det \mathbf{g}, \]

(3.17)

which expands to

\[ \det (\mathbf{I} + \alpha \mathbf{q}^3) = (1 + \alpha_{11} \mathbf{q}^3)(1 + \alpha_{22} \mathbf{q}^3) - \alpha_{12} \alpha_{21} (\mathbf{q}^3)^2 \]

(3.18)

Further expansion gives

\[
|\mathbf{I} + \alpha \mathbf{q}^3| &= 1 + \mathbf{I} + \alpha_{22} \mathbf{q}^3 + \mathbf{I} + \alpha_{11} \mathbf{q}^3 + \mathbf{I} + \alpha_{11} \mathbf{I} + \alpha_{22} (\mathbf{q}^3)^2 - \mathbf{I} + \alpha_{12} \mathbf{I} + \alpha_{21} (\mathbf{q}^3)^2, \\
&= 1 + (\mathbf{I} + \alpha_{11} + \mathbf{I} + \alpha_{22}) \mathbf{q}^3 + (\mathbf{I} + \alpha_{11} \mathbf{I} + \alpha_{22} - \mathbf{I} + \alpha_{12} \mathbf{I} + \alpha_{21}) (\mathbf{q}^3)^2, \\
&= 1 + \text{Tr} \alpha \mathbf{q}^3 + \det \alpha (\mathbf{q}^3)^2.
\]

(3.19)

Thus we have a function \( f \) that satisfies

\[ \sqrt{f} = |\mathbf{I} + \alpha \mathbf{q}^3| = 1 + 2 \mathbf{M} \mathbf{q}^3 + K(\mathbf{q}^3)^2. \]

(3.20)

Orthonormality of the normal coordinate with the tangent subspace means that the full metric has the form

\[
\mathbf{G} = \begin{bmatrix}
G_{11} & G_{12} & 0 \\
G_{12} & G_{22} & 0 \\
0 & 0 & 1
\end{bmatrix}.
\]

(3.21)
3.1.1.3 Schrödinger equation

We now introduce the Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V_\lambda \psi = i\hbar \frac{\partial \psi}{\partial t}. \quad (3.22)$$

Using Ref. [15], which is nearly as old as quantum mechanics itself, we use the three-dimensional Laplace-Beltrami operator. It is

$$\nabla^2 \psi = \frac{1}{\sqrt{G}} [\sqrt{G} G^{ij} \psi_j]_i \quad (3.23)$$

where the metric tensor of the surrounding space is given by

$$G^{ij} = \frac{1}{g} \begin{bmatrix} G_{22} & -G_{12} & 0 \\ -G_{12} & G_{11} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (3.24)$$

and its determinant is

$$G = G_{11} G_{22} - (G_{12})^2. \quad (3.25)$$

So the Schrödinger equation expands to

$$-\frac{\hbar^2}{2m} \frac{1}{\sqrt{G}} [\sqrt{G} G^{ij} \psi_j]_i + V_\lambda \psi = i\hbar \psi_t, \quad \text{Ref. [15]}$$

$$-\frac{\hbar^2}{2m} \frac{1}{G} G_{i\lambda} G^{ij} \psi_j - \frac{\hbar^2}{2m} \frac{1}{G} G^{ij} \psi_j - \frac{\hbar^2}{2m} G^{ij} \psi_{ji} + V_\lambda \psi = i\hbar \psi_t, \quad (3.26)$$
Noting that $G^{33} = 1$ we then have
\begin{align*}
- \frac{\hbar^2}{2m} \frac{1}{2G} G_{,i} G^{ij} \psi_{,j} - \frac{\hbar^2}{2m} G^{ij}_{,j} \psi_{,j} - \frac{\hbar^2}{2m} G^{ij} \psi_{,ji} \\
- \frac{\hbar^2}{2m} G_{3} \psi_{,3} - \frac{\hbar^2}{2m} \psi_{,33} + V \psi = i\hbar \psi_t. \tag{3.27}
\end{align*}

Next utilize the identity
\[ [\ln \sqrt{G}]_{,3} = \frac{G_{,3}}{2G} \tag{3.28} \]
and separate the $q^3$ variables to get
\begin{align*}
\sum_{i,j=1}^{2} - \frac{\hbar^2}{2m} \frac{1}{2G} G_{,i} G^{ij} \psi_{,j} - \frac{\hbar^2}{2m} G^{ij}_{,j} \psi_{,j} - \frac{\hbar^2}{2m} G^{ij} \psi_{,ji} \\
- \frac{\hbar^2}{2m} \frac{1}{2G} [\ln \sqrt{G}]_{,3} \psi_{,3} - \frac{\hbar^2}{2m} \psi_{,33} + V \psi = i\hbar \psi_t, \\
- \frac{\hbar^2}{2m} \sum_{i,j=1}^{2} \left\{ \frac{1}{2G} G_{,i} G^{ij} \psi_{,j} + G^{ij}_{,j} \psi_{,j} + G^{ij} \psi_{,ji} \right\} \\
- \frac{\hbar^2}{2m} \left\{ \psi_{,33} + [\ln \sqrt{G}]_{,3} \psi_{,3} \right\} + V \psi = i\hbar \psi_t, \\
- \frac{\hbar^2}{2m} \sum_{i,j=1}^{2} \left\{ \frac{1}{2G} G_{,i} G^{ij} \psi_{,j} + G^{ij}_{,j} \psi_{,j} + G^{ij} \psi_{,ji} \right\} \\
- \frac{\hbar^2}{2m} \left\{ \psi_{,33} + [\ln \sqrt{G}]_{,3} \psi_{,3} \right\} + V \psi = i\hbar \psi_t \tag{3.29}
\end{align*}

The tangential terms can be combined to form a new operator
\[ \mathcal{D}(q^1, q^2, q^3)[\psi] = \frac{1}{2G} G_{,i} G^{ij} \psi_{,j} + G^{ij}_{,j} \psi_{,j} + G^{ij} \psi_{,ji}, \tag{3.30} \]
shortening the Schrödinger equation to
\begin{align*}
- \frac{\hbar^2}{2m} \mathcal{D}(q^1, q^2, q^3)[\psi] - \frac{\hbar^2}{2m} \psi_{,33} + [\ln \sqrt{G}]_{,3} \psi_{,3} + V \psi = i\hbar \psi_t. \tag{3.31}
\end{align*}
3.1.1.4 Separation of variables

We now look to separate this equation into an equation tangential to the surface and an equation normal to the surface. To separate the equation, define a function

\[ \chi(q^1, q^2, q^3) = \chi_t(q^1, q^2)\chi_n(q^3) \]

(3.32)

and relate it to \( \psi \) by

\[ \chi(q^1, q^2, q^3) = \sqrt{f(q^1, q^2, q^3)}\psi(q^1, q^2, q^3), \]

(3.33)

such that we can define the surface probability density as

\[ P = |\chi_t|^2 \int |\chi_n|^2 dq^3. \]

(3.34)

We require a function \( f(q^1, q^2, q^3) \) that has the volume element

\[ dV = \sqrt{G}dq^1dq^2dq^3. \]

(3.35)

Defining \( dS = \sqrt{G}dq^1dq^2 \), we have

\[ dV = f(q^1, q^2, q^3)\sqrt{G}dq^1dq^2dq^3. \]

(3.36)

We can write the function derived above as

\[ f = \left\{ 1 + \text{Tr} (\alpha)q^3 + \text{det} (\alpha)(q^3)^2 \right\}^2. \]

(3.37)
Next plug $\psi = \frac{\chi}{\sqrt{f}}$ into the Schrödinger equation and expand it:

$$
-\frac{\hbar^2}{2m} \nabla \left( \frac{\chi}{\sqrt{f}} \right) - \frac{\hbar^2}{2m} \left\{ \frac{\partial^2}{\partial (q^3)^2} \left( \frac{\chi}{\sqrt{f}} \right) + \frac{\partial}{\partial q^3} \left[ \ln \sqrt{G} \right] \frac{\partial}{\partial q^3} \left( \frac{\chi}{\sqrt{f}} \right) \right\} \\
+ V_\lambda \frac{\chi}{\sqrt{f}} = i \hbar \frac{\partial \chi}{\partial t}, \quad (3.38)
$$

$$
-\sqrt{f} \frac{\hbar^2}{2m} \nabla \left( \frac{\chi}{\sqrt{f}} \right) - \frac{\hbar^2}{2m} \left\{ \sqrt{f} \frac{\partial^2}{\partial (q^3)^2} \left( \frac{\chi}{\sqrt{f}} \right) + \sqrt{f} \frac{\partial}{\partial q^3} \left[ \ln \sqrt{G} \right] \frac{\partial}{\partial q^3} \left( \frac{\chi}{\sqrt{f}} \right) \right\} \\
+ V_\lambda \chi = i \hbar \frac{\partial \chi}{\partial t}, \quad (3.39)
$$

$$
-\sqrt{f} \frac{\hbar^2}{2m} \nabla \left( \frac{\chi}{\sqrt{f}} \right) - \frac{\hbar^2}{2m} \left\{ \sqrt{f} \frac{\partial}{\partial q^3} \frac{\partial}{\partial q^3} \left( \frac{\chi}{\sqrt{f}} \right) + \sqrt{f} \frac{G_3}{2G} \frac{\partial}{\partial q^3} \left( \frac{\chi}{\sqrt{f}} \right) \right\} \\
+ V_\lambda \chi = i \hbar \frac{\partial \chi}{\partial t}. \quad (3.40)
$$

The central term evaluates to

$$
\frac{\partial}{\partial q^3} \left( \frac{\chi}{\sqrt{f}} \right) = \frac{1}{f} \left[ \chi_3 \sqrt{f} - \frac{\chi f_3}{2 \sqrt{f}} \right] = \left[ \frac{\chi_3}{\sqrt{f}} - \frac{\chi f_3}{2 f^{32}} \right], \quad (3.41)
$$

which converts the Schrödinger equation to

$$
-\sqrt{f} \frac{\hbar^2}{2m} \nabla \left( \frac{\chi}{\sqrt{f}} \right) - \frac{\hbar^2}{2m} \left\{ \sqrt{f} \left[ \frac{\partial}{\partial q^3} \frac{\chi_3}{\sqrt{f}} - \frac{1}{2} \frac{\partial}{\partial q^3} \frac{\chi f_3}{f^{32}} \right] + \sqrt{f} \frac{G_3}{2G} \left[ \frac{\chi_3}{\sqrt{f}} - \frac{\chi f_3}{2 f^{32}} \right] \right\} \\
+ V_\lambda \chi = i \hbar \frac{\partial \chi}{\partial t}, \quad (3.42)
$$
\[-\sqrt{f} \frac{\hbar^2}{2m} \mathcal{D} \left( \frac{\chi}{\sqrt{f}} \right) - \frac{\hbar^2}{2m} \left\{ \sqrt{f} \left[ \frac{\chi_{,33}}{\sqrt{f}} - \frac{\chi_{,3} f_{,3}}{2 f_{,2}^2} - \frac{\chi_{,3} f_{,3}}{2 f_{,2}^2} - \frac{\chi f_{,33}}{4 f^3} \sqrt{f} \right] \right\} + \frac{3}{4 f^3} \chi \sqrt{f} (f_{,3})^2 \right\} + V_{\lambda \chi} = i \hbar \frac{\partial \chi}{\partial t}. \]

(3.43)

Noting that $G_{3,3} = 2 f f_{,3} g$,

\[-\sqrt{f} \frac{\hbar^2}{2m} \mathcal{D} \left( \frac{\chi}{\sqrt{f}} \right) - \frac{\hbar^2}{2m} \left\{ \chi_{,33} - \frac{\chi_{,3} f_{,3}}{2 f} - \frac{\chi_{,3} f_{,3}}{2 f} - \frac{\chi f_{,33}}{2 f} \right\} + \frac{3}{4 f^2} (f_{,3})^2 \right\} + V_{\lambda \chi} = i \hbar \frac{\partial \chi}{\partial t}. \]

(3.44)

\[-\sqrt{f} \frac{\hbar^2}{2m} \mathcal{D} \left( \frac{\chi}{\sqrt{f}} \right) - \frac{\hbar^2}{2m} \left\{ \chi_{,33} + \frac{3}{4 f^2} (f_{,3})^2 - \frac{1}{2 f^2} (f_{,3})^2 \chi \right\} + \frac{f_{,33}}{2 f} \chi - \frac{f_{,3}}{f} \chi_{,3} + \frac{f_{,3}}{f} \chi_{,3} \right\} + V_{\lambda \chi} = i \hbar \frac{\partial \chi}{\partial t}. \]

(3.45)

\[-\sqrt{f} \frac{\hbar^2}{2m} \mathcal{D} \left( \frac{\chi}{\sqrt{f}} \right) - \frac{\hbar^2}{2m} \left\{ \chi_{,33} \right\} + \left[ \frac{3}{4 f^2} (f_{,3})^2 - \frac{2}{4 f^2} (f_{,3})^2 - f f_{,33} \frac{4 f^2}{4 f^2} \chi \right\} + V_{\lambda \chi} = i \hbar \frac{\partial \chi}{\partial t}. \]

(3.46)

\[\sqrt{f} \left[ -\frac{\hbar^2}{2m} \mathcal{D} \left( \frac{\chi}{\sqrt{f}} \right) \right] - \frac{\hbar^2}{2m} \left\{ \chi_{,33} \right\} + \left[ \frac{1}{4 f^2} [(f_{,3})^2 - 2 f f_{,33}] \chi \right\} + V_{\lambda \chi} = i \hbar \frac{\partial \chi}{\partial t}. \]

(3.47)
Since we are only interested in the surface, we can take the limit $d \to 0$ and $q^3 \to 0$, except for the $V_\lambda$ term where it is important, and take $V_0 \to \infty$. Then $f \to 1$ and

\[
f_{,3} = \lim_{q^3 \to 0} \left[ \text{Tr} (\alpha) + 2 \det (\alpha) q^3 \right] = \text{Tr} \alpha, \tag{3.49}
\]

\[
f_{,33} = 2 \det \alpha, \tag{3.50}
\]

\[
\left[ -\frac{\hbar^2}{2m} \mathcal{D}(\chi) \right] - \frac{\hbar^2}{2m} \left\{ \frac{\partial^2 \chi}{\partial (q^3)^2} + \frac{1}{4} \left( \text{Tr} \alpha \right)^2 - 4 \det \alpha \right\} \chi + V_\lambda \chi = i\hbar \frac{\partial \chi}{\partial t} \tag{3.51}
\]

\[
\left[ -\frac{\hbar^2}{2m} \mathcal{D}(\chi) \right] - \frac{\hbar^2}{2m} \frac{\partial^2 \chi}{\partial (q^3)^2} + \left( \frac{1}{2} \text{Tr} \alpha \right)^2 - \det \alpha \right\} \chi + V_\lambda \chi = i\hbar \frac{\partial \chi}{\partial t} \tag{3.52}
\]

\[
\left[ -\frac{\hbar^2}{2m} \mathcal{D}(\chi) \right] - \frac{\hbar^2}{2m} \frac{\partial^2 \chi}{\partial (q^3)^2} - \frac{\hbar^2}{2m} (M^2 - K) \chi + V_\lambda \chi = i\hbar \frac{\partial \chi}{\partial t} \tag{3.53}
\]

Next we look at the $\mathcal{D}$ operator.

\[
\mathcal{D}(q^1, q^2, q^3)[\psi] = \frac{1}{2G} G_{ij} \psi_j \psi_j + G^{ij} \psi_j \psi_j + G^{ij} \psi_j \psi_j, \tag{3.54}
\]

where

\[
G_{ij} = g_{ij} + [\alpha g + (\alpha g)^T]_{ij} q^3 + (\alpha g^T)_{ij} (q^3)^2. \tag{3.55}
\]

In the limit $q^3 \to 0$, $G_{ij} = g_{ij}$, $G^{ij} = g^{ij}$, and $G = f^2 g = g$, so we have

\[
\mathcal{D}(q^1, q^2, q^3)[\psi] = \frac{1}{2G} g_{ij} \psi_j \psi_j + G^{ij} \psi_j \psi_j + g^{ij} \psi_j \psi_j = \frac{1}{\sqrt{G}} [\sqrt{G} g^{ij} \psi_j]_i. \tag{3.56}
\]

Thus

\[
\mathcal{D}(q^1, q^2, q^3)[\psi] = \sum_{i,j=1}^2 \frac{1}{\sqrt{G}} \frac{\partial}{\partial q^i} \left[ \sqrt{G} g^{ij} \frac{\partial \psi}{\partial q^j} \right] = \nabla^2_{LB} \psi. \tag{3.57}
\]
Let $\chi(q^1, q^2, q^3, t) = \chi_t(q^1, q^2, t)\chi_n(q^3, t)$. Then

$$ -\frac{1}{\chi_t} \frac{\hbar^2}{2m} \frac{\partial}{\partial q^i} \left( \sqrt{G} g^{ij} \frac{\partial \chi_t}{\partial q^j} \right) - \frac{\hbar^2}{2m} (M^2 - K) - \frac{i\hbar}{\chi_t} \frac{\partial \chi_t}{\partial t} = \frac{1}{\chi_n} \frac{\hbar^2}{2m} \frac{\partial^2 \chi_n}{\partial (q^3)^2} - V_\lambda + \frac{i\hbar}{\chi_n} \frac{\partial \chi_n}{\partial t} $$

Thus the equations separate to

$$ -\frac{\hbar^2}{2m} \frac{1}{\sqrt{G}} \frac{\partial}{\partial q^i} \left( \sqrt{G} g^{ij} \frac{\partial \chi_t}{\partial q^j} \right) - \frac{\hbar^2}{2m} (M^2 - K) \chi_t = i\hbar \frac{\partial \chi_t}{\partial t}, $$

and

$$ -\frac{\hbar^2}{2m} \frac{\partial^2 \chi_n}{\partial (q^3)^2} + V_\lambda \chi_n = i\hbar \frac{\partial \chi_n}{\partial t}. $$

The first equation is an infinite square well. The second will have energy eigenvalues $\epsilon$. The energy eigenvalues of the full PDE are given by

$$ E = \frac{\hbar^2 n^2 \pi^2}{2md^2} + \epsilon. $$

Because it produces infinite energy eigenvalues as the range of $q^3$ goes to zero, we can ignore the first term for the case of a constrained particle, leaving $\epsilon$. Using the Weingarten equations the potential in the second equation can be written as

$$ -\frac{\hbar^2}{2m} \left( \frac{1}{2} \text{Tr} (\alpha_{ij}) \right)^2 - \det (\alpha_{ij}) = -\frac{\hbar^2}{2m} (M^2 - K), $$

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

Thus the Laplace-Beltrami operator $\mathcal{D}$ (which is also denoted by the usual $\nabla^2$ or $\nabla_{LB}^2$), mean curvature $M$, and Gaussian curvature $K$ combine to form the curved-space Schrödinger equation:

$$ -\frac{\hbar^2}{2m} \left( \mathcal{D} + (M^2 - K) \right) \chi_t (q^1, q^2) = E \chi_t (q^1, q^2). $$
This is the equation that is used for solving particles constrained to curved surfaces as a two-dimensional problem. Note that if this derivation is not done correctly (for example, by taking a three-dimensional equation and simply holding one coordinate fixed with zero derivative at that value), the curvature terms will not show up in the Schrödinger equation.

### 3.1.1.5 Particle constrained to a circle

As a preliminary example, we study a particle constrained to a circle of radius \(a\). Although this is a space curve and not a surface, and thus has a slightly different curvature term (Ref. [2]), it highlights a nontrivial effect of using the differential geometric formalism.

For a particle constrained to a circle of radius \(a\), the parameterization is

\[
\mathbf{r} = \begin{bmatrix}
a \cos \theta \\
a \sin \theta 
\end{bmatrix}
\]  

(3.64)

Its derivatives are given by

\[
\frac{\partial \mathbf{r}}{\partial \theta} = a \begin{bmatrix} -\sin \theta \\ \cos \theta \end{bmatrix}.
\]  

(3.65)

Thus the metric is

\[
g = a^2 \begin{bmatrix} -\sin \theta & -\sin \theta \\ \cos \theta & \cos \theta \end{bmatrix} = a^2.
\]  

(3.66)

The Laplace-Beltrami operator is

\[
\nabla^2 \psi = \frac{1}{a^2} \frac{\partial^2 \psi}{\partial \theta^2}.
\]  

(3.67)
and the curvature is
\[ k = \frac{1}{a}. \]  
(3.68)

For a space curve, the Schrödinger equation is [2]

\[ -\frac{\hbar^2}{2ma^2} \frac{\partial^2 \psi}{\partial \theta^2} - \frac{\hbar^2 k^2}{2m} \psi = E \psi, \]  
(3.69)

so the Schrödinger equation becomes

\[ -\frac{\hbar^2}{2ma^2} \frac{\partial^2 \psi}{\partial \theta^2} - \frac{\hbar^2}{8ma^2} \psi = E \psi. \]  
(3.70)

This can be written as

\[ \frac{\partial^2 \psi}{\partial \theta^2} = -\left( \frac{1}{4} + \frac{2ma^2E}{\hbar^2} \right) \psi, \]  
(3.71)

which is the Helmholtz equation with \( k^2 \) equal to the quantity in parenthesis on the right hand side.

This has energy levels

\[ E = \frac{\hbar^2}{2ma^2} \left( n^2 - \frac{1}{4} \right) \]  
(3.72)

where \( n \in \mathbb{N} \).

Note that this energy has a shift of \( \Delta E = -\frac{\hbar^2}{8ma^2} \) from the traditional solution in numerous quantum mechanics textbooks. [21; 22; 23; 24] However, since it is a constant shift, it does not affect the differences between energy levels and therefore has a negligible physical effect because it merely moves the zero-point energy.

3.1.2 Encinosa and Etimadi (Ref. [3])

Ref. [3] uses differential forms to derive the same Schrödinger equation as Refs. [2]. Rather than using classical differential geometry, one first forms the line element \( ds \)
and from it uses the exterior derivative and Hodge star operator to derive a Laplacian and the curvature energy shift. This produces equations identical to the method of Ref. [2] above.

### 3.1.2.1 Derivation of the Laplacian operator via differential forms

The derivation of the distortion potential begins with a parameterization of the two-dimensional surface in question and its embedding into a three-dimensional space. The coordinate system is defined as two surface-parallel coordinates $q_1$ and $q_2$, and an orthogonal coordinate $q_3$. The parameterization is

$$r(q_1, q_2, q_3) = x(q_1, q_2) + q_3 \hat{e}_3.$$  \hspace{1cm} (3.73)

The next step is to take the exterior derivative. It is

$$dr = dx + d(q_3 \hat{e}_3) = dx + dq_3 \hat{e}_3,$$  \hspace{1cm} (3.74)

where $dq_3$ is the infinitesimal displacement normal to the surface. The exterior derivative can be projected onto a coordinate basis by

$$dx = x_1 dq_1 + x_2 dq_2 = \sigma_1 \hat{e}_1 + \sigma_2 \hat{e}_2,$$  \hspace{1cm} (3.75)

where the $\hat{e}_i$'s are unit basis vectors and the $\sigma_i$'s are one-forms on . From this it can be deduced that

$$x_1 dq_1 + x_2 dq_2 = \frac{\sigma_1}{|x_1|} + \frac{\sigma_2}{|x_2|},$$  \hspace{1cm} (3.76)

so that $\sigma_1 = |x_1| dq_1$ and $\sigma_2 = |x_2| dq_2$. 

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For a zero-form $\chi$, the exterior derivative is [3; 17]

\[
\begin{align*}
d\chi &= \frac{\partial \chi}{\partial x_1} dx_1 + \frac{\partial \chi}{\partial x_2} dx_2 + \frac{\partial \chi}{\partial x_3} dx_3 \\
&= \frac{\partial \chi}{\partial x_1} x_{11} dq_1 + \frac{\partial \chi}{\partial x_2} x_{12} dq_2 + \frac{\partial \chi}{\partial x_3} dq_3 \\
&= \frac{\partial \chi}{\partial x_1} \sigma_1 + \frac{\partial \chi}{\partial x_2} \sigma_2 + \frac{\partial \chi}{\partial x_3} dq_3 \\
&= a_1 \sigma_1 + a_2 \sigma_2 + a_3 dq_3,
\end{align*}
\]

(3.77)

where the $a_i$ functions are zero forms. Its Hodge dual gives

\[
* d\chi = *(a_1 \sigma_1 + a_2 \sigma_2 + a_3 dq_3) = a_1 \sigma_2 \wedge dq_3 + a_2 dq_3 \wedge \sigma_1 + a_3 \sigma_1 \wedge \sigma_2.
\]

(3.78)

Applying the exterior derivative of this gives

\[
d* d\chi = d(a_1 \sigma_2 \wedge dq_3) + d(a_2 dq_3 \wedge \sigma_1) + d(a_3 \sigma_1 \wedge \sigma_2).
\]

(3.79)

Noting $d^2 x = 0$, $a \wedge a = 0$, and $d(a \wedge b) = da \wedge b + (-1)^p a \wedge db$, where $a$ is a $p$-form,

\[
\begin{align*}
d* d\chi &= d(a_1 \sigma_2) \wedge dq_3 + d(a_2 dq_3) \wedge \sigma_1 + d(a_3 \sigma_1) \wedge \sigma_2 + a_1 \sigma_2 \wedge d(dq_3) \\
&+ a_2 dq_3 \wedge d\sigma_1 + a_3 \sigma_1 \wedge d\sigma_2, \\
&= da_1 \sigma_2 \wedge dq_3 + da_2 dq_3 \wedge \sigma_1 + da_3 \sigma_1 \wedge \sigma_2 + a_1 d_2 \wedge dq_3 + a_3 d_1 \wedge d_2 + a_2 dq_3 \wedge d\sigma_1 + a_3 \sigma_1 \wedge d\sigma_2.
\end{align*}
\]

(3.80)

Noting that $d_i = 0$ because $\frac{\partial \sigma_i}{\partial x_j} = 0$ for all $(i, j)$,

\[
\begin{align*}
d* d\chi &= \chi_{11} \sigma_1 \wedge \sigma_2 \wedge dq_3 + \chi_{12} \sigma_2 \wedge dq_3 \wedge \sigma_1 + \chi_{33} dq_3 \wedge \sigma_1 \wedge \sigma_2, \\
&= \chi_{11} \sigma_1 \wedge \sigma_2 \wedge dq_3 + \chi_{22} \sigma_2 \wedge dq_3 \wedge \sigma_1 + \chi_{33} dq_3 \wedge \sigma_1 \wedge \sigma_2, \\
&= (\nabla^2 \chi) \sigma_1 \wedge \sigma_2 \wedge dq_3.
\end{align*}
\]

(3.81)
Taking the Hodge operator once more gives

\[ *d * d\chi = \nabla^2 \chi. \quad (3.82) \]

Thus we have derived the Laplacian operator for this coordinate system via differential forms.

### 3.1.2.2 Cylindrical coordinates

Now that this has been derived, the parameterization is modified slightly such that in cylindrical coordinates it is described by the Monge form

\[ \mathbf{r} = \rho \cos \phi \hat{i} + \rho \sin \phi \hat{j} + S(\rho) \hat{k}. \quad (3.83) \]

The arc length is given by

\[ \frac{1}{Z} = \sqrt{1 + S^2(\rho)}. \quad (3.84) \]

This has cylindrical symmetry. The unit basis vectors are then given by

\[ \hat{e}_1 = \frac{\mathbf{r}_\rho}{|\mathbf{r}_\rho|} = (\cos \phi, \sin \phi, S(\rho)) Z, \quad (3.85) \]

\[ \hat{e}_2 = \frac{\mathbf{r}_\phi}{|\mathbf{r}_\phi|} = \frac{1}{\rho} (-\rho \sin \phi, \rho \cos \phi, 0) = (- \sin \phi, \cos \phi, 0), \quad (3.86) \]

\[ \hat{e}_3 = (-S(\rho) \cos \phi, -S(\rho) \sin \phi, 1) Z. \quad (3.87) \]
The exterior derivative of the parameterization is

\[ \text{dr} = \sigma_1 \hat{e}_1 + \sigma_2 \hat{e}_2 + \sigma_3 \hat{e}_3 = r_\rho \, d\rho + r_\phi \, d\phi + z_z \, dz, \]

\[ \Rightarrow \begin{align*}
  &\quad (\cos \phi, \sin \phi, S, \rho \, d\rho) \\
  &\quad + (\rho \, d\rho, 0) (\cos \phi, \sin \phi, -S, \rho \, d\rho) \\
  &\quad + (\rho \, d\rho, 0) (\cos \phi, \sin \phi, -S, \rho \, d\rho) Z \sigma_3.
\end{align*} \]

(3.88)

This implies that \( \sigma_1 = \frac{d\rho}{Z}, \sigma_2 = \rho d\phi, \) and \( \sigma_3 = dq_3. \)

Taking the Hodge dual of the exterior derivative gives

\[ * \left( \frac{d\rho}{Z} \right) = \rho d\phi \wedge dq_3, * \rho d\phi = \frac{1}{Z} dq_3 \wedge d\rho, \text{ and } * dq_3 = \rho d\rho \wedge d\phi. \] (3.89)

The next step is to derive the Laplacian operator.

\[ d\chi = \frac{\partial \chi}{\partial \rho} d\rho + \frac{\partial \chi}{\partial \phi} d\phi + \frac{\partial \chi}{\partial q_3} dq_3, \]

\[ = Z \frac{\partial \chi}{\partial \rho} d\rho + \frac{1}{\rho} \frac{\partial \chi}{\partial \phi} \rho d\phi + \frac{\partial \chi}{\partial q_3} dq_3. \] (3.90)

Taking the Hodge dual of this gives

\[ * d\chi \begin{align*}
  &\quad = Z \frac{\partial \chi}{\partial \rho} \rho d\phi \wedge dq_3 + \frac{1}{\rho} \frac{\partial \chi}{\partial \phi} dq_3 \wedge \frac{d\rho}{Z} + \frac{\partial \chi}{\partial q_3} \frac{d\rho}{Z} \wedge \rho d\phi, \\
  &\quad = d \left( \rho Z \frac{\partial \chi}{\partial \rho} d\phi \wedge \frac{d\rho}{Z} \right) + d \left( \frac{1}{Z} \rho \frac{\partial \chi}{\partial \phi} dq_3 \wedge d\rho \right) + d \left( \frac{\rho}{Z} \frac{\partial \chi}{\partial q_3} dq_3 \wedge d\rho \right), \\
  &\quad = \frac{\partial}{\partial \rho} \left( \rho Z \frac{\partial \chi}{\partial \rho} \right) d\phi \wedge dq_3 + \frac{\partial}{\partial \phi} \left( \frac{1}{Z} \rho \frac{\partial \chi}{\partial \phi} \right) dq_3 \wedge d\rho + \frac{\partial}{\partial q_3} \left( \frac{\rho}{Z} \frac{\partial \chi}{\partial q_3} \right) dq_3 \wedge d\rho \\
  &\quad + \frac{\partial}{\partial q_3} \left( \frac{\rho}{Z} \frac{\partial \chi}{\partial q_3} \right) dq_3 \wedge d\phi, \\
  &\quad = \frac{Z}{\rho} \left[ \frac{\partial}{\partial \rho} \left( \rho Z \frac{\partial \chi}{\partial \rho} \right) + \frac{\partial}{\partial \phi} \left( \frac{1}{Z} \rho \frac{\partial \chi}{\partial \phi} \right) + \frac{\partial}{\partial q_3} \left( \frac{\rho}{Z} \frac{\partial \chi}{\partial q_3} \right) \right] \left( \frac{d\rho}{Z} \wedge \rho d\phi \wedge dq_3 \right).\end{align*} \] (3.91)
The second Hodge dual gives

\[ *d*d\chi = \frac{Z}{\rho} \frac{\partial}{\partial \rho} \left( \rho Z \frac{\partial \chi}{\partial \rho} \right) + \frac{Z}{\rho} \frac{\partial}{\partial \phi} \left( \frac{1}{Z \rho} \frac{\partial \chi}{\partial \phi} \right) + \frac{Z}{\rho} \frac{\partial}{\partial q_3} \left( \frac{\rho}{Z} \frac{\partial \chi}{\partial q_3} \right), \]

\[ = Z^2 \chi_{,\rho\rho} + \frac{Z}{\rho} (Z + \rho Z_{,\rho}) \chi_{,\rho} + \frac{1}{\rho^2} \chi_{,\phi\phi} + \chi_{,33} \]  \hspace{1cm} (3.92)

\[ \nabla^2 \chi = Z^2 \chi_{,\rho\rho} + \left( \frac{Z^2}{\rho} + Z Z_{,\rho} \right) \chi_{,\rho} + \frac{1}{\rho^2} \chi_{,\phi\phi} + \chi_{,33}. \]  \hspace{1cm} (3.93)

Now that the Laplacian is derived, we use it to derive equation 13 in Ref. [3].

\[ \nabla^2 \chi = Z^2 \chi_{,\rho\rho} + Z \left( \frac{Z}{\rho} + Z_{,\rho} \right) \chi_{,\rho} + \frac{1}{\rho^2} \chi_{,\phi\phi} + \chi_{,33} = \nabla^2_t \chi + \chi_{,33}, \]  \hspace{1cm} (3.94)

where

\[ \nabla^2_t \chi = Z^2 \chi_{,\rho\rho} + Z \left( \frac{Z}{\rho} + Z_{,\rho} \right) \chi_{,\rho} + \frac{1}{\rho^2} \chi_{,\phi\phi}. \]  \hspace{1cm} (3.95)

Noting that, setting \( \lambda^2 = G_{11} \) and \( \mu^2 = G_{22} \),

\[ \nabla^2 \chi \]  \hspace{1cm} (3.96)

Using the identity

\[ \left[ \ln \sqrt{G} \right]_3 = \frac{G_{,3}}{2G}, \]  \hspace{1cm} (3.97)
we have
\[
\nabla^2 \chi = \sum_{i,j=1}^{2} \frac{1}{2} GG_{ij} \chi_{,ij} + G_{,i} \chi_{,j} + G_{,j} \chi_{,i} + \left[ \ln \sqrt{G} \right]_{,3} \chi_{,3} + \chi_{,33},
\]
\[
= \frac{1}{\lambda^2} \chi_{,\rho\rho} + \frac{\partial}{\partial \rho} \left( \frac{\mu}{\lambda} \right) \chi_{,\rho} + \frac{1}{\mu^2} \chi_{,\phi\phi} + \left[ \ln (\lambda \mu) \right]_{,3} \chi_{,3} + \chi_{,33},
\]
\[
= \nabla^2 \chi + \left[ \ln (\lambda \mu) \right]_{,3} \chi_{,3} + \chi_{,33},
\]
\[
= \frac{1}{\lambda^2} \chi_{,\rho\rho} + \frac{\partial}{\partial \rho} \left( \frac{\mu}{\lambda} \right) \chi_{,\rho} + \frac{1}{\mu^2} \chi_{,\phi\phi}
\]
(3.98)

The differential form derivation shows
\[
\nabla^2 \chi = Z^2 \chi_{,\rho\rho} + Z \left( \frac{Z}{\rho} + Z_{,\rho} \right) \chi_{,\rho} + \frac{1}{\rho^2} \chi_{,\phi\phi}
\]
\[
= \frac{1}{\lambda^2} \chi_{,\rho\rho} + \frac{\partial}{\partial \rho} \left( \frac{\mu}{\lambda} \right) \chi_{,\rho} + \frac{1}{\mu^2} \chi_{,\phi\phi}.
\]
(3.99)

So \( \lambda = \frac{1}{Z} \) and \( \mu = \rho \).

On the surface, \( q_3 = 0 \) and the second fundamental form is
\[
h_{11} = (0, 0, S_{,\rho\rho}) \cdot (-S_{,\rho} \cos \phi, -S_{,\rho} \sin \phi, 1) Z,
\]
\[
= Z S_{,\rho\rho},
\]
(3.100)

and
\[
h_{22} = (-\rho \cos \phi, -\rho \sin \phi, 0) \cdot (-S_{,\rho} \cos \phi, -S_{,\rho} \sin \phi, 1) Z
\]
\[
= \rho S_{,\rho} Z.
\]
(3.101)

The metric tensor on the surface is diagonal with components \( \lambda^2, \mu^2 \) and is given
by

\[ g_{11} = \lambda^2 = |r, \rho|^2 = \cos^2 \phi + \sin^2 \phi + S^2 = 1 + S^2, \]
\[ = \frac{1}{\rho^2}, \quad (3.102) \]

\[ g_{22} = \mu^2 = |r, \phi|^2 = \rho^2 \sin^2 \phi + \rho^2 \cos^2 \phi \]
\[ = \rho^2, \quad (3.103) \]

and

\[ g_{33} = 1. \quad (3.104) \]

The discriminant is

\[ \sqrt{g} = \frac{\rho}{\rho^2}. \quad (3.105) \]

The Laplacian derived using this method is

\[ \nabla^2 \chi = \frac{Z}{\rho} \left[ \frac{\rho}{Z} Z^2 \chi_{,\rho} \right]_{,\rho} + \frac{Z}{\rho} \left[ \frac{1}{Z} \frac{1}{\rho^2} \chi_{,\phi} \right]_{,\phi} + \frac{Z}{\rho} \left[ \frac{\rho}{Z} \chi_{,3} \right]_{,3}, \]
\[ = \frac{Z}{\rho} \left[ \rho Z \chi_{,\rho} \right]_{,\rho} + \frac{1}{\rho^2} \chi_{,\phi \phi} + \chi_{,33}, \]
\[ = Z^2 \chi_{,\rho \rho} + Z \left( \frac{Z}{\rho} + Z_{,\rho} \right) \chi_{,\rho} + \frac{1}{\rho^2} \chi_{,\phi \phi} + \chi_{,33}. \quad (3.106) \]

As before, compare with the more general derivation

\[ \nabla^2 \chi = \frac{1}{\lambda^2} \chi_{,\rho \rho} + \frac{\partial}{\partial \rho} \left( \frac{\mu}{\lambda} \right) \chi_{,\rho} + \frac{1}{\mu^2} \chi_{,\phi \phi} + \chi_{,33} \quad (3.107) \]

to get \( \lambda = 1/Z \) and \( \mu = \rho \).

From the first and second fundamental forms we can calculate the shape operator
and get the principal curvatures from that.

\[ \alpha = -\frac{1}{g} \begin{bmatrix} g_{22} h_{11} & 0 \\ 0 & h_{22} g_{11} \end{bmatrix} = - \begin{bmatrix} \frac{s_{\rho \rho} Z}{\lambda^3} & 0 \\ 0 & \frac{\rho s_{\rho \rho} Z}{\mu^3} \end{bmatrix} = - \begin{bmatrix} S_{\rho \rho} Z^3 & 0 \\ 0 & \frac{s_{\rho \rho} Z}{\rho} \end{bmatrix}. \]  

(3.108)

Thus the principal curvatures are

\[ k_1 = -\frac{S_{\rho} Z}{\rho} \]  

(3.109)

and

\[ k_2 = -\frac{S_{\rho \rho}}{\lambda^3} = -S_{\rho \rho} Z^3. \]  

(3.110)

The Gaussian and mean curvatures are

\[ K = k_1 k_2 = \frac{S_{\rho} S_{\rho \rho} Z^4}{\rho}, \]  

(3.111)

and

\[ M = -\frac{Z}{2} \left( \frac{S_{\rho}}{\rho} + Z^2 S_{\rho \rho} \right). \]  

(3.112)

In the surrounding space, the metric tensor has additional components proportional to the distance from the surface and the principal curvatures. Hence

\[ \lambda = \frac{1 + q_3 k_2}{Z}, \]  

(3.113)

and

\[ \mu = \rho (1 + q_3 k_1). \]  

(3.114)

3.1.2.3 Schrödinger equation

We finally derive the Schrödinger equation. From here, this is simply an application of Ref. [2]. Equations 17 through 26 in Ref. [3] is a derivation identical to
equations 6 through 15 in Ref. [2].

Equation 27 is straightforward,

\[
V_D = -\frac{\hbar^2}{2m} (H^2 - K) = -\frac{\hbar^2}{2m} \left[ \frac{Z^2}{4} \left( \frac{S_\rho + \rho S_{\rho\rho} Z^2}{\rho} \right)^2 - \frac{S_\rho S_{\rho\rho} Z^4}{\rho} \right],
\]

\[
= -\frac{\hbar^2}{2m} \left[ \frac{Z^2}{4\rho^2} (S_\rho + \rho S_{\rho\rho} Z^2)^2 - \frac{4\rho S_\rho S_{\rho\rho} Z^4}{4\rho^2} \right],
\]

\[
= -\frac{\hbar^2}{2m} \frac{Z^2}{4\rho^2} \left( S_\rho^2 + 2\rho S_\rho S_{\rho\rho} Z^2 + \rho^2 S_{\rho\rho}^2 Z^4 - 4\rho S_\rho S_{\rho\rho} Z^2 \right),
\]

\[
= -\frac{\hbar^2}{2m} \frac{Z^2}{4\rho^2} \left( S_\rho^2 - 2\rho S_\rho S_{\rho\rho} Z^2 + \rho^2 S_{\rho\rho}^2 Z^4 \right),
\]

\[
= -\frac{\hbar^2}{2m} \frac{Z^2}{4\rho^2} (S_\rho - \rho S_{\rho\rho} Z^2)^2. \tag{3.115}
\]

The kinetic energy operator for a particle with only radial dependence is

\[
-\frac{\hbar^2}{2m} \nabla^2 \psi = -\frac{\hbar^2}{2m} \left\{ Z^2 \chi_{\rho\rho} + \left( \frac{Z^2}{\rho} + Z Z_\rho \right) \chi_\rho \right\}. \tag{3.116}
\]

But

\[
Z_\rho = \left[ (1 + S_\rho^2)^{-12} \right]_{\rho} = -S_\rho S_{\rho\rho} (1 + S_\rho^2)^{-32} = -Z^3 S_\rho S_{\rho\rho}. \tag{3.117}
\]

So

\[
-\frac{\hbar^2}{2m} \nabla^2 \psi = -\frac{\hbar^2}{2m} \left\{ Z^2 \chi_{\rho\rho} + \frac{Z^2}{\rho} \chi_\rho - Z^4 S_\rho S_{\rho\rho} \chi_\rho \right\},
\]

\[
= -\frac{\hbar^2}{2m} \left\{ Z^2 \left( \chi_{\rho\rho} + \frac{1}{\rho} \chi_\rho \right) - Z^4 S_\rho S_{\rho\rho} \chi_\rho \right\}. \tag{3.118}
\]

The Schrödinger equation for the surface in question is now ready for analysis.
3.1.3 Ley-Koo and Castillo-Animas (Ref. [4])

Ref. [4] takes a more straightforward approach. Rather than try to apply differential geometry, it begins by defining the spheroidal coordinate system, and identifying the constants of the motion. Among them are two constants similar to a sphere’s angular momentum which are quantized using canonical quantization to form a quantum operator \( \hat{\Lambda} \).

While this approach works well for a particle confined to a sphere, this shows certain pitfalls (detailed below in chapter IV). The Laplace-Beltrami operator of the surface does not produce the same equation as the Laplace operator of the surrounding space, although the two surfaces have similar qualities. The sphere hides these differences because the normal coordinate has a metric component equal to one, and the constant curvature of the surface nullifies the curvature energy shift. However, under certain conditions where the normal coordinate’s metric tensor element does have a value equal to one, this approach can be used as an unperturbed state for an additional curvature energy shift treated as a perturbation, described below.

The Hamiltonian operator is found to produce the prolate spheroidal wave equation while the \( \hat{\Lambda} \) operator produces a similar equation. The Hamiltonian is separated and the \( \xi \) component of the wavefunction is set to a constant value. The energy eigenvalues are then computed down to a parameter \( \lambda \). The remaining eigenfunctions and energy levels are described by Ref. [25].

However, Ref. [4] then continues to derive the energy levels using the \( \hat{\Lambda} \) operator. The method involves constructing a matrix of the operator in a basis of associated Legendre polynomials [26; 23] and diagonalizing it. The result is a representation of the wavefunction as a linear combination of spherical harmonics. A computer is used to numerically solve the eigenvalues for the various coefficients of the series and finding the intersections of the curves created by the parameters at various values with the straight lines identified with the energy levels from the Hamiltonian.
This method does not consider an energy shift due to curvature, and it handles the operator-ordering problem by using half of the anticommutator bracket. It has the advantage of relative simplicity compared to the differential geometric approach. However, it is questionable as to whether this equation is correct, as it is different from Refs. [2; 15; 5; 3].

3.1.3.1 Derivation of operators

The relevant operators of this quantum mechanical system in curved coordinates are

\[ \hat{r}_i = r_i, \] (3.119)
\[ \hat{p}_j = -i\hbar \sum_m \left( \frac{\partial r_j}{\partial q_m} \right) \frac{1}{h_m} \frac{\partial}{\partial q_m}, \] (3.120)
\[ \hat{p}_j^2 = -\hbar^2 \sum_{m,u} \left( \frac{\partial r_j}{\partial q_m} \right) \frac{1}{h_m} \frac{\partial}{\partial q_m} \left[ \left( \frac{\partial r_j}{\partial q_u} \right) \frac{1}{h_u} \frac{\partial}{\partial q_u} \right], \] (3.121)
\[ \hat{\ell}^2 = -\hbar^2 \nabla^2, \] (3.122)

and

\[ \hat{\ell}_k = \hat{r}_i \hat{p}_j \varepsilon_{ijk} = -i\hbar \sum_{i,j,m} \frac{\partial r_j}{\partial q_m} \frac{\varepsilon_{ijk}}{h_m} \frac{\partial}{\partial q_m} = -i\hbar \sum_m \begin{bmatrix} y \frac{z_m}{h_m} \frac{\partial}{\partial q_m} - z \frac{y_m}{h_m} \frac{\partial}{\partial q_m} \\ x \frac{z_m}{h_m} \frac{\partial}{\partial q_m} - z \frac{x_m}{h_m} \frac{\partial}{\partial q_m} \\ x \frac{y_m}{h_m} \frac{\partial}{\partial q_m} - y \frac{x_m}{h_m} \frac{\partial}{\partial q_m} \end{bmatrix}, \] (3.123)
\[ \hat{\ell}^2 = -\hbar^2 \sum_{ijkmuvw} \left\{ r_i \frac{\partial r_j}{\partial q_m} \frac{\varepsilon_{ijk}}{h_m} \frac{\partial}{\partial q_m} \left[ r_u \frac{\partial r_v}{\partial q_w} \frac{\varepsilon_{uvk}}{h_w} \frac{\partial}{\partial q_w} \right] \right\}. \] (3.124)

3.1.3.2 Coordinate system

There are two angular momenta that combine to be a constant of motion for the prolate spheroid. [4] First define 2f as the distance between the two foci (which lie along the z-axis), and define r₁ and r₂ as the distance between a point and each respec-
tive focus. Figure 3.2 shows a diagram of this system. Then the prolate spheroidal coordinates are defined as [4]

\[
\begin{align*}
\xi &= \frac{r_1 + r_2}{2f}, \\
\eta &= \frac{r_1 - r_2}{2f},
\end{align*}
\]

(3.125, 3.126)

and \(\phi\), where \(\xi \in [1, \infty), \eta \in [-1, 1]\), and \(\phi \in [1, 2\pi]\).

3.1.3.3 Invariants of the system

We next look for invariants in the system. For the free particle they are the energy, the \(z\)-component of the angular momentum, and a third not so immediately found. First define

\[
\mathbf{l}_1 = \mathbf{r}_1 \times \mathbf{p} = (\mathbf{r} + \mathbf{f}) \times \mathbf{p}
\]

(3.127)
and

\[ l_2 = r_2 \times p = (r - f) \times p. \] (3.128)

For a sphere, \( l_1 = l_2 \) and \( l \cdot l \) is a constant of the motion. Therefore we look at \( l_1 \cdot l_2 \). Taking its time derivative, we have

\[ \frac{\partial}{\partial t} \{l_1 \cdot l_2\} = \frac{\partial}{\partial t} \{[(r + f) \times p] \cdot [(r - f) \times p]\}. \] (3.129)

We can evaluate this using the identities

\[ \frac{\partial}{\partial t} \{l_1 \cdot l_2\} = \frac{\partial l_1}{\partial t} \cdot l_2 + l_1 \cdot \frac{\partial l_2}{\partial t} \] (3.130)

and, because \( \frac{\partial p}{\partial t} = 0 \),

\[ \frac{\partial}{\partial t} \{f \times p\} = \frac{\partial f}{\partial t} \times p. \] (3.131)

Combining these we have

\[
\begin{align*}
\frac{\partial}{\partial t} \{l_1 \cdot l_2\} &= \left(\frac{\partial f}{\partial t} \times p\right) \cdot [(r + f) \times p] - [(r - f) \times p] \cdot \left(\frac{\partial f}{\partial t} \times p\right) \\
&= \left(\frac{\partial f}{\partial t} \times p\right) \cdot \left(\left(r \times p - f \times p - r \times p - f \times p\right)\right) \\
&= \left(\frac{\partial f}{\partial t} \times p\right) \cdot (-2f \times p) \\
&= -2 \left(\frac{\partial f}{\partial t} \times p\right) \cdot (f \times p) \\
&= 0.
\end{align*}
\] (3.132)

Now that the time variation of this operator is known, we construct a quantum operator for it. Since we do not know which order is the correct order of operation,
we take the average of \( l_1 \cdot l_2 \) and \( l_2 \cdot l_1 \):

\[
\hbar^2 \hat{\Lambda}_p = \frac{1}{2} [l_1 \cdot l_2 + l_2 \cdot l_1]
\]

\[
= \frac{1}{2} \{(r + f) \times p \} \cdot [(r - f) \times p] + [(r - f) \times p] \cdot [(r + f) \times p]
\]

\[
= \frac{1}{2} \{(r \times p + f \times p) \cdot (r \times p - f \times p) + (r \times p - f \times p) \cdot (r \times p + f \times p)
\]

\[
+ (r \times p) \cdot (r \times p) - (f \times p) \cdot (r \times p) + (r \times p) \cdot (f \times p) - (f \times p) \cdot (f \times p)
\]

\[
= \frac{1}{2} \{ 2 \|r \times p\|^2 - 2 \|f \times p\|^2 \}
\]

\[
= l^2 - \|f \times p\|^2.
\]  

(3.133)

This can be further expanded noting that \( f_x = f_y = 0 \):

\[
l^2 - \|f \times p\|^2 = l^2 - (-f_z p_y)^2 - (f_z p_x)^2
\]

\[
= l^2 - [f_z p_y f_z p_y + f_z p_x f_z p_x].
\]  

(3.134)

Before continuing, we note that \( f \), being the distance between the foci, is just a constant. Therefore they can be pulled to the left:

\[
l^2 - \|f \times p\|^2 = l^2 - f_z^2 p_y^2 - f_z^2 p_x^2
\]

\[
= l^2 - f_z^2 (p_x^2 + p_y^2)
\]

\[
= l^2 - f_z^2 (p_x^2 + p_y^2 + p_z^2) + f_z^2 p_z^2
\]

\[
= l^2 - (f_x^2 + f_y^2 + f_z^2) (p_x^2 + p_y^2 + p_z^2) + f_z^2 p_z^2
\]

\[
= l^2 - f_z^2 p_x^2 + (f_x^2 + f_y^2 + f_z^2) p_z^2
\]

\[
= l^2 - f_z^2 (p_z^2 - \hat{p}_z^2).
\]  

(3.135)
3.1.3.4 Geometric constructions

The next step is to calculate the geometric constructions. These are the parameterization vector, the unit vectors, the scale factors $h_i = \sqrt{g_{ii}}$, gradient and Laplacian, and finally the momentum operator and its square.

Letting $\mathbf{r} = (x(\xi, \eta, \phi), y(\xi, \eta, \phi), z(\xi, \eta, \phi))$, the geometry indicates that

$$
\begin{bmatrix}
x \\
y \\
z
\end{bmatrix} = f
\begin{bmatrix}
\sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \cos \phi \\
\sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \sin \phi \\
\xi \eta
\end{bmatrix},
\tag{3.136}
$$

and

$$
\hat{e}_\xi = \frac{1}{h_\xi} (\hat{e}_x x, \xi + \hat{e}_y y, \xi + \hat{e}_z z, \xi),
$$

$$
\hat{e}_\eta = \frac{1}{h_\eta} (\hat{e}_x x, \eta + \hat{e}_y y, \eta + \hat{e}_z z, \eta),
$$

$$
\hat{e}_\phi = \frac{1}{h_\phi} (\hat{e}_x x, \phi + \hat{e}_y y, \phi + \hat{e}_z z, \phi),
\tag{3.137}
$$

where $\hat{e}_x, \hat{e}_y, \hat{e}_z$ are the Cartesian unit vectors $\hat{i}, \hat{j}, \text{and } \hat{k}$, respectively.

The scale factors are

$$
h_\xi = \sqrt{\left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2 + \left(\frac{\partial z}{\partial \xi}\right)^2} = \frac{f \sqrt{\xi^2 - \eta^2}}{\sqrt{\xi^2 - 1}},
$$

$$
h_\eta = \sqrt{\left(\frac{\partial x}{\partial \eta}\right)^2 + \left(\frac{\partial y}{\partial \eta}\right)^2 + \left(\frac{\partial z}{\partial \eta}\right)^2} = \frac{f \sqrt{\xi^2 - \eta^2}}{\sqrt{1 - \eta^2}},
$$

$$
h_\phi = \sqrt{\left(\frac{\partial x}{\partial \phi}\right)^2 + \left(\frac{\partial y}{\partial \phi}\right)^2 + \left(\frac{\partial z}{\partial \phi}\right)^2} = f \sqrt{(\xi^2 - 1)(1 - \eta^2)}. \tag{3.138}
$$
These produce the gradient operator

\[ \nabla = \sum_i \frac{\hat{e}_i}{h_i \partial q_i} \frac{\partial}{\partial q_i} = \hat{e}_\xi \frac{\partial}{\partial \xi} + \hat{e}_\eta \frac{\partial}{\partial \eta} + \hat{e}_\phi \frac{\partial}{\partial \phi} \]

\[ = \left( \hat{e}_x \frac{\partial}{\partial \xi} x + \hat{e}_y \frac{\partial}{\partial \eta} y + \hat{e}_z \frac{\partial}{\partial \phi} z \right) \frac{1}{h_\xi \partial \xi} + \left( \hat{e}_x \frac{\partial}{\partial \eta} x + \hat{e}_y \frac{\partial}{\partial \eta} y + \hat{e}_z \frac{\partial}{\partial \eta} z \right) \frac{1}{h_\eta \partial \eta} \]

\[ + \left( \hat{e}_x \frac{\partial}{\partial \phi} x + \hat{e}_y \frac{\partial}{\partial \phi} y + \hat{e}_z \frac{\partial}{\partial \phi} z \right) \frac{1}{h_\phi \partial \phi} \]

\[ = \begin{bmatrix} \frac{x \xi}{h_\xi \partial \xi} + \frac{x \eta}{h_\eta \partial \eta} + \frac{x \phi}{h_\phi \partial \phi} \\ \frac{y \xi}{h_\xi \partial \xi} + \frac{y \eta}{h_\eta \partial \eta} + \frac{y \phi}{h_\phi \partial \phi} \\ \frac{z \xi}{h_\xi \partial \xi} + \frac{z \eta}{h_\eta \partial \eta} + \frac{z \phi}{h_\phi \partial \phi} \end{bmatrix} \cdot \quad (3.139) \]

However, \((x, y, z) = (x(\xi, \eta, \phi), y(\xi, \eta, \phi), z(\xi, \eta, \phi))\). The next step is therefore to calculate the Jacobian matrix and the coefficients of each of the above derivatives.

The Jacobian matrix is

\[ J = \begin{bmatrix} x_\xi & x_\eta & x_\phi \\ y_\xi & y_\eta & y_\phi \\ z_\xi & z_\eta & z_\phi \end{bmatrix} = f \begin{bmatrix} \xi \sqrt{1-\eta^2} \cos \phi & -\eta \sqrt{\xi^2-1} \cos \phi & -\sqrt{\xi^2-1} \sqrt{1-\eta^2} \sin \phi \\ \xi \sqrt{1-\eta^2} \sin \phi & \eta \sqrt{\xi^2-1} \sin \phi & \sqrt{\xi^2-1} \sqrt{1-\eta^2} \cos \phi \\ \eta & \xi & 0 \end{bmatrix} \cdot \quad (3.140) \]

Using equation (3.137), we can project the basis vectors onto the Cartesian basis as

\[ \hat{e}_\xi = \frac{\sqrt{\xi^2-1}}{\sqrt{\xi^2-\eta^2}} \begin{bmatrix} \xi \sqrt{1-\eta^2} \cos \phi \\ \xi \sqrt{1-\eta^2} \sin \phi \\ \eta \end{bmatrix} = \begin{bmatrix} \xi \sqrt{1-\eta^2} \cos \phi \\ \xi \sqrt{1-\eta^2} \sin \phi \\ \sqrt{\xi^2-1} \sqrt{1-\eta^2} \eta \end{bmatrix}, \quad (3.141) \]

\[ \hat{e}_\eta = \begin{bmatrix} -\eta \sqrt{\xi^2-1} \cos \phi \\ -\eta \sqrt{\xi^2-1} \sin \phi \\ \sqrt{1-\eta^2} \xi \end{bmatrix}, \quad (3.142) \]
\[ \hat{e}_\phi = \frac{1}{\sqrt{(\xi^2 - 1)(1 - \eta^2)}} \begin{bmatrix} -\sqrt{\xi^2 - 1}\sqrt{1 - \eta^2} \sin \phi \\ \sqrt{\xi^2 - 1}\sqrt{1 - \eta^2} \cos \phi \\ 0 \end{bmatrix} = \begin{bmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{bmatrix}. \] (3.143)

The gradient operator is calculated to be
\[
\nabla = e_\xi \frac{\sqrt{\xi^2 - 1}}{\sqrt{\xi^2 - \eta^2}} \frac{\partial}{\partial \xi} + e_\eta \frac{\sqrt{1 - \eta^2}}{\sqrt{\xi^2 - \eta^2}} \frac{\partial}{\partial \eta} + e_\phi \frac{1}{f \sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi}. \] (3.144)

When projected into Cartesian space it becomes
\[
\nabla = \begin{bmatrix} \frac{\xi \sqrt{1 - \eta^2}}{\sqrt{\xi^2 - \eta^2}} \cos \phi \\ \frac{\xi \sqrt{1 - \eta^2}}{\sqrt{\xi^2 - \eta^2}} \sin \phi \\ \frac{\sqrt{\xi^2 - 1}}{\sqrt{\xi^2 - \eta^2}} \eta \end{bmatrix} \frac{\sqrt{\xi^2 - 1}}{\sqrt{\xi^2 - \eta^2}} \frac{\partial}{\partial \xi} + \begin{bmatrix} -\eta \frac{\sqrt{\xi^2 - 1}}{\sqrt{\xi^2 - \eta^2}} \cos \phi \\ -\eta \frac{\sqrt{\xi^2 - 1}}{\sqrt{\xi^2 - \eta^2}} \sin \phi \\ \frac{\sqrt{1 - \eta^2}}{\sqrt{\xi^2 - \eta^2}} \xi \end{bmatrix} \frac{\sqrt{1 - \eta^2}}{\sqrt{\xi^2 - \eta^2}} \frac{\partial}{\partial \eta} + \begin{bmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{bmatrix} \frac{1}{f \sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi}. \] (3.145)

When it is simplified and multiplied by \(-i\hbar\), it gives the momentum operator,
\[
\hat{p} = -i\hbar \nabla
\]
\[
= -i\hbar \begin{bmatrix} \xi \sqrt{1 - \eta^2} \sqrt{\xi^2 - 1} \cos \phi \frac{\partial}{\partial \xi} - \eta \sqrt{\xi^2 - 1} \sqrt{\xi^2 - \eta^2} \frac{\cos \phi}{\sqrt{\xi^2 - \eta^2}} \frac{\partial}{\partial \eta} - \sin \phi \frac{\sin \phi}{f \sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \\ \xi \sqrt{1 - \eta^2} \sqrt{\xi^2 - 1} \sin \phi \frac{\partial}{\partial \xi} - \eta \sqrt{\xi^2 - 1} \sqrt{\xi^2 - \eta^2} \frac{\sin \phi}{\sqrt{\xi^2 - \eta^2}} \frac{\partial}{\partial \eta} + \cos \phi \frac{\cos \phi}{f \sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \\ \eta \frac{\sqrt{\xi^2 - 1}}{\sqrt{\xi^2 - \eta^2}} \frac{\partial}{\partial \xi} + \frac{1 - \eta^2}{\xi^2 - \eta^2} \frac{\partial}{\partial \eta} \end{bmatrix}. \] (3.146)

This will be used in calculating the angular momentum and in the \( \Lambda \) operator. Its
\[ \hat{p}^2 = -\hbar^2 \nabla^2 \]
\[ = -\frac{\hbar^2}{f^2 \xi^2 - \eta^2} \left\{ \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] \right. \]
\[ + \left. \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2}{\partial \phi^2} \right\} . \tag{3.147} \]

Another part of this that will be needed is the z-component of the momentum squared. It is
\[ \hat{p}_z^2 = -\hbar^2 \left[ \eta^2 \frac{\xi^2 - 1}{\xi^2 - \eta^2} \frac{\partial}{\partial \xi} \left( \frac{\xi^2 - 1}{\xi^2 - \eta^2} \frac{\partial}{\partial \xi} \right) + \eta \frac{(\xi^2 - 1)(1 - \eta^2)}{\xi^2 - \eta^2} \frac{\partial}{\partial \xi} \left( \frac{\xi}{\xi^2 - \eta^2} \frac{\partial}{\partial \eta} \right) \right. \]
\[ + \left. \frac{(1 - \eta^2)(\xi^2 - 1)}{\xi^2 - \eta^2} \xi \frac{\partial}{\partial \eta} \left( \frac{\eta}{\xi^2 - \eta^2} \frac{\partial}{\partial \xi} \right) + \frac{1 - \eta^2}{\xi^2 - \eta^2} \xi \frac{\partial^2}{\partial \eta^2} \left( \frac{1 - \eta^2}{\xi^2 - \eta^2} \frac{\partial}{\partial \xi} \right) \right] . \tag{3.148} \]

This is used to construct the Hamiltonian operator.

### 3.1.3.5 Laplacian and Hamiltonian operator

Next we construct the Hamiltonian operator in prolate spheroidal coordinates. The Hamiltonian derives from the Laplacian. The Laplacian is given in Ref. [13] as
\[ \nabla^2 = \frac{1}{f^2(\xi^2 - \eta^2)} \left\{ \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2}{\partial \phi^2} \right\} , \tag{3.149} \]
which is identical to the one given in Ref. [4].

The Laplacian is given by
\[ \nabla^2 = \frac{1}{h_{\xi} h_{\eta} h_{\phi}} \left[ \frac{\partial}{\partial \xi} \left( \frac{h_{\eta} h_{\phi}}{h_{\xi}} \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( \frac{h_{\xi} h_{\phi}}{h_{\eta}} \frac{\partial}{\partial \eta} \right) + \frac{\partial}{\partial \phi} \left( \frac{h_{\xi} h_{\eta}}{h_{\phi}} \frac{\partial}{\partial \phi} \right) \right] . \tag{3.150} \]
Its derivation follows:

\[
\nabla^2 = \frac{\sqrt{\xi^2 - 1} \sqrt{1 - \eta^2}}{f \sqrt{\xi^2 - \eta^2} f \sqrt{\xi^2 - \eta^2} f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2}} \times \left[ \frac{\partial}{\partial \xi} \left( \frac{f \sqrt{\xi^2 - \eta^2} f \sqrt{(\xi^2 - 1) (1 - \eta^2)}}{\sqrt{1 - \eta^2}} \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( \frac{f \sqrt{\xi^2 - \eta^2} f \sqrt{(\xi^2 - 1) (1 - \eta^2)}}{\sqrt{\xi^2 - 1}} \frac{\partial}{\partial \eta} \right) + \frac{\partial}{\partial \phi} \left( \frac{f \sqrt{\xi^2 - \eta^2} f \sqrt{\xi^2 - \eta^2}}{f \sqrt{(\xi^2 - 1) (1 - \eta^2)}} \frac{\partial}{\partial \phi} \right) \right] \]

\begin{align*}
\nabla^2 &= \frac{\sqrt{\xi^2 - 1} \sqrt{1 - \eta^2}}{f \sqrt{\xi^2 - \eta^2} f \sqrt{\xi^2 - \eta^2} f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2}} \times \\
&\quad \left[ \frac{\partial}{\partial \xi} \left( \frac{f \sqrt{\xi^2 - \eta^2} f \sqrt{(\xi^2 - 1) (1 - \eta^2)}}{\sqrt{1 - \eta^2}} \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( \frac{f \sqrt{\xi^2 - \eta^2} f \sqrt{(\xi^2 - 1) (1 - \eta^2)}}{\sqrt{\xi^2 - 1}} \frac{\partial}{\partial \eta} \right) + \frac{\partial}{\partial \phi} \left( \frac{f \sqrt{\xi^2 - \eta^2} f \sqrt{\xi^2 - \eta^2}}{f \sqrt{(\xi^2 - 1) (1 - \eta^2)}} \frac{\partial}{\partial \phi} \right) \right] \\
&= \frac{1}{f^3(\xi^2 - \eta^2)} \left[ \frac{\partial}{\partial \xi} \left( \frac{f(\xi^2 - 1) \partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left( f(1 - \eta^2) \frac{\partial}{\partial \eta} \right) + \frac{\partial}{\partial \phi} \left( \frac{f(\xi^2 - \eta^2) \partial}{(\xi^2 - 1)(1 - \eta^2) \partial \phi} \right) \right], \\
\end{align*}

(3.152)

which finally results in

\[
\nabla^2 = \frac{1}{f^2(\xi^2 - \eta^2)} \left\{ \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + \frac{\partial}{\partial \phi} \left[ \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)} \frac{\partial}{\partial \phi} \right] \right\}. \]

(3.153)
Multiplying by the Schrödinger factor to get the Schrödinger operator we have the Hamiltonian operator for a free particle:

\[ \hat{H}_p = \frac{\hbar^2}{2\mu} \nabla^2 \]
\[ = \frac{\hbar^2}{2\mu f^2} \frac{1}{\xi^2 - \eta^2} \left\{ \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2}{\partial \phi^2} \right\} . \]

\[ (3.154) \]

3.1.3.6 Angular momentum operators

Now that the Hamiltonian is derived, the angular momentum operator is derived. A large amount of algebra shows shows that the angular momentum operator in the \(z\) direction is simply \( \hat{L}_z = -i\hbar \frac{\partial}{\partial \phi} \), while for \( x \) and \( y \) it is

\[ \hat{L}_x = -i\hbar \left[ f \frac{\sqrt{\xi^2 - 1} \sqrt{1 - \eta^2}}{\xi^2 - \eta^2} \sin \phi \left( \xi \frac{\partial}{\partial \eta} - \eta \frac{\partial}{\partial \xi} \right) - \frac{\xi \eta \cos \phi}{\sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \right] . \]

\[ (3.155) \]

\[ \hat{L}_y = -i\hbar \left[ f \frac{\sqrt{1 - \eta^2} \sqrt{\xi^2 - 1}}{\xi^2 - \eta^2} \cos \phi \left( \eta \frac{\partial}{\partial \xi} - \xi \frac{\partial}{\partial \eta} \right) - \frac{\xi \eta \sin \phi}{\sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \right] . \]

\[ (3.156) \]
Combining these terms using $L^2 = L_x^2 + L_y^2 + L_z^2$ produces the lengthy equation

$$L^2 = -\hbar^2 \left\{ \frac{f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2}}{\xi^2 - \eta^2} \sin \phi \left( \xi \frac{\partial}{\partial \eta} \left[ \frac{f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2}}{\xi^2 - \eta^2} \sin \phi \left( \xi \frac{\partial}{\partial \eta} - \eta \frac{\partial}{\partial \xi} \right) \right] \right) \right. \\
- \frac{\xi \eta \cos \phi}{\sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \left[ \frac{f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2}}{\xi^2 - \eta^2} \sin \phi \left( \xi \frac{\partial}{\partial \eta} - \frac{\xi \eta \cos \phi}{\sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \right) \right] \right) \\
- \xi \frac{\partial}{\partial \xi} \left[ \frac{f \sqrt{1 - \eta^2} \sqrt{\xi^2 - 1}}{\xi^2 - \eta^2} \cos \phi \left( \eta \frac{\partial}{\partial \xi} \left[ \frac{f \sqrt{1 - \eta^2} \sqrt{\xi^2 - 1}}{\xi^2 - \eta^2} \cos \phi \left( \eta \frac{\partial}{\partial \xi} - \xi \frac{\partial}{\partial \eta} \right) \right] \right) \right. \\
- \frac{\xi \eta \sin \phi}{\sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \left[ \frac{f \sqrt{1 - \eta^2} \sqrt{\xi^2 - 1}}{\xi^2 - \eta^2} \cos \phi \left( \eta \frac{\partial}{\partial \xi} - \frac{\xi \eta \sin \phi}{\sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \right) \right] \right) \right) \\
- \eta \frac{\partial}{\partial \xi} \left[ \frac{f \sqrt{1 - \eta^2} \sqrt{\xi^2 - 1}}{\xi^2 - \eta^2} \cos \phi \left( \eta \frac{\partial}{\partial \xi} - \frac{\xi \eta \sin \phi}{\sqrt{(\xi^2 - 1)(1 - \eta^2)}} \frac{\partial}{\partial \phi} \right) \right] \right) \right) \\
+ \frac{\partial^2}{\partial \phi^2} \right\} \\
+ \left( 3.157 \right)$$

This equation is so long as to be nearly useless unless one uses a computer algebra system such as Mathematica. However, it can be used in conjunction with the momentum operator to derive a symmetry operator to the Hamiltonian. This operator, called $\hat{\Lambda}_p$, is given by

$$\hat{\Lambda}_p = \hat{l}^2 - f^2 (\hat{p}_x^2 - \hat{p}_z^2). \quad (3.158)$$

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Plugging in equations (3.147) and (3.148), and simplifying gives
\[
\hat{\Lambda}_p = \frac{\eta^2}{\xi^2 - \eta^2} \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial}{\partial \xi} \right] + \frac{\xi^2}{\xi^2 - \eta^2} \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + \frac{\xi^2 + \eta^2 - 1}{(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2}{\partial \phi^2}.
\]
This operator is a symmetry operator of the Hamiltonian.

3.1.3.7 Separation of variables

We begin by assuming that the wavefunction has the form
\[
\psi(\xi, \eta, \phi) = \Xi(\xi) H(\eta) \Phi(\phi),
\]
and then carrying out the process of separation of variables of the Schrödinger equation, which results in
\[
\frac{\hbar^2}{2 \mu f^2} \frac{1}{\xi^2 - \eta^2} \left\{ \frac{1}{\Xi} \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial \Xi}{\partial \xi} \right] + \frac{1}{H} \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial H}{\partial \eta} \right] \right. \\
\left. + \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)} \frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} \right\} = E,
\]
Letting
\[
\frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} = m^2
\]
and
\[
E = \frac{\hbar^2 k^2}{2 \mu}.
\]
then we have
\[
\frac{1}{\Xi} \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial \Xi}{\partial \xi} \right] + \frac{1}{H} \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial H}{\partial \eta} \right] = f^2 k^2 (\xi^2 - \eta^2) - \frac{m^2 (\xi^2 - \eta^2)}{(\xi^2 - 1)(1 - \eta^2)}.
\]
Factoring the far right term gives

\[
\frac{1}{\Xi} \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial \Xi}{\partial \xi} \right] + \frac{1}{H} \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial H}{\partial \eta} \right] = f^2 k^2 (\xi^2 - \eta^2) - m^2 \left[ \frac{1}{\xi^2 - 1} + \frac{1}{1 - \eta^2} \right].
\]

Adding \(\lambda - \lambda\) for the eigenvalue of the \(\hat{\Lambda}_\mu\) and rearranging gives

\[
\left\{ \frac{1}{\Xi} \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial \Xi}{\partial \xi} \right] - f^2 k^2 \xi^2 + \frac{m^2}{\xi^2 - 1} - \lambda \right\} + \left\{ \frac{1}{H} \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial H}{\partial \eta} \right] + f^2 k^2 \eta^2 + \frac{m^2}{1 - \eta^2} + \lambda \right\} = 0. \tag{3.166}
\]

The separated equations are therefore

\[
\left\{ \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial}{\partial \xi} \right] - f^2 k^2 \xi^2 + \frac{m^2}{\xi^2 - 1} - \lambda \right\} \Xi = 0, \tag{3.167}
\]

and

\[
\left\{ \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + f^2 k^2 \eta^2 + \frac{m^2}{1 - \eta^2} + \lambda \right\} H = 0. \tag{3.168}
\]

### 3.1.3.8 Solution of the separated system

Now that the equation is separated, we then seek to solve the resulting separated ODEs. The prolate spheroid is a surface of constant \(\xi\); therefore we take as our boundary condition

\[
\Xi(\xi) = \Xi(\xi_0) = \text{constant}, \tag{3.169}
\]

and

\[
\frac{d\Xi}{d\xi} = 0. \tag{3.170}
\]

The solution to the \(\Xi\) equation is therefore

\[
\left\{ f^2 k^2 \xi_0^2 + \frac{m^2}{\xi_0^2 - 1} - \lambda \right\} \Xi(\xi_0) = 0, \tag{3.171}
\]

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which reduces to
\[ E_{\lambda m} = \frac{h^2 k^2}{2\mu} = \frac{h^2}{2\mu} \frac{1}{f^2 \xi_0^2} \left( \lambda - \frac{m^2}{\xi_0^2 - 1} \right). \] (3.172)

This leaves the other equation:
\[ \left\{ \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + f^2 k^2 \eta^2 + \frac{m^2}{1 - \eta^2} + \lambda \right\} H = 0. \] (3.173)

This is the spheroidal wave equation, and is well-documented (Ref. [25]). In that reference, \( H(\eta) = S_{mn}(c, \eta) \), where \( c = f k \). The solutions are called prolate angular functions, come in two varieties, and have the form
\[ S_{mn}^{(1)}(f k, \eta) = \sum_{r=0,1}^{\infty} d_r^{mn}(f k) P_{m+r}(\eta), \] (3.174)
\[ S_{mn}^{(2)}(f k, \eta) = \sum_{s=-\infty}^{\infty} d_r^{mn}(f k) Q_{m+r}(\eta), \] (3.175)
where \( P_{m+r}(\eta) \) and \( Q_{m+r}(\eta) \) are Legendre functions of the first and second kinds.

Derivation of the \( d_r^{mn}(f k) \) coefficients is lengthy and beyond the scope of this paper. There are several normalization schemes to choose from.

The energy eigenvalues are determined from equation (3.172) by the intersections of
\[ \lambda = \xi_0^2 k^2 f^2 + \frac{m^2}{\xi_0^2 - 1} \] (3.176)
and
\[ y(k^2 f^2) = \xi_0^2 k^2 f^2 + \frac{m^2}{\xi_0^2 - 1}. \] (3.177)

Ref. [4] performs this calculation using a computer and produces plots of the curves produced by the equations above.
CHAPTER IV

Some Common Pitfalls

The non-relativistic quantum mechanics of particles constrained to curves and surfaces is a problem which occasionally finds its place in textbooks (e.g., Ref. [27]) and lecture notes. The simplest example is that of a particle moving on the surface of a sphere, and this problem is often mapped onto the rigid rotator problem. It is also of fundamental importance in the formal theory of quantum mechanics since it has been understood that the standard canonical quantization prescription in Cartesian coordinates breaks down in curved space[7]. The problem was probably first solved by Jensen and Koppe in 1971 [1], and clarified in more detail in the early nineteen eighties by da Costa [2].

Despite this, there are two mistakes that authors occasionally make when working in the field. For example, see Ref. [4], which assumes that the Schrödinger problem can be constrained by simply holding one coordinate constant in the three-dimensional Schrödinger equation.

Both mistakes are possibly related to the simplicity and prevalence of the problem for a particle constrained to the surface of a sphere. The purpose of this chapter is to clarify the procedure to prevent these mistakes from being made in the future.

The first mistake, made in Ref. [4], is to assume that the Laplacian for the surface is simply the Laplacian of the three-dimensional problem with the term containing
the derivative with respect to the constrained coordinate removed, and setting it to a constant value throughout the remainder of the operator. It will be shown that this not the case, because removing one term from the metric tensor will change the determinant of the metric tensor, and therefore the Laplace-Beltrami operator as well. So while the metric tensor of the surface is a subspace of the metric tensor of the space it is imbedded in, the Laplace-Beltrami operator for the surface is sufficiently different from the Laplacian of its surrounding space to require the Laplace-Beltrami operator to be derived.

One special case is for a particle constrained to a sphere, for which the Laplace-Beltrami operator is the same as for full three-dimensional spherical coordinates without the radial term. This is because the metric is diagonal, and the constrained coordinate has a scale factor equal to one. Therefore the determinant remains the same.

The second mistake is to neglect the potential energy due to the curvature of the surface. It is shown in the literature [1; 2] that, when constraining a particle to an embedded surface, there is an effective potential energy well on that surface, dependent on its parameterization, that is generated by its curvature. Again, the particle constrained to the surface of a sphere is a special case, because the mean curvature squared minus the Gaussian curvature is zero, resulting in it safely being neglected from the equation. For most surfaces, this term is nonzero, so it cannot be neglected. Both mistakes will be worked out in more detail below.
4.1 Formulation of the Laplace-Beltrami Operator for the Surface from the Laplace Operator of the Embedded Coordinate System

Let $\mathcal{M}$ be a metric space in $\mathbb{E}^3$ and then let

$$x(Q) : \mathbb{E}^3 \to \mathcal{M} : Q \mapsto x.$$  \hspace{1cm} (4.1)

be a coordinate chart from Cartesian coordinates to $\mathcal{M}$. The metric tensor of $\mathcal{M}$ is then

$$G_{ij} = \frac{\partial x}{\partial Q^i} \cdot \frac{\partial x}{\partial Q^j}. \hspace{1cm} (4.2)$$

If we now hold $Q^3$ constant, we have a coordinate system $q := (Q^1, Q^2) : (q^1, q^2)$ and a parametrized surface $\mathcal{N} \subset \mathbb{E}^2$ with $\mathcal{N} \in \mathcal{M}$ and parametrization $x(q) : \mathbb{E}^3 \to \mathcal{M} : x(q) = (x(q), y(q), z(q))$. The metric tensor of $\mathcal{N}$ is then

$$g_{ij} = \frac{\partial x}{\partial q^i} \cdot \frac{\partial x}{\partial q^j}. \hspace{1cm} (4.3)$$

From this we see that

$$G_{ij} = g_{ij} : i, j = 1, 2. \hspace{1cm} (4.4)$$

While the metric tensor of $\mathcal{N}$ is a subspace of the metric tensor of $\mathcal{M}$, the component will generally produce a different metric discriminant. That is,

$$G := \det[G_{ij}] \neq \det[g_{ij}] =: g. \hspace{1cm} (4.5)$$

unless $G_{33} = 1$. 

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For orthogonal coordinate systems, in which $G_{ij} = 0 : i \neq j$, we have

$$G = G_{33}g.$$  \hfill (4.6)

The Laplacian operator for $\mathcal{M}$ is defined as

$$\nabla^2 f(Q) := \sum_{i,j=1}^{3} \frac{1}{\sqrt{G}} \frac{\partial}{\partial Q^i} \left( \sqrt{G} G^{ij} \frac{\partial f}{\partial Q^j} \right),$$ \hfill (4.7)

while the Laplace-Beltrami operator for $\mathcal{N}$ is

$$\nabla^2_{LB} f(q) := \sum_{i,j=1}^{2} \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^i} \left( \sqrt{g} g^{ij} \frac{\partial f}{\partial q^j} \right),$$ \hfill (4.8)

Finally, $\nabla^2_{LB} f(q)$ in terms of $\nabla^2 f(Q)$ is

$$\nabla^2_{LB} f(q) = \nabla^2 f(Q) - \frac{1}{\sqrt{G}} \frac{\partial}{\partial Q^3} \left( \sqrt{G} G^{33} \frac{\partial f}{\partial Q^3} \right) - \sum_{i,j=1}^{2} G^{ij} \frac{\partial G_{33}}{\partial Q^i} \frac{\partial f}{\partial Q^j} - \frac{1}{\sqrt{G}} \sum_{i=1}^{2} \left[ \frac{\partial}{\partial Q^i} \left( \sqrt{G} G^{3i} \frac{\partial f}{\partial Q^3} \right) + \frac{\partial}{\partial Q^i} \left( \sqrt{G} G^{3i} \frac{\partial f}{\partial Q^3} \right) \right].$$ \hfill (4.9)

For orthogonal coordinate systems this becomes

$$\nabla^2_{LB} f(q) = \nabla^2 f(Q) - \sum_{i,j=1}^{2} G^{ij} \frac{\partial G_{33}}{\partial Q^i} \frac{\partial f}{\partial Q^j} - \frac{1}{\sqrt{G}} \frac{\partial}{\partial Q^3} \left( \sqrt{G} G^{33} \frac{\partial f}{\partial Q^3} \right).$$ \hfill (4.10)

Therefore it is not trivial to formulate the Laplace-Beltrami operator of the surface from the Laplacian of the coordinate system in which the surface is embedded.

### 4.2 The Effect of Curvature on Potential Energy

It is occasionally assumed that the Laplacian is the only component that needs to be modified for the Schrödinger equation. But it has been shown that there is an
effective potential induced by the curvature of the surface. This potential energy is

\[ V_S = -\frac{\hbar^2}{2\mu} (M^2 - K), \]  

(4.11)

where \( \mu \) is the mass of the particle, \( M \) is the mean curvature, and \( K \) is the Gaussian curvature.

For a plane curve (such as a circular or elliptic ring), the effective potential is instead given by [18]

\[ V_D = -\frac{\hbar^2}{8\mu} \kappa^2, \]  

(4.12)

where \( \kappa \) is the curvature, defined for a parametrization in Cartesian coordinates \( (x, y) \) as [14]

\[ \kappa = \left| \frac{x'y'' - y'x''}{(x'^2 + y'^2)^{3/2}} \right|. \]  

(4.13)

### 4.3 A Note on Spherical Coordinates

Spherical coordinates form a special case, and are noteworthy because they are central to discussion of angular momentum in nearly all quantum mechanics courses. It appears that the mistakes mentioned above happen because the sphere masks them.

For the sphere, the constrained coordinate is typically the radial coordinate \( r \).

The full metric tensor for spherical coordinates is

\[
G_{ij} = \begin{bmatrix}
1 & 0 & 0 \\
0 & r^2 & 0 \\
0 & 0 & r^2 \sin^2 \theta
\end{bmatrix}.
\]  

(4.14)
When constraining the radial coordinate, this becomes

\[ g_{ij} = \begin{bmatrix} r^2 & 0 \\ 0 & r^2 \sin^2 \theta \end{bmatrix}. \tag{4.15} \]

Thus for the sphere, we have \( G = g \) and the constrained component is one and the constrained component is one. Therefore, for the sphere,

\[ \nabla^2_{LB} f(\theta, \phi) = \nabla^2 f(a, \theta, \phi) - \frac{1}{\sqrt{G}} \frac{\partial}{\partial r} \left( \sqrt{G} \frac{\partial f}{\partial r} \right), \tag{4.16} \]

which is simply the Laplace operator with the radial term removed. This produces the illusion that one can simply remove the constrained term from the Laplace operator to obtain a suitable Laplace-Beltrami operator for the surface.

The situation is compounded by the fact that, for a sphere of radius \( a \),

\[ V_S = M^2 - K = \frac{1}{a^2} - \frac{1}{a^2} = 0. \tag{4.17} \]

Because of this triviality, the curvature term typically does appear in discussions of angular momentum in quantum mechanics textbooks. This means that the concept of potential energy from curvature is not as well known, and therefore often neglected.

### 4.4 On Separation Constants

One advantage of the two-dimensional Laplace-Beltrami approach, instead of applying a function of constraint to the full three-dimensional Schrödinger equation, is that the two-dimensional approach produces two separated equations instead of three. This in turn produces one less constant of separation.

For closed surfaces like spheres, there will still be two quantum numbers in the final solution. One of the quantum numbers will appear as the constant of separation,
and the other will be hidden inside the energy term.

For example, the spherical coordinate Schrödinger equation is traditionally solved with the orbital quantum number appearing in the radial equation [23]. In the two-dimensional case, the radial equation does not exist. The orbital quantum number instead appears when the constraint is applied that the wavefunction must be finite: the Legendre equation only has finite solutions for eigenvalues \( \lambda \) that satisfy

\[
\lambda = \frac{2mE}{\hbar^2} = l(l + 1).
\]  \hspace{1cm} (4.18)

Two common mistakes made when constraining particles to curved surfaces are examined and clarified. A comment is made regarding the simplicity of the problem of the particle constrained to the surface of a sphere. A table of metric tensors and Laplace-Beltrami operators for various coordinate systems and their constrained counterparts is listed.
CHAPTER V

Analysis of a Sphere

In this chapter, the sphere problem is derived rigorously and fully using the differential geometric technique. The sphere is the simplest closed surface to solve for due to its symmetry and constant curvature. It is a standard problem covered in many quantum mechanics textbooks. It will be the first of three surfaces studied.

5.1 Analytical Solution

The parameterization of a sphere with radius $a$ in spherical coordinates is

$$
\begin{bmatrix}
  x \\
  y \\
  z
\end{bmatrix} =
\begin{bmatrix}
  a \sin \theta \cos \phi \\
  a \sin \theta \sin \phi \\
  a \cos \theta
\end{bmatrix}.
$$

(5.1)

The Jacobian is

$$
J =
\begin{bmatrix}
  a \cos \theta \cos \phi & -a \sin \theta \sin \phi \\
  a \cos \theta \sin \phi & a \sin \theta \cos \phi \\
-a \sin \theta & 0
\end{bmatrix}
$$

(5.2)
The associated metric tensor is

\[
g_{ij} = \begin{bmatrix} a^2 & 0 \\ 0 & a^2 \sin^2 \theta \end{bmatrix}.
\] (5.3)

The Laplace-Beltrami operator is

\[
\nabla^2 \psi = \frac{1}{a^2 \sin \theta} \partial_\theta [\sin \theta \partial_\theta \psi] + \frac{1}{a^2 \partial_\phi^2 \psi}.
\] (5.4)

The normal vector is

\[
N = \begin{bmatrix} a^2 \sin^2 \theta \cos \phi \\ a^2 \sin^2 \theta \sin \phi \\ a^2 \sin \theta \cos \theta \end{bmatrix}.
\] (5.5)

Its norm is

\[
\|N\| = a^2 \sin \theta.
\] (5.6)

Therefore the unit normal vector is

\[
n = \begin{bmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{bmatrix}.
\] (5.7)

The Hessian matrix is

\[
H = \begin{bmatrix} -a \sin \theta \cos \phi & -a \cos \theta \sin \phi & -a \sin \theta \cos \phi \\ -a \sin \theta \sin \phi & a \cos \theta \cos \phi & -a \sin \theta \sin \phi \\ -a \cos \phi & 0 & 0 \end{bmatrix}.
\] (5.8)
Therefore the second fundamental form is

\[
h_{ij} = \begin{bmatrix}
-a & 0 \\
0 & -a \sin^2 \theta
\end{bmatrix}.
\] (5.9)

This puts the Gaussian curvature at

\[
K = \frac{h}{g} = \frac{a^2 \sin^2 \theta}{a^4 \sin^2 \theta} = \frac{1}{a^2}.
\] (5.10)

The mean curvature is

\[
M = \frac{1}{2g} (g_{11} h_{22} + g_{22} h_{11} - 2g_{12} h_{12}) = -\frac{a^3}{a^4} = \frac{1}{a}.
\] (5.11)

Therefore

\[
M^2 - K = 0.
\] (5.12)

Putting these elements together gives the Schrödinger equation

\[
\frac{1}{a^2} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{\cos \theta}{a^2 \sin \theta} \frac{\partial \psi}{\partial \theta} + \frac{1}{a^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} = -\frac{2\mu E}{\hbar^2} \psi.
\] (5.13)

Multiply both sides by \(a^2 \sin^2 \theta\) to get

\[
\sin^2 \theta \frac{\partial^2 \psi}{\partial \theta^2} + \sin \theta \cos \theta \frac{\partial \psi}{\partial \theta} + \frac{\partial \psi}{\partial \phi^2} = -a^2 \sin^2 \theta \frac{2\mu E}{\hbar^2} \psi.
\] (5.14)

This is slightly different from the traditional angular momentum derivation in that the energy is present rather than being separated out as part of the radial equation. Separating the variables gives

\[
\frac{1}{\Theta} \sin^2 \theta \frac{d^2 \Theta}{d\theta^2} + \frac{1}{\Theta} \sin \theta \cos \theta \frac{d\Theta}{d\theta} + a^2 \sin^2 \theta \frac{2\mu E}{\hbar^2} = -\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = m^2.
\] (5.15)
where \( m \) is a separation constant. These become

\[
\sin^2 \theta \frac{d^2 \Theta}{d\theta^2} + \sin \theta \cos \theta \frac{d\Theta}{d\theta} + a^2 \sin^2 \theta \frac{2\mu E}{\hbar^2} \Theta = m^2 \Theta, \quad (5.16)
\]

and

\[
\frac{d^2 \Phi}{d\phi^2} = -m^2 \Phi. \quad (5.17)
\]

Equation (5.17) has the solution

\[
\Phi(\phi) = Ae^{im\phi} + Be^{-im\phi}. \quad (5.18)
\]

Equation (5.16) is

\[
\sin^2 \theta \frac{d^2 \Theta}{d\theta^2} + \sin \theta \cos \theta \frac{d\Theta}{d\theta} + \frac{2\mu a^2 E}{\hbar^2} \sin^2 \theta \Theta = m^2 \Theta. \quad (5.19)
\]

This is Legendre’s differential equation,

\[
\sin^2 \theta \frac{d^2 \Theta}{d\theta^2} + \sin \theta \cos \theta \frac{d\Theta}{d\theta} + \lambda \sin^2 \theta \Theta = m^2 \Theta, \quad (5.20)
\]

with

\[
\lambda = \frac{2\mu a^2 E}{\hbar^2}. \quad (5.21)
\]

To ensure that solutions are nonsingular for integer \( m \) we must have the identity

\[
\lambda = l(l + 1) : l \in \mathbb{N}. \quad (5.22)
\]

The solution is then the associated Legendre polynomials, which we expected:

\[
\Theta(\theta) = AP^m_l(\cos \theta). \quad (5.23)
\]
The associated Legendre functions of the second kind have singularities present, and so are not part of the solution. Combining this with \( \Phi \) gives

\[
\psi_{lm}(\theta, \phi) = P^m_l(\cos \theta) \left( A_{lm}e^{im\phi} + B_{lm}e^{-im\phi} \right).
\] (5.24)

The boundary conditions and the normalization constraint \(|\psi|^2 = 1\) result in the solution being the spherical harmonics:

\[
\psi_{lm}(\theta, \phi) = A_{lm}P^m_l(\cos \theta) e^{im\phi} = Y_{lm}(\theta, \phi).
\] (5.25)

This is the standard solution covered in most quantum mechanics textbooks.

5.2 Shell Method

The sphere was used to calibrate calculations using the shell squeezing method. This method removes the singularities by working with a three-dimensional volume problem in Cartesian coordinates. Thus it is hoped that the method will yield the correct energy levels and remove any ambiguity as to which method is correct.

5.2.1 Summary of the method

Throughout this section, energy given by an \( E \) or \( \epsilon \) are given in electron volts and energy values given by an \( \epsilon \) are given in units where \( \hbar^2/2m = 1 \). They are related by the equation

\[
\epsilon = \frac{2mE}{\hbar^2}.
\] (5.26)

Furthermore, note that

\[
\frac{\hbar^2}{2m} = 3.810099 \ \text{eV} \cdot \text{Å}.
\] (5.27)
The solution to the energy levels for a particle constrained to a sphere of radius $a$ is

$$\varepsilon = \frac{l(l + 1)}{a^2}. \quad (5.28)$$

Ref. [1] shows that the energy of a particle constrained to a surface can be calculated from a particle constrained between two parallel surfaces separated by uniform distance $d$ using the formula

$$\epsilon = \lim_{d \to 0} \left( E - \frac{\pi^2 \hbar^2}{2Md^2} \right), \quad (5.29)$$

and throwing out the singular term as being unphysical.

5.2.2 Calibration using the sphere

The first step was to calibrate a single set of concentric spheres to the analytical solution. The Schrödinger equation for a particle constrained to a spherical shell of inner radius $a$ and outer radius $b$ with no internal potential energy is a combination of a spherical well with a hard sphere inside it. The general solution is

$$\psi(r, \theta, \phi) = \sum_{n=1}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[ A_{nlm} j_l(k_{nl}r) + B_{nlm} y_l(k_{nl}r) \right] Y_{lm}(\theta, \phi), \quad (5.30)$$

where

$$k_{nl} = \frac{n\pi}{b - a}. \quad (5.31)$$

The zeros of the spherical Bessel functions and spherical Neumann functions occur at integer multiples of $\pi$, hence the energy contribution from the radial component is identical to an infinite square well. Because the volume of interest does not include the origin and does not extend to infinity, we must keep both the spherical Bessel functions and spherical Neumann functions in the general solution. The solution is based on the moment of inertia of the classical shell of nonzero, finite thickness.
Table 5.1: Analytical Energy levels for concentric spheres

\[ n = 1, \]
\[ (a - b) \quad l = 0, m = 0 \quad 1,1,0 \quad 1,1,-1 \quad 1,1,1 \quad 1,2,0 \quad 1,2,2 \]

<table>
<thead>
<tr>
<th>l</th>
<th>(1,1,0)</th>
<th>(1,1,-1)</th>
<th>(1,1,1)</th>
<th>(1,2,0)</th>
<th>(1,2,2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.094010</td>
<td>0.095135</td>
<td>0.095135</td>
<td>0.097383</td>
<td>0.097383</td>
</tr>
<tr>
<td>10</td>
<td>0.376042</td>
<td>0.377180</td>
<td>0.377180</td>
<td>0.379457</td>
<td>0.379457</td>
</tr>
</tbody>
</table>

The moment of inertia for a spherical shell with inner radius \(a\) and outer radius \(b\) is [28]

\[ I = \frac{2}{5} M \frac{b^5 - a^5}{b^3 - a^3}. \]  

Two values that are needed are shown in Table 5.1.

Combining the equation

\[ E_{nl} = \frac{\hbar^2 k^2}{2I}, \]

with the equation

\[ k_l^2 = l(l + 1), \]

produces the formula

\[ E_l = 5 \frac{\hbar^2}{M} l(l + 1) \frac{(b^3 - a^3)}{(b^5 - a^5)}. \]

FEMLAB was used to calculate the solution for a particle constrained to move between two concentric spherical shells, one with radius 110 Å and one with radius 90 Å. These were then moved closer together by 5 Å each. The energy levels calculated by FEMLAB agree with the analytical solution to within \((-0.7 \pm 0.6)\)%.

Further convergence to the analytical value of 0.376042 eV is shown in Table 5.3 for spheres 10 Å apart by the number of mesh refinements. Beyond two refinements, the calculation time neared one hour for one pair of shells. At three refinements for the 110 Å and 95 Å pair, there were over three hundred thousand degrees of freedom in the finite element system. The eigenfunction closely resembled the spherical harmonics, with only the lowest order Bessel functions contributing to the radial portions.
Table 5.2: FEMLAB Energy levels for concentric spheres

<table>
<thead>
<tr>
<th>Refinements</th>
<th>(a - b)</th>
<th>(l = 0, m = 0)</th>
<th>1,1,0</th>
<th>1,1,1</th>
<th>1,1,1</th>
<th>1,2,0</th>
<th>1,2,2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>20</td>
<td>0.0954</td>
<td>0.0964</td>
<td>0.0964</td>
<td>0.0964</td>
<td>0.0984</td>
<td>0.0985</td>
</tr>
<tr>
<td>1</td>
<td>20</td>
<td>0.0949</td>
<td>0.0957</td>
<td>0.0958</td>
<td>0.0958</td>
<td>0.0974</td>
<td>0.0974</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>0.0944</td>
<td>0.0952</td>
<td>0.0952</td>
<td>0.0952</td>
<td>0.0967</td>
<td>0.0968</td>
</tr>
</tbody>
</table>

Table 5.3: Convergence of FEMLAB runs on concentric spheres by refinements

<table>
<thead>
<tr>
<th>Refinements</th>
<th>Degrees of freedom</th>
<th>Calculation Time (s)</th>
<th>Calculated energy</th>
<th>Absolute Error</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>13995</td>
<td>13.516</td>
<td>0.381196</td>
<td>−0.005154</td>
<td>−1.37%</td>
</tr>
<tr>
<td>1</td>
<td>36948</td>
<td>99.844</td>
<td>0.380061</td>
<td>−0.004019</td>
<td>−1.07%</td>
</tr>
<tr>
<td>2</td>
<td>103927</td>
<td>662.922</td>
<td>0.378353</td>
<td>−0.002311</td>
<td>−0.61%</td>
</tr>
<tr>
<td>3</td>
<td>301380</td>
<td>3036.328</td>
<td>0.377162</td>
<td>−0.00112</td>
<td>−0.30%</td>
</tr>
</tbody>
</table>

5.2.3 Varying the distance between the spheres

Five sets of two concentric spherical shells were constructed in FEMLAB with a mean radius of 100 Å in each set. These shells were treated as infinite barriers which the particle could not escape, i.e., given two concentric shells of radii \(a\) and \(b\), \(\psi(a) = \psi(b) = 0\). Each set of concentric spheres used different values of \(a\) and \(b\) while keeping their average constant. Energy levels were noted for each set of spheres.

Once the energy levels were tabulated, they were placed in Excel and plotted, and a linear trendline was added to the plot using \(d^{-2}\) as the linear component. This produced a fit of the form

\[
\varepsilon_{tot} = \frac{B}{d^2} + A. \tag{5.36}
\]

In all runs, \(B \approx \pi^2\), indicating a good fit, and \(A\) is the energy (in units of \(\varepsilon\)) of the constrained particle, because it is the only term that is not divergent as \(d \to 0\).

Table 5.4 shows the total energy levels by \(d\) for the analytical solution and for the numerical runs, respectively, with the coefficients of the fits for each below them.
Table 5.4: The Sphere

<table>
<thead>
<tr>
<th>Total Energy</th>
<th>$d$</th>
<th>Calculated</th>
<th>Analytical</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_{00}$</td>
<td>20</td>
<td>0.024914</td>
<td>0.024674</td>
</tr>
<tr>
<td>$\varepsilon_{00}$</td>
<td>40</td>
<td>0.006180</td>
<td>0.006169</td>
</tr>
<tr>
<td>$\varepsilon_{00}$</td>
<td>60</td>
<td>0.002743</td>
<td>0.002742</td>
</tr>
<tr>
<td>$\varepsilon_{00}$</td>
<td>80</td>
<td>0.001542</td>
<td>0.001542</td>
</tr>
<tr>
<td>$\varepsilon_{00}$</td>
<td>100</td>
<td>0.000987</td>
<td>0.000987</td>
</tr>
<tr>
<td>$\varepsilon_{10}$</td>
<td>20</td>
<td>0.025122</td>
<td>0.024874</td>
</tr>
<tr>
<td>$\varepsilon_{10}$</td>
<td>40</td>
<td>0.006383</td>
<td>0.006369</td>
</tr>
<tr>
<td>$\varepsilon_{10}$</td>
<td>60</td>
<td>0.002950</td>
<td>0.002942</td>
</tr>
<tr>
<td>$\varepsilon_{10}$</td>
<td>80</td>
<td>0.001755</td>
<td>0.001742</td>
</tr>
<tr>
<td>$\varepsilon_{10}$</td>
<td>100</td>
<td>0.001207</td>
<td>0.001187</td>
</tr>
<tr>
<td>$\varepsilon_{11}$</td>
<td>20</td>
<td>0.025128</td>
<td>0.024874</td>
</tr>
<tr>
<td>$\varepsilon_{11}$</td>
<td>40</td>
<td>0.006384</td>
<td>0.006369</td>
</tr>
<tr>
<td>$\varepsilon_{11}$</td>
<td>60</td>
<td>0.002950</td>
<td>0.002942</td>
</tr>
<tr>
<td>$\varepsilon_{11}$</td>
<td>80</td>
<td>0.001755</td>
<td>0.001742</td>
</tr>
<tr>
<td>$\varepsilon_{11}$</td>
<td>100</td>
<td>0.001207</td>
<td>0.001187</td>
</tr>
<tr>
<td>$A_{00}$</td>
<td>0.000</td>
<td>0.000000</td>
<td></td>
</tr>
<tr>
<td>$A_{10}$</td>
<td>0.0002</td>
<td>0.00020</td>
<td></td>
</tr>
<tr>
<td>$A_{11}$</td>
<td>0.0002</td>
<td>0.00020</td>
<td></td>
</tr>
</tbody>
</table>

(listed as $A_{ij}$ and $B_{ij}/\pi$). The convergence of the ground state is shown in this table.

It can be seen that the value for $A_{00} = 0$. Therefore, the shell method works well for the sphere to about three digits of accuracy.

5.2.4 Calibration using a finite cylinder

Let us now consider the finite cylinder as another test case of the shell squeezing technique. Reference [80] lists the energy of a particle with mass $m$ constrained to a hollow cylinder with thickness $2\epsilon$, radius $R$, and length $L$ as

$$E_{HC} = \frac{\hbar^2}{2m} \left[ \left( \frac{n\pi}{2\epsilon} \right)^2 + \left( \frac{k\pi}{L} \right)^2 + (1 + \delta) \frac{4l^4 - 1}{4R^2} \right],$$

(5.37)
Table 5.5: Fit values for energy in the surface limit for a cylinder using the shell method

<table>
<thead>
<tr>
<th>l</th>
<th>$\Delta E_{DG}$</th>
<th>$\Delta E_{HC}$</th>
<th>$\Delta E_{HC} - \Delta E_{DG}$</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-0.25</td>
<td>-0.000</td>
<td>0.250</td>
<td>-0.999</td>
</tr>
<tr>
<td>1</td>
<td>0.75</td>
<td>0.660</td>
<td>-0.090</td>
<td>-0.119</td>
</tr>
<tr>
<td>1</td>
<td>0.75</td>
<td>0.659</td>
<td>-0.091</td>
<td>-0.122</td>
</tr>
<tr>
<td>2</td>
<td>3.75</td>
<td>3.824</td>
<td>0.074</td>
<td>0.020</td>
</tr>
<tr>
<td>2</td>
<td>3.75</td>
<td>3.821</td>
<td>0.071</td>
<td>0.019</td>
</tr>
<tr>
<td>3</td>
<td>8.75</td>
<td>8.563</td>
<td>-0.187</td>
<td>-0.021</td>
</tr>
</tbody>
</table>

where $l \in \mathbb{N}$ is a quantum number and $\delta$ is the error of the numerical solution of the 3-D equation and the differential geometric dimensional reduction method. The authors of Ref. [80] found that for their runs, for the $n = 1$ state, $\delta = 3.9 \times 10^n$, where $n = -9$ for $\epsilon = 10^{-4}$, $-7$ for $\epsilon = 10^{-3}$, $-5$ for $\epsilon = 10^{-2}$, and $-3$ for $\epsilon = 10^{-1}$. Thus it was found in that reference that the differential geometric approach had good agreement with the numerical calculation.

FEMLAB was used to calculate both $\delta$ and to use the shell squeezing method to approximate the energy using the form

$$E = \frac{A}{(2\epsilon)^2} + C.$$  \hfill (5.38)

At the limit $\epsilon \to 0$, only the $C$ term remains finite and thus the divergent term is thrown out as being unphysical. Thus this corresponds to the energy of the particle constrained to the surface. The results (in units where $\hbar/2m = 1$) are listed in Table 5.5. Numerical simulation did not reproduce the negative energy shift predicted by the differential geometric method. However, the shift was simulated for the excited states. The reason for this is unknown. The calculations produced a maximum error of 0.18 from the differential geometric method and are shown in Figure 5.1.
Figure 5.1: Overlay of shell method energy levels for cylinders with Differential Geometric analytical values

5.3 Summary

The sphere was shown to have an analytical solution and zero curvature term. The shell method was introduced and shown to agree with the sphere, but to disagree with the finite cylinder for the ground state and agree with it for the excited states. The reason for the zero ground state for the cylinder is unknown. However, this technique will be used again later when the spheroid and ellipsoid are studied.
Analysis of the Prolate and Oblate Spheroids

In this chapter, the symmetry of the sphere is relaxed and prolate and oblate spheroids are studied. It should be noted that the technique used in some references such as Ref. [4] produces different results because the problem is solved as a three-dimensional problem with one component of the separated wavefunction held constant. Thus the energy shift due to curvature is neglected. This results in a ground state with zero energy, whereas the curvature prohibits this when using the two-dimensional equation.

The goal of this chapter is to derive the two-dimensional equation and find its solutions. These are compared with Cantele’s work (Ref. [5]), which is shown to be equivalent.

6.1 Formulation of Schrödinger Equation

6.1.1 Fundamental forms and Laplace operator

The parameterization of the prolate spheroid is

\[
\begin{bmatrix}
    f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \cos \phi \\
    f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \sin \phi \\
    f \xi \eta
\end{bmatrix}
\]

\[ (6.1) \]
The Jacobian matrix is
\[
\frac{\partial (x, y, z)}{\partial (\eta, \phi)} = \begin{bmatrix}
-\eta f \sqrt{\xi^2 - 1} \cos \phi & -f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \sin \phi \\
-\eta f \sqrt{\xi^2 - 1} \sin \phi & f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \cos \phi \\
f \xi & 0
\end{bmatrix}.
\] (6.2)

From this the metric tensor can be calculated. It is
\[
g_{ij} = \begin{bmatrix}
f^2 \xi^2 - \eta^2 \\
0 \\
0 & f^2(\xi^2 - 1)(1 - \eta^2)
\end{bmatrix}.
\] (6.3)

Its determinant is
\[
g = f^4(\xi^2 - \eta^2)(\xi^2 - 1).
\] (6.4)

This is sufficient information to derive the tangential portion of the Laplace-Beltrami operator. It is
\[
\mathcal{D}[\chi_t(u, v)] = \frac{1}{f^2(\xi^2 - \eta^2)^2} \frac{\partial}{\partial \eta} \left[ \frac{f^2}{\sqrt{\xi^2 - \eta^2}} \frac{\partial \chi_t}{\partial \eta} \right] + \frac{1}{f^2(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2 \chi_t}{\partial \phi^2}
\]
\[
= \frac{1 - \eta^2}{f^2(\xi^2 - \eta^2)^2} \frac{\partial^2 \chi_t}{\partial \eta^2} + \frac{\eta(\eta^2 - 2\xi^2 + 1)}{f^2(\xi^2 - \eta^2)^2} \frac{\partial \chi_t}{\partial \eta}
\]
\[
+ \frac{1}{f^2(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2 \chi_t}{\partial \phi^2}.
\] (6.5)

The next object to calculate is the second fundamental form. This requires the Hessian matrix and the unit normal vector. The unit normal vector is
\[
n = -\frac{1}{f^2(\xi^2 - \eta^2)} \begin{bmatrix}
\pm \frac{\sqrt{1 - \eta^2}}{\sqrt{\xi^2 - 1}} \xi \cos \phi \\
\pm \frac{\sqrt{1 - \eta^2}}{\sqrt{\xi^2 - 1}} \xi \sin \phi \\
\eta
\end{bmatrix},
\] (6.6)
and the Hessian matrix is

\[
H = \begin{bmatrix}
-f \sqrt{\xi^2 - 1} \cos \phi \left( \frac{1}{\sqrt{1-\eta^2}} - \frac{\eta^2}{(1-\eta^2)^2} \right) & \eta f \sqrt{\xi^2 - 1} \sin \phi & -f \sqrt{\xi^2 - 1} \sqrt{1-\eta^2} \cos \phi \\
-f \sqrt{\xi^2 - 1} \sin \phi \left( \frac{1}{\sqrt{1-\eta^2}} - \frac{\eta^2}{(1-\eta^2)^2} \right) & \eta f \sqrt{\xi^2 - 1} \cos \phi & -f \sqrt{\xi^2 - 1} \sqrt{1-\eta^2} \sin \phi \\
0 & 0 & 0 \\
\end{bmatrix}.
\]

(6.7)

With these values calculated, the second fundamental form can be calculated. It is

\[
h_{ij} = \begin{bmatrix}
\frac{\xi(1-3\eta^2)}{f(\xi^2-\eta^2)(1-\eta^2)} & 0 \\
0 & \frac{(1-\eta^2)\xi}{f(\xi^2-\eta^2)} \\
\end{bmatrix}.
\]

(6.8)

Its determinant is

\[
h = \frac{\xi^2(1-3\eta^2)}{f^2(\xi^2-\eta^2)^2}.
\]

(6.9)

With the fundamental forms calculated, the curvatures can be derived.

### 6.1.2 Mean and Gaussian curvatures

The mean curvature is

\[
M = \frac{\xi}{2f^3(\xi^2-\eta^2)} \left[ \frac{1}{\xi^2 - 1} + \frac{(1-\eta^2)^2}{\xi^2 - \eta^2} \right],
\]

(6.10)

and the Gaussian curvature is

\[
K = \frac{\xi^2(1-3\eta^2)}{f^6(\xi^2-\eta^2)^3(\xi^2 - 1)}.
\]

(6.11)

These combine to form the effective potential

\[
V_S = -\frac{\hbar^2}{2\mu} \frac{\xi^2}{4f^6(\xi^2 - 1)(\xi^2 - \eta^2)^2} \left[ \frac{(\eta^2 - 1)^4 + 1}{\xi^2 - 1} + \frac{\eta^2(2\eta^2 - 1) + 1}{\xi^2 - \eta^2} \right].
\]

(6.12)

Figure 6.1 plots \(M^2 - K\) as a function of \(\eta\) for the case \(f = 2.2, \xi = 1.1\). Thus the
potential is attractive at the poles. Figure 6.2 shows a three-view plot of this value.

We are now ready to formulate the Schrödinger equation.

6.1.3 Formulation and separation of the Schrödinger equation

The full Schrödinger equation for a particle constrained to the surface of a prolate spheroid is

\[
\frac{1}{f^2\sqrt{\xi^2 - \eta^2}} \frac{\partial}{\partial \eta} \left[ \frac{1 - \eta^2}{\sqrt{\xi^2 - \eta^2}} \frac{\partial \chi_t}{\partial \eta} \right] + \frac{1}{f^2(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2 \chi_t}{\partial \phi^2} \\
+ \frac{\xi^2}{4f^6(\xi^2 - 1)(\xi^2 - \eta^2)^2} \left[ \frac{(\eta^2 - 1)^4 + 1}{\xi^2 - 1} + \frac{\eta^2(2\eta^2 - 1) + 1}{\xi^2 - \eta^2} \right] \chi_t \\
= -k^2 \chi_t, \quad (6.13)
\]

where \( k^2 = \frac{2mE}{\hbar^2} \).

This equation, although formidable, is separable. Let \( \chi_t(\eta, \phi) = H(\eta)\Phi(\phi) \). Then
Figure 6.2: (Color in electronic version) $M^2 - K$ for a prolate spheroid with $f = 2.2, \xi = 1.1$
equation (6.13) becomes

\[
\frac{1}{H} \left( \xi^2 - 1 \right) \left( 1 - \eta^2 \right)^2 \frac{d^2 H}{d \eta^2} + \frac{1}{H (\xi^2 - \eta^2)} \left[ \frac{(1 - \eta^2)^2}{(\xi^2 - \eta^2)^2} - 2 \frac{\eta (1 - \eta^2)}{\xi^2 - \eta^2} \right] \frac{dH}{d\eta} + \frac{\xi^2 (1 - \eta^2)}{4 f^4 (\xi^2 - \eta^2)^2} \left[ (\eta^2 - 1)^4 + 1 \right] + \frac{\eta^2 (2 \eta^2 - 1) + 1}{\xi^2 - \eta^2} + f^2 (1 - \eta^2) (\xi^2 - 1) \frac{2 \mu E}{\hbar^2} \right] \frac{dH}{d\eta} + \\
\left\{ \frac{\xi^2}{4 f^6 (\xi^2 - 1)(\xi^2 - \eta^2)^2} \left[ 1 + (1 - \eta^2)^4 + \frac{1 - \eta^2 (1 - 2 \eta^2)}{\xi^2 - \eta^2} \right] \right. \\
\left. + \frac{m^2}{f^2 (\xi^2 - 1)(1 - \eta^2)} \right\} H = - \frac{2 \mu E}{\hbar^2} H, \quad (6.14)
\]

This separates into the equations

\[
\frac{1 - \eta^2}{f^2 (\xi^2 - \eta^2)} \frac{d^2 H}{d \eta^2} + \frac{1}{f^2 (\xi^2 - \eta^2)} \left[ \frac{1 - \eta^2}{\xi^2 - \eta^2} - 2 \eta \right] \frac{dH}{d\eta} + \\
\frac{\xi^2}{4 f^6 (\xi^2 - 1)(\xi^2 - \eta^2)^2} \left[ 1 + (1 - \eta^2)^4 + \frac{1 - \eta^2 (1 - 2 \eta^2)}{\xi^2 - \eta^2} \right] \right. \\
\left. + \frac{m^2}{f^2 (\xi^2 - 1)(1 - \eta^2)} \right\} H = - \frac{2 \mu E}{\hbar^2} H, \quad (6.15)
\]

and

\[
\frac{d^2 \Phi}{d \phi^2} = - m^2 \Phi. \quad (6.16)
\]

Since equation 6.16 is nearly trivial, we will solve it first. It is

\[
\Phi(\phi) = A e^{im \phi} + B e^{-im \phi} : m \in \mathbb{Z}, \quad (6.17)
\]

where \(A\) and \(B\) are constants.

This leaves the \(H(\eta)\) equation. This will be shown to be identical with equation (24) from Ref. [5], which was solved numerically using the shooting method and the software package NAG.
6.2 Equivalence of the Two-Dimensional Equation with Ref. [5]

We now turn to duplicate the results of Ref. [5] using the full two-dimensional equation, equation (6.13). To do so, we must first prove that it is equivalent to the equation used in that reference.

6.2.1 Statement of the problem

Given the map

\[
\begin{bmatrix}
  x \\
  y \\
  z
\end{bmatrix} = \begin{bmatrix}
  f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \cos \phi \\
  f \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \sin \phi \\
  f \xi \eta
\end{bmatrix} = \begin{bmatrix}
  a \sin \theta \cos \phi \\
  a \sin \theta \sin \phi \\
  c \cos \phi
\end{bmatrix},
\]

where \(a = f \sinh \alpha\) and \(c = f \cosh \alpha\) for \(\alpha \geq 0\), [13] show that the \((\xi, \eta, \phi)\) equation

\[
\frac{1 - \eta^2}{f^2(\xi^2 - \eta^2)} \frac{\partial^2 \sigma}{\partial \eta^2} - \frac{\eta(\xi^2 - \eta^2) + (\xi^2 - 1) \partial \sigma}{f^2(\xi^2 - \eta^2)^2} \frac{\partial \sigma}{\partial \eta} + \frac{1}{f^2(\xi^2 - 1)(\xi^2 - \eta^2)^2} \frac{\partial^2 \sigma}{\partial \eta^2}
\]

\[
\frac{\xi^2}{4f^6(\xi^2 - 1)(\xi^2 - \eta^2)^2} \left[ \frac{(\eta^2 - 1)^4}{\xi^2 - 1} + \frac{\eta^2(2\eta^2 - 1) + 1}{\xi^2 - \eta^2} \right] \sigma
\]

\[
= -\varepsilon^S \sigma,
\]

is equivalent to

\[
- \frac{1}{g_{11}} \frac{\partial^2 \sigma}{\partial \theta^2} - \frac{1}{\sqrt{g_{11}g_{22}}} \frac{\partial}{\partial \theta} \left[ \sqrt{\frac{g_{22}}{g_{11}}} \frac{\partial \sigma}{\partial \theta} - \frac{1}{g_{22}} \frac{\partial^2 \sigma}{\partial \phi^2} - \left( \frac{T^2}{4} - D \right) \sigma \right] = \frac{2m}{\hbar^2} (E^S - E_n^S) \sigma,
\]

where

\[
g_{11} = a^2 \cos^2 \theta + c^2 \sin^2 \theta, \quad \text{(6.21)}
\]

\[
g_{22} = a^2 \sin^2 \theta, \quad \text{(6.22)}
\]
\[ x = \frac{c}{a}, \quad (6.23) \]
\[ e = \frac{f}{c}, \quad (6.24) \]
\[ \varepsilon^S = \frac{2m(E^S - E^S_n)}{\hbar^2}, \quad (6.25) \]

and
\[ m^S(\theta) = \frac{m(1 + \chi^2 \tan^2 \theta)}{\chi^2(1 + \tan^2 \theta)}, \quad (6.26) \]

under the transform
\[ \sigma = \left( \frac{a^2 \cos^2 \theta + c^2 \sin^2 \theta}{a^2 \sin^2 \theta} \right)^{1/4} t(\theta). \quad (6.27) \]

### 6.2.2 Choice of substitution

Inspection of equation (6.18) shows some similarities between the prolate spheroidal coordinates and the spherical coordinates. Specifically, the coordinate charts reduce to
\[ \sqrt{\xi^2 - 1} = \sinh \alpha \sin \theta, \quad (6.28) \]

and
\[ \xi \eta = \cosh \alpha \cos \theta, \quad (6.29) \]

which cannot be analytically solved. However, there are similarities in domains: \( \xi > 1, \alpha > 1, \eta \in [-1, 1], \) and \( \theta \in [0, 2\pi] \). We also note that \( \cos \theta \in [-1, 1] \). By applying intuition to the coordinate domains, we find that \( \xi \) roughly corresponds to \( \alpha \) and \( \eta \) to \( \theta \). Therefore we propose the relationships
\[ \sqrt{\xi^2 - 1} = \sinh \alpha, \quad (6.30) \]
\[ \xi = \cosh \alpha, \quad (6.31) \]
\[ \sqrt{1 - \eta^2} = \sin \theta, \quad (6.32) \]
\[ \eta = \cos \theta. \]  

(6.33)

Trying this map gives

\[ \cosh^2 \alpha - \sinh^2 \alpha = 1 \]  

(6.34)

\[ \sin^2 \theta + \cos^2 \theta = 1. \]  

(6.35)

These are just the Pythagorean Theorem for hyperbolic functions and Euler’s identity, respectively. Therefore this system is consistent and might work.

### 6.2.3 Proof of equivalence

Begin with equation (6.20) and let \( M = \frac{T}{2}, \) \( K = D, \) and \( \varepsilon^S = \frac{2m}{\hbar^2} (E^S - E^S_n). \) Then

\[
- \frac{1}{a^2 \cos^2 \theta} \frac{1}{1 + \chi \tan^2 \theta} \frac{\partial^2 \sigma}{\partial \theta^2} - \frac{a^2 \cos \theta}{\sin \theta (a^2 \cos^2 \theta + c^2 \sin^2 \theta)^2} \frac{\partial \sigma}{\partial \theta} - \frac{1}{a^2 \sin^2 \theta} \frac{\partial^2 \sigma}{\partial \phi^2} - (M^2 - K) \sigma = \varepsilon^S \sigma \quad (6.36)
\]

Using the change of variables \( \eta = \cos \theta, \) \( \xi = \cosh \alpha = \frac{\xi}{f}, \) then

\[ 1 - \eta^2 = \sin^2 \theta, \]  

(6.37)

\[ \xi^2 - 1 = \sinh^2 \alpha = \frac{a^2}{f^2} = \frac{c^2}{f^2} - 1, \]  

(6.38)

\[ \frac{1 - \eta^2}{\eta^2} = \tan^2 \theta, \]  

(6.39)

\[ \xi^2 - \eta^2 = \frac{a^2}{f^2} + \sin^2 \theta = \frac{c^2}{f^2} - \cos^2 \theta = \frac{a^2}{f^2} + \xi^2 - 1 = \frac{c^2}{f^2} - \eta^2, \]  

(6.40)

\[ a^2 = f^2 (\xi^2 - 1) \]  

(6.41)

and

\[ f^2 + a^2 = c^2. \]  

(6.42)
Finally,
\[ \frac{f^2}{a^2} + 1 = \chi^2. \]  
(6.43)

The derivatives are
\[ \frac{\partial}{\partial \theta} = \frac{\partial \eta}{\partial \theta} \frac{\partial}{\partial \eta} = -\sqrt{1 - \eta^2} \frac{\partial}{\partial \eta}, \]  
(6.44)

\[ \frac{\partial}{\partial \eta} = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta}, \]  
(6.45)

\[ \frac{\partial^2}{\partial \theta^2} = \frac{\partial \eta}{\partial \theta} \frac{\partial}{\partial \eta} \left[ \frac{\partial \eta}{\partial \theta} \frac{\partial}{\partial \eta} \right] = (\frac{\partial \eta}{\partial \theta})^2 \frac{\partial^2}{\partial \eta^2} + \frac{\partial \eta}{\partial \theta} \frac{\partial^2}{\partial \eta^2} \frac{\partial}{\partial \eta}, \]  
(6.46)

\[ \frac{\partial^2}{\partial \eta^2} = (1 - \eta^2) \frac{\partial^2}{\partial \eta^2} + \eta \frac{\partial}{\partial \eta}, \]  
(6.47)

and
\[ \frac{\partial^2}{\partial \eta^2} = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \theta^2} + \frac{2}{\sin^3 \theta \tan \theta} \frac{\partial}{\partial \theta}. \]  
(6.48)

Plugging in all of these substitutions into equation (6.36) gives
\[ -\frac{1}{f^2(\xi^2 - 1)\eta^2} \left[ 1 + \left( \frac{f^2(\xi^2 - 1)}{f^2(\xi^2 - 1) + 1} \right) \frac{1 - \eta^2}{\eta^2} \right] \left[ (1 - \eta^2) \frac{\partial^2}{\partial \eta^2} + \eta \frac{\partial}{\partial \eta} \right] \]
\[ - \frac{f^2(\xi^2 - 1)\eta^2}{\sqrt{1 - \eta^2} \left\{ f^2(\xi^2 - 1)\eta^2 + [f^2 + f^2(\xi^2 - 1)](1 - \eta^2) \right\}^2} \left[ -\sqrt{1 - \eta^2} \frac{\partial}{\partial \eta} \right] \]
\[ - \frac{1}{f^2(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2 \sigma}{\partial \phi^2} - (M^2 - K) \sigma = \varepsilon S \sigma \]  
(6.49)

Cleaning this up gives
\[ -\frac{1 - \eta^2}{f^2(\xi^2 - \eta^2)} \frac{\partial^2 \sigma}{\partial \eta^2} + \frac{\eta}{f^2(\xi^2 - \eta^2)} \left[ \frac{\xi^2 - 1}{\xi^2 - \eta^2} - 1 \right] \frac{\partial \sigma}{\partial \eta} - \frac{1}{f^2(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2 \sigma}{\partial \phi^2} \]
\[ - (M^2 - K) \sigma = \varepsilon S \sigma. \]  
(6.50)

Thus the first and third terms are proved. All that remains is to show that the
curvatures are equal and that
\[
\frac{\eta}{f^2(\xi^2 - \eta^2)} \left[ \frac{\xi^2 - 1}{\xi^2 - \eta^2} - 1 \right] = -\frac{\eta[(\xi^2 - \eta^2) + (\xi^2 - 1)]}{f^2(\xi^2 - \eta^2)^2}
\] (6.51)

This means that we need to prove
\[
\frac{\xi^2 - 1}{\xi^2 - \eta^2} - 1 = \frac{(\xi^2 - \eta^2) + (\xi^2 - 1)}{\xi^2 - \eta^2}
\] (6.52)

Observe that
\[
\frac{\xi^2 - 1 + \xi^2 - \eta^2}{\xi^2 - \eta^2} - 1 = \frac{(\xi^2 - \eta^2) + (\xi^2 - 1)}{\xi^2 - \eta^2}
\] (6.53)

Therefore equation (6.19) and equation (6.20) are equivalent up to the Laplace-Beltrami operator. Unfortunately, Ref. [5] does not give the formulas for the curvatures. However, they can be derived, so the two equations can be proved. The Jacobian of the spherical coordinate representation of equation (6.18) is
\[
\frac{\partial (x, y, z)}{\partial (\theta, \phi)} = \begin{bmatrix}
a \cos \theta \cos \phi & a \sin \theta \sin \phi \\
a \cos \theta \sin \phi & -a \sin \theta \cos \phi \\
-c \sin \theta & 0
\end{bmatrix},
\] (6.54)

with Hessian matrix
\[
H = \begin{bmatrix}
-a \sin \theta \cos \phi & a \cos \theta \sin \phi & a \sin \theta \cos \phi \\
-a \sin \theta \sin \phi & -a \cos \theta \cos \phi & a \sin \theta \sin \phi \\
-c \cos \theta & 0 & 0
\end{bmatrix}.
\] (6.55)
The normal vector is

\[
N = \begin{bmatrix}
(-a \sin \theta \cos \phi)(-c \sin \theta) - (a \cos \theta \sin \phi)(0) \\
(0)(a \cos \theta \cos \phi) - (a \sin \theta \sin \phi)(-c \sin \theta) \\
(a \sin \theta \sin \phi)(a \cos \theta \sin \phi) - (a \cos \theta \cos \phi)(-a \sin \theta \cos \phi)
\end{bmatrix},
\]

which simplifies to

\[
N = \begin{bmatrix}
ac \sin^2 \theta \cos \phi \\
ac \sin^2 \theta \sin \phi \\
a^2 \sin \theta \cos \theta
\end{bmatrix}.
\]

Its norm is

\[
N = a \sqrt{c^2 \sin^4 \theta + a^2 \sin^2 \theta \cos^2 \theta}.
\]

The metric tensor is given by equations (6.21) and (6.22). The second fundamental form is

\[
h_{\theta\theta} = \frac{-ac \sin \theta}{\sqrt{c^2 \sin^4 \theta + a^2 \sin^2 \theta \cos^2 \theta}},
\]

\[
h_{\phi\phi} = \frac{acsin^3\theta}{\sqrt{c^2 \sin^4 \theta + a^2 \sin^2 \theta \cos^2 \theta}},
\]

\[
h_{\theta\phi} = 0,
\]

and its determinant is

\[
h = \frac{-a^2 c^2 \sin^4 \theta}{c^2 \sin^4 \theta + a^2 \sin^2 \theta \cos^2 \theta}.
\]

The metric discriminant is its square root,

\[
g = a^2 \sin^2 \theta(a^2 \cos^2 \theta + c^2 \sin^2 \theta).
\]

Therefore the Gaussian curvature is

\[
K = -\frac{\chi^2}{a^2 \sin^4 \theta(cot^2 \theta + \chi^2)^2},
\]

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and the Mean curvature is
\[ M = \frac{\chi (\chi^2 - 1)}{2a \sin \theta} \left( \frac{1}{(\cot^2 \theta + \chi^2)^{\frac{3}{2}}} \right). \] (6.65)

Now that the mean and Gaussian curvatures have been calculated, Theorem (A.76) and Theorem (A.79) from section A can be used to transform equations (6.64) and (6.65). The Jacobian matrix for transforming from prolate spheroidal coordinates to spherical coordinates is
\[ J = \begin{bmatrix} -\sin \theta & 0 \\ 0 & 1 \end{bmatrix}. \] (6.66)

Therefore the metric tensor transforms as
\[ g' = g \sin^2 \theta. \] (6.67)

The corresponding Hessian matrix is
\[ H'[u] = \begin{bmatrix} -\cos \theta & 0 \\ 0 & 0 \end{bmatrix}. \] (6.68)

Using these formulas in Theorem (A.76) and defining \( u^p \) as the \( p \)-th component of the parameterization in spherical coordinates and \( x^p \) as the same component of the parameterization in spheroidal coordinates gives
\[ h' = \left[ \left( \partial'_{11} u^p \right) n_k (\partial_p x^k) + J^i_{11} J^j_{12} h_{ij} \right] \left[ \left( \partial'_{22} u^q \right) n_b (\partial_p x^b) + J^g_{22} J^h_{23} h_{gh} \right] \\
- \left[ \left( \partial'_{12} u^c \right) n_d (\partial_p x^d) + J^i_{11} J^j_{13} h_{ij} \right] \left[ \left( \partial'_{22} u^q \right) n_b (\partial_p x^b) + J^g_{22} J^h_{23} h_{gh} \right] \\
= \left[ -\cos \theta n_k (\partial_1 x^k) + \sin^2 \theta h_{11} \right] [h_{22}]. \] (6.69)
A closer look at the normal vector dotted with the $\eta$ derivative shows

$$n_k(\partial_1 x^k) = -\frac{1}{f^2(\xi^2 - \eta^2)} \left\{ -\frac{f\eta\sqrt{\xi^2 - 1}}{\sqrt{1 - \eta^2}} \cos \phi \sqrt{\frac{1 - \eta^2}{\xi^2 - 1}} \xi \cos \phi \\
-\frac{f\eta\sqrt{\xi^2 - 1}}{\sqrt{1 - \eta^2}} \sin \phi \sqrt{\frac{1 - \eta^2}{\xi^2 - 1}} \xi \sin \phi + f\xi \eta \right\}$$

$$= -\frac{1}{f^2(\xi^2 - \eta^2)} \left\{ -f\eta \xi \cos^2 \phi - f\eta \xi \sin^2 \phi + f\xi \eta \right\}$$

$$= -\frac{1}{f^2(\xi^2 - \eta^2)} \left\{ -f\xi \eta + f\xi \eta \right\}$$

$$= 0. \quad (6.70)$$

Filling this value in gives

$$h' = h_{11} h_{22} \sin^2 \theta. \quad (6.71)$$

Plugging into the definition of Gaussian curvature shows

$$K' = \frac{h'}{g'} = \frac{h_{11} h_{22} \sin^2 \theta}{g \sin^2 \theta} = \frac{h}{g} = K. \quad (6.72)$$

Therefore the Gaussian curvature is equivalent.

Next we check the mean curvature term. Plugging our coordinates into Theorem (A.79) gives

$$M' = \frac{1}{2 \sin^2 \theta g} \left\{ \sin^2 \theta g_{11} \left[ n_k (\partial'_{22} u^m) (\partial_m x^k) + h_{22} \right] + g_{22} \left[ n_k (\partial'_{11} u^p) (\partial_p x^k) + \sin^2 \theta h_{11} \right] \right\}. \quad (6.73)$$

Recalling that

$$\partial'_{\phi \phi} u^m = 0, \quad (6.74)$$

$$\partial'_{\theta \theta} u^p = \begin{bmatrix} \sin \theta \\ 0 \end{bmatrix}, \quad (6.75)$$
and
\[ n_k \partial_1 x^k = n_\eta \partial_1 x^k = 0 \] (6.76)

means that
\[ M' = \frac{1}{2 \sin^2 \theta g} [g_{11} h_{22} \sin^2 \theta + g_{22} h_{11} \sin^2 \theta] = \frac{1}{2g} [g_{11} h_{22} + g_{22} h_{11}] = M. \] (6.77)

Therefore the mean curvature is also invariant under this coordinate transform. It follows that equation (6.19) is equivalent to equation (6.20).

This ends the proof.

6.3 Derivation of Equation (24) in Ref. [5]

The next step is to derive equation (24) in Ref. [5] from the base metric. The Laplacian is given by

\[
\nabla^2 \sigma = \frac{1}{\sqrt{g}} \partial_i \left[ g^{ij} \sqrt{g} \partial_j \sigma \right] \\
= \frac{1}{\sqrt{g}} \partial_1 \left[ g^{11} \sqrt{g} \partial_1 \sigma \right] + \frac{1}{\sqrt{g}} \partial_2 \left[ g^{22} \sqrt{g} \partial_2 \sigma \right] \\
= \frac{1}{\sqrt{g_{11}g_{22}}} \partial_1 \left[ \frac{g_{22}}{g_{11}} \partial_1 \sigma \right] + \frac{1}{\sqrt{g_{11}g_{22}}} \partial_2 \left[ \frac{g_{11}}{g_{22}} \partial_2 \sigma \right] \\
= \frac{1}{g_{11}} \partial_1 [\partial_1 \sigma] + \frac{1}{g_{22}} \partial_2 [\partial_2 \sigma] + \frac{1}{2g_{11}g_{22}} \partial_1 \left[ \frac{g_{22}}{g_{11}} \right] \partial_1 \sigma + \frac{1}{2g_{11}} \partial_2 \left[ \frac{g_{11}}{g_{22}} \right] \partial_2 \sigma,
\] (6.78)

So the Schrödinger equation becomes

\[
\partial_1 [\partial_1 \sigma] + \frac{g_{11}}{g_{22}} \partial_2 [\partial_2 \sigma] + \frac{g_{11}}{2g_{22}} \partial_1 \left[ \frac{g_{22}}{g_{11}} \right] \partial_1 \sigma + \frac{1}{2} \partial_2 \left[ \frac{g_{11}}{g_{22}} \right] \partial_2 \sigma + g_{11}(M^2 - K) \sigma = -g_{11} \varepsilon \sigma,
\] (6.79)

Now substitute
\[
\partial_1 = \frac{\partial}{\partial \theta},
\] (6.80)
\[ \partial_2 = \frac{\partial}{\partial \phi}, \quad (6.81) \]

and
\[ \sigma = \left( \frac{g_{11}}{g_{22}} \right)^{1/4} t(\theta) e^{im\phi}. \quad (6.82) \]

Then
\[ \partial_1 \sigma = \frac{1}{4} \left( \frac{g_{22}}{g_{11}} \right)^{3/4} \partial_1 \left( \frac{g_{11}}{g_{22}} \right) t + \left( \frac{g_{11}}{g_{22}} \right)^{1/4} \partial_1 t e^{im\phi}, \quad (6.83) \]
\[ \partial_1 [\partial_1 \sigma] = \partial_1 \left[ \frac{1}{4} \left( \frac{g_{22}}{g_{11}} \right)^{3/4} \partial_1 \left( \frac{g_{11}}{g_{22}} \right) t \right] + \left( \frac{g_{11}}{g_{22}} \right)^{1/4} \partial_1 t e^{im\phi}, \quad (6.84) \]

and
\[ \partial_1 [\partial_1 \sigma] = \left\{ \left( \frac{g_{11}}{g_{22}} \right)^{1/4} \partial_1 t + \left[ \frac{1}{4} \left( \frac{g_{22}}{g_{11}} \right)^{3/4} \partial_1 \left( \frac{g_{11}}{g_{22}} \right) + \frac{1}{4} \left( \frac{g_{22}}{g_{11}} \right)^{3/4} \partial_1 \left( \frac{g_{11}}{g_{22}} \right) \right] \partial_1 t \right. \]
\[ + \frac{1}{4} \left[ \frac{3}{4} \left( \frac{g_{11}}{g_{22}} \right)^{1/4} \partial_1 \left( \frac{g_{22}}{g_{11}} \right) \partial_1 \left( \frac{g_{11}}{g_{22}} \right) + \left( \frac{g_{22}}{g_{11}} \right)^{3/4} \partial_1 \partial_1 \left( \frac{g_{11}}{g_{22}} \right) \right] t \left. \right\} e^{im\phi}. \quad (6.85) \]

Since \( g_{11} \) and \( g_{22} \) do not depend on \( \phi \),
\[ \partial_2 \sigma = im \left( \frac{g_{11}}{g_{22}} \right)^{1/4} t e^{im\phi}, \quad (6.86) \]

and
\[ \partial_2 [\partial_2 \sigma] = -m^2 \left( \frac{g_{11}}{g_{22}} \right)^{1/4} t e^{im\phi}, \quad (6.87) \]
and we get

\[
\left\{ \frac{1}{4} \left[ \left( \frac{g_{11}}{g_{22}} \right)^{3/4} \left( \frac{g_{11}}{g_{22}} \right)^{1/4} \partial_1 \left( \frac{g_{22}}{g_{11}} \right) \partial_1 \left( \frac{g_{11}}{g_{22}} \right) + \left( \frac{g_{22}}{g_{11}} \right)^{3/4} \partial_1 \partial_1 \left( \frac{g_{11}}{g_{22}} \right) \right] t(\theta) \right. \\
+ \left. \frac{1}{4} \left[ \left( \frac{g_{22}}{g_{11}} \right)^{3/4} \partial_1 \left( \frac{g_{11}}{g_{22}} \right) \right] \partial_1 t(\theta) + \partial_1 \left( \frac{g_{11}}{g_{22}} \right)^{1/4} \partial_1 t + \left( \frac{g_{11}}{g_{22}} \right)^{1/4} \partial_1 \partial_1 \right\} e^{i \mu \phi} \\
+ \frac{g_{11}}{2g_{22}} \partial_1 \left( \frac{g_{22}}{g_{11}} \right) \left\{ \frac{1}{4} \left( \frac{g_{22}}{g_{11}} \right)^{3/4} \partial_1 \left( \frac{g_{11}}{g_{22}} \right) t(\theta) + \left( \frac{g_{11}}{g_{22}} \right)^{1/4} \partial_1 t \right\} e^{i \mu \phi} \\
+ im \frac{1}{2} \partial_2 \left( \frac{g_{11}}{g_{22}} \right) \left( \frac{g_{11}}{g_{22}} \right)^{1/4} t(\theta) e^{i \mu \phi} + g_{11}(M^2 - K) \left( \frac{g_{11}}{g_{22}} \right)^{1/4} t(\theta) e^{i \mu \phi} \\
= -g_{11} \varepsilon \left( \frac{g_{11}}{g_{22}} \right)^{1/4} t(\theta) e^{i \mu \phi}. \quad (6.88) 
\]

Cleaning up gives

\[
\partial_1 \partial_1 t + \left[ \frac{1}{2} g_{22} \partial_1 \left( \frac{g_{11}}{g_{22}} \right) + \frac{1}{2} g_{11} \partial_1 \left( \frac{g_{22}}{g_{11}} \right) \right] \partial_1 t(\theta) \\
+ \left[ \frac{5}{16} \partial_1 \left( \frac{g_{22}}{g_{11}} \right) \partial_1 \left( \frac{g_{11}}{g_{22}} \right) + \frac{1}{4} \partial_2 \partial_1 \left( \frac{g_{11}}{g_{22}} \right) - m^2 \frac{g_{11}}{g_{22}} + g_{11}(M^2 - K) \right] t(\theta) \\
= -\varepsilon g_{11} t(\theta). \quad (6.89) 
\]

Focusing on the first derivative term,

\[
\partial_1 \left( \frac{g_{11}}{g_{22}} \right) = \frac{g_{22} \partial_1 g_{11} - g_{11} \partial_1 g_{22}}{\left(g_{22}\right)^2}, \quad (6.90) 
\]

and

\[
\partial_1 \left( \frac{g_{22}}{g_{11}} \right) = \frac{g_{11} \partial_1 g_{22} - g_{22} \partial_1 g_{11}}{\left(g_{11}\right)^2}. \quad (6.91) 
\]
So
\[
\frac{g_{11} g_{22} g_{22} \partial_1 g_{11}}{(g_{11})^2 (g_{22})^2} - \frac{g_{11} g_{22} g_{22} \partial_1 g_{11}}{(g_{11})^2 (g_{22})^2} + \frac{g_{22} \partial_1 \left( \frac{g_{11}}{g_{22}} \right)}{g_{11}} + \frac{g_{11} \partial_1 \left( \frac{g_{22}}{g_{11}} \right)}{g_{22}} = 0. \tag{6.92}
\]

Therefore
\[
\frac{1}{4} g_{22} \partial_1 \partial_1 \left( \frac{g_{11}}{g_{22}} \right) + g_{11} (M^2 - K) - m^2 \frac{g_{11}}{g_{22}} \right] t(\theta) = -\varepsilon g_{11} t(\theta). \tag{6.93}
\]

Now, we have to calculate several values that will be used the next few steps:

\[
\cos^2 \theta = \frac{1}{1 + \tan^2 \theta}, \tag{6.94}
\]

\[
\sin^2 \theta = \frac{\tan^2 \theta}{1 + \tan^2 \theta}, \tag{6.95}
\]

\[
H = \begin{bmatrix}
-a \sin \theta \cos \phi & \partial_\theta \phi x & -a \sin \theta \cos \phi \\
a \sin \theta \sin \phi & \partial_\theta \phi y & -a \sin \theta \sin \phi \\
-c \cos \theta & \partial_\theta \phi z & 0
\end{bmatrix}, \tag{6.96}
\]

\[
\mathbf{n} = \begin{bmatrix}
\frac{\chi \tan \theta \cos \phi}{\sqrt{1 + \chi^2 \tan^2 \theta}} \\
\frac{\chi \tan \theta \sin \phi}{\sqrt{1 + \chi^2 \tan^2 \theta}} \\
\frac{1}{\sqrt{1 + \chi^2 \tan^2 \theta}}
\end{bmatrix}, \tag{6.97}
\]

\[
g_{11} = a^2 \cos^2 \theta + c^2 \sin^2 \theta = \frac{c^2 (1 + \chi^2 \tan^2 \theta)}{\chi^2 (1 + \tan^2 \theta)}, \tag{6.98}
\]

\[
g_{22} = a^2 \sin^2 \theta = \frac{c^2 \tan^2 \theta}{\chi^2 (1 + \tan^2 \theta)}, \tag{6.99}
\]

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\[ h_{11} = -\frac{c \cos \theta (\tan^2 \theta + 1)}{\sqrt{1 + \chi^2 \tan^2 \theta}} = -c \sqrt{1 + \tan^2 \theta}, \quad (6.100) \]
\[ h_{22} = -\frac{c \sin \theta \tan \theta}{\sqrt{1 + \chi^2 \tan^2 \theta}} = -\frac{c \tan \theta}{\sqrt{1 + \chi^2 \tan^2 \theta} \sqrt{1 + \tan^2 \theta}}. \quad (6.101) \]
\[ h = \frac{c^2 \tan^2 \theta}{1 + \chi^2 \tan^2 \theta}, \quad (6.102) \]
\[ g = \frac{c^4 \tan^2 \theta (1 + \chi^2 \tan^2 \theta)}{\chi^4 (1 + \tan^2 \theta)^2}, \quad (6.103) \]
\[ K = \frac{c^2 \tan^2 \theta}{1 + \chi^2 \tan^2 \theta} \quad \frac{\chi^4 (1 + \tan^2 \theta)^2}{c^4 \tan^2 \theta (1 + \chi^2 \tan^2 \theta)} = \frac{\chi^4 (1 + \tan^2 \theta)^2}{c^2 (1 + \chi^2 \tan^2 \theta)^2}, \quad (6.104) \]

\[ M = \frac{1}{2g} (g_{11} h_{22} + g_{22} h_{11}) \]
\[ = \frac{1}{2} \frac{\chi^4 (1 + \tan^2 \theta)^2}{c^4 \tan^2 \theta (1 + \chi^2 \tan^2 \theta)} \left[ \frac{c^2 (1 + \chi^2 \tan^2 \theta)}{\chi^2 (1 + \tan^2 \theta)^2} \frac{-c \tan \theta}{\sqrt{1 + \chi^2 \tan^2 \theta} \sqrt{1 + \tan^2 \theta}} \right. \]
\[ + \left. \frac{c^2 \tan^2 \theta}{\chi^2 (1 + \tan^2 \theta)^2} \frac{-c \sqrt{1 + \tan^2 \theta}}{\sqrt{1 + \chi^2 \tan^2 \theta}} \right] \]
\[ = -\frac{\chi^2 \sqrt{1 + \tan^2 \theta}}{2c \sqrt{1 + \chi^2 \tan^2 \theta}} \left[ \frac{1 + \chi^2 \tan^2 \theta + 1 + \tan^2 \theta}{1 + \chi^2 \tan^2 \theta} \right], \quad (6.105) \]

and

\[ M^2 - K = \left\{ \frac{-\chi^2 \sqrt{1 + \tan^2 \theta}}{2c \sqrt{1 + \chi^2 \tan^2 \theta}} \left[ \frac{1 + \chi^2 \tan^2 \theta + 1 + \tan^2 \theta}{1 + \chi^2 \tan^2 \theta} \right] \right\}^2 - \frac{\chi^4 (1 + \tan^2 \theta)}{c^2 (1 + \chi^2 \tan^2 \theta)^2} \]
\[ = \frac{\chi^4 (1 + \tan^2 \theta)}{4c^2 (1 + \chi^2 \tan^2 \theta)^3} \left[ (1 + \chi^2 \tan^2 \theta)^2 + 2(1 + \chi^2 \tan^2 \theta)(1 + \tan^2 \theta) \right. \]
\[ + (1 + \tan^2 \theta)^2 \right] - \frac{4\chi^4 (1 + \tan^2 \theta)}{4c^2 (1 + \chi^2 \tan^2 \theta)^2} \]
\[ = \frac{\chi^4 (1 + \tan^2 \theta)(1 + \chi^2 \tan^2 \theta)^2}{4c^2 (1 + \chi^2 \tan^2 \theta)^3} + \frac{2\chi^4 (1 + \tan^2 \theta)^2 (1 + \chi^2 \tan^2 \theta)}{4c^2 (1 + \chi^2 \tan^2 \theta)^3} \]
\[ + \frac{\chi^4 (1 + \tan^2 \theta)^3}{4c^2 (1 + \chi^2 \tan^2 \theta)^3} - \frac{4\chi^4 (1 + \tan^2 \theta)}{4c^2 (1 + \chi^2 \tan^2 \theta)^3} \left. \right]. \quad (6.106) \]
So
\[
\frac{g_{11}}{g_{22}} = \chi^2 + \frac{1}{\tan^2 \theta}, \tag{6.107}
\]
\[
\frac{g_{22}}{g_{11}} = \frac{\tan^2 \theta}{1 + \chi^2 \tan^2 \theta}, \tag{6.108}
\]
\[
\partial_1 \left( \frac{g_{11}}{g_{22}} \right) = \partial_1 \left( \frac{1 + \chi^2 \tan^2 \theta}{\tan^2 \theta} \right) = -\frac{1 + \tan^2 \theta}{\tan^3 \theta}, \tag{6.109}
\]
\[
\partial_1 \left( \frac{g_{22}}{g_{11}} \right) = \partial_1 \left( \frac{\tan^2 \theta}{1 + \chi^2 \tan^2 \theta} \right) = \frac{2 \tan \theta (1 + \tan^2 \theta)}{(1 + \chi^2 \tan^2 \theta)^2}, \tag{6.110}
\]
and
\[
\partial_1 \partial_1 \left( \frac{g_{11}}{g_{22}} \right) = \partial_1 \left( \frac{-2(1 + \tan^2 \theta)}{\tan^3 \theta} \right) = \frac{4(1 + \tan^2 \theta) + 2(1 + \tan^2 \theta)^2}{\tan^4 \theta}. \tag{6.111}
\]

Plugging all of these into the Schrödinger equation
\[
\partial_1 \partial_1 t + \left\{ \frac{5}{16} \partial_1 \left( \frac{g_{22}}{g_{11}} \right) \partial_1 \left( \frac{g_{11}}{g_{22}} \right) + \frac{1}{4} \frac{g_{22}}{g_{11}} \partial_1 \partial_1 \left( \frac{g_{11}}{g_{22}} \right) + g_{11}(M^2 - K) - m^2 \frac{g_{11}}{g_{22}} \right\} t = -\varepsilon g_{11} t, \tag{6.112}
\]
gives
\[
\partial_1 \partial_1 t + \left\{ \frac{5}{16} \left[ \frac{2 \tan \theta (1 + \tan^2 \theta)}{1 + \chi^2 \tan^2 \theta)^2} \right] - \frac{2(1 + \tan^2 \theta)}{\tan^3 \theta} \right\} + \frac{1}{4} \left[ \frac{\tan^2 \theta}{1 + \chi^2 \tan^2 \theta} \right] \left[ \frac{4(1 + \tan^2 \theta) + 2(1 + \tan^2 \theta)^2}{\tan^4 \theta} \right] + \frac{\chi^2}{4c^2} \left[ \frac{1 + \chi^2 \tan^2 \theta}{1 + \tan^2 \theta} \right] \left[ \frac{\chi^4 (1 + \tan^2 \theta) (1 + \chi^2 \tan^2 \theta)^2}{4c^2 (1 + \chi^2 \tan^2 \theta)^3} \right] + \frac{2\chi^4 (1 + \tan^2 \theta)^2 (1 + \chi^2 \tan^2 \theta)}{4c^2 (1 + \chi^2 \tan^2 \theta)^3} + \frac{\chi^4 (1 + \tan^2 \theta)^3}{4c^2 (1 + \chi^2 \tan^2 \theta)^3} \right) \right] - m^2 \left( \frac{1 + \chi^2 \tan^2 \theta}{\tan^2 \theta} \right) t(\theta) = -\frac{\varepsilon c^2}{\chi^2} \frac{1 + \chi^2 \tan^2 \theta}{1 + \tan^2 \theta} t(\theta), \tag{6.113}
\]

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which simplifies to

\[
\partial_1 \partial_1 t + \left\{ \frac{4 + 4 \chi^2 \tan^2 \theta + 4 \tan^2 \theta + 4 \chi^2 \tan^4 \theta + 2 + 2 \chi^2 \tan^2 \theta + 4 \tan^2 \theta + 4 \chi^2 \tan^4 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \right. \\
+ \frac{2 \tan^4 \theta + 2 \chi^2 \tan^6 \theta - 5 - 10 \tan^2 \theta - 5 \tan^4 \theta + \chi^2 \tan^2 \theta + 2 \chi^4 \tan^4 \theta + \chi^6 \tan^6 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \\
+ \frac{\chi^2 \tan^2 \theta + 2 \chi^2 \tan^4 \theta + 2 \chi^2 \tan^2 \theta + 2 \chi^2 \tan^4 \theta + 2 \chi^4 \tan^4 \theta - 2 \chi^4 \tan^6 \theta + \chi^2 \tan^6 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \\
+ \frac{-4 \chi^2 \tan^2 \theta - 4 \chi^4 \tan^4 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} - m^2 \left( \frac{1 + \chi^2 \tan^2 \theta}{\tan^2 \theta} \right) \left\} \right. \\
+ t(\theta) = -\frac{\varepsilon c^2}{\chi^2} \frac{1 + \chi^2 \tan^2 \theta}{1 + \tan^2 \theta} t(\theta), \\
\tag{6.114}
\]

and further to

\[
\partial_1 \partial_1 t + \left\{ \frac{-1 + 2 + 4 \tan^2 \theta + 4 \tan^2 \theta - 10 \tan^2 \theta + 6 \chi^2 \tan^2 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \\
+ \frac{2 \chi^2 \tan^2 \theta + 2 \chi^2 \tan^2 \theta - 4 \chi^2 \tan^2 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \\
+ \frac{4 \chi^2 \tan^4 \theta + 4 \chi^2 \tan^4 \theta + 4 \chi^2 \tan^4 \theta + 2 \chi^4 \tan^4 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \\
+ \frac{-4 \chi^4 \tan^4 \theta + 2 \chi^4 \tan^4 \theta + 2 \tan^4 \theta - 5 \tan^4 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \\
+ \frac{2 - 2 \chi^2 + 1 + \chi^4}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \chi^2 \tan^6 \theta - m^2 \left( \frac{1 + \chi^2 \tan^2 \theta}{\tan^2 \theta} \right) \right\} \right. \\
t(\theta) = -\frac{\varepsilon c^2}{\chi^2} \frac{1 + \chi^2 \tan^2 \theta}{1 + \tan^2 \theta} t(\theta). \\
\tag{6.115}
\]
Still more simplification gives

\[
\frac{\partial}{\partial t} \left( \frac{\partial t}{\partial \theta} \right) + \left\{ \frac{1 + (6\chi^2 - 2) \tan^2 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} + \frac{(8\chi^2 - 3) \tan^4 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \right. \\
+ \left. \frac{\chi^2 (3 - 2\chi^2 + \chi^4) \tan^6 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} - m^2 \left( \frac{1 + \chi^2 \tan^2 \theta}{\tan^2 \theta} \right) \right\} t(\theta) \\
= - \frac{\varepsilon c^2 1 + \chi^2 \tan^2 \theta}{\chi^2 1 + \tan^2 \theta} t(\theta).
\]

(6.116)

Finally, this becomes

\[
- \frac{\partial^2 t}{\partial \theta^2} - \left[ \frac{1 + (6\chi^2 - 2) \tan^2 \theta + (8\chi^2 - 3) \tan^4 \theta + \chi^2 (3 + \chi^4 - 2\chi^2) \tan^6 \theta}{4(1 + \chi^2 \tan^2 \theta)^2 \tan^2 \theta} \right. \\
\left. - m^2 \left( \chi^2 + \frac{1}{\tan^2 \theta} \right) \right] t = \frac{\varepsilon c^2 1 + \chi^2 \tan^2 \theta}{\chi^2 1 + \tan^2 \theta} t,
\]

(6.117)

which is Canteles equation (24).

This ends the proof.

### 6.4 Numerical Validation of Ref. [5]

The next step is to compare the results of a numerical solution of equation 24 in Ref. [5] to the results plotted in Figure 4a of that reference. To do so, the equation must be entered into a boundary value problem solver with the correct conditions.

For each value of \(\chi\), corresponding values of \(\xi\) and \(f\) were calculated using the formulas

\[
\xi = \frac{\chi}{\sqrt{\chi^2 - 1}}, \quad (6.118)
\]

and

\[
f = \left[ \frac{3V}{4\pi \xi (\xi^2 - 1)} \right]^{1/3}, \quad (6.119)
\]
Figure 6.3: Numerical solution of $|\sigma_{00}|^2$ for $\chi = 0.5$ for the spheroid using ODE

where $V$ is the volume of the ellipsoid (set equal to 216 nm$^3$ or 512 nm$^3$).

One of the authors of Ref. [5] kindly provided his source code. However, the software package he used, NAG, was not available. Therefore FEMLAB was used to attempt to model the boundary conditions and geometry as accurately as possible. The results are shown in Figures 6.3, 6.4, 6.14, and 6.6.

These results are validated to six decimal places for the $m = \pm 1$ state, but vary from Ref. [5] by up to ten percent for the $m = 0$ states, partially because there are second order poles at $\eta = \pm 1$. However, they are close.

6.5 Numerical Validation of Ref. [4]

6.5.1 Extraction of data values in the reference material

Energy levels were extracted from the plots in Ref. [4] by taking screen shots of the plots, then finding the pixel index of each bar in the plots, and matching them to the pixels of the tick marks on the axes. These plots had a nominal pixel resolution of 0.11628\v per pixel.

The results in Ref. [4] were validated in two ways. The first was using the spheroidal wave equation, which was the equation used in that reference. The second
Figure 6.4: Numerical solution of $|\sigma_{10}|^2$ for $\chi = 2.5$ for the spheroid using ODE

Figure 6.5: Numerical solution of $|\sigma_{00}|^2$ for $\chi = 4$ for the spheroid using ODE
method used the 2-D equation in prolate spheroidal coordinates. It was found that the spheroidal wave equation produced eigenvalues whose mean error was within 0.1% of Ref. [4], and whose standard deviation of error was 7% from that reference. Using the correct unperturbed Hamiltonian (equation (6.15)) produced results that deviated significantly from those in Ref. [4].

A first run was made to validate the energy levels in the reference paper, using the equation in the paper. This equation is

\[
- \frac{\hbar^2}{2\mu f^2} \left\{ \frac{1}{\xi^2 - \eta^2} \left\{ \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial \psi}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial \psi}{\partial \eta} \right] \right\} + \frac{1}{(\xi^2 - 1)(1 - \eta^2)} \frac{\partial^2 \psi}{\partial \phi^2} \right\} = \varepsilon \psi.
\]

(6.120)

which, after separation and calculation of \( \lambda \) from the \( \xi \) equation, becomes the latitu-
Figure 6.7: $|\sigma|^2$ for $\xi = 1.1, f = 10, m = 0, 1, 2, 3$.

The straight line corresponds to $m = 0$, and as $m$ increases, the wavefunction more closely resembles a Gaussian distribution. Figures 6.8 through 6.10 show the calculated energy levels overlaid with Ref. [4]. This is sufficient to validate the energy levels in Ref. [4]. It does not validate that the technique is accurate; only that the solutions to the equation used in that source are.
Figure 6.8: Energy levels for a prolate spheroid with $\xi = 1.1$ overlaid with Ref. [4]

Figure 6.9: Energy levels for a prolate spheroid with $\xi = 1.25$ overlaid with Ref. [4]
6.5.2 Using the two-dimensional equation

We now attempt to compare the energy levels for a prolate spheroid using the unperturbed two-dimensional Hamiltonian operator to that in Ref. [4]. The equation modeled is

$$\frac{1}{\sqrt{\xi_0^2 - \eta^2}} \frac{\partial}{\partial \eta} \left[ \frac{1 - \eta^2}{\sqrt{\xi_0^2 - \eta^2}} \frac{\partial S}{\partial \eta} \right] + \lambda S - m^2 S = 0 \quad (6.122)$$

where

$$\lambda = \frac{2\mu f^2}{\hbar^2} E. \quad (6.123)$$
The one-dimensional FEMLAB system is

\[
\begin{aligned}
&d_a \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( -c \frac{\partial u}{\partial x} - \alpha u - \gamma \right) + \beta \frac{\partial u}{\partial x} + au = f \quad \text{on } \Omega \\
hu = r & \quad \text{on } \partial \Omega \text{ (Dirichlet)} \\
n \cdot \left( -c \frac{\partial u}{\partial x} - \alpha u - \gamma \right) + qu = g - h\mu & \quad \text{on } \partial \Omega \text{ (Generalized Neumann)}. 
\end{aligned}
\]

(6.124)

For the equation we are studying, the FEMLAB parameters are

\[
\begin{aligned}
d_a &= \sqrt{\xi^2 - \eta^2}, \\
\alpha &= \beta = \gamma = f = 0, \\
c &= -\frac{1 - \eta^2}{\sqrt{\xi^2 - \eta^2}}, \\
a &= -m^2 \sqrt{\xi^2 - \eta^2}. 
\end{aligned}
\]

(6.125-6.128)

The energies displayed must be scaled due to the values of \( h, c, \) and the particle mass \( \mu. \) These constants are given in eV·Å. For these calculations, \( f = 1 \) and \( \xi \) was varied. The line segment was set to go from -1 to 1, so that a simple correspondence between \( x \) and \( \eta \) could be made. Therefore the calculations must be scaled to correspond with the actual arc length in Å.

The arc length is half of the circumference of an ellipse and can therefore be given by the Gauss-Kummer series expansion

\[
L = \frac{1}{2} \pi (a + b) \sum_{n=0}^{\infty} (0.5 \mid n)^2 \left[ \frac{(a - b)^2}{(a + b)^2} \right]^n,
\]

(6.129)

where \( a \) and \( b \) are the semimajor axes, given by

\[
a = f\xi,
\]

(6.130)
and

\[ b = f \sqrt{\xi^2 - 1}, \quad (6.131) \]

and the binomial coefficient is calculated as

\[ (0.5 \mid n) = \frac{\Gamma \left( \frac{3}{2} \right)}{\Gamma(n+1)\Gamma \left( \frac{3}{2} - n \right)} \quad (6.132) \]

Note that the eccentricity of the cross-sectional ellipse is in fact the inverse of \( \xi \):

\[ e = \frac{f}{a} = \frac{1}{\xi}. \quad (6.133) \]

Because the FEMLAB line segment has a length of two units, the scale factor in the Schrödinger factor becomes

\[
L = \frac{1}{2} \pi f \left( \xi + \sqrt{\xi^2 - 1} \right) \sum_{n=0}^{\infty} (0.5 \mid n)^2 \left[ \frac{(\xi - \sqrt{\xi^2 - 1})^2}{(\xi + \sqrt{\xi^2 - 1})^2} \right]^n.
\]

This series converges very quickly and expands to

\[
L = \frac{1}{2} \pi f \left( \xi + \sqrt{\xi^2 - 1} \right) \left \{ 1 + \frac{1}{4} \left[ \frac{(\xi - \sqrt{\xi^2 - 1})^2}{(\xi + \sqrt{\xi^2 - 1})^2} \right] + \frac{1}{64} \left[ \frac{(\xi - \sqrt{\xi^2 - 1})^2}{(\xi + \sqrt{\xi^2 - 1})^2} \right]^2 + \frac{1}{256} \left[ \frac{(\xi - \sqrt{\xi^2 - 1})^2}{(\xi + \sqrt{\xi^2 - 1})^2} \right]^3 + O(h^4) \right \}.
\]

Because the line segment FEMLAB has length 2, the ratio of the lengths is therefore \( L/2 \). \( f \) has units of length and \( \xi \) is dimensionless, so this is a linear scale factor. Once this factor is used to scale the data, an accurate comparison can be made with the reference material.
6.6 Application of the Shell Method to the Spheroid

Numerical analysis was done for several sets of confocal spheroidal shells with an average z-intercept 100 Å and varying χ. For the numerical runs, the units used were in ε so as to compare with Ref. [5]. For each value of χ, the calculation was made with five different sets of confocal spheroids with different values of d, with constant mean d. The data was fit to the same formula as for the sphere.

The energy ε was then converted to electron Volts via

$$
\epsilon = \frac{2ME}{h^2}. \quad (6.136)
$$

Table 6.1 shows the values of A and B/π² for several spheroids. χ = 2.5 produced an outlier with energies in the proper range but the B coefficient is a factor of 4 too small. All other fits showed B ≈ 1. The values of A are plotted in Figure 6.15.

6.6.1 Spherical limit

The predicted value for the ground state angular energy in the spherical limit is zero, as it was with the finite cylinder. Energies are given in Table 6.2 and shown
Figure 6.11: Plot of $E$ vs. $\chi$ in meV showing the spherical limit
in Figure 6.11. The analytical energies for the sphere are shown in the plot along $\chi = 1$, which is the spherical limit. The error in calculation for the ground state energy is because the raw value of the numerical run was $\varepsilon = 2.5 \times 10^{-5}$, which when scaled to the same radius as the spheroids studied and converted to meV, results in a ground state energy of $-0.9$ meV. Thus at this scale the precision of the method is approximately 1 meV.

6.6.2 Comparison with Ref. [5]

Data values are shown side by side with those of Ref. [5] in Tables 6.2 through 6.4 and plotted in Figure 6.15. A scalar factor unit conversion of $100^2 = 10^4$ was applied to account for the fact that the spheroids calculated used a distance scale of 100 Å while Ref. [5] used a distance scale of 1.
Table 6.2: Energy comparison with Ref. [5]

<table>
<thead>
<tr>
<th>$\chi$</th>
<th>Perturbative $\varepsilon$</th>
<th>Ref. [5]</th>
<th>1D</th>
<th>Shell</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-0.316</td>
<td>-2.225</td>
<td>-2.225</td>
<td>-</td>
</tr>
<tr>
<td>0.2</td>
<td>-0.276</td>
<td>-0.588</td>
<td>-0.588</td>
<td>-</td>
</tr>
<tr>
<td>0.3</td>
<td>-0.226</td>
<td>-0.303</td>
<td>-0.298</td>
<td>-</td>
</tr>
<tr>
<td>0.4</td>
<td>-0.174</td>
<td>-0.197</td>
<td>-0.183</td>
<td>-</td>
</tr>
<tr>
<td>0.5</td>
<td>-0.125</td>
<td>-0.132</td>
<td>-0.106</td>
<td>0.838</td>
</tr>
<tr>
<td>0.6</td>
<td>-0.082</td>
<td>-0.084</td>
<td>-0.047</td>
<td>-</td>
</tr>
<tr>
<td>0.7</td>
<td>-0.047</td>
<td>-0.047</td>
<td>0.000648</td>
<td>-0.228</td>
</tr>
<tr>
<td>0.8</td>
<td>-0.021</td>
<td>-0.021</td>
<td>0.038</td>
<td>-0.119</td>
</tr>
<tr>
<td>0.9</td>
<td>-0.005</td>
<td>-0.005</td>
<td>0.065</td>
<td>-0.275</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0.081</td>
<td>-0.000</td>
</tr>
<tr>
<td>1.1</td>
<td>-0.005</td>
<td>-0.005</td>
<td>0.085</td>
<td>-0.102</td>
</tr>
<tr>
<td>1.2</td>
<td>-0.021</td>
<td>-0.021</td>
<td>0.079</td>
<td>-0.114</td>
</tr>
<tr>
<td>1.3</td>
<td>-0.048</td>
<td>-0.048</td>
<td>0.062</td>
<td>-0.204</td>
</tr>
<tr>
<td>1.4</td>
<td>-0.086</td>
<td>-0.086</td>
<td>0.033</td>
<td>-</td>
</tr>
<tr>
<td>1.5</td>
<td>-0.135</td>
<td>-0.135</td>
<td>-0.007</td>
<td>-0.086</td>
</tr>
<tr>
<td>1.6</td>
<td>-0.194</td>
<td>-0.194</td>
<td>-0.057</td>
<td>-0.055</td>
</tr>
<tr>
<td>1.7</td>
<td>-0.264</td>
<td>-0.264</td>
<td>-0.119</td>
<td>-</td>
</tr>
<tr>
<td>1.8</td>
<td>-0.344</td>
<td>-0.345</td>
<td>-0.191</td>
<td>-</td>
</tr>
<tr>
<td>1.9</td>
<td>-0.436</td>
<td>-0.436</td>
<td>-0.273</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>-0.537</td>
<td>-0.538</td>
<td>-0.366</td>
<td>-</td>
</tr>
<tr>
<td>2.5</td>
<td>-1.203</td>
<td>-1.204</td>
<td>-1.014</td>
<td>-0.400</td>
</tr>
<tr>
<td>3</td>
<td>-2.127</td>
<td>-2.137</td>
<td>-1.854</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>-4.742</td>
<td>-4.929</td>
<td>-4.400</td>
<td>-0.326</td>
</tr>
<tr>
<td>5</td>
<td>-8.369</td>
<td>-9.540</td>
<td>-8.385</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.3: Spheroid Energy Eigenstates for $l = 1, m = 0$

<table>
<thead>
<tr>
<th>$\chi$</th>
<th>Ref. [5]</th>
<th>1-D</th>
<th>Shell</th>
<th>1-D error</th>
<th>Shell error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>0.922352</td>
<td>1.028</td>
<td>1.5</td>
<td>0.106</td>
<td>0.6</td>
</tr>
<tr>
<td>0.7</td>
<td>1.412780</td>
<td>1.577</td>
<td>0.9</td>
<td>0.164</td>
<td>-0.5</td>
</tr>
<tr>
<td>0.8</td>
<td>1.631530</td>
<td>1.825</td>
<td>1.3</td>
<td>0.193</td>
<td>-0.3</td>
</tr>
<tr>
<td>0.9</td>
<td>1.827760</td>
<td>2.049</td>
<td>1.5</td>
<td>0.222</td>
<td>-0.3</td>
</tr>
<tr>
<td>1</td>
<td>2.000000</td>
<td>2.249</td>
<td>1.9</td>
<td>0.249</td>
<td>-0.1</td>
</tr>
<tr>
<td>1.1</td>
<td>2.147690</td>
<td>2.423</td>
<td>2.2</td>
<td>0.275</td>
<td>0.1</td>
</tr>
<tr>
<td>1.2</td>
<td>2.270850</td>
<td>2.572</td>
<td>2.4</td>
<td>0.301</td>
<td>0.1</td>
</tr>
<tr>
<td>1.3</td>
<td>2.369740</td>
<td>2.695</td>
<td>2.5</td>
<td>0.325</td>
<td>0.1</td>
</tr>
<tr>
<td>1.5</td>
<td>2.496940</td>
<td>2.869</td>
<td>3.1</td>
<td>0.372</td>
<td>0.6</td>
</tr>
<tr>
<td>1.6</td>
<td>2.526420</td>
<td>2.920</td>
<td>3.4</td>
<td>0.394</td>
<td>0.9</td>
</tr>
</tbody>
</table>
Figure 6.13: (Color in electronic copy) $|\psi|^2$ for the first three eigenfunctions for an oblate spheroid with $\chi = 0.5$
Figure 6.14: (Color in electronic copy) $|\psi|^2$ for the ground state for a prolate spheroid with $\chi = 4$
6.7 Time-Independent Perturbation Theory Approach

A final look at the spheroid uses the Schrödinger equation for a sphere, and applies the curvature term as a perturbation. This does not account for the spheroid’s shape, just the curvature. Had the spheroidal coordinate Laplace-Beltrami operator been used, the shape would have been accounted for as well. Therefore, in this case, there will still be a deviation in energy as the spheroid deviates from the sphere. However, near the sphere, it should produce close results.

6.7.1 Perturbation using the spheroidal coordinate Schrödinger equation

Ideally, using time-independent perturbation theory assuming that the energy shift due to curvature is a perturbation gives the unperturbed equation system

\[
\frac{d}{d\eta} \left[ \frac{1 - \eta^2}{\sqrt{\xi^2 - \eta^2}} \frac{dS^0}{d\eta} \right] - \left( m^2 - \frac{\sqrt{\xi^2 - \eta^2}}{(\xi^2 - 1)(1 - \eta^2)} \right) S^0 = -f^2 \sqrt{\xi^2 - \eta^2} \varepsilon^0 S^0 \tag{6.137}
\]

and

\[ \Phi = Ae^{im\phi} + Be^{-im\phi} : m \in \mathbb{Z}. \tag{6.138} \]
The perturbation shift is then applied via [23]

\[
\varepsilon^1 = \frac{\xi^2}{4f^4} \langle S^0 | \sqrt{\xi^2 - \eta^2} \left[ \frac{1 - 3\eta^2}{(\xi^2 - \eta^2)^2} - \frac{1}{(\xi^2 - \eta^2)(\xi^2 - 1)} \right]^2 | S^0 \rangle,
\]

(6.139)

where \( S^0 \) is the two-dimensional equation without the curvature, which is the Helmholtz equation

\[
\frac{d^2 S^0}{d\eta^2} + \left[ \frac{\eta}{\xi^2 - \eta^2} - \frac{2\eta}{1 - \eta^2} \right] \frac{dS^0}{d\eta} - m^2 \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)^2} S^0 = -f^2 \xi^2 - \eta^2 \varepsilon^0 S^0 \tag{6.140}
\]

6.7.2 Energy shift due to curvature as a perturbation from a sphere

Rather than use the full spheroidal wave functions as the unperturbed state, it is much simpler to use a sphere. The drawback of this is that it becomes less applicable as the spheroid becomes further from the spherical limit. Nonetheless it produces values very close to those in Ref. [5] for values of \( \chi \) between 0.5 and 1.5.

The effective potential energy due to curvature \( V \) is given by

\[
V = -\frac{\hbar^2}{2m} \left( M^2 - K \right).
\tag{6.141}
\]

For the ground state of a sphere, the wavefunction is constant. The curvature energy shift for an ellipsoidal surface \( \mathcal{M} \) can be taken as a perturbation of a sphere, and is given by the equation

\[
E = -\frac{\hbar^2}{2m A} \iint_{\mathcal{M}} \left( M^2 - K \right) dA,
\tag{6.142}
\]

where \( A \) is the surface area of the surface, \( M \) is the mean curvature, and \( K \) is the Gaussian curvature.

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Furthermore, by the Gauss-Bonnet theorem [29],

$$\int\int_{M} K dA = 2\pi \chi(M),$$  \hspace{1cm} (6.143)

where \(\chi(M)\) is the Euler characteristic of the surface. For a closed genus 0 surface its value is two. This is a topological invariant.

The surface integral of the squared mean curvature is known as the Willmore Energy [30], given by the formula

$$\mathcal{W} = \int\int_{M} M^2 dA.$$ \hspace{1cm} (6.144)

Plugging this into equation gives

$$E = -\frac{\hbar^2}{2mA} (\mathcal{W} - 4\pi).$$  \hspace{1cm} (6.145)

Notice that the Willmore energy is dependent on the embedding. Note also that the Willmore energy is dimensionless and is not an energy in the physical sense. However, when multiplied by the Schrödinger factor and divided by the surface area, physical energy values are obtained.

These values were calculated in Mathematica and compared with Ref. [5]. The results are shown in Table 6.2. Note that more extreme eccentricities show deviation from the analysis. This is likely due to the fact that we are treating the energy shift as a perturbation of the ground state of a sphere, and the curvature potential is significant enough at these values that the perturbation technique begins to break.

The perturbative result raises the question about the applicability of the shell method to constrained quantum mechanics. The formula does follow the results of [1], but the technique appears to have sufficient numerical error that its results are unreliable. The plot also shows that the 1D FEMLAB approach produced similar
results as Ref. [5], and was in fact more accurate than that reference for $\chi = 5$. This suggests that the perturbative technique is still valid to that level of prolateness.

The energy shift for the spheroid is proportional to the Willmore energy minus the integral curvature, and is given by

$$\Delta E = -\frac{\hbar^2 \chi^2 (\chi^2 - 1)^2}{16\pi m E(\pi|\chi^2 - 1|)} \int_0^{2\pi} \int_0^\pi \frac{\sin^6 \theta + 3\chi^4 \sin^4 \theta \cos^2 \theta + 3\chi^2 \sin^2 \theta \cos^4 \theta + \cos^6 \theta}{\chi^6 \sin^6 \theta + 3\chi^4 \sin^4 \theta \cos^2 \theta + 3\chi^2 \sin^2 \theta \cos^4 \theta + \cos^6 \theta} \, d\theta d\phi,$$

where $E(\pi|\chi^2 - 1|)$ is an elliptic integral of the second kind.

These results are very close to Ref. [5], which is expected since it is an equivalent
formulation.

6.8 Conclusions

Unfortunately, the shell method did not produce results with sufficient precision to produce the proper spherical limit. This means that it cannot be used to determine whether the differential geometric method or the method in Ref. [4] is the correct one. Nonetheless, the fact that the differential geometric method can be derived from the Dirac bracket quantization lends support for that method over Ref. [4], and is further supported by the wealth of literature on the differential geometric method.
CHAPTER VII

Analysis of the Triaxial Ellipsoid

In this chapter, the symmetry of the spheroid is further reduced to the most general surface in its family, the triaxial ellipsoid. This surface has not been studied in this context before. First, a formulation in ellipsoidal coordinates [31; 13] is considered. This will be seen to produce an equation for which the Laplace-Beltrami operator is separable but the curvature potential is not. A parameterization in spherical coordinates will then be considered and subjected to numerical study. The shell method will then be considered as it was for the spheroid, and finally the curvature will be treated as a perturbation of a sphere.

The approach of Ref. [2] takes into account the energy shift due to curvature. New first and second fundamental forms must be constructed for the parameterized surface, with a corresponding Laplace-Beltrami Operator tangential to the surface. The mean and Gaussian curvatures are derived, and from these the kinetic energy due to curvature is calculated.
7.1 Ellipsoidal Coordinate Formulation

7.1.1 Fundamental forms and tangential Laplace-Beltrami operator

The parameterization of the ellipsoid with intercepts \((x_0, y_0, z_0)\) is [32]

\[
\mathbf{r} = \begin{pmatrix}
    a \sqrt{a^2 - b^2} \frac{\xi_1^{2} - a^2}{\sqrt{\xi_2^{2} - b^2}} \\
    b \sqrt{a^2 - b^2} \frac{\xi_1^{2} - b^2}{\sqrt{\xi_2^{2} - a^2}} \\
    z_0 \frac{\xi_1^{3}}{ab}
\end{pmatrix}
\]

(7.1)

We begin by calculating the first and second derivatives of the parameterization, from which the rest of the constructs may be derived. The Jacobian of this parameterization is

\[
\mathbf{J} = \pm \begin{pmatrix}
    a \sqrt{a^2 - b^2} \frac{\xi_1^{2} - a^2}{\sqrt{\xi_2^{2} - b^2}} & a \sqrt{a^2 - b^2} \frac{\xi_1^{2} - a^2}{\sqrt{\xi_2^{2} - b^2}} & a \sqrt{a^2 - b^2} \frac{\xi_1^{2} - a^2}{\sqrt{\xi_2^{2} - b^2}} \\
    b \sqrt{a^2 - b^2} \frac{\xi_1^{2} - b^2}{\sqrt{\xi_2^{2} - a^2}} & b \sqrt{a^2 - b^2} \frac{\xi_1^{2} - b^2}{\sqrt{\xi_2^{2} - a^2}} & b \sqrt{a^2 - b^2} \frac{\xi_1^{2} - b^2}{\sqrt{\xi_2^{2} - a^2}} \\
    z_0 \frac{\xi_1^{3}}{ab} & z_0 \frac{\xi_1^{3}}{ab} & z_0 \frac{\xi_1^{3}}{ab}
\end{pmatrix}
\]

(7.2)
and its Hessian matrix is
\[
\mathbf{H} = \pm \begin{bmatrix}
-x_0 \frac{\sqrt{\xi_2^2 - a^2}}{\sqrt{a^2 - b^2}} & x_0 \xi_3 \frac{\sqrt{\xi_2^2 - a^2}}{\sqrt{a^2 - b^2}} & -ax_0 \frac{\sqrt{\xi_2^2 - a^2}}{\sqrt{a^2 - b^2}} \\
- \frac{by_0 \sqrt{\xi_3^2 - b^2}}{\sqrt{a^2 - b^2} \xi_2^2 - b^2)} & \frac{by_0 \xi_2 \xi_3}{\sqrt{a^2 - b^2} \xi_2^2 - b^2)} & 0 \\
0 & \frac{\xi_0}{ab} & 0
\end{bmatrix}.
\]  

(7.3)

Its metric tensor is then found to be
\[
g_{ij} = \begin{bmatrix}
\frac{(z_0^2 - \xi_2^2)(z_0^2 - \xi_3^2)}{(a^2 - \xi_2^2)(\xi_2^2 - b^2)} & 0 & 0 \\
0 & \frac{(z_0^2 - \xi_2^2)(\xi_2^2 - \xi_3^2)}{(a^2 - \xi_2^2)(b^2 - \xi_3^2)} & 0 \\
0 & 0 & \frac{\xi_0}{ab}
\end{bmatrix}.
\]  

(7.4)

This metric is orthogonal as is expected. It has the metric discriminant
\[
g = \frac{(z_0^2 - \xi_2^2)(z_0^2 - \xi_3^2)(\xi_2^2 - \xi_3^2)^2}{(a^2 - \xi_2^2)(\xi_2^2 - b^2)(a^2 - \xi_2^2)(b^2 - \xi_3^2)}.
\]  

(7.5)

The surface-tangent portion of the Laplace-Beltrami operator is [2]
\[
\mathcal{D}[\chi_t(\xi_2, \xi_3)] = \sqrt{(a^2 - \xi_2^2)(\xi_2^2 - b^2)} \frac{\xi_0}{\xi_2^2 - \xi_3^2} \frac{\sqrt{a^2 - \xi_2^2}(\xi_2^2 - b^2)}{\xi_2^2 - \xi_3^2} \frac{\partial_2}{\sqrt{z_0^2 - \xi_2^2}} \frac{\partial_2 \chi_t}{\partial_2 \chi_t} + \sqrt{(a^2 - \xi_2^2)(b^2 - \xi_3^2)} \frac{\xi_0}{\xi_2^2 - \xi_3^2} \frac{\xi_0}{\xi_2^2 - \xi_3^2} \frac{\sqrt{a^2 - \xi_2^2}(b^2 - \xi_3^2)}{\xi_2^2 - \xi_3^2} \frac{\partial_3 \chi_t}{\partial_3 \chi_t}.
\]  

(7.6)

The surface normal vector is [33]
\[
n = \pm \frac{\frac{x}{x_0}, \frac{y}{y_0}, \frac{z}{z_0}}{\sqrt{\frac{x^2}{z_0^2} - \frac{x^2}{x_0} - \frac{y^2}{y_0}}}
\]  

\[
= \pm \frac{\sqrt{\xi_2^2 - a^2} \frac{\sqrt{\xi_3^2 - a^2}}{a^2 - b^2} - \frac{\xi_2^2}{a^2} - \frac{\xi_3^2}{b^2}}{\sqrt{\xi_2^2 a^2 + \frac{(\xi_2^2 - a^2)(\xi_2^2 - a^2)}{a^2 - b^2} - \frac{(\xi_3^2 - b^2)(\xi_3^2 - b^2)}{b^2 - a^2}}}
\]  

(7.7)

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For brevity we denote the normalizing factor of the normal vector as the quantity

\[ N = ab\sqrt{a^2 - b^2} \sqrt{\frac{\xi_2^2\xi_3^2}{a^2b^2} + \frac{(\xi_2^2 - a^2)(\xi_3^2 - a^2)}{a^2(a^2 - b^2)}} - \frac{(\xi_2^2 - b^2)(\xi_3^2 - b^2)}{b^2(a^2 - b^2)} \]

\[ = \sqrt{\xi_2^2\xi_3^2(a^2 - b^2) - b^2(\xi_2^2 - a^2)(\xi_3^2 - a^2) - a^2(\xi_2^2 - b^2)(\xi_3^2 - b^2)}, \quad (7.8) \]

which shortens equations considerably. The scale factor at the beginning is to simplify calculations further.

The second fundamental form is

\[ h_{22} = -\frac{x_0y_0z_0}{\sqrt{\xi_2^2 - z_0^2\sqrt{\xi_3^2}} - z_0^2 [\xi_2^2(\xi_2^2 - a^2 - b^2) - a^2b^2]}, \quad (7.9) \]

\[ h_{23} = h_{32} = 0, \quad (7.10) \]

\[ h_{33} = \frac{x_0y_0z_0}{\sqrt{\xi_3^2 - z_0^2\sqrt{\xi_2^2}} - z_0^2 [\xi_3^2(\xi_3^2 + a^2 + b^2) - a^2b^2]}, \quad (7.11) \]

To attempt to clean these up more, we now focus on the denominator term,

\[ \xi_i^2 \left[ \xi_i^2 \mp (a^2 + b^2) \right] - a^2b^2 = \xi_i^4 \mp \xi_i^2(a^2 + b^2) - a^2b^2. \quad (7.12) \]

Letting \( u_i = \xi_i^2 \) gives

\[ u_i^2 \mp (a^2 + b^2)u_i - a^2b^2. \quad (7.13) \]

This has the four solutions

\[ u_2 = \xi_2^2 = \frac{a^2 + b^2}{2} \pm \frac{1}{2} \sqrt{(a^2 + b^2)^2 - 4a^2b^2}, \quad (7.14) \]

and

\[ u_3 = \xi_3^2 = -\frac{a^2 + b^2}{2} \pm \frac{1}{2} \sqrt{(a^2 + b^2)^2 - 4a^2b^2}. \quad (7.15) \]
Letting
\[ D_{\pm} = \frac{a^2 + b^2 \pm (a^2 - b^2)}{2} = \begin{cases} a^2, & +, \\ b^2, & -, \end{cases} \] (7.16)
then equation (7.12) may be written
\[ \xi_i^2 [\xi_i^2 \mp (a^2 + b^2)] - a^2 b^2 = (\xi_i^2 \mp a^2)(\xi_i^2 \mp b^2). \] (7.17)

The second fundamental form is therefore
\[ h_{22} = -\frac{x_0 y_0 z_0}{\sqrt{z_0^2 - \xi_2^2 + \sqrt{z_0^2 - \xi_3^2} a^2 - \xi_2^2}} a^2(\xi_2^2 - b^2), \] (7.18)
\[ h_{23} = h_{32} = 0, \] (7.19)
\[ h_{33} = -\frac{x_0 y_0 z_0}{\sqrt{z_0^2 - \xi_2^2 + \sqrt{z_0^2 - \xi_3^2} a^2 + \xi_3^2}} b^2(\xi_3^2 + \xi_2^2). \] (7.20)
The determinant is
\[ h = \frac{x_0^2 y_0^2 z_0^2 (\xi_2^2 - \xi_3^2)^2}{(z_0^2 - \xi_2^2)(z_0^2 - \xi_3^2)(a^2 - \xi_2^2)(\xi_2^2 - b^2)(a^2 + \xi_3^2)(b^2 + \xi_2^2)}. \] (7.21)

We now have all the components necessary to calculate the potential due to curvature and the Schrödinger equation.

### 7.1.2 Calculation of mean and Gaussian curvature

The mean curvature can be calculated in several ways, the simplest of which is [2]
\[ M = \frac{1}{2g} (g_{22} h_{33} + g_{33} h_{22} - 2g_{23} h_{23}) = \frac{g_{22} h_{33} + g_{33} h_{22}}{2g}. \] (7.22)
Expanding in all terms gives

\[
M = -\frac{(\xi_0^2-\xi_2^2)(\xi_2^2-\xi_3^2)}{(a^2-\xi_2^2)(\xi_2^2-b^2)} \frac{x_0 y_0 z_0}{\xi_2^2} \frac{\xi_2^2-\xi_3^2}{\xi_2^2-\xi_3^2} \frac{1}{(a^2+\xi_3^2)(b^2+\xi_3^2)}
\]

\[
-\frac{2}{(a^2-\xi_2^2)(\xi_2^2-b^2)} \frac{(z^2_0-\xi_2^2)(\xi_2^2-\xi_3^2)}{(a^2+\xi_3^2)(b^2+\xi_3^2)} \frac{x_0 y_0 z_0}{\xi_2^2} \frac{\xi_2^2-\xi_3^2}{\xi_2^2-\xi_3^2} \frac{1}{(a^2+\xi_3^2)(b^2+\xi_3^2)}
\]

\[
(7.23)
\]

This further simplifies to

\[
M = -\frac{x_0 y_0 z_0}{2\sqrt{z^2_0 - \xi_2^2} \sqrt{z^2_0 - \xi_3^2}} \left( \frac{1}{z^2_0 - \xi_2^2} + \frac{1}{(z^2_0 - \xi_3^2)} \frac{(a^2 - \xi_3^2)(b^2 - \xi_3^2)}{(a^2 + \xi_3^2)(b^2 + \xi_3^2)} \right). \quad (7.24)
\]

The Gaussian curvature can be calculated via the fundamental forms as [33]

\[
K = \frac{h}{g} = \frac{x_0^2 y_0^2 z_0^2 (\xi_2^2 - \xi_3^2)^2}{(z^2_0 - \xi_2^2)(z^2_0 - \xi_3^2)(a^2 - \xi_3^2)(b^2 - \xi_3^2)(a^2+\xi_3^2)(b^2+\xi_3^2)}
\]

\[
= \frac{\xi_0^2 y_0^2 z_0^2}{(z^2_0 - \xi_2^2)(z^2_0 - \xi_3^2)^2} \frac{(a^2 - \xi_3^2)(b^2 - \xi_3^2)}{(a^2 + \xi_3^2)(b^2 + \xi_3^2)}. \quad (7.25)
\]

Ref. [34] gives the equivalent Cartesian coordinate form

\[
K = \frac{1}{x^2_0 y^2_0 z^2_0} \left( \frac{x^2}{x^2_0} + \frac{y^2}{y^2_0} + \frac{z^2}{z^2_0} \right)^{-2}. \quad (7.26)
\]

Combined with the mean curvature, the effective energy potential due to curvature is

\[
V = -\frac{\hbar^2}{8m} \frac{x_0^2 y_0^2 z_0^2}{(z^2_0 - \xi_2^2)(z^2_0 - \xi_3^2)} \left( \frac{1}{z^2_0 - \xi_2^2} - \frac{1}{(z^2_0 - \xi_3^2)} \frac{(a^2 - \xi_3^2)(b^2 - \xi_3^2)}{(a^2 + \xi_3^2)(b^2 + \xi_3^2)} \right)^2. \quad (7.27)
\]

Letting

\[
v(\xi_2) = \frac{1}{z^2_0 - \xi_2^2}. \quad (7.28)
\]

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$w(\xi_3) = \frac{1}{z_0^2 - \xi_3^2} \frac{(a^2 - \xi_3^2)(b^2 - \xi_3^2)}{(a^2 + \xi_3^2)(b^2 + \xi_3^2)}$, \hspace{1cm} (7.29)

$C = -\frac{\hbar^2}{8m} x_0^2 y_0^2 z_0^2$, \hspace{1cm} (7.30)

then

\begin{align*}
V &= C \frac{(v + w)^2 - 4vw}{(z_0^2 - \xi_2^2)(z_0^2 - \xi_3^2)} \\
&= C \frac{v^2 - 2vw + w^2}{(z_0^2 - \xi_2^2)(z_0^2 - \xi_3^2)} \\
&= C \frac{(v(\xi_2) - w(\xi_3))^2}{(z_0^2 - \xi_2^2)(z_0^2 - \xi_3^2)}. \hspace{1cm} (7.31)
\end{align*}

Figure 7.2 shows a four-view plot of $M^2 - K$ for an ellipsoid with $x_0 = 1, y_0 = 1.5, z_0 = 2$. 

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7.1.3 Formulation of the Schrödinger equation

The curved-surface Schrödinger equation is [2]

\[-\frac{\hbar^2}{2m} \{\mathcal{D} - (M^2 - K)\} \chi_t(\xi_2, \xi_3) = E\chi_t(\xi_2, \xi_3). \tag{7.32}\]

Filling in the fundamental forms and potential gives

\[
\sqrt{(a^2 - \xi_2^2)(\xi_2^2 - b^2)} \left( \frac{\sqrt{(a^2 - \xi_2^2)(\xi_2^2 - b^2)}}{(\xi_2^2 - \xi_3^2)\sqrt{z_0^2 - \xi_2^2}} \partial_2 \right) \left[ \frac{\sqrt{(a^2 - \xi_2^2)(\xi_2^2 - b^2)}}{(\xi_2^2 - \xi_3^2)\sqrt{z_0^2 - \xi_2^2}} \partial_2 \chi_t \right] 
+ \sqrt{(a^2 - \xi_3^2)(b^2 - \xi_3^2)} \left( \frac{\sqrt{(a^2 - \xi_3^2)(b^2 - \xi_3^2)}}{(\xi_2^2 - \xi_3^2)\sqrt{z_0^2 - \xi_3^2}} \partial_3 \chi_t \right) 
+ \frac{x_0^2 y_0^2 z_0^2}{4(z_0^2 - \xi_2^2)(z_0^2 - \xi_3^2)} \left( \frac{1}{z_0^2 - \xi_2^2} \right) \chi_t + \frac{2mE}{\hbar^2} \chi_t = 0. \tag{7.33}\]

This equation is not separable. Furthermore, only one octant of the ellipsoid may be described by this equation, leading to a problem of determining initial boundary conditions. Therefore the curvature term must be considered as a perturbation, or another parameterization is required. The latter will be tried first.

7.2 Longitude-Colatitude Coordinate Formulation

It was found that parameterizing the triaxial ellipsoid in angular coordinates $(\phi, \theta) \in [0, 2\pi] \otimes [0, \pi]$ eliminates the boundary condition problem, in that the full ellipsoid can be described with one partial differential equation. However, this parameterization does not have an orthogonal metric, which makes the Laplace-Beltrami operator more complex due to the presence of cross terms. Furthermore, the resulting Schrödinger equation is not separable. However, the potential energy term for the Schrödinger equation is not separable in ellipsoidal coordinates, either. Therefore
the angular presents itself as a potential contender for two-dimensional numerical analysis.

The parameterization for a triaxial ellipsoid with semimajor axes $x = x_0$, $y = y_0$, and $z = z_0$ is \([35]\)

$$
\mathbf{r} = \begin{bmatrix}
  x_0 \sin \theta \cos \phi \\
  y_0 \sin \theta \sin \phi \\
  z_0 \cos \theta
\end{bmatrix}.
$$

(7.34)

A plot of this surface is shown in Figure 7.1.

Its Jacobian matrix is

$$
\frac{\partial(x, y, z)}{\partial(\phi, \theta)} = \begin{bmatrix}
  -x_0 \sin \theta \sin \phi & x_0 \cos \theta \cos \phi \\
  y_0 \sin \theta \cos \phi & y_0 \cos \theta \sin \phi \\
  0 & -z_0 \sin \theta
\end{bmatrix}.
$$

(7.35)

This produces the metric tensor

$$
g_{\phi\phi} = \left[ x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi \right] \sin^2 \theta, \quad (7.36)
$$

$$
g_{\theta\theta} = \cos^2 \theta \left[ x_0^2 \cos^2 \phi + y_0^2 \sin^2 \phi + z_0^2 \tan^2 \theta \right], \quad (7.37)
$$

$$
g_{\phi\theta} = g_{\theta\phi} = \frac{y_0^2 - x_0^2}{4} \sin 2\theta \sin 2\phi. \quad (7.38)
$$

Its determinant is

$$
g = \left[ x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi \right] \sin^2 \theta \left[ x_0^2 \cos^2 \phi + y_0^2 \sin^2 \phi \right] \cos^2 \theta + z_0^2 \sin^2 \theta \\
-\frac{(y_0^2 - x_0^2)^2}{16} \sin^2 2\theta \sin^2 2\phi. \quad (7.39)
$$
This can be rewritten as
\[
g = \frac{x_0^2 y_0^2 \tan^6 \phi + (x_0^2 + y_0^2)^2 \tan^4 \theta - x_0^2 y_0^2 \tan^2 \theta + z_0^2 (1 + \tan^2 \theta)^4 \sin^2 \theta}{(1 + \tan^2 \theta)^4}. \tag{7.40}
\]

Using this the upstairs metric is
\[
g^{\theta \theta} = \frac{[x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi] \sin^2 \theta (1 + \tan^2 \theta)^4}{x_0^2 y_0^2 \tan^6 \phi + (x_0^2 + y_0^2)^2 \tan^4 \theta - x_0^2 y_0^2 \tan^2 \theta + z_0^2 (1 + \tan^2 \theta)^4 \sin^2 \theta}, \tag{7.41}
\]
\[
g^{\phi \phi} = \frac{[x_0^2 \cos^2 \phi + y_0^2 \sin^2 \phi + z_0^2 \tan^2 \theta] (1 + \tan^2 \theta)^4 \cos^2 \theta}{x_0^2 y_0^2 \tan^6 \phi + (x_0^2 + y_0^2)^2 \tan^4 \theta - x_0^2 y_0^2 \tan^2 \theta + z_0^2 (1 + \tan^2 \theta)^4 \sin^2 \theta}, \tag{7.42}
\]
and
\[
g^{\phi \theta} = -\frac{(y_0^2 - x_0^2) \sin 2 \theta \sin 2 \phi (1 + \tan^2 \theta)^4}{4 \left[ x_0^2 y_0^2 \tan^6 \phi + (x_0^2 + y_0^2)^2 \tan^4 \theta - x_0^2 y_0^2 \tan^2 \theta + z_0^2 (1 + \tan^2 \theta)^4 \sin^2 \theta \right]}.	ag{7.43}
\]

The non-normalized normal vector is
\[
N = \begin{bmatrix}
y_0 z_0 \sin^2 \theta \cos \phi \\
x_0 z_0 \sin^2 \theta \sin \phi \\
\frac{1}{2} x_0 y_0 \sin 2 \theta
\end{bmatrix}. \tag{7.44}
\]

Its norm is
\[
N = \left[ z_0^2 \sin^4 \theta \left( x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi \right) + \frac{x_0^2 y_0^2}{4} \sin^2 2 \theta \right]^{1/2}. \tag{7.45}
\]

The unit normal vector is therefore
\[
n = \left[ z_0^2 \sin^4 \theta \left( x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi \right) + \frac{x_0^2 y_0^2}{4} \sin^2 2 \theta \right]^{-1/2} \begin{bmatrix}
y_0 z_0 \sin^2 \theta \cos \phi \\
x_0 z_0 \sin^2 \theta \sin \phi \\
\frac{1}{2} x_0 y_0 \sin 2 \theta
\end{bmatrix}. \tag{7.46}
\]
The second derivatives of the parameterization are

\[
\frac{\partial^2 r}{\partial \phi^2} = \begin{bmatrix}
-x_0 \sin \theta \cos \phi \\
-y_0 \sin \theta \sin \phi \\
0
\end{bmatrix}, \quad (7.47)
\]

\[
\frac{\partial^2 r}{\partial \phi \partial \theta} = \begin{bmatrix}
-x_0 \cos \theta \sin \phi \\
y_0 \cos \theta \cos \phi \\
0
\end{bmatrix}, \quad (7.48)
\]

and

\[
\frac{\partial^2 r}{\partial \theta^2} = \begin{bmatrix}
-x_0 \sin \theta \cos \phi \\
-y_0 \sin \theta \sin \phi \\
-z_0 \cos \theta
\end{bmatrix}. \quad (7.49)
\]

Dotting these with the normal vector gives the components of the second fundamental form:

\[
h_{\phi\phi} = -\frac{x_0 y_0 z_0 \tan^2 \theta}{z_0^2 \tan^2 \theta \left( x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi \right) + x_0^2 y_0^2} \tan^2 \theta, \quad (7.50)
\]

\[
h_{\phi\theta} = 0, \quad (7.51)
\]

and

\[
h_{\theta\theta} = -\frac{x_0 y_0 z_0}{\cos \theta \left[ z_0^2 \tan^2 \theta \left( x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi \right) + x_0^2 y_0^2 \right]^{1/2}} \tan^2 \theta. \quad (7.52)
\]

The fact that \(h_{\phi\theta} = 0\) indicates that these coordinates may not be orthogonal but they are conjugate.

Its determinant is

\[
h = -\frac{x_0^2 y_0^2 z_0^2 \tan^2 \theta}{\cos \theta \left[ z_0^2 \tan^2 \theta \left( x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi \right) + x_0^2 y_0^2 \right]^{1/2}}. \quad (7.53)
\]
The Gaussian curvature is therefore

\[
K = \frac{x_0^2 y_0^2 z_0^2 \tan^2 \theta (1 + \tan^2 \theta)^4}{\cos \theta \left[ z_0^2 \tan^2 \theta \left( x_0^2 \sin^2 \phi + y_0^2 \cos^2 \phi \right) + x_0^2 y_0^2 \right]^4} \times \frac{1}{\left[ x_0^2 y_0^2 \tan^6 \phi + (x_0^2 + y_0^2)^2 \tan^4 \theta - x_0^2 y_0^2 \tan^2 \theta + z_0^2 (1 + \tan^2 \theta)^4 \sin^2 \theta \right]}.
\]

(7.54)

The mean curvature and Laplace-Beltrami operators are very long formulas best implemented in a computer from the metric and second fundamental form.

Using the prolate spheroid as an example, we can establish the following mixed boundary conditions: periodic conditions in \( \phi \),

\[
\sigma(\phi', \theta) = \sigma(\phi' + 2\pi, \theta),
\]

(7.55)

\[
\frac{\partial \sigma}{\partial \phi} \bigg|_{\phi=\phi'} = \frac{\partial \sigma}{\partial \phi} \bigg|_{\phi=\phi'+2\pi},
\]

(7.56)

and Dirichlet conditions on \( \theta \),

\[
\sigma(\phi, \pi) = \pm \sigma(\phi, 0) \neq 0,
\]

(7.57)

and

\[
\frac{\partial \sigma}{\partial \theta} \bigg|_{\theta=0} = - \frac{\partial \sigma}{\partial \theta} \bigg|_{\theta=\pi},
\]

(7.58)

FEMLAB runs were attempted for \((x_0, y_0, z_0) = (1, 1, 1)\) (a sphere), \((x_0, y_0, z_0) = (1, 1, 2)\) (a prolate spheroid), and \((x_0, y_0, z_0) = (1, 1.5, 2)\) (a triaxial ellipsoid). However, none of the results appeared satisfactory enough to explore further. Therefore another method was tried.
Table 7.1: Ellipsoid energy levels using the shell method

| $\chi_1$ | $\chi_2$ | $|\chi|$ | $\varepsilon_{00}$ | $\varepsilon_{10}$ | $\varepsilon_{11}$ |
|----------|----------|----------|-----------------|-----------------|-----------------|
| 1        | 1        | 1.000000 | −0.3            | 1.9             | 1.9             |
| 0.9      | 1.1      | 1.004988 | −0.1            | 1.9             | 2.0             |
| 0.8      | 1.2      | 1.019804 | 0.0             | 1.9             | 2.0             |
| 1.1      | 1.2      | 1.151086 | −0.2            | 2.1             | 2.3             |
| 1.2      | 1.3      | 1.251000 | −0.1            | 2.5             | 2.8             |
| 1.5      | 2        | 1.767767 | 0.3             | 1.1             | 1.3             |

7.3 Shell Method

The shell method explored using the spheroid was applied to the triaxial ellipsoid. The method applied was identical to that of the spheroid, except for the geometry. The method was calibrated to within one meV for the sphere, so that must be taken into consideration. The results are tabulated in Table 7.1. An ellipsoid has not one but two independent values of $\chi$; one for the $xz$-axis, and one for the $xy$-axis. A third $\chi$ may be calculated from the other two for the $yz$-axis. We will name the two independent ones $\chi_1$ and $\chi_2$.

From Table 7.1, it can be seen that the precision for this method was poor, giving a ground state energy of $\varepsilon = −0.3$ for the sphere, which should have a zero value. This is from the sphere’s calculation where the raw value was $\varepsilon = 2.5 \times 10^{-5}$. Multiplying it by $10^4$ to account for unit radius as opposed to a radius of 100 Å accounts for this disparity from zero.

7.4 Time-Independent Perturbation Approach

Finally, time-independent perturbation theory is applied to the ellipsoid. The unperturbed state is considered to be a sphere, and the curvature term is applied. Since this formulation only considers the effect of curvature and not the effect of the shape of the ellipsoid, only states near the sphere are considered.
Table 7.2: Perturbative $\varepsilon$ for ellipsoids near spherical limit

<table>
<thead>
<tr>
<th>$\chi_1$</th>
<th>0.7</th>
<th>0.8</th>
<th>0.9</th>
<th>$\chi_2$</th>
<th>1.0</th>
<th>1.1</th>
<th>1.2</th>
<th>1.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>-0.093</td>
<td>-0.092</td>
<td>-0.103</td>
<td>-0.126</td>
<td>-0.164</td>
<td>-0.219</td>
<td>-0.294</td>
<td></td>
</tr>
<tr>
<td>0.6</td>
<td>-0.064</td>
<td>-0.058</td>
<td>-0.062</td>
<td>-0.079</td>
<td>-0.109</td>
<td>-0.155</td>
<td>-0.219</td>
<td></td>
</tr>
<tr>
<td>0.7</td>
<td>-0.046</td>
<td>-0.034</td>
<td>-0.033</td>
<td>-0.043</td>
<td>-0.067</td>
<td>-0.105</td>
<td>-0.160</td>
<td></td>
</tr>
<tr>
<td>0.8</td>
<td>-0.038</td>
<td>-0.021</td>
<td>-0.014</td>
<td>-0.019</td>
<td>-0.036</td>
<td>-0.068</td>
<td>-0.115</td>
<td></td>
</tr>
<tr>
<td>0.9</td>
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<td>-0.017</td>
<td>-0.005</td>
<td>-0.005</td>
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<td>-0.041</td>
<td>-0.081</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>-0.051</td>
<td>-0.023</td>
<td>-0.006</td>
<td>0.000</td>
<td>-0.006</td>
<td>-0.025</td>
<td>-0.059</td>
<td></td>
</tr>
<tr>
<td>1.1</td>
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<td>-0.038</td>
<td>-0.016</td>
<td>-0.005</td>
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<td>-0.046</td>
<td></td>
</tr>
<tr>
<td>1.2</td>
<td>-0.101</td>
<td>-0.062</td>
<td>-0.035</td>
<td>-0.018</td>
<td>-0.014</td>
<td>-0.022</td>
<td>-0.043</td>
<td></td>
</tr>
<tr>
<td>1.3</td>
<td>-0.139</td>
<td>-0.110</td>
<td>-0.062</td>
<td>-0.040</td>
<td>-0.031</td>
<td>-0.033</td>
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<td></td>
</tr>
<tr>
<td>1.4</td>
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<td>-0.136</td>
<td>-0.098</td>
<td>-0.071</td>
<td>-0.055</td>
<td>-0.053</td>
<td>-0.063</td>
<td></td>
</tr>
<tr>
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<td>-0.089</td>
<td>-0.081</td>
<td>-0.086</td>
<td></td>
</tr>
</tbody>
</table>

The surface area of an ellipsoid with semimajor axes $a$, $b$, and $c$, is given by [35]

$$S = 2\pi \left[ c^2 + \frac{bc^2 \theta}{\sqrt{a^2 - c^2}} + b\sqrt{a^2 - c^2} E(\text{am}(\theta)|k) \right]. \quad (7.59)$$

This value will be needed for normalizing the perturbation energy shift more accurately than using the average of the semimajor axes as the radius of a sphere and using the surface area of that sphere.

The Willmore energy for an ellipsoid is a very complicated function and was calculated using a computer algebra system. This result was converted into MATLAB code and integrated over the surface using Simpson’s rule twice. Some of the results are given in Table 7.2. This table has values of $\varepsilon$ which is given in units where $\hbar^2/2m = 1$.

It can be clearly seen from Table 7.2 and Figure 7.3 that the curvature energy shift goes to zero in the spherical limit $\chi_1 = \chi_2 = 1$. The energy is quadratic with various values of $\chi_1$ and $\chi_2$. Its maximum is zero at the spherical limit, and is lowest when $\chi_1 \gg 1$ and $\chi_2 \ll 1$ or vice versa.
Figure 7.3: Perturbative $\varepsilon$ for the triaxial ellipsoid for various values of $\chi_1$ and $\chi_2$
7.4.1 Application of the perturbation

The energy shift due to the perturbation is

\[ \varepsilon_1 = \frac{x_0^2 y_0^2 z_0^2}{4} \langle \psi^0 \mid \left\{ \frac{1}{z_0^2 - \xi_2^2} - \frac{1}{\xi_3^2} \left[ \frac{1}{z_0^2 - \xi_2^2} - \frac{1}{\xi_3^2} \frac{(a^2 - \xi_3^2)(b^2 - \xi_3^2)}{(a^2 + \xi_3^2)(b^2 + \xi_3^2)} \right]^2 \right\} \mid \psi^0 \rangle. \]

(7.60)

This is the integral

\[ \varepsilon_1 = \frac{x_0^2 y_0^2 z_0^2}{4} \int_b^a \left\{ \left( A e^{\sqrt{\lambda_2 + \xi_2}} + B e^{\sqrt{\lambda_2 - \xi_2}} \right)^2 \int_0^b \left\{ \left( C e^{\sqrt{\lambda_3 + \xi_3}} + D e^{\sqrt{\lambda_3 - \xi_3}} \right)^2 \left( \frac{1}{z_0^2 - \xi_2^2} - \frac{1}{\xi_3^2} \left[ \frac{1}{z_0^2 - \xi_2^2} - \frac{1}{\xi_3^2} \frac{(a^2 - \xi_3^2)(b^2 - \xi_3^2)}{(a^2 + \xi_3^2)(b^2 + \xi_3^2)} \right]^2 \right\} d\xi_3 \right\} d\xi_2 \].

(7.61)

This integral was evaluated numerically using MATLAB. A contour plot of the results are plotted in Figure 7.3.

7.5 Conclusions

This analysis shows several difficulties with the triaxial ellipsoid. Ellipsoidal coordinates produce a separable Laplace-Beltrami operator but the curvature term is not separable. The spherical coordinate parameterization is complicated and nonseparable, and further does not lend itself well to numerical analysis. The shell method produces low-precision results while simultaneously being computationally expensive. Finally, the perturbation approach produces acceptable results but is limited to small eccentricities. However, it can be shown using the first three methods that the particle tends to be isolated towards the areas of low curvature, and all show that the energy shift becomes greater as the eccentricity increases.
CHAPTER VIII

Conclusions

This thesis has studied various methods of quantization on curved surfaces, and paid heavy emphasis on the differential geometric method (Refs. [2; 3]) and on the shell method (Ref. [1]). Unfortunately, the results of the shell method were not precise enough to determine more than a single digit of accuracy, and therefore no direct conclusion can be made regarding which of the various methods is the correct method. However, the following can be said about the approaches studied.

The differential geometric approach was found in Ref. [11] to be equivalent to the Dirac bracket formalism using certain constraints in the latter formalism. This lends support to this method, as does its ability to produce the angular momentum operator in the spherical limit. However, it often leads to nonseparable equations which must be solved by various means, such as numerical methods or perturbation theory. In addition, the equations are prone to singularities that make numerical analysis problematic and sensitive.

The method of setting the surface normal wavefunction and associated coordinate to constants produces positive eigenvalues but does not appear to be consistent with the differential geometric or perturbative methods except for the case of the sphere. Energy shifts are positive for the spheroid, similar to the shell method.

The shell method does not have the singularities present, but requires several finite
element runs with a high number of elements, resulting in very slow and cumbersome calculations. This method is also prone to statistical error during the quadratic fit of the data. However, despite this lack of precision, this method has a coarse correlation with the differential geometric method for excited states. But the ground state for this method is approximately zero for both the spheroid and finite cylinder, which tends to support the method of setting one of the separated wavefunctions constant.

The perturbation method produces results that closely match the differential geometric approach, but the applicability of this method is limited to a smaller domain. However, these results match most closely because the differential geometric approach was used in determining the perturbation. Therefore it is not a formulation but a method of solving the Schrödinger equation once it is derived.

Overall, the equations were much more difficult to solve than anticipated. The singularities for the spheroid, lack of separability for the ellipsoid, and ground state energy for the shell method produced numerous complications. Taken as a whole, the Dirac formalism and shell methods tend to support the differential geometric method for the spheroid, while the method of Ref. [4] is in general disagreement with the other three methods other than the ground state. Despite that, the overall strongest argument is that the differential geometric method is the correct method for quantization on curved surfaces. However, more research is needed on the unresolved issues uncovered herein.
APPENDICES
APPENDIX A

Transformation Properties of the First and Second Fundamental Forms for Orthogonal Coordinates under Conformal Mappings

This section uses more rigor than in previous sections in order to derive the transformation properties of the first and second fundamental forms and their determinants.

A.1 Definitions of the System

Remark A.1. The Einstein summation convention is used throughout this section.

Definition A.2. Let $S \subset \mathbb{R}^2$ be a surface embedded in $\mathbb{R}^3$.

Definition A.3. Let $\mathcal{M} \subset S$ be a basis on $S$.

Definition A.4. Let $\mathcal{N} \subset S$ be a basis on $S$.

Definition A.5. Let $\mathbf{x} := (x^1, x^2, x^3) : x^i \in \mathbb{R}$ be the lengths along the Cartesian coordinate axes in $\mathbb{R}^3$. 
Definition A.6. Let \( u := (u^1, u^2) : u^i \in \mathbb{R}, u^i \in \mathcal{M} \) be the lengths along the basis vectors in the \( \mathcal{M} \) basis.

Definition A.7. Let \( v := (v^1, v^2) : v^i \in \mathbb{R}, v \in \mathcal{N} \) be the lengths along basis vectors in the \( \mathcal{N} \) basis.

Definition A.8. Let \( R : \mathbb{R}^3 \to \mathcal{M} ; R = x(u) \) be a parametrization of \( S \) in the \( \mathcal{M} \) basis.

Definition A.9. Let \( S : \mathbb{R}^3 \to \mathcal{N} ; S = x(v) \) be a parametrization of \( S \) in the \( \mathcal{N} \) basis.

Definition A.10. Let \( R^{-1} : \mathcal{M} \to \mathbb{R}^3 ; R^{-1} = u(x) \) be the pullback of \( R \).

Definition A.11. Let \( S^{-1} : \mathcal{N} \to \mathbb{R}^3 ; S^{-1} = v(x) \) be the pullback of \( S \).

Definition A.12. Let \( C : \mathcal{M} \to \mathcal{N} ; C = u(v) \) be a coordinate chart mapping points on \( \mathcal{M} \) to points on \( \mathcal{N} \).

Definition A.13. Let \( C^{-1} : \mathcal{N} \to \mathcal{M} ; C^{-1} = v(u) \) be the pullback of \( C \).

Remark A.14. The following diagram commutes.

\[
\begin{array}{ccc}
\mathbb{R}^3 & \xrightarrow{R} & \mathcal{M} \\
\downarrow{\mathcal{S}} & & \downarrow{C} \\
\mathcal{N} & \xrightarrow{C^{-1}} & \mathcal{M}
\end{array}
\]

Definition A.15. Denote the partial derivative in \( \mathcal{M} \) by \( \partial_j f = \frac{\partial f}{\partial u^j} \).

Definition A.16. Denote the partial derivative in \( \mathcal{N} \) by \( \partial'_j f = \frac{\partial f}{\partial v^j} \).

Definition A.17. Let \( \nabla \) be the gradient operator in \( \mathcal{M} \).

Definition A.18. Let \( \nabla' \) be the gradient operator in \( \mathcal{N} \).
Definition A.19. The Jacobian matrix of $C$ is given by $J = J_j^i = \partial_j^i u^i$.

Definition A.20. Let $J = \det J$ be the determinant of the Jacobian matrix of $C$.

Definition A.21. Let $J_{C^{-1}}$ be the Jacobian matrix of $C^{-1}$.

Definition A.22. Let $J^{-1}$ be the inverse of the Jacobian matrix of $C$.

Lemma A.23. $J_{C^{-1}} (C(p)) = J^{-1}(p) : \forall p \in \mathcal{M}$. (A.1)

Proof. This is the inverse function theorem. See Ref. [36] for details.


Proof. $J = J_j^i = \partial_j^i u^i = \partial_j^i u^j = J_i^j = J^T$.

Lemma A.25. Then $\partial_j^i f = J_{j}^k \partial_k f$.

Proof. By the chain rule, $\partial_j^i f = \partial_j^i u^k \partial_k f. \partial_j^i u^k = J_{j}^k$.

Corollary A.26. Then $\nabla' f = J^T \nabla f$.

A.2 Metric Tensor

Definition A.27. Let $g$ be the metric tensor in $\mathcal{M}$.

Definition A.28. Let $g'$ be the metric tensor in $\mathcal{N}$.

Definition A.29. Let $g_{ij} = \delta_{km} \partial_i x^m \partial_j x^k$ be the component in the i-th row and j-th column of the metric tensor in $\mathcal{M}$.

Definition A.30. Let $g'_{ij} = \delta_{km} \partial'_i x^m \partial'_j x^k$ be the component in the i-th row and j-th column of the metric tensor in $\mathcal{N}$.

Lemma A.31. Then $g'_{ij} = J_{i}^m g_{mk} J_{j}^k$ under a change of basis from $\mathcal{M}$ to $\mathcal{N}$.
Proof.

\[ g'_{ij} = \delta_{km} \delta_{i}^{m} x^{m} \partial'_{j} x^{k} = \delta_{pq} J_{i}^{m} \partial_{m} x^{q} J_{j}^{k} \partial_{k} x^{p} = J_{i}^{m} \delta_{pq} \partial_{m} x^{q} \partial_{k} x^{p} J_{j}^{k} = J_{i}^{m} g_{mk} J_{j}^{k}. \]

(A.2)

Corollary A.32. Then \( g' = J^{T} g J \) under a change of basis from \( \mathcal{M} \) to \( \mathcal{N} \).

Definition A.33. Let \( g = \det g \) be the metric discriminant in \( \mathcal{M} \).

Definition A.34. Let \( g' = \det g' \) be the metric discriminant in \( \mathcal{N} \).

Lemma A.35. \( g' = J^{2} g \).

Proof.

\[ g' = \det g' = \det (J^{T} g J) = \det (J g J) = \det J \det g \det J = J g J = J^{2} g. \]

(A.3)

\[ \square \]

A.3 Normal Vector

Definition A.36. Let \( N \) be the normal vector in \( \mathcal{M} \).

Definition A.37. Let \( N' \) be the normal vector in \( \mathcal{N} \).

Definition A.38. Let \( N^{k} = \varepsilon_{ij} k \partial_{1} x^{i} \partial_{2} x^{j} \) be the k-th component of the normal vector in \( \mathcal{M} \).

Definition A.39. Let \( N'^{k} = \varepsilon_{ij} k \partial'_{1} x^{i} \partial'_{2} x^{j} \) be the k-th component of the normal vector in \( \mathcal{N} \).

Lemma A.40. Then \( N' = J N \).
Proof. Temporarily renaming coordinates \((x^1, x^2, x^3) = (x, y, z)\), \((u^1, u^2) = (u, v)\) and \((v^1, v^2) = (u', v')\), the normal vector can be written as

\[
\mathbf{N} = \frac{\partial r}{\partial u} \times \frac{\partial r}{\partial v} = \begin{bmatrix}
\frac{\partial y}{\partial u} \frac{\partial z}{\partial v} - \frac{\partial y}{\partial v} \frac{\partial z}{\partial u} \\
\frac{\partial z}{\partial u} \frac{\partial x}{\partial v} - \frac{\partial z}{\partial v} \frac{\partial x}{\partial u} \\
\frac{\partial x}{\partial u} \frac{\partial y}{\partial v} - \frac{\partial x}{\partial v} \frac{\partial y}{\partial u}
\end{bmatrix}.
\] (A.4)

This transforms by the chain rule as

\[
\mathbf{N'} = \begin{bmatrix}
(\frac{\partial u}{\partial u'} \frac{\partial y}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial y}{\partial u'}) (\frac{\partial u}{\partial u'} \frac{\partial z}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial z}{\partial u'}) - (\frac{\partial u}{\partial u'} \frac{\partial y}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial y}{\partial u'}) (\frac{\partial u}{\partial u'} \frac{\partial z}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial z}{\partial u'}) \\
(\frac{\partial u}{\partial u'} \frac{\partial z}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial z}{\partial u'}) (\frac{\partial u}{\partial u'} \frac{\partial x}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial x}{\partial u'}) - (\frac{\partial u}{\partial u'} \frac{\partial z}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial z}{\partial u'}) (\frac{\partial u}{\partial u'} \frac{\partial x}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial x}{\partial u'}) \\
(\frac{\partial u}{\partial u'} \frac{\partial x}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial x}{\partial u'}) (\frac{\partial u}{\partial u'} \frac{\partial y}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial y}{\partial u'}) - (\frac{\partial u}{\partial u'} \frac{\partial x}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial x}{\partial u'}) (\frac{\partial u}{\partial u'} \frac{\partial y}{\partial v'} + \frac{\partial v}{\partial v'} \frac{\partial y}{\partial u'})
\end{bmatrix},
\] (A.5)

which can be written as

\[
\mathbf{N'} = \begin{bmatrix}
(J_{11} \frac{\partial y}{\partial u} + J_{21} \frac{\partial y}{\partial v}) (J_{12} \frac{\partial z}{\partial u} + J_{22} \frac{\partial z}{\partial v}) - (J_{11} \frac{\partial z}{\partial u} + J_{21} \frac{\partial z}{\partial v}) (J_{12} \frac{\partial y}{\partial u} + J_{22} \frac{\partial y}{\partial v}) \\
(J_{11} \frac{\partial z}{\partial u} + J_{21} \frac{\partial z}{\partial v}) (J_{12} \frac{\partial x}{\partial u} + J_{22} \frac{\partial x}{\partial v}) - (J_{11} \frac{\partial x}{\partial u} + J_{21} \frac{\partial x}{\partial v}) (J_{12} \frac{\partial z}{\partial u} + J_{22} \frac{\partial z}{\partial v}) \\
(J_{11} \frac{\partial x}{\partial u} + J_{21} \frac{\partial x}{\partial v}) (J_{12} \frac{\partial y}{\partial u} + J_{22} \frac{\partial y}{\partial v}) - (J_{11} \frac{\partial y}{\partial u} + J_{21} \frac{\partial y}{\partial v}) (J_{12} \frac{\partial x}{\partial u} + J_{22} \frac{\partial x}{\partial v})
\end{bmatrix}.
\] (A.6)

Expanding terms and rearranging the scalars gives

\[
N'_{x} = J_{11} \left( \frac{\partial y}{\partial u} \frac{\partial z}{\partial v} - \frac{\partial z}{\partial u} \frac{\partial y}{\partial v} \right) J_{12} + J_{11} \left( \frac{\partial y}{\partial u} \frac{\partial z}{\partial v} - \frac{\partial y}{\partial v} \frac{\partial z}{\partial u} \right) J_{22} + J_{21} \left( \frac{\partial y}{\partial v} \frac{\partial z}{\partial u} - \frac{\partial z}{\partial v} \frac{\partial y}{\partial u} \right) J_{12} + J_{21} \left( \frac{\partial y}{\partial v} \frac{\partial z}{\partial u} - \frac{\partial z}{\partial v} \frac{\partial y}{\partial u} \right) J_{22}
\] (A.7)

\[
N'_{y} = J_{11} \left( \frac{\partial z}{\partial u} \frac{\partial x}{\partial v} - \frac{\partial x}{\partial u} \frac{\partial z}{\partial v} \right) J_{12} + J_{11} \left( \frac{\partial z}{\partial u} \frac{\partial x}{\partial v} - \frac{\partial x}{\partial u} \frac{\partial z}{\partial v} \right) J_{22} + J_{21} \left( \frac{\partial z}{\partial v} \frac{\partial x}{\partial u} - \frac{\partial x}{\partial v} \frac{\partial z}{\partial u} \right) J_{12} + J_{21} \left( \frac{\partial z}{\partial v} \frac{\partial x}{\partial u} - \frac{\partial x}{\partial v} \frac{\partial z}{\partial u} \right) J_{22}
\] (A.8)

\[
N'_{z} = J_{11} \left( \frac{\partial x}{\partial u} \frac{\partial y}{\partial v} - \frac{\partial y}{\partial u} \frac{\partial x}{\partial v} \right) J_{12} + J_{11} \left( \frac{\partial x}{\partial u} \frac{\partial y}{\partial v} - \frac{\partial y}{\partial u} \frac{\partial x}{\partial v} \right) J_{22} + J_{21} \left( \frac{\partial x}{\partial v} \frac{\partial y}{\partial u} - \frac{\partial y}{\partial v} \frac{\partial x}{\partial u} \right) J_{12} + J_{21} \left( \frac{\partial x}{\partial v} \frac{\partial y}{\partial u} - \frac{\partial y}{\partial v} \frac{\partial x}{\partial u} \right) J_{22},
\] (A.9)
which consolidates to

\[ \mathbf{N}' = \begin{bmatrix} J_{11} J_{22} \left( \frac{\partial y}{\partial u} \frac{\partial z}{\partial v} - \frac{\partial y}{\partial v} \frac{\partial z}{\partial u} \right) - J_{21} J_{12} \left( \frac{\partial y}{\partial u} \frac{\partial z}{\partial v} - \frac{\partial y}{\partial v} \frac{\partial z}{\partial u} \right) \\
J_{11} J_{22} \left( \frac{\partial x}{\partial u} \frac{\partial z}{\partial v} - \frac{\partial x}{\partial v} \frac{\partial z}{\partial u} \right) - J_{21} J_{12} \left( \frac{\partial x}{\partial u} \frac{\partial z}{\partial v} - \frac{\partial x}{\partial v} \frac{\partial z}{\partial u} \right) \\
J_{11} J_{22} \left( \frac{\partial x}{\partial u} \frac{\partial y}{\partial v} - \frac{\partial x}{\partial v} \frac{\partial y}{\partial u} \right) - J_{21} J_{12} \left( \frac{\partial x}{\partial u} \frac{\partial y}{\partial v} - \frac{\partial x}{\partial v} \frac{\partial y}{\partial u} \right) \end{bmatrix}, \quad (A.10) \]

and then simplifies to

\[ \mathbf{N}' = \begin{bmatrix} (J_{11} J_{22} - J_{21} J_{12}) \left( \frac{\partial y}{\partial u} - \frac{\partial y}{\partial v} \right) \\
(J_{11} J_{22} - J_{21} J_{12}) \left( \frac{\partial x}{\partial u} - \frac{\partial x}{\partial v} \right) \\
(J_{11} J_{22} - J_{21} J_{12}) \left( \frac{\partial x}{\partial u} - \frac{\partial x}{\partial v} \right) \end{bmatrix}, \quad (A.11) \]

which is just

\[ \mathbf{N}' = J \mathbf{N}. \quad (A.12) \]

This ends the proof. \(\square\)

**Corollary A.41.** Then \(N^k = J N^k\).

**Definition A.42.** Let \( N = \sqrt{(N^1)^2 + (N^2)^2 + (N^3)^2} \) be the norm of the normal vector in \(\mathcal{M}\).

**Definition A.43.** Let \( N' = \sqrt{(N'^1)^2 + (N'^2)^2 + (N'^3)^2} \) be the norm of the normal vector in \(\mathcal{N}\).

**Definition A.44.** Let \( \mathbf{n} \) be the unit normal vector in \(\mathcal{M}\).

**Definition A.45.** Let \( \mathbf{n}' \) be the unit normal vector in \(\mathcal{N}\).

**Definition A.46.** Let \( n^k = \frac{N^k}{N} \) be the k-th component of the unit normal vector in \(\mathcal{M}\).

**Definition A.47.** Let \( n'^k = \frac{N'^k}{N'} \) be the k-th component of the unit normal vector in \(\mathcal{N}\).
Lemma A.48. Then $n^k = n'^k$.

Proof.

\[ n'^k = N'^k \frac{N^k}{\|JN\|} = JN^k \|JN\| = N^k n^k. \quad \text{(A.13)} \]

\[ \Box \]

Corollary A.49. Then $n = n'$.

A.4 Second Derivatives

Definition A.50. Denote the second partial derivative in $M$ by \( \partial_{ij}f = \frac{\partial^2 f}{\partial u_i \partial u_j} \).

Definition A.51. Denote the partial derivative in $N$ by \( \partial'_{ij}f = \frac{\partial^2 f}{\partial v_i \partial v_j} \).

Definition A.52. Denote \( \partial_{ii}f = \partial^2_i f \).

Definition A.53. Let $H[f]$ be the Hessian matrix of $f$ in $M$.

Definition A.54. Let $H'[f]$ be the Hessian matrix of $f$ in $N$.

Definition A.55. Define the component of the Hessian matrix in $M$ in the $i$-th row and $j$-th columns as $H_{ij}[f] = \partial_{ij}f$.

Definition A.56. Define the component of the Hessian matrix in $N$ in the $i$-th row and $j$-th columns as $H'_{ij}[f] = \partial'_{ij}f$.

Definition A.57. Let $H[u]$ be the Hessian matrix of $u$ in $M$.

Definition A.58. Define the Hessian matrix of a vector as a vector of Hessian matrices of the components of the vector such that $H[u]_{ijk} = H_{ij}[u^k]$.

Definition A.59. Let the dot product between a vector and Hessian behave as \( \{n \cdot H[u]\}_{ij} = n_k H_{ij}[u^k] \).

Definition A.60. Let $H'[u]$ be the Hessian matrix of $u$ in $N$. 

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Lemma A.61. Then \( \{H^\prime\}_{ij} \left[f\right] = (\partial'_{ij} u^n) (\partial_n f) + J^m_i J^n_j H_{mn} \left[f\right] \).

Proof. 

\[
\begin{align*}
\partial'_{ij} f &= J^m_i \partial_m (J^n_j \partial_n f) \\
&= J^m_i (\partial_m J^n_j) \partial_n f + J^m_i J^n_j \partial_{mn} f \\
&= J^m_i (\partial_m J^n_j) \partial_n f + J^m_i (\partial_{mn} f) J^n_j \\
&= J^m_i (\partial_n f) (\partial_m \partial'_{j} u^n) + J^m_i (\partial_{mn} f) J^n_j \\
&= (\partial_n f) J^m_i (J^{-1})^n_i p \partial'_{pj} u^n + J^m_i (\partial_{mn} f) J^n_j \\
&= \delta_p^i (\partial_n f) (\partial'_{pj} u^n) + J^m_i (\partial_{mn} f) J^n_j \\
&= (\partial'_{ij} u^n) (\partial_n f) + J^m_i J^n_j H_{mn} \left[f\right].
\end{align*}
\] (A.14)

\[ \Box \]

Corollary A.62. Then \( H'[f] = H'[u] \cdot \nabla f + J^T H[f] J \).

A.5 Second Fundamental Form

Definition A.63. Lower the index of the unit normal vector by applying a Euclidean metric using \( n_k = \delta_{km} n^m \).

Definition A.64. Define the second fundamental form of \( S \) in \( M \) as \( h \).

Definition A.65. Define the second fundamental form of \( S \) in \( N \) as \( h' \).

Definition A.66. Define the component of the i-th row and j-th column of the second fundamental form in \( M \) as \( h_{ij} = n_k \partial_{ij} x^k \).

Definition A.67. Define the component of the i-th row and j-th column of the second fundamental form in \( N \) as \( h'_{ij} = n_k \partial'_{ij} x^k \).
Lemma A.68. Then 
\[ h'_{ij} = (\partial'_{ij}u^p)n_k(\partial_p x^k) + J^m_i h_{mp}J^p_j. \]

Proof.
\[
h'_{ij} = \delta_{km}n^m\partial'_{ij}x^k = \delta_{kp}n^p [(\partial'_{ij}u^n)(\partial_n x^k) + J^m_i J^m_j (\partial_{mn} x^k)]
\]
\[
= \delta_{kp}n^p (\partial'_{ij}u^n)(\partial_n x^k) + J^m_i J^m_j \delta_{kp}n^p (\partial_{mn} x^k)
\]
\[
= n_k (\partial'_{ij}u^n)(\partial_n x^k) + J^m_i h_{mn}J^m_j. \quad (A.15)
\]

\[\square\]

Corollary A.69. Then 
\[ h' = H'[u] \cdot [((\nabla x)u)] + J^T hJ. \]

Definition A.70. Define the determinant of the second fundamental form of \( M \) as 
\[ h = \det h. \]

Definition A.71. Define the determinant of the second fundamental form of \( N \) as 
\[ h' = \det h'. \]

Lemma A.72. Then 
\[
h' = \left[ (\partial'_{11}u^a)n_k(\partial_n x^k) + J^e_1 J^f_1 h_{ef} \right] \left[ (\partial'_{22}u^a)n_b(\partial_a x^b) + J^g_2 J^h_2 h_{gh} \right]
\]
\[
- \left[ (\partial'_{12}u^c)n_d(\partial_c x^d) + J^i_1 J^j_2 h_{ij} \right] \left[ (\partial'_{12}u^p)n_q(\partial_p x^q) + J^r_1 J^s_2 h_{rs} \right]. \quad (A.16)
\]

Proof.
\[
h = \det h
\]
\[
= n_k \partial_{11} x^k n_m \partial_{22} x^m - n_p \partial_{12} x^p n_q \partial_{12} x^q. \quad (A.17)
\]
\[ h' = \det h' = h'_{11} h'_{22} - (h'_{12})^2 \]
\[ = \left[ (\partial'_{11} u^n) n_k (\partial_a x^k) + J'_1 J'_1 h_{ef} \right] [(\partial'_{22} u^a) n_b (\partial_a x^b) + J'_2 J'_2 h_{gh}] \]
\[ - [(\partial'_{12} u^n) n_d (\partial_c x^d) + J'_1 J'_2 h_{ij}] [(\partial'_{12} u^a) n_q (\partial_p x^q) + J'_1 J'_2 h_{rs}] \]  (A.18)

\[ h' = \det \{ H'[u] \cdot (n^T \nabla x) + J^T hJ \} \]
\[ = \det \{ H'[u] \cdot (n^T \nabla x) + J^T hJ \}. \]  (A.19)

### A.6 Gaussian Curvature

**Definition A.74.** Define the Gaussian curvature of \( \mathcal{M} \) as \( K = \frac{h}{g} \). \[37\]

**Definition A.75.** Define the Gaussian curvature of \( \mathcal{N} \) as \( K' = \frac{h'}{g'} \).

**Theorem A.76.** Then the Gaussian curvature of \( \mathcal{S} \) transforms from \( \mathcal{M} \) to \( \mathcal{N} \) via
\[ K' = \frac{\det \{ H'[u] \cdot (n^T \nabla x) + J^T hJ \}}{J^2 g}. \]  (A.20)

**Proof.**
\[ K' = \frac{h'}{g'} = \frac{\det \{ H'[u] \cdot (n^T \nabla x) + J^T hJ \}}{J^2 g}. \]  (A.21)

### A.7 Mean Curvature

**Definition A.77.** Define the mean curvature of \( \mathcal{M} \) as \( M = \frac{1}{2g} (g_{11} h_{22} + g_{22} h_{11} - 2g_{12} h_{12}) \). \[37\]
Definition A.78. Define the mean curvature of $\mathcal{N}$ as

$$M' = \frac{1}{2g'} (g'_{11} h'_2 2 + g'_{22} h'_1 11 - 2g'_{12} h'_1 12).$$

Theorem A.79. Then the mean curvature of $\mathcal{S}$ transforms from $\mathcal{M}$ to $\mathcal{N}$ via

$$M' = \frac{1}{2J^2 g} \left\{ J'^p_{1g} g'^q_{1} \left[ n_k (\partial'_{22} u^n) (\partial_n x^k) + J^m_{2} h_{mn} J^n_{2} \right] ight. \\
+ J'^p_{2g} g'^q_{2} \left[ n_k (\partial'_{11} u^n) (\partial_n x^k) + J^m_{1} h_{mn} J^n_{1} \right] \\
- 2 J'^p_{1g} g'^q_{2} \left[ n_k (\partial'_{12} u^n) (\partial_n x^k) + J^m_{1} h_{mn} J^n_{2} \right] \right\}. \quad (A.22)$$

Proof. .

$$M' = \frac{1}{2J^2 g} (g'_{11} h'_2 2 + g'_{22} h'_1 11 - 2g'_{12} h'_1 12), \quad (A.23)$$

$$M' = \frac{1}{2J^2 g} \left\{ J'^p_{1g} g'^q_{1} \left[ n_k (\partial'_{22} u^n) (\partial_n x^k) + J^m_{2} h_{mn} J^n_{2} \right] ight. \\
+ J'^p_{2g} g'^q_{2} \left[ n_k (\partial'_{11} u^n) (\partial_n x^k) + J^m_{1} h_{mn} J^n_{1} \right] \\
- 2 J'^p_{1g} g'^q_{2} \left[ n_k (\partial'_{12} u^n) (\partial_n x^k) + J^m_{1} h_{mn} J^n_{2} \right] \right\}. \quad (A.24)$$

This ends the proof.
APPENDIX B

Use of FEMLAB

This section provides a walk-through for performing the analysis of the cylinder in FEMLAB 3.0a, in order to aid the reader in duplicating the results of this thesis if desired.

B.1 Startup

We begin our analysis by starting FEMLAB. The first screen after the splash screen is the Model Navigator (Figure B.1). Select PDE Modes, then coefficient form, then stationary state analysis. Add this to the multiphysics list on the right (Figure B.2). Press OK, and the geometry editor will appear (Figure B.3).

B.2 Geometry

Draw a rectangle 100 high and 628 wide, with one corner at the origin, by selecting the square with a red dot at the bottom corner, then clicking and dragging a rectangle. Double click on it, and specify 100 as the height and 628 as the width (Figure B.4). Press the zoom to extents button (with an arrow crosshair icon) to scale (Figure B.5).
Figure B.1: Model Navigator

Figure B.2: Model Navigator with physics added
Figure B.3: Geometry Editor

Figure B.4: Rectangle Editor
B.3 Options

B.3.1 Summary

The equation used by FEMLAB 3.0a is given as

\[
\begin{aligned}
  d_a \frac{\partial u}{\partial t} + \nabla \cdot (-c \nabla u - \alpha u - \gamma) + \beta \cdot \nabla u + au &= f & \quad \text{on } \Omega, \\
  hu &= r & \quad \text{on } \partial \Omega \ (\text{Dirichlet}), \\
  \hat{n} \cdot (-c \nabla u - \alpha u - \gamma) + qu &= g - h^T \mu & \quad \text{on } \partial \Omega \ (\text{Neumann}),
\end{aligned}
\]  

(B.1)
which can be expanded into

\[
\begin{aligned}
&d_u \frac{\partial u}{\partial t} + \nabla \cdot \left( - \begin{bmatrix} c_{xx} & c_{xy} \\ c_{yx} & c_{yy} \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{bmatrix} - \begin{bmatrix} \alpha_x \\ \alpha_y \end{bmatrix} u - \begin{bmatrix} \gamma_x \\ \gamma_y \end{bmatrix} \right) + \beta_x \frac{\partial u}{\partial x} + \beta_y \frac{\partial u}{\partial y} + au = f \\
&h u = r \\
&\hat{n} \cdot \left( - \begin{bmatrix} c_{xx} & c_{xy} \\ c_{yx} & c_{yy} \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{bmatrix} - \begin{bmatrix} \alpha_x \\ \alpha_y \end{bmatrix} u - \begin{bmatrix} \gamma_x \\ \gamma_y \end{bmatrix} \right) + qu = g - h^T \mu \\
\end{aligned}
\]

on \( \Omega \),

\[
\begin{aligned}
&h u = r \\
&\hat{n} \cdot \left( - \begin{bmatrix} c_{xx} & c_{xy} \\ c_{yx} & c_{yy} \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{bmatrix} - \begin{bmatrix} \alpha_x \\ \alpha_y \end{bmatrix} u - \begin{bmatrix} \gamma_x \\ \gamma_y \end{bmatrix} \right) + qu = g - h^T \mu \\
\end{aligned}
\]

on \( \partial \Omega \) (Dirichlet)

\[
\begin{aligned}
&h u = r \\
&\hat{n} \cdot \left( - \begin{bmatrix} c_{xx} & c_{xy} \\ c_{yx} & c_{yy} \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{bmatrix} - \begin{bmatrix} \alpha_x \\ \alpha_y \end{bmatrix} u - \begin{bmatrix} \gamma_x \\ \gamma_y \end{bmatrix} \right) + qu = g - h^T \mu \\
\end{aligned}
\]

on \( \partial \Omega \) (Neumann),

\[
\begin{aligned}
&B.2
\end{aligned}
\]

Filling in the Schrödinger equation for a particle constrained to a surface gives

\[
\begin{aligned}
&i\hbar \frac{\partial u}{\partial t} + \nabla \cdot \left( - \frac{\hbar^2}{2m} \begin{bmatrix} 1 & 0 \\ 0 & R^{-2} \end{bmatrix} \nabla u - 0 u - 0 \right) + 0 \cdot \nabla u + RV u = 0 \\
&1 u = 0 \\
&\hat{n} \cdot \left( - \frac{\hbar^2}{2m} R \begin{bmatrix} 1 & R^{-2} \end{bmatrix} \nabla u - 0 u - 0 \right) + 0 u = g - h^T \mu \\
\end{aligned}
\]

on \( \Omega \)

\[
\begin{aligned}
&B.3
\end{aligned}
\]

on \( \partial \Omega \) (Dirichlet)

\[
\begin{aligned}
&B.3
\end{aligned}
\]

on \( \partial \Omega \) (Neumann).

The following settings must be set in FEMLAB.

### B.3.2 Constants and expressions

#### B.3.2.1 Constants

These are accessible in FEMLAB from the Options menu (Figure B.6 and Figure B.7). Enter the constants listed in Table B.1.
### Table B.1: Constants for the Cylinder

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>m</td>
<td>510998.913</td>
<td>Mass of electron in $\text{eV} \div c^2$</td>
</tr>
<tr>
<td>hbar_c</td>
<td>1973.269631</td>
<td>$\hbar c$ in $\text{eV} \text{Å}$</td>
</tr>
<tr>
<td>R</td>
<td>100</td>
<td>The radius of the cylinder in Å</td>
</tr>
<tr>
<td>L</td>
<td>100</td>
<td>The length of the cylinder in Å</td>
</tr>
</tbody>
</table>

![Figure B.6: Constants Menu Item](image1.png)

![Figure B.7: Constants after editing](image2.png)
Table B.2: Expressions for the Cylinder

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>cfactor</td>
<td>$(\hbar c)^2(2^4 m)$</td>
<td>Diffusive flux factor $\frac{\hbar^2 c^2}{2m c^2}$</td>
</tr>
<tr>
<td>Vs</td>
<td>$c factor/(4^2 R^2)$</td>
<td>Effective potential energy due to curvature</td>
</tr>
<tr>
<td>Vext</td>
<td>0</td>
<td>Non-geometric potential energy</td>
</tr>
<tr>
<td>V</td>
<td>$Vs + Vext$</td>
<td>Potential energy of the system</td>
</tr>
</tbody>
</table>

Figure B.8: Scalar Expressions

B.3.2.2 Expressions

These are accessed from the options menu as well (Figure B.8 and Figure B.9). Enter the expressions listed in Table B.2.

B.4 Physics Menu

B.4.1 Subdomain coefficients

These are accessible by selecting Subdomain Settings from the physics Menu (Figure B.10). Select subdomain 1 and enter the coefficients listed in Table B.3 (Figure B.11 and Figure B.12):
Figure B.9: Scalar Expressions after editing

Table B.3: Subdomain Coefficients for the Cylinder

<table>
<thead>
<tr>
<th>Term</th>
<th>Name</th>
<th>FEMLAB variables</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_a E u$</td>
<td>Mass</td>
<td>dau</td>
<td>1</td>
</tr>
<tr>
<td>$c \nabla u$</td>
<td>Diffusive flux</td>
<td>cu1x, cu2x, cu1y, cu2y</td>
<td>$\begin{bmatrix} \text{cfactor}/R^2 &amp; 0 \ 0 &amp; \text{cfactor} \end{bmatrix}$</td>
</tr>
<tr>
<td>$a u$</td>
<td>Conservative flux source</td>
<td>gax, gay</td>
<td>$\begin{bmatrix} 0 \ 0 \end{bmatrix}$</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Convection</td>
<td>beu1, beu2</td>
<td>$\begin{bmatrix} 0 \ 0 \end{bmatrix}$</td>
</tr>
<tr>
<td>$\beta \cdot \nabla u$</td>
<td>Absorption</td>
<td>au</td>
<td>$\begin{bmatrix} 0 \end{bmatrix}$</td>
</tr>
<tr>
<td>$a u$</td>
<td>Source</td>
<td>f</td>
<td>0</td>
</tr>
</tbody>
</table>
Figure B.10: Subdomain Settings Menu Item

Figure B.11: Subdomain Settings diffusion coefficient tensor entry
Figure B.12: Subdomain Settings after editing

Table B.4: Boundary Conditions for the Cylinder

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Type</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,4</td>
<td>Dirichlet</td>
<td>[Use defaults]</td>
</tr>
<tr>
<td>1,3</td>
<td>Neumann</td>
<td>[Use defaults]</td>
</tr>
</tbody>
</table>

B.4.2 Boundary conditions

These are also accessible from the Physics menu, by selecting Boundary Conditions (Figure B.13). Select the boundaries specified and enter the settings listed in Table B.4 (Figure B.14 and Figure B.15):

B.4.3 Periodic boundary conditions

These are accessible from the Physics menu, selecting Periodic Conditions (Figure B.16). This is a little more involved than previous tasks. Periodic boundary conditions for the cylinder are listed in Table B.5

Select boundaries 1 and 4 and enter the following expressions: u and u_x, as shown in Figure B.17. Then select u and click on the Destination tab.
Figure B.13: Boundary Settings Menu Item

Figure B.14: Boundary conditions for periodic edges

Table B.5: Periodic Boundary Conditions for the Cylinder

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Source boundary</th>
<th>Dest. boundary</th>
<th>Source points</th>
<th>Dest. points</th>
</tr>
</thead>
<tbody>
<tr>
<td>pconstr1</td>
<td>u</td>
<td>1</td>
<td>3</td>
<td>3,4</td>
<td>1,2</td>
</tr>
<tr>
<td>pconstr2</td>
<td>uₓ</td>
<td>1</td>
<td>3</td>
<td>3,4</td>
<td>1,2</td>
</tr>
</tbody>
</table>
Figure B.15: Boundary conditions for edge of cylinder

Figure B.16: Periodic Boundary Conditions menu item

Figure B.17: Periodic Boundary Conditions Source Tab
Check boundaries 1 and 4, and check them. In Expression, type \( u \) and then select `pconstr1` (Figure B.18). Then click on the Source Vertices Tab (Figure B.19).

Copy vertices 1 and 2 in order as shown in Figure B.19, then click on the Destination Vertices Tab (Figure B.20) and select vertices 3 and 4, in that order.

Now return to the Source tab, select \( u_x \), and repeat the process detailed above for \( u \). The only difference is in the destination tab (Figure B.21), enter \( u_x \) as the Expression and select `pconstr2` in the Constraint name drop-down box.

### B.5 Mesh Generation and Refinement

Next click on the initialize mesh button (Figure B.22), then refine the mesh by clicking on the button to its right (Figure B.23).
Figure B.20: Periodic Boundary Conditions Destination Vertices Tab

Figure B.21: Periodic Boundary Conditions Destination Tab for $u_x$

Figure B.22: Initialized Mesh
B.6 Solver Parameters

Select the Solver Parameters menu item (Figure B.24). The Solver Parameters Screen (Figure B.25) will appear. Select the Eigenvalue solver, and then increase the desired number of Eigenvalues to 20 or more. Press OK to save settings.

B.7 Solve the Problem

We are now ready to solve the problem. Select Solve Problem from the Solve menu (Figure B.26) and the progress screen (Figure B.27) will appear. This may take several minutes depending on the complexity of the problem.

B.8 Postprocessing

Once the results are calculated, the first solution will be displayed. The screen will look similar to Figure B.28.

To view other eigenstates, select Plot Parameters from the Postprocessing menu (Figure B.29). This brings up the Plot Parameters screen (Figure B.30).
Figure B.24: Solver Parameters menu item

Figure B.25: Solver Parameters Screen
Figure B.26: Solve Problem menu item

Figure B.27: Solve Problem Progress screen
Figure B.28: Postprocessing Mode

Figure B.29: Plot Parameters Menu
On this screen, there are many options. Expression is the expression to plot. The default is $u$, but any valid expression may be entered. Several expressions are predefined as well. The General tab (Figure B.31) allows for the selection of which Eigenstate to plot.
Figure B.31: Plot Parameters General Tab
APPENDIX C

Tables of Extracted Data

The following table contains data extracted from Ref. [4] alongside the results of the numerical analysis performed in sections 6.5 and 6.4.

Table C.1: Extracted Energies and Numerically Calculated Energies From Ref. [4]

<table>
<thead>
<tr>
<th>$\xi$</th>
<th>$m$</th>
<th>$\lambda$</th>
<th>Ref. [4] $E$ (eV)</th>
<th>$E$ (eV)</th>
<th>Scaled $E$ (eV)</th>
<th>Error (eV)</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>0</td>
<td>0</td>
<td>0.00</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1.1</td>
<td>0</td>
<td>1</td>
<td>2.91</td>
<td>0.031635</td>
<td>3.16</td>
<td>−0.255</td>
<td>−8.79%</td>
</tr>
<tr>
<td>1.1</td>
<td>0</td>
<td>2</td>
<td>9.54</td>
<td>0.094945</td>
<td>9.49</td>
<td>4.38</td>
<td>0.46%</td>
</tr>
<tr>
<td>1.1</td>
<td>0</td>
<td>3</td>
<td>18.6</td>
<td>0.187801</td>
<td>18.8</td>
<td>−0.169</td>
<td>−0.91%</td>
</tr>
<tr>
<td>1.1</td>
<td>0</td>
<td>4</td>
<td>30.9</td>
<td>0.311366</td>
<td>31.1</td>
<td>−0.195</td>
<td>−0.63%</td>
</tr>
<tr>
<td>1.1</td>
<td>1</td>
<td>0</td>
<td>6.40</td>
<td>0.065313</td>
<td>6.53</td>
<td>−0.134</td>
<td>−2.09%</td>
</tr>
<tr>
<td>1.1</td>
<td>1</td>
<td>1</td>
<td>12.9</td>
<td>0.129898</td>
<td>13.0</td>
<td>−0.0781</td>
<td>−0.61%</td>
</tr>
<tr>
<td>1.1</td>
<td>1</td>
<td>2</td>
<td>22.6</td>
<td>0.223277</td>
<td>22.3</td>
<td>0.239</td>
<td>1.06%</td>
</tr>
<tr>
<td>1.1</td>
<td>1</td>
<td>3</td>
<td>34.1</td>
<td>0.346395</td>
<td>34.6</td>
<td>−0.557</td>
<td>−1.64%</td>
</tr>
<tr>
<td>1.1</td>
<td>2</td>
<td>0</td>
<td>23.0</td>
<td>0.228103</td>
<td>22.8</td>
<td>0.221</td>
<td>0.96%</td>
</tr>
<tr>
<td>1.1</td>
<td>2</td>
<td>1</td>
<td>33.0</td>
<td>0.331407</td>
<td>33.1</td>
<td>−0.106</td>
<td>−0.32%</td>
</tr>
</tbody>
</table>
Table C.1: Extracted Energies and Numerically Calculated Energies From Ref. [4]

<table>
<thead>
<tr>
<th>$\xi$</th>
<th>$m$</th>
<th>$\lambda$</th>
<th>E (eV)</th>
<th>Scaled E (eV)</th>
<th>Error (eV)</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.25</td>
<td>0</td>
<td>0</td>
<td>0.00</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1.25</td>
<td>0</td>
<td>1</td>
<td>2.10</td>
<td>0.02043</td>
<td>2.04</td>
<td>0.0586</td>
</tr>
<tr>
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<td>0</td>
<td>2</td>
<td>5.60</td>
<td>0.060416</td>
<td>6.04</td>
<td>−0.437</td>
</tr>
<tr>
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<td>0</td>
<td>3</td>
<td>11.8</td>
<td>0.118998</td>
<td>11.9</td>
<td>−0.107</td>
</tr>
<tr>
<td>1.25</td>
<td>0</td>
<td>4</td>
<td>19.3</td>
<td>0.196645</td>
<td>19.7</td>
<td>−0.400</td>
</tr>
<tr>
<td>1.25</td>
<td>0</td>
<td>5</td>
<td>24.9</td>
<td>0.293025</td>
<td>29.3</td>
<td>−4.43</td>
</tr>
<tr>
<td>1.25</td>
<td>1</td>
<td>0</td>
<td>2.80</td>
<td>0.027486</td>
<td>2.75</td>
<td>0.0536</td>
</tr>
<tr>
<td>1.25</td>
<td>1</td>
<td>1</td>
<td>6.54</td>
<td>0.067072</td>
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<td>−0.169</td>
</tr>
<tr>
<td>1.25</td>
<td>1</td>
<td>2</td>
<td>12.6</td>
<td>0.125962</td>
<td>12.6</td>
<td>0.0135</td>
</tr>
<tr>
<td>1.25</td>
<td>1</td>
<td>3</td>
<td>20.4</td>
<td>0.204081</td>
<td>20.4</td>
<td>0.0243</td>
</tr>
<tr>
<td>1.25</td>
<td>1</td>
<td>4</td>
<td>30.4</td>
<td>0.301387</td>
<td>30.1</td>
<td>0.218</td>
</tr>
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<td>1.25</td>
<td>2</td>
<td>0</td>
<td>8.87</td>
<td>0.09138</td>
<td>9.14</td>
<td>−0.265</td>
</tr>
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<td>1.25</td>
<td>2</td>
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<td>0.151656</td>
<td>15.2</td>
<td>−0.221</td>
</tr>
<tr>
<td>1.25</td>
<td>2</td>
<td>2</td>
<td>22.8</td>
<td>0.230636</td>
<td>23.1</td>
<td>−0.296</td>
</tr>
<tr>
<td>1.25</td>
<td>2</td>
<td>3</td>
<td>33.3</td>
<td>0.328628</td>
<td>32.9</td>
<td>0.413</td>
</tr>
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<td>1.25</td>
<td>3</td>
<td>0</td>
<td>18.8</td>
<td>0.190921</td>
<td>19.1</td>
<td>−0.294</td>
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<td>1.25</td>
<td>3</td>
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<td>27.2</td>
<td>−0.256</td>
</tr>
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<td>1.25</td>
<td>3</td>
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<td>39.2</td>
<td>−1.94</td>
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<td>−0.238</td>
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<td>−2.38</td>
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<td>2</td>
<td>0</td>
<td>1</td>
<td>0.595</td>
<td>0.005889</td>
<td>0.0589</td>
<td>0.00642</td>
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<td>1.55</td>
<td>0.017525</td>
<td>1.75</td>
<td>−0.205</td>
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<td>2</td>
<td>0</td>
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<td>3.45</td>
<td>0.033984</td>
<td>3.40</td>
<td>0.0545</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>4</td>
<td>6.07</td>
<td>0.057414</td>
<td>5.74</td>
<td>0.331</td>
</tr>
</tbody>
</table>
Table C.1: Extracted Energies and Numerically Calculated Energies From Ref. [4]

<table>
<thead>
<tr>
<th>ξ</th>
<th>m</th>
<th>λ</th>
<th>Ref. [4] E (eV)</th>
<th>Scaled Energy E (eV)</th>
<th>Scaled E (eV)</th>
<th>Error (eV)</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
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Tables of Metric Tensors and Laplace-Beltrami Operators for Selected Coordinate Systems

The following tables give the metric tensors and Laplace-Beltrami operators for several coordinate systems. These are provided to demonstrate the differences between the Laplace-Beltrami operators between coordinate systems and their constrained counterparts, and to provide a convenient reference for those studying potentials in these coordinate systems. These coordinate systems are detailed in several mathematical physics textbooks. (Refs. [13; 31; 38])

D.1 Metric Tensors

When constraining coordinates, the metric tensor of the constrained system is simply the cofactor of the constrained coordinate in the full metric tensor. The following table provides the metric tensors for several coordinate systems and constrained systems.

2-D Cartesian:

\[
G_{ij} = \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix}
\]  \hspace{1cm} (D.1)
3-D Cartesian:

\[ G_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]  (D.2)

2-D polar:

\[ G_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & r^2 \end{bmatrix} \]  (D.3)

3-D circular cylindrical:

\[ G_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]  (D.4)

2-D circular cylindrical constrained to a constant radius \( a \):

\[ g_{ij} = \begin{bmatrix} a^2 & 0 \\ 0 & 1 \end{bmatrix} \]  (D.5)

2-D elliptical:

\[ G_{ij} = \begin{bmatrix} f^2 \sin^2 v \cosh^2 u + f^2 \cos^2 v \sinh^2 u & 0 \\ 0 & f^2 \sin^2 v \cosh^2 u + f^2 \cos^2 v \sinh^2 u \end{bmatrix} \]  (D.6)

3-D elliptical cylindrical:

\[ G_{ij} = \begin{bmatrix} f^2 (\sinh^2 u + \sin^2 v) & 0 & 0 \\ 0 & f^2 (\sinh^2 u + \sin^2 v) & 0 \\ 0 & 0 & 1 \end{bmatrix} \]  (D.7)
2-D elliptical cylindrical constrained to constant $u$:

\[
g_{ij} = \begin{bmatrix}
    f^2 (\sinh^2 u + \sin^2 v) & 0 \\
    0 & 1
\end{bmatrix}
\]  \hspace{1cm} (D.8)

2-D parabolic:

\[
G_{ij} = \begin{bmatrix}
    \mu^2 + \nu^2 & 0 \\
    0 & \mu^2 + \nu^2
\end{bmatrix}
\]  \hspace{1cm} (D.9)

3-D parabolic cylindrical:

\[
G_{ij} = \begin{bmatrix}
    \mu^2 + \nu^2 & 0 & 0 \\
    0 & \mu^2 + \nu^2 & 0 \\
    0 & 0 & 1
\end{bmatrix}
\]  \hspace{1cm} (D.10)

2-D parabolic cylindrical constrained to constant $\mu$:

\[
g_{ij} = \begin{bmatrix}
    \mu^2 + \nu^2 & 0 \\
    0 & 1
\end{bmatrix}
\]  \hspace{1cm} (D.11)

3-D circular spherical:

\[
G_{ij} = \begin{bmatrix}
    1 & 0 & 0 \\
    0 & r^2 & 0 \\
    0 & 0 & r^2 \sin^2 \theta
\end{bmatrix}
\]  \hspace{1cm} (D.12)

2-D spherical constrained to a constant radius $a$:

\[
g_{ij} = \begin{bmatrix}
    a^2 & 0 \\
    0 & a^2 \sin^2 \theta
\end{bmatrix}
\]  \hspace{1cm} (D.13)
3-D prolate spheroidal:

\[
G_{ij} = \begin{bmatrix}
\frac{f^2\xi^2 - \eta^2}{\xi^2 + 1} & 0 & 0 \\
0 & \frac{f^2\xi^2 - \eta^2}{1 - \eta^2} & 0 \\
0 & 0 & f^2 (\xi^2 - 1) (1 - \eta^2)
\end{bmatrix}
\]  
(D.14)

2-D prolate spheroid constrained to constant \(\xi\):

\[
G_{ij} = \begin{bmatrix}
\frac{f^2\xi^2 - \eta^2}{1 - \eta^2} & 0 \\
0 & f^2 (\xi^2 - 1) (1 - \eta^2)
\end{bmatrix}
\]  
(D.15)

3-D oblate spheroidal:

\[
G_{ij} = \begin{bmatrix}
\frac{f^2\xi^2 + \eta^2}{\xi^2 + 1} & 0 & 0 \\
0 & \frac{f^2\xi^2 + \eta^2}{1 - \eta^2} & 0 \\
0 & 0 & f^2 (\xi^2 + 1) (1 - \eta^2)
\end{bmatrix}
\]  
(D.16)

2-D oblate spheroid with constant \(\xi\):

\[
g_{ij} = \begin{bmatrix}
\frac{f^2\xi^2 + \eta^2}{1 - \eta^2} & 0 \\
0 & f^2 (\xi^2 + 1) (1 - \eta^2)
\end{bmatrix}
\]  
(D.17)

3-D triaxial ellipsoidal:

\[
G_{ij} = \begin{bmatrix}
\frac{\xi_1(\xi_1^2 - \xi_2^2)(\xi_1^2 - \xi_3^2)}{(\xi_1^2 - a^2)(\xi_1^2 - b^2)(\xi_1^2 - c^2)} & 0 & 0 \\
0 & \frac{\xi_2(\xi_2^2 - \xi_1^2)(\xi_2^2 - \xi_3^2)}{(a^2 - \xi_1^2)(\xi_2^2 - b^2)(\xi_2^2 - c^2)} & 0 \\
0 & 0 & \frac{\xi_3(\xi_3^2 - \xi_1^2)(\xi_3^2 - \xi_2^2)}{(a^2 - \xi_1^2)(b^2 - \xi_2^2)(\xi_3^2 - c^2)}
\end{bmatrix}
\]  
(D.18)
2-D triaxial ellipsoid with constant $\xi_1$:

\[
g_{ij} = \begin{bmatrix}
\frac{\xi_1^2(\xi_2^2-\xi_3^2)(\xi_3^2-\xi_1^2)}{(a^2-\xi_1^2)(b^2-\xi_1^2)(c^2-\xi_1^2)} & 0 \\
0 & \frac{\xi_3^2(\xi_1^2-\xi_2^2)(\xi_1^2-\xi_3^2)}{(a^2-\xi_1^2)(b^2-\xi_1^2)(c^2-\xi_1^2)}
\end{bmatrix} \tag{D.19}
\]

3-D parabolic rotational:

\[
G_{ij} = \begin{bmatrix}
\eta^2 + \xi^2 & 0 & 0 \\
0 & \eta^2 + \xi^2 & 0 \\
0 & 0 & \eta^2 \xi^2
\end{bmatrix} \tag{D.20}
\]

2-D parabolic rotational with constant $\xi$:

\[
g_{ij} = \begin{bmatrix}
\eta^2 + \xi^2 & 0 \\
0 & \eta^2 \xi^2
\end{bmatrix} \tag{D.21}
\]

3-D conic:

\[
G_{ij} = \begin{bmatrix}
1 & 0 & 0 \\
0 & \frac{r^2(\lambda^2-\theta^2)}{b^4-(b^2+c^2)^2b^2c^2} & 0 \\
0 & 0 & -\frac{r^2(\lambda^2-\theta^2)}{\lambda^4-(b^2+c^2)^2\lambda^2+b^2c^2}
\end{bmatrix} \tag{D.22}
\]

2-D cone with constant $\theta$:

\[
g_{ij} = \begin{bmatrix}
1 & 0 \\
0 & \frac{-r^2(\lambda^2-\theta^2)}{\lambda^4-(b^2+c^2)^2\lambda^2+b^2c^2}
\end{bmatrix} \tag{D.23}
\]

3-D paraboloidal:

\[
G_{ij} = \begin{bmatrix}
\frac{(\lambda-\mu)(\nu-\mu)}{(b-\mu)(c-\mu)} & 0 & 0 \\
0 & \frac{(\lambda-\nu)(\mu-\nu)}{(b-\nu)(c-\nu)} & 0 \\
0 & 0 & \frac{(\lambda-\mu)(\nu-\lambda)}{(\lambda-b)(\lambda-c)}
\end{bmatrix} \tag{D.24}
\]
2-D paraboloidal with constant $\mu$:

$$g_{ij} = \begin{bmatrix} \frac{(\lambda-\nu)(\mu-\nu)}{(b-\nu)(c-\nu)} & 0 \\ 0 & \frac{(\lambda-\mu)(\nu-\lambda)}{(\lambda-b)(\lambda-c)} \end{bmatrix}$$  \hspace{0.5cm} (D.25)

### D.2 Laplacian and Laplace-Beltrami Operators

The Laplace-Beltrami operator changes between the full three-dimensional coordinate system and the constrained two dimensional system, because one of the variables has been removed.

2-D Cartesian:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$  \hspace{0.5cm} (D.26)

3-D Cartesian:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$  \hspace{0.5cm} (D.27)

2-D polar:

$$\nabla^2 = r^2 \frac{\partial^2}{\partial r^2} + r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}$$  \hspace{0.5cm} (D.28)

3-D circular cylindrical:

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}$$  \hspace{0.5cm} (D.29)

2-D circular cylinder with constant radius $a$:

$$\nabla_{LB}^2 = \frac{1}{a^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}$$  \hspace{0.5cm} (D.30)

2-D elliptical:

$$\nabla^2 = \frac{1}{f^2 (\sinh^2 u + \sin^2 v)} \left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right)$$  \hspace{0.5cm} (D.31)
3-D elliptical cylindrical:
\[
\nabla^2 = \frac{1}{f^2 (\sinh^2 u + \sin^2 v)} \left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right) + \frac{\partial^2}{\partial z^2} \quad (D.32)
\]

2-D elliptical cylinder with constant \( u \):
\[
\nabla^2_{LB} = \frac{1}{f^2 \sqrt{\sinh^2 u + \sin^2 v}} \frac{\partial}{\partial v} \left( \frac{1}{\sqrt{\sinh^2 u + \sin^2 v}} \frac{\partial}{\partial v} \right) + \frac{\partial^2}{\partial z^2} \quad (D.33)
\]

2-D parabolic:
\[
\nabla^2 = \frac{1}{\mu^2 + \nu^2} \left( \frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2} \right) \quad (D.34)
\]

3-D parabolic cylindrical:
\[
\nabla^2 = \frac{1}{\mu^2 + \nu^2} \left( \frac{\partial^2}{\partial \mu^2} + \frac{\partial^2}{\partial \nu^2} \right) + \frac{\partial^2}{\partial z^2} \quad (D.35)
\]

2-D parabolic cylindrical with constant \( \mu \):
\[
\nabla^2_{LB} = \frac{1}{\sqrt{\mu^2 + \nu^2}} \frac{\partial}{\partial \nu} \left( \frac{1}{\sqrt{\mu^2 + \nu^2}} \frac{\partial}{\partial \nu} \right) + \frac{\partial^2}{\partial z^2} \quad (D.36)
\]

3-D circular spherical:
\[
\nabla^2 = \frac{1}{r^2 \sin \theta} \left[ \sin \theta \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad (D.37)
\]

2-D sphere with constant radius \( a \):
\[
\nabla^2_{LB} = \frac{1}{a^2 \sin \theta} \left[ \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2}{\partial \phi^2} \right] \quad (D.38)
\]
3-D prolate spheroidal:

\[ \nabla^2 = \frac{1}{f^2 (\xi^2 - \eta^2)} \times \left\{ \frac{\partial}{\partial \xi} \left[ (\xi^2 - 1) \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + \frac{\xi^2 - \eta^2}{(\xi^2 - 1) (1 - \eta^2)} \frac{\partial^2}{\partial \phi^2} \right\} \]

(D.39)

2-D prolate spheroid with constant \( \xi \):

\[ \nabla^2_{LB} = \frac{1}{f^2 \sqrt{\xi^2 - \eta^2}} \left\{ \frac{\partial}{\partial \eta} \left[ 1 - \eta^2 \frac{\partial}{\partial \eta} \right] + \frac{\xi^2 - \eta^2}{(\xi^2 - 1) (1 - \eta^2)} \frac{\partial^2}{\partial \phi^2} \right\} \]

(D.40)

3-D oblate spheroidal:

\[ \nabla^2 = \frac{1}{f^2 (\xi^2 + \eta^2)} \times \left\{ \frac{\partial}{\partial \xi} \left[ (\xi^2 + 1) \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ (1 - \eta^2) \frac{\partial}{\partial \eta} \right] + \frac{\xi^2 + \eta^2}{(\xi^2 + 1) (1 - \eta^2)} \frac{\partial^2}{\partial \phi^2} \right\} \]

(D.41)

2-D oblate spheroid with constant \( \xi \):

\[ \nabla^2_{LB} = \frac{1}{f^2 \sqrt{\xi^2 + \eta^2}} \left\{ \frac{\partial}{\partial \eta} \left[ 1 - \eta^2 \frac{\partial}{\partial \eta} \right] + \frac{\xi^2 + \eta^2}{(\xi^2 + 1) (1 - \eta^2)} \frac{\partial^2}{\partial \phi^2} \right\} \]

(D.42)

3-D triaxial ellipsoidal:

\[ \nabla^2 = \frac{\sqrt{(\xi_1^2 - a^2) (\xi_1^2 - b^2) (\xi_1^2 - c^2)}}{\xi_1 (\xi_1^2 - \xi_2^2) (\xi_1^2 - \xi_3^2)} \frac{\partial}{\partial \xi_1} \left[ \frac{\sqrt{(\xi_1^2 - a^2) (\xi_1^2 - b^2) (\xi_1^2 - c^2)}}{\xi_1} \frac{\partial}{\partial \xi_1} \right]
\]

\[ + \frac{\sqrt{(a^2 - \xi_2^2) (\xi_2^2 - b^2) (\xi_2^2 - c^2)}}{\xi_2 (\xi_1^2 - \xi_2^2) (\xi_2^2 - \xi_3^2)} \frac{\partial}{\partial \xi_2} \left[ \frac{\sqrt{(a^2 - \xi_2^2) (\xi_2^2 - b^2) (\xi_2^2 - c^2)}}{\xi_2} \frac{\partial}{\partial \xi_2} \right]
\]

\[ + \frac{\sqrt{(a^2 - \xi_3^2) (b^2 - \xi_3^2) (c^2 - \xi_3^2)}}{\xi_3 (\xi_1^2 - \xi_3^2) (\xi_2^2 - \xi_3^2)} \frac{\partial}{\partial \xi_3} \left[ \frac{\sqrt{(a^2 - \xi_3^2) (b^2 - \xi_3^2) (c^2 - \xi_3^2)}}{\xi_3} \frac{\partial}{\partial \xi_3} \right]
\]

(D.43)
2-D triaxial ellipsoid with constant $\xi_1$:

$$\nabla_{LB}^2 = \frac{\sqrt{(a^2 - \xi_2^2)(b^2 - \xi_2^2)(c^2 - \xi_2^2)}}{\xi_2 \sqrt{\xi_1^2 - \xi_2^2}} \frac{\partial}{\partial \xi_2} \left[ \frac{\sqrt{(a^2 - \xi_2^2)(b^2 - \xi_2^2)(c^2 - \xi_2^2)}}{\xi_2 \sqrt{\xi_1^2 - \xi_2^2}} \frac{\partial}{\partial \xi_2} \right]$$

$$+ \frac{\sqrt{(a^2 - \xi_3^2)(b^2 - \xi_3^2)(c^2 - \xi_3^2)}}{\xi_3 \sqrt{\xi_1^2 - \xi_3^2}} \frac{\partial}{\partial \xi_3} \left[ \frac{\sqrt{(a^2 - \xi_3^2)(b^2 - \xi_3^2)(c^2 - \xi_3^2)}}{\xi_3 \sqrt{\xi_1^2 - \xi_3^2}} \frac{\partial}{\partial \xi_3} \right]$$

(D.44)

3-D parabolic rotational:

$$\nabla^2 = \frac{1}{\xi^2 + \eta^2} \left[ \frac{1}{\xi} \frac{\partial}{\partial \xi} \left( \xi \frac{\partial}{\partial \xi} \right) + \frac{1}{\eta} \frac{\partial}{\partial \eta} \left( \eta \frac{\partial}{\partial \eta} \right) \right] + \frac{1}{\xi^2 \eta^2} \frac{\partial^2}{\partial \phi^2}$$

(D.45)

2-D parabolic rotational with constant $\xi$:

$$\nabla_{LB}^2 = \frac{1}{\eta \sqrt{\xi^2 + \eta^2}} \left[ \frac{\eta}{\sqrt{\xi^2 + \eta^2}} \frac{\partial}{\partial \eta} \frac{\partial}{\partial \eta} \right] + \frac{1}{\xi^2 \eta^2} \frac{\partial^2}{\partial \phi^2}$$

(D.46)

3-D conic:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial}{\partial r} \right]$$

$$+ \frac{\sqrt{(\theta^2 - b^2)(c^2 - \theta^2)}}{r^2 (\theta^2 - \lambda^2)} \frac{\partial}{\partial \theta} \left[ \frac{\sqrt{(\theta^2 - b^2)(c^2 - \theta^2)}}{r^2 (\theta^2 - \lambda^2)} \frac{\partial}{\partial \theta} \right]$$

$$+ \frac{\sqrt{(b^2 - \lambda^2)(c^2 - \lambda^2)}}{r^2 (\theta^2 - \lambda^2)} \frac{\partial}{\partial \lambda} \left[ \frac{\sqrt{(b^2 - \lambda^2)(c^2 - \lambda^2)}}{r^2 (\theta^2 - \lambda^2)} \frac{\partial}{\partial \lambda} \right]$$

(D.47)

2-D cone with constant $\theta$:

$$\nabla_{LB}^2 = \frac{1}{r} \frac{\partial}{\partial r} \left[ r \frac{\partial}{\partial r} \right]$$

$$+ \frac{\sqrt{\lambda^4 - (b^2 + c^2) \lambda^2 + b^2 c^2}}{r^2 \sqrt{\theta^2 - \lambda^2}} \frac{\partial}{\partial \lambda} \left[ \frac{\sqrt{\lambda^4 - (b^2 + c^2) \lambda^2 + b^2 c^2}}{r^2 \sqrt{\theta^2 - \lambda^2}} \frac{\partial}{\partial \lambda} \right]$$

(D.48)
3-D paraboloidal:

\[
\nabla^2 = \sqrt{(\mu - b)(\mu - c)(\mu - \nu)(\mu - \lambda)\partial\mu} \left[ \sqrt{(\mu - b)(\mu - c)\partial\mu} \right] \\
+ \sqrt{(b - \nu)(c - \nu)(\mu - \nu)(\lambda - \nu)\partial\nu} \left[ \sqrt{(b - \nu)(c - \nu)\partial\nu} \right] \\
+ \sqrt{(b - \lambda)(\lambda - c)(\lambda - \nu)(\mu - \lambda)\partial\lambda} \left[ \sqrt{(b - \lambda)(\lambda - c)\partial\lambda} \right] \\
\]

(D.49)

2-D paraboloidal with constant \( \mu \):

\[
\nabla_{LB}^2 = \sqrt{(b - \nu)(c - \nu)(\mu - \nu)(\lambda - \nu)\partial\nu} \left[ \sqrt{(b - \nu)(c - \nu)\partial\nu} \right] \\
+ \sqrt{(\lambda - b)(\lambda - c)(\lambda - \nu)(\lambda - \mu)\partial\lambda} \left[ \sqrt{(\lambda - b)(\lambda - c)\partial\lambda} \right] \\
\]

(D.50)
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