

# Path Integrals and the Quantum Routhian

by

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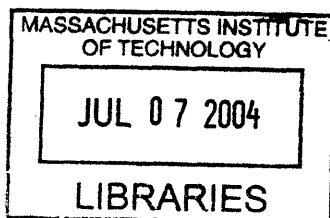
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## Abstract

In this thesis, we consider the use of the Routhian in quantum mechanics, which is an object halfway between a Lagrangian and a Hamiltonian expressing the dynamics of a system in terms of conserved momentum and non-cyclic coordinates. Starting from the phase space path integral, we derive an expression for the quantum mechanical propagator of a system written in terms of its Routhian. We then go on to show how this formalism can provide calculational simplifications in simple situations such as a free particle on a line or a circle, and we demonstrate that for a particle in a constant magnetic field, by using conserved momentum it is possible to obtain a positive definite measure after Wick rotating to imaginary time. By doing this, we are able to obtain the quantum corrections to the partition function. Finally, we attempt to develop a general method for approximating the partition function for a particle on a sphere if there is a conserved azimuthal momentum, and consider in detail the free particle on a sphere. We reduce the problem to having to solve a complicated differential equation, obtaining an answer very close to the exact result in the simplest approximation.

Thesis Supervisor: Frank Wilczek

Title: Herman Feshbach Professor of Physics



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# Chapter 1

## Introduction

There are two major approaches to formulating the dynamics of classical systems. The first is using the Lagrangian, which is a function of coordinates and their derivatives, and for which the equations of motion are a set of second order differential equations. The second is using the Hamiltonian, which is a function of coordinates and momenta, and for which the equations of motion are a system of coupled first order differential equations. Each of these approaches has their advantages and disadvantages - the Hamiltonian allows us to work with first order differential equations, but at the cost of having twice as many of them. However, if some of the system's momenta are conserved, then the differential equations associated with these momenta are trivial, and the Hamiltonian formulation offers clear advantages. One of the simplest ways that momenta can be conserved is if the Hamiltonian or Lagrangian is cyclic in (independent of) their conjugate coordinates.

It was the idea of Routh in the late 19th century to try to have the best of both worlds - he constructed a function that behaves like a Hamiltonian in the cyclic coordinates and a Lagrangian in the non-cyclic coordinates. This function is called the Routhian, and it was soon found to be useful in the study of deviations from steady motion (such as planetary oscillations around periodic orbits) [9]. However, it never gained the popularity that its counterparts did, perhaps because it had the flavor of a mere mathematical formality.

Meanwhile, quantum mechanics was also developing in two major ways. The first

is the canonical approach, in which the coordinates and their conjugate momenta are promoted to operators acting on a Hilbert space. The Hamiltonian is primarily used in this approach. The second approach is that of the path integral, which expresses the propagator (probability amplitude) for a particle to travel between two points in terms of an integral over all possible paths between those points. This can be written either in terms of the Hamiltonian (as an integral over phase space) or the Lagrangian (as an integral over coordinate space). This is also closely related to the statistical mechanics partition function.

The purpose of this thesis is to first formulate the quantum mechanics of a general system in terms of its Routhian, and then to look at some simple examples in order to try to determine how this might be useful. In order to do this, we adopt the path integral approach, and we show how we can simplify the path integral by isolating the contributions from classically conserved momenta. Then we show how doing this can provide basic calculational simplifications for the free particle on a line and on a circle.

More interestingly, we also consider the propagator for a particle confined to a plane when in the presence of a constant magnetic field and a potential that is independent of one of the coordinates. We find that by using the Routhian formulation, we are able to avoid the difficulty mentioned in [1] of magnetic fields giving rise to imaginary terms in the path integral measure when Wick rotating to imaginary time. We show how we can calculate the quantum corrections to the classical partition function using this method.

Finally, we attempt to calculate the partition function for a free particle confined to a sphere using the Routhian formalism, with the aim of constructing a general method of approximating the partition function for a particle in the presence of a potential that is independent of the azimuthal coordinate. In order to do this, we use a semiclassical approximation, and we reduce the problem to the calculation of an operator determinant, which involves the solution of a nontrivial differential equation. Although it is difficult to solve exactly, we show that if we approximate this determinant to that of a free particle (valid for small azimuthal momentum), we

obtain a partition function that is very close to the exact result.



## Chapter 2

# General Theory of the Classical Routhian

We will now go over the construction of the classical Routhian. Suppose we begin with a classical system whose Lagrangian is independent of some subset of the generalized coordinates used to describe the system. Calling these cyclic coordinates  $y_i$ , and the rest of the non-cyclic coordinates  $x_i$ , we write this as:

$$L(x^i, y^i, \dot{x}^i, \dot{y}^i; t) = L(x^i, \dot{x}^i, \dot{y}^i; t) \quad (2.1)$$

In order to construct the Routhian, we perform a Legendre transformation on the cyclic coordinates so as to write the system in terms of the conserved conjugate momentum (using the standard summation convention for repeated indices):

$$R(x^i, \dot{x}^i, p_i; t) = L - p_i \dot{y}^i \quad (2.2)$$

where  $p_i$  is the conjugate momentum to  $y^i$ :

$$p_i = \frac{\partial L}{\partial \dot{y}^i} \quad (2.3)$$

The equations of motion of the system in terms of its Routhian are like Euler-Lagrange equations for the non-cyclic coordinates, and like Hamilton's equations for the cyclic coordinates. In addition, the conjugate momenta  $p_i$  is conserved:

$$\frac{d}{dt} \left( \frac{\partial R}{\partial \dot{x}^i} \right) - \frac{\partial R}{\partial x^i} = 0 \quad (2.4)$$

$$\frac{\partial R}{\partial p_i} = -\dot{y}^i \quad (2.5)$$

$$\dot{p}_i = 0 \quad (2.6)$$

Alternatively, if we start with the Hamiltonian  $H(x^i, p_i, q_i)$  of some system, where  $q_i$  are the conserved momentum, and  $p_i$  are the momentum conjugate to the non-cyclic coordinates, we can construct the Routhian:

$$R(x^i, \dot{x}^i, q_i) = p_i \dot{x}^i - H \quad (2.7)$$

As a simple example, let us consider a particle in two dimensions with a potential that is independent of one of the coordinates. Its Lagrangian has the form:

$$L(x, y, \dot{x}, \dot{y}) = \frac{m}{2} \dot{x}^2 + \frac{m}{2} \dot{y}^2 - V(x) \quad (2.8)$$

The potential is independent of  $y$ , and therefore its conjugate momentum is conserved. The Routhian is given by:

$$R(x, \dot{x}, p) = \frac{m}{2} \dot{x}^2 - \frac{p^2}{2m} - V(x) \quad (2.9)$$

On some level, writing classical mechanics in terms of the Routhian is just a mathematical formality. However, its use comes in recognizing that we can simplify certain kinds of situations by utilizing conserved momenta, while at the same time not over-complicating things by introducing non-conserved momenta. In classical mechanics, one of the ways this has proved most useful has been in considering deviations from steady motion. In other words, we can consider small perturbations around steady solutions in the non-cyclic directions using states with fixed momentum [9]. However, we are not able to generalize these sorts of calculations easily to quantum mechanical situations because in those cases we need to consider contributions from all paths,

not just the steady classical paths, and so we will not further consider these kinds of examples.





## Chapter 3

# General Theory of the Quantum

## Routhian

We now wish to consider how the Routhian can be used in quantum mechanics. We will see that its usefulness comes in simplifying problems by separating out contributions to amplitudes from conserved momentum. Conventionally, there have been two major approaches to quantum mechanics. The first approach promotes the Hamiltonian to an operator acting on a Hilbert space, whereas the second approach writes the propagator as an integral over all paths between two points, weighted by the exponential of the classical action. It is this latter approach that enables us to easily isolate contributions from fixed momentum.

It is most convenient to start from the Hamiltonian formulation of the path integral. We will consider a quantum mechanical system described by coordinates  $x^i(t)$ , momentum  $p_j(t)$ , and Hamiltonian  $H(x^i, p_i)$ . The probability amplitude for a particle to propagate from  $x_I^i$  to  $x_F^i$  in time  $T$  is given by a sum over all paths in phase space connecting those points:

$$K(x_F^i, x_I^i, T) = \int_{x^i(0)=x_I^i}^{x^i(T)=x_F^i} Dx^i(t) \int Dp_i(t) e^{\frac{i}{\hbar} \int_0^T dt (p_i \dot{x}^i - H(x^i, p_i))} \quad (3.1)$$

Note that we use the notation  $\int Dx^i(t)$  to indicate path integrals over all variables  $x^i(t)$ . In addition, we will suppress writing the  $t$  dependence of these integration

variables. Now we assume that the Hamiltonian is independent of some subset of the coordinates  $y^i$  with conjugate momentum  $q_i$ . We will now use  $x^i$  to refer to the non-cyclic coordinates, and  $p_i$  to refer to their conjugate momentum. We wish to perform the integral over the cyclic coordinates, but before we can do this we must integrate by parts:

$$K(x_F^i, y_F^i, x_I^i, y_I^i, T) = \int Dx^i \int Dy^i \int Dp_i \int Dq_i e^{\frac{i}{\hbar}(q_i(T)y^i(T) - q_i(0)y^i(0) + \int_0^T dt(-\dot{q}_i y^i + p_i \dot{x}^i - H(x^i, p_i, q_i)))} \quad (3.2)$$

Now we can perform the integral over  $y^i(t)$ , yielding  $\delta$  functionals setting each  $\dot{q}_i$  to 0 at each  $t$ :

$$K(x_F^i, y_F^i, x_I^i, y_I^i, T) = \int Dx^i \int Dp_i \int Dq_i \delta[\dot{q}_i(t)] e^{\frac{i}{\hbar}(q_i(T)y^i(T) - q_i(0)y^i(0) + \int_0^T dt(p_i \dot{x}^i - H(x^i, p_i, q_i)))} \quad (3.3)$$

We can now perform the integral over  $q_i(t)$ , in which the  $\delta$  functionals set the momentum to be a constant. In particular,  $q_i(T) = q_i(0)$ . After performing this integration, we are left with a normal integral over the fixed momentum:

$$K(x_F^i, y_F^i, x_I^i, y_I^i, T) = \int_{-\infty}^{\infty} \frac{dq_i}{2\pi\hbar} \int Dx^i \int Dp_i e^{\frac{i}{\hbar}(q_i(y_F^i - y_I^i) + \int_0^T dt(p_i \dot{x}^i - H(x^i, p_i, q_i)))} \quad (3.4)$$

Note that the integrand is the exponential of the Routhian expressed in terms of  $x^i, p_i$ , and  $q_i$  rather than  $x^i, \dot{x}^i$ , and  $q_i$ . However, if we assume that the Hamiltonian is quadratic in  $p_i$ , we can perform the gaussian  $p_i(t)$  functional integral and obtain the path integral in terms of the classical Routhian:

$$K(x_F^i, y_F^i, x_I^i, y_I^i, T) = \int_{-\infty}^{\infty} \frac{dq_i}{2\pi\hbar} e^{\frac{i}{\hbar}q_i(y_F^i - y_I^i)} \int Dx^i e^{\frac{i}{\hbar} \int_0^T dt R(x^i, \dot{x}^i, q_i)} \quad (3.5)$$

By taking advantage of the symmetry of the original Hamiltonian, the path integral has been reduced to an integration only over variables that do not have conserved conjugate momenta. Given that the dependence on the conserved momenta is usually quadratic, we can in most situations perform the gaussian  $q_i$  integration. However,

doing this makes it very difficult to proceed with the remaining path integral, and we shall see that by leaving things in terms of an integral over the fixed momenta until the very end, we can obtain distinct calculational advantages.



# Chapter 4

## Examples of the Quantum Routhian

### 4.1 Free Particle

Now we shall consider some examples of the Quantum Routhian. Perhaps the simplest example of all is the free particle in one dimension, so we shall look at this first before proceeding to more complicated situations.

The Routhian in the free particle case is the negative of the Hamiltonian:

$$R(p) = -\frac{p^2}{2m} \quad (4.1)$$

Since there are no non-cyclic coordinates, the Routhian path integral reduces to:

$$K(x_I, x_F, T) = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar}(p(x_F-x_I) - \int_0^T dt \frac{p^2}{2m})} \quad (4.2)$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar}(p(x_F-x_I) - \frac{p^2 T}{2m})} \quad (4.3)$$

$$(4.4)$$

This gaussian integral can be readily done to yield the free particle propagator:

$$K(x_I, x_F, T) = \sqrt{\frac{m}{2\pi\hbar iT}} e^{-\frac{m(x_F-x_I)^2}{2\hbar iT}} \quad (4.5)$$

This result was slightly easier to obtain than it would have been had we simply done the coordinate path integral, as we avoided having to compute the determinant of a differential operator.

## 4.2 Free Particle on a circle

Now we consider a slightly more interesting example, in which we also see how utilizing conserved momentum can lead to calculational simplifications - that of a free particle confined to a circle. In order to do this, we first must deal with some subtleties related to path integral quantization on multiply connected spaces, and path integral quantization in polar coordinates. The main subtlety of the latter is that the quantum Hamiltonian operator in polar coordinates contains an extra term that comes about when we use the correct quantum mechanical forms of the radial and angular momentum operators. We will not go through the derivation, but for future reference we write down the result in d-dimensions:

$$\hat{H} = \frac{\hat{P}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2} + \frac{\hbar^2}{2m} \frac{(d-1)(d-3)}{4r^2} \quad (4.6)$$

This is the operator that must be used in the derivation of the path integral, and hence an extra term must be added to the classical action. This extra term can also be derived by directly changing variables in the path integral ([4],[2]). In addition, the terms in the measure  $dx(t)dy(t)$  becomes  $r(t)dr(t)d\theta(t)$ , and  $dp_x(t)dp_y(t)$  becomes  $\frac{1}{r(t)}dp_r(t)dp_{\theta(t)}$  at each point in time t. We would expect that the propagator for the free particle in 2 dimensions is thus:

$$K(r_F, \theta_F, r_I, \theta_I, T) = \int Dr \int D\theta \int Dp_r \int Dp_{\theta} e^{\frac{i}{\hbar} \int_0^T dt (p_r \dot{r} + p_{\theta} \dot{\theta} - \frac{p_r^2}{2m} - \frac{p_{\theta}^2}{2mr^2} + \frac{\hbar^2}{8mr^2})} \quad (4.7)$$

In this expression the limits of integration should run from 0 to  $2\pi$  for  $\theta$  and from 0 to  $\infty$  for r. However, this expression does not correctly take into account the boundary conditions at  $\theta = 0, 2\pi$  and  $r = 0$  ([3]). We can see this by noting that the particle can change coordinates from 0 to  $2\pi$  without moving, and so there will be

an incorrect contribution to the weight of the measure because of the large change in coordinate values. In addition, it does not seem that we are correctly taking into account paths that make full loops around the origin in a short amount of time.

In order to fix these problems, we can take the coordinates to range from  $-\infty$  to  $\infty$  and then sum over equivalent final points ([8]). By projecting these coordinates onto a line, a small change in coordinate values always accompanies a small change in location, and we distinguish between paths that loop around the origin many times (moving from  $\theta$  to  $\theta + 2\pi m$  means we have wrapped around  $m$  times). In other words, we define  $K^\infty$  to be the propagator given in (4.7) but with limits of integration going from  $-\infty$  to  $\infty$  in both  $r$  and  $\theta$ . The point  $(r, \theta)$  is equivalent to  $(r, \theta + 2\pi m)$  and  $(-r, \theta + \pi + 2\pi m)$ . The full propagator is given by:

$$K(r_F, \theta_F, r_I, \theta_I, T) = \sum_{m=-\infty}^{\infty} K^\infty(r_F, \theta_F + 2\pi m, r_I, \theta_I, T) + K^\infty(-r_F, \theta_F + \pi + 2\pi m, r_I, \theta_I, T) \quad (4.8)$$

Now, confining the particle to a circle fixes  $r$  to a constant, and sets  $p_r$  to 0. Imposing these conditions on the above propagator, we obtain the propagator for a particle on a circle:

$$K(\theta_F, \theta_I, T) = \sum_{n=-\infty}^{\infty} K^\infty(\theta_F + 2\pi n, \theta_I, T) \quad (4.9)$$

where

$$K^\infty(\theta_F, \theta_I, T) = \int D\theta \int Dp_\theta e^{\frac{i}{\hbar} \int_0^T dt (p_\theta \dot{\theta} - \frac{p_\theta^2}{2mr^2} + \frac{\hbar^2}{8mr^2})} \quad (4.10)$$

This is just the path integral for a free particle with an extra constant added to the Hamiltonian. The usual way of proceeding would be to use the free particle propagator (4.5) and compute the sum (4.9) using the Poisson resummation formula ([8]). However, we would like to show that if we instead use (4.2), which expresses the propagator as an integral over fixed values of the conserved momentum, the calculation becomes simpler and more physically insightful. First we write  $K^\infty$  as an integral over angular momentum:

$$K^\infty(\theta_F + 2\pi n, \theta_I, T) = \int_{-\infty}^{\infty} dp_\theta e^{\frac{i}{\hbar}(p_\theta(\theta_F - \theta_I + 2\pi n) - \frac{(p_\theta^2 - \frac{\hbar^2}{4})T}{2mr^2})} \quad (4.11)$$

Finally we perform the sum over  $n$ :

$$K(\theta_F, \theta_I, T) = \int_{-\infty}^{\infty} dp_\theta \left( \sum_{n=-\infty}^{\infty} e^{2\pi i \frac{p_\theta}{\hbar} n} \right) e^{\frac{i}{\hbar}(p_\theta(\theta_F - \theta_I) - \frac{(p_\theta^2 - \frac{\hbar^2}{4})T}{2mr^2})} \quad (4.12)$$

$$= \int_{-\infty}^{\infty} dp_\theta \left( \sum_{n=-\infty}^{\infty} \delta\left(n - \frac{p_\theta}{\hbar}\right) \right) e^{\frac{i}{\hbar}(p_\theta(\theta_F - \theta_I) - \frac{(p_\theta^2 - \frac{\hbar^2}{4})T}{2mr^2})} \quad (4.13)$$

$$= \sum_{n=-\infty}^{\infty} e^{in(\theta_F - \theta_I) - \frac{i\hbar T(n^2 - \frac{1}{4})}{2mr^2}} \quad (4.14)$$

$$(4.15)$$

We have obtained the standard result ([2]), but in doing so we have seen explicitly how the quantization of angular momentum comes about from summing over equivalent final points.

### 4.3 2-D Particle in a Magnetic Field

Finally we consider an example of a situation where utilizing conserved momentum allows us to do something that we would not otherwise easily be able to do. We look at a particle confined to a plane (the  $x$  and  $y$  directions), in the presence of a constant transverse magnetic field (pointing in the  $z$  direction). In addition, we place the particle in a potential  $V(y)$  that is independent of one of the coordinates. We shall see that by utilizing conserved the conserved momentum of the system, we are able to Wick rotate to Euclidian time (working with  $\tau = it$ ) and obtain the exponential of a positive definite quantity, with no imaginary part. This in turn allows us to use approximations that we would not otherwise be able to use. If we had tried to do this without utilizing the Routhian approach, the magnetic field term would have been imaginary, since it is coupled to the time derivative of the coordinate.

The Hamiltonian of this system is given by:

$$H = \frac{1}{2m} (\vec{p} - e\vec{A})^2 + V(y) \quad (4.16)$$



We are free to choose any vector potential  $\vec{A}$  that satisfies:

$$\vec{B} = B_0 \hat{z} = \nabla \times \vec{A} \quad (4.17)$$

In order to make the Hamiltonian independent of the x coordinate, we choose:

$$\vec{A} = -B_0 y \hat{x} \quad (4.18)$$

The Hamiltonian is then:

$$H = \frac{(p_x + eB_0 y)^2}{2m} + \frac{p_y^2}{2m} + V(y) \quad (4.19)$$

And the Routhian becomes:

$$R = \frac{m}{2} \dot{y}^2 - \frac{(p_x + eB_0 y)^2}{2m} - V(y) \quad (4.20)$$

Now, using the expression for the propagator in terms of the Routhian, we obtain:

$$K(x_F, y_F, x_I, y_I, T) = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar} p(x_F - x_I)} \int Dy e^{\frac{i}{\hbar} \int_0^T dt (\frac{m}{2} \dot{y}^2 - \frac{(p + eB_0 y)^2}{2m} - V(y))} \quad (4.21)$$

Now, suppose we perform a Wick rotation to Euclidian time, setting  $\tau = it$ . We then have:

$$K(x_F, y_F, x_I, y_I, T) = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar} p(x_F - x_I)} \int Dy e^{\frac{-1}{\hbar} \int_0^{\beta\hbar} d\tau (\frac{m}{2} \dot{y}^2 + \frac{(p + eB_0 y)^2}{2m} + V(y))} \quad (4.22)$$

We can see that the exponential term in the path integral is of the form  $e^{-ax}$  where  $a$  is a positive definite quantity. If we had started from the Lagrangian formulation of the path integral, the vector potential would have been coupled to the first time derivative of the coordinate, which would have led to an imaginary term when we performed the Wick rotation.

We are now at liberty to use approximations that are justified for path integrals with a positive definite measure. As an example of this, we will show how we can easily calculate the quantum mechanical corrections to the partition function by comparison

with the standard one dimensional result. The partition function is obtained by setting  $x_F = x_I$  and  $y_F = y_I$ , and then integrating over the mean position.

In order to proceed, we first quote the standard result ([1]). If the partition function is given by integrating  $K(y, \beta)$  over the mean value of  $y$ ,  $\bar{y}$ , where:

$$K(\bar{y}, \beta) = \int_{y(0)=y(\tau)=\bar{y}} Dy e^{\frac{-1}{\hbar} \int_0^{\beta\hbar} d\tau (\frac{m}{2} \dot{y}^2 + V(y))} \quad (4.23)$$

Then we can use the following expansion in powers of  $\hbar$  for the partition function  $Z$ :

$$Z = \sqrt{\frac{m}{2\pi\beta\hbar^2}} \int d\bar{y} e^{-\beta V(\bar{y})} (1 - \frac{\beta^2 \hbar^2}{24m} V''(\bar{y}) + \dots) \quad (4.24)$$

The higher order terms are functions of the second and higher derivatives of  $V$ . After setting  $x_F = x_I$  and  $y_F = y_I$ , we see that (4.22) looks like (4.23), but with an additional  $p$  integration, and an additional "effective potential" term  $V_{eff}(y) = \frac{(p+eB_0y)^2}{2m}$ . We can easily write down the partition function correction:

$$Z = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \sqrt{\frac{m}{2\pi\beta\hbar^2}} \int d\bar{y} e^{-\beta(V(\bar{y}) + \frac{(p+eB_0\bar{y})^2}{2m})} (1 - \frac{\beta^2 \hbar^2}{24m} (V''(\bar{y}) + \frac{e^2 B_0^2}{m}) + \dots) \quad (4.25)$$

We can at last perform the gaussian  $p$  integration:

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{-\beta \frac{(p+eB_0\bar{y})^2}{2m}} = \sqrt{\frac{m}{2\pi\beta\hbar^2}} \quad (4.26)$$

We finally obtain the result for the partition function of this system:

$$Z = \frac{m}{2\pi\beta\hbar^2} \int d\bar{y} e^{-\beta V(\bar{y})} (1 - \frac{\beta^2 \hbar^2}{24m} (V''(\bar{y}) + \frac{e^2 B_0^2}{m}) + \dots) \quad (4.27)$$

This example was deliberately simple so as to illustrate the principles of our approach without getting distracted by tedious calculations. However, it is clear that the above approach can be fairly easily generalized to more complicated magnetic fields, as long as we can choose the vector potential to be independent of one of the coordinates.

## 4.4 Free Particle on a Sphere

We now look at one final example attempting to generalize the calculation of the propagator for the free particle on a circle. Specifically, we look at the free particle on a sphere, and attempt to calculate its partition function using a semi-classical approximation, with the aim of constructing a general method that will work if we add additional potential terms that are independent of the azimuthal angle. We are presently unable to complete the calculation due to difficulty in solving a differential equation, but we show how a simple limit leads to a result that is very close to the exact answer.

In general, the propagator for a particle on a sphere can be written as a sum over equivalent points of propagators on a plane, just as in the case of the circle. This allows us to take the limits of integration on the angles (using standard spherical coordinates) to range from  $-\infty$  to  $\infty$ . On this plane, the point  $(\theta, \phi)$  is equivalent to the points  $(\theta + 2\pi m, \phi + 2\pi n)$  and  $(-\theta + 2\pi m, \phi + \pi + 2\pi n)$  for all integers  $m$  and  $n$ . Thus we write the propagator as:

$$K(\theta_f, \phi_f, \theta_i, \phi_i, T) = \sum_{m,n} K^\infty(\theta_f + 2\pi m, \phi_f + 2\pi n, \theta_i, \phi_i, T) + K^\infty(-\theta_f + 2\pi m, \phi_f + \pi + 2\pi n, \theta_i, \phi_i, T) \quad (4.28)$$

where  $K^\infty$  is given by the following phase space path integral ( $-\infty < \theta, \phi < \infty$ ):

$$K^\infty(\theta_f, \phi_f, \theta_i, \phi_i, T) = \int D\theta \int D\phi \int Dp_\theta \int Dp_\phi e^{\frac{i}{\hbar} \int_0^T dt (p_\theta \dot{\theta} + p_\phi \dot{\phi} - H)} \quad (4.29)$$

over functions satisfying  $\theta(0) = \theta_i, \theta(T) = \theta_f, \phi(0) = \phi_i, \phi(T) = \phi_f$ .

For the free particle, we have:

$$H = \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2 \sin^2 \theta} \quad (4.30)$$

Note that there is no additional  $1/r^2$  term added like in the 2-dimensional case because it happens to vanish in 3 dimensions (see 4.6). Using the standard Routhian procedure, the path integral can be simplified to a simple integral over azimuthal momentum and a path integral over  $\theta$ :

$$K^\infty(\theta_f, \phi_f, \theta_i, \phi_i, T) = \int_{-\infty}^{\infty} \frac{dp_\phi}{2\pi\hbar} \int D\theta e^{\frac{i}{\hbar}(p_\phi(\phi_f - \phi_i) + \int_0^T dt (\frac{1}{2}mr^2\dot{\theta}^2 - \frac{p_\phi^2}{2mr^2\sin^2\theta}))} \quad (4.31)$$

Even in the free particle case, this integral over  $\theta$  is quite difficult to perform. However, we have managed to simplify the problem to a path integral over one variable, with an additional effective potential. We wish to have a general method of evaluating this path integral that can also be used when there is an additional potential that depends only on  $\theta$ .

We now consider one approach to this problem - using a semiclassical approximation. In this approximation, we consider the effect of quadratic fluctuations around each classical path. In other words, we expand the path as  $\theta(t) = \theta_{cl}(t) + \alpha(t)$  where we assume  $\alpha(t)$  is small, keeping quadratic terms. The gaussian integration over  $\alpha(t)$  is performed, and we sum the result over each classical path. The resulting approximation is:

$$\int D\theta e^{\frac{i}{\hbar}S[\theta(t)]} \approx \sum_{cl} e^{\frac{i}{\hbar}S[\theta_{cl}(t)]} \det\left(-\frac{i}{2\pi\hbar} \frac{\delta^2 S}{\delta\theta^2} \Big|_{\theta_{cl}}\right)^{-\frac{1}{2}} \quad (4.32)$$

We can now use this approximation to evaluate the  $\theta$  integral:

$$K^\infty(\theta_f, \phi_f, \theta_i, \phi_i, T) \approx \int_{-\infty}^{\infty} dp_\phi e^{\frac{i}{\hbar}(p_\phi(\phi_f - \phi_i))} \sum_{\theta_{cl}} e^{\frac{i}{\hbar}S[\theta_{cl}]} \det(\hat{O})^{-\frac{1}{2}} \quad (4.33)$$

where the sum goes over all classical paths connecting  $\theta_i$  to  $\theta_f$  in time  $T$ , and the operator in the determinant is:

$$\hat{O} = -\frac{1}{2}mr^2\partial_t^2 - \frac{d^2}{d\theta^2} \left( \frac{p_\phi^2}{2mr^2\sin^2\theta} \right) \Big|_{\theta_{cl}} \quad (4.34)$$

Note that we are ignoring overall prefactors in the propagator (such as  $\frac{1}{2\pi\hbar}$ ) as they can be fixed later by normalization. The classical equation of motion is:

$$\frac{1}{2}mr^2\ddot{\theta} - \frac{p_\phi^2}{2mr^2} \frac{\cos\theta}{\sin^3\theta} = 0 \quad (4.35)$$

We can utilize the conservation of energy to help solve this equation, requiring us to solve the equation:

$$\frac{1}{2}mr^2\dot{\theta}^2 + \frac{p_\phi^2}{2mr^2\sin^2\theta} = E \quad (4.36)$$

The general solution to this equation is:

$$\cos(\theta) = A \cos(\beta t + c) \quad (4.37)$$

where A and  $\beta$  are related to the energy of the solution via:

$$A = \sqrt{1 - \frac{p_\phi^2}{2Emr^2}} = \sqrt{1 - \alpha^2}, \beta = \sqrt{\frac{2E}{mr^2}} \quad (4.38)$$

Boundary conditions fix the values of c and E. The classical action can be calculated to give:

$$S[\theta_{cl}] = ET - p_\phi \left[ \tan^{-1} \left( \frac{\tan(\beta T + c)}{\alpha} \right) - \tan^{-1} \left( \frac{\tan c}{\alpha} \right) \right] \quad (4.39)$$

In order to tackle a simpler problem than finding the propagator, we attempt to calculate the partition function. In order to do this, we will set  $\theta_f = \theta_i, \phi_f = \phi_i$ , and integrate over all coordinates. In addition, we will perform a Wick rotation to imaginary time. When we set  $\theta_f = \theta_i$ , the second term in (4.39) disappears, and we are left with  $S[\theta_{cl}] = ET$ .

This condition also leads to  $A \cos(c) = A \cos(\beta T + c)$ , which implies that  $\beta T = 2\pi\ell$  for integer  $\ell$ . This leads to a discrete classical energy spectrum:

$$E_\ell = \frac{2\pi^2 mr^2}{T^2} \ell^2 \quad (4.40)$$

In addition, since  $E = \frac{1}{2}mr^2\dot{\theta}^2 + \frac{p_\phi^2}{2mr^2\sin^2\theta}$ , classical solutions can only exist if  $E \geq \frac{p_\phi^2}{2mr^2}$ .

Using these conditions, we obtain the following form for  $K^\infty$ :

$$K^\infty(\theta_i, \phi_i + 2\pi n, \theta_i, \phi_i, T) \approx \sum_{\ell=-\infty}^{\infty} \int_{p_\phi^2 \leq 2mr^2 E_\ell} dp_\phi e^{\frac{i}{\hbar}(2\pi n p_\phi + E_\ell T)} \det(\hat{O}) \quad (4.41)$$

As long as  $0 < \theta_i < \pi$ , there are no classical paths connecting to a  $\theta_f$  outside of this range due to the infinite potential barrier, so we don't have to worry about

summing over  $\theta_f + 2\pi m$ , or the term setting  $\theta_f = -\theta_i$  in the sum (4.28). In other words, in this approximation, we have:

$$K^\infty(\theta_i + 2\pi m, \phi_f, \theta_i, \phi_i, T) \approx K^\infty(-\theta_i + 2\pi m, \phi_f, \theta_i, \phi_i, T) \approx 0 \quad (4.42)$$

for any nonzero  $m$ . We obtain the following expression for the partition function (still in real time):

$$Z \approx \int_0^{2\pi} d\phi \int_0^\pi d\theta \sum_{n=-\infty}^{\infty} \sum_{\ell=-\infty}^{\infty} \int_{p_\phi^2 \leq 2mr^2 E_t} dp_\phi e^{(2\pi i n \frac{p_\phi}{\hbar} + \frac{i E_t T}{\hbar})} \det(\hat{O})^{-\frac{1}{2}} \quad (4.43)$$

Performing the sum over  $n$  gives a sum over  $\delta(n - \frac{p_\phi}{\hbar})$  just as with the free particle on a circle, and we can easily do the  $p_\phi$  integral (which sets  $p_\phi = n\hbar$ ) and the trivial  $\phi$  integral:

$$Z \approx \sum_{\ell=-\infty}^{\infty} \sum_{n^2 \leq \frac{(2\pi)^2 m^2 r^4 \ell^2}{\hbar^2 T^2}} e^{-\frac{2\pi^2 m r^2 \ell^2}{i T \hbar}} \int_0^\pi d\theta \det(\hat{O})^{-\frac{1}{2}} \quad (4.44)$$

Finally, we can perform a Wick rotation to imaginary time (setting  $\tau = it$  and  $\tau_f = iT$ ). Note that the restriction on the  $n$  sum will still make sense, since now  $\tau_f$  will be an imaginary quantity. Clearly in order to proceed, we must actually calculate the determinant, as it can potentially depend on  $n, \ell, \tau_f$ , and  $\theta$ . Substituting the classical solution into (4.34) and rearranging gives (up to a constant):

$$\hat{O} = \partial_\tau^2 - \frac{2n^2 \hbar^2}{m^2 r^4} \frac{1 + 2A^2 \cos^2(2\pi \ell \frac{\tau}{\tau_f} + c)}{(1 - A^2 \cos^2(2\pi \ell \frac{\tau}{\tau_f} + c))^2} \quad (4.45)$$

with:

$$A^2 = 1 + \frac{n^2 \hbar^2 (\tau_f)^2}{(2\pi)^2 m^2 r^4 \ell^2} \quad (4.46)$$

$$\cos(\theta) = A \cos(c) \quad (4.47)$$

In calculating the determinant, this operator acts on all functions satisfying  $\theta(0) = \theta(\tau_f) = 0$ . Now, in order to actually calculate this determinant, we can try to use the

technique developed in [5]. Using these methods, we are able to express the ratio of the determinants of two operators in terms of the ratio of solutions of their associated homogenous differential equations. In other words, if we start with two operators  $\hat{O}_1$  and  $\hat{O}_2$  acting on functions  $g(x)$  with  $0 \leq x \leq 1$  and satisfying  $g(0) = g(1) = 0$  then the ratio of determinants is:

$$\frac{\det(\hat{O}_1)}{\det(\hat{O}_2)} = \frac{f_1(1)}{f_2(1)} \quad (4.48)$$

where  $f_i(x)$  is the solution to  $\hat{O}_i f_i(x) = 0$  satisfying  $f_i(0) = 0$  and  $f'_i(0) = 1$ .

In order to use this, we must rescale our operator so that we use the variable  $x = \frac{r}{r_f}$ . After doing this and dividing out overall constants, the operator becomes:

$$\hat{O}_s = \partial_x^2 - \frac{2\tau_f^2 n^2 \hbar^2}{m^2 r^4} \frac{1 + 2A^2 \cos^2(2\pi \ell x + c)}{(1 - A^2 \cos^2(2\pi \ell x + c))^2} \quad (4.49)$$

Using this operator, we write  $\det(\hat{O}) = \frac{\det(\hat{O}_s)}{\det(\hat{O}_s^{free})} \det(\hat{O}^{free})$  where  $O_s^{free} = \partial_x^2$ . The subscript s means scaled, and the scaling that we've done to  $\hat{O}$  is exactly cancelled by the scaling we do to get from the actual free particle operator to  $O_s^{free}$ .  $\det(\hat{O}^{free})^{-\frac{1}{2}}$  is just the prefactor of the free particle propagator. In addition, the solution to  $\hat{O}_s^{free} f(x) = 0$  satisfying  $f(0) = 0$  and  $f'(0) = 1$  is  $f(x) = x$ , so we have  $f(1) = 1$ . This gives us:

$$\det(\hat{O})^{-\frac{1}{2}} = \frac{1}{\sqrt{g(1)}} \sqrt{\frac{m}{2\pi \hbar \tau_f}} \quad (4.50)$$

where  $g(x)$  is the solution to  $\hat{O}_s g(x) = 0$  satisfying  $g(0) = 0$  and  $g'(0) = 1$ . This is a difficult differential equation to solve, and we have not yet been able to find an exact solution. The simplest way to proceed is to just ignore the effective potential term, and we expect that doing this will approximate the real answer when  $\frac{\tau_f^2 n^2 \hbar^2}{m^2 r^4} \ll 1$ . This will stop being valid when we get to terms with high azimuthal momentum (large n) or large times. However, although this is not the ideal kind of approximation that we would like to make, it is instructive to work through this limit.

In this situation, the determinant gives simply  $\det(\hat{O})^{-\frac{1}{2}} \approx \sqrt{\frac{m}{2\pi \hbar \tau_f}}$ , and we obtain, up to a  $\tau_f$  independent constant:

$$Z \approx \frac{1}{\sqrt{\tau_f}} \sum_{\ell=-\infty}^{\infty} \sum_{n^2 \leq \frac{(2\pi i)^2 m^2 r^4 \ell^2}{\hbar^2 \tau_f^2}} e^{-\frac{2\pi^2 m r^2 \ell^2}{\tau_f \hbar}} \quad (4.51)$$

$$\approx \frac{1}{\sqrt{\tau_f}} \sum_{\ell=-\infty}^{\infty} \left( 2 \left( \frac{2\pi i m r^2 \ell}{\tau_f} \right) + 1 \right) e^{-\frac{2\pi^2 m r^2 \ell^2}{\tau_f \hbar}} \quad (4.52)$$

$$(4.53)$$

Using the Poisson resummation formula ( $\sum_n e^{-\pi a n^2 + 2\pi i b n} = \frac{1}{\sqrt{a}} \sum_n e^{-\frac{\pi(n-b)^2}{a}}$ ) and its derivative with respect to  $b$ , we can finally rewrite this as:

$$Z \approx \sum_{\ell=-\infty}^{\infty} (2\ell + 1) e^{-\frac{\ell^2 \hbar \tau_f}{2m r^2}} \quad (4.54)$$

We have obtained an answer very close to the exact result (the only difference being  $\ell(\ell + 1)$  in the exact result is replaced by  $\ell^2$  here). Unfortunately, it is hard to justify the above manipulation, as our approximation may break down for terms with very large  $n$  (and hence very large  $\ell$ ). Because of this problem, we tentatively propose that it may be possible to come up with a better approximation scheme for solutions to the differential equation using the WKB method. We note that because we performed the Wick rotation before attempting to solve the differential equation, the WKB method will yield solutions that are exponential rather than oscillatory due to the change in sign of the effective potential term, and we hope that this extra exponential dependence may provide a more accurate correction to the resulting energy levels.

Nevertheless, we have seen how we can obtain a good approximation to the quantum spectrum by considering the energies of periodic classical orbits, and this was made possible by the use of conserved azimuthal momentum. Once an approximation scheme to solving the problematic differential equation can be found that is valid for all values of  $n$ , we hope to use this same procedure in more complicated situations. For example, it would be interesting to attempt to calculate the partition function for a quantum spherical pendulum (i.e., as above, but with an additional potential  $V(\theta) = mg \cos(\theta)$ ). The classical solutions in this case correspond to elliptic functions, and we could try to find the classical energy spectrum of periodic orbits in a



similar fashion as above. We then hope to find an approximation to the partition function using this spectrum.



# Chapter 5

## Conclusions

In this thesis we have explored a few examples of how the Routhian can be used in quantum mechanics. We have seen how writing the propagator or partition function of a system in terms of its conserved momentum can simplify calculations, avoid coupling magnetic fields to velocities, and make progress in deriving the partition function for a particle confined to a sphere using periodic classical orbits.

Clearly there is much more that can be done with this idea, such as considering more complicated magnetic fields and adding extra potential terms to the particle confined to a sphere. In particular, in the future we would like to try to consider a particle in a magnetic field in the presence of a radial potential, so that by using conserved angular momentum, we can perhaps perform a path integral derivation of the Zeeman effect. In addition, we would like to consider the use of the WKB approximation in calculating the kinds of operator determinants that appear in the semiclassical approximation of a particle confined to a sphere. We expect that this kind of approximation will be usable in more complicated situations, such as a gravitational potential.

In addition, it is worth exploring whether this kind of procedure can work in situations with different kinds of symmetries - symmetries that do not necessarily manifest themselves in the form of cyclic coordinates. We would like to determine if there is a general method for simplifying a path integral by making use of a system's conserved Noether currents, or if it must be done on a case by case basis. It is at

least clear that the use of conserved quantities in the calculation of path integrals has not yet been exploited to its fullest extent, and we hope that this thesis has helped to show that further exploration along these lines may be fruitful.

# Bibliography

- [1] R. Feynman and A. Hibbs, "Quantum mechanics and path integrals", McGraw-Hill, New York, 1965.
- [2] M. Gutzwiller, et al., "Path integrals from meV to MeV", World Scientific, Philadelphia, 1986.
- [3] A. Kapoor, P. Sharan "Hamiltonian path integral quantization in polar coordinates", 1998, arxiv:quant-ph/9804037
- [4] D. Khandekar, S. Lawande, and K. Bhaqwat, "Path-integral methods and their applications", World Scientific, River Edge, NJ, 1993.
- [5] K. Kirsten and A. McKane, "Functional determinants by contour integration methods", 2003, arxiv:math-ph/0305010
- [6] S. Lundquist, et al., "Path summation: achievements and goals", World Scientific, Teaneck, NJ, 1988.
- [7] G. Paz, "On the Connection between The Radial Momentum Operator and the Hamiltonian in n Dimensions", 2001, arxiv:quant-ph/0009046
- [8] L. Schulman, "Techniques and applications of path integration", Wiley, New York, 1981.
- [9] D. Wells "Theory and Problems of Lagrangian Dynamics" McGraw-Hill, New York, 1967.