Quantum Dynamics barring the Schrodinger Equation

A Theory on the Unification of the Foundations of Quantum Fluid Dynamics with Path Integrals

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In India, at the Undergraduate level, there might be many programmes that offer a student with exposure to research. But I doubt if any of them even have the potential of actually shaping the life of a young scientist like NIUS does.

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[2]A pre-print of a manuscript prepared for publication in peer-reviewed journal can be accessed at: `https://arxiv.org/abs/2002.00255`

This thesis is Dedicated to

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Abstract

In 1927, soon after the discovery of Schrodinger Equation, Madelung had recast it into a hydrodynamic structure that deals with only real and observable quantities like probability density and current density. The hydrodynamic formulation of Quantum Mechanics, which started off from the shore of de Broglie's pilot wave theory, was later expanded and founded as Quantum Fluid Dynamics (QFD) by David Bohm. Since then, QFD has attracted attention of physicists and chemists, particularly owing to its parallelism to classical fluid dynamics, in the subject areas of Theoretical Chemistry, Condesed Matter Physics and Material Sciences. It has been used in problems as varied as simulating solutions of Gross-Pitaevskii equations in the study of Quantum Superfluids, In the foundations of many body Density functional Theory (DFT), In theoretical formulation and study of Quantum Nonlocality, In studying the Bogoliubov dispersions in experimental systems of Quantum Superfluid of Light and experimental observation of Hawking Radiations in acoustic black holes.

The dynamical problem of QFD is posed as a system of coupled nonlinear first order partial differential equations (PDE)s. One of them is the continuity equation, the other being a Quantum Mechanical analogue of the Hamilton Jacobi (H-J) equation. The key ingredient of QFD is the Quantum Potential (QP), which serves as the quantum correction to the classical framework, and as is argued, being the only quantity depending explicitly on Plancks constant, it brings in all the quantum effects to the dynamical system,

The computation of QP, for a general system, however, have posed serious challenges in QFD. David Bohm had suggested that the best way to obtain the QP is to solve the time dependent Schrodinger Equation followed by the Madelung transformation. However this poses a question of practicality as the wave-function itself can provide one with the same data. Several numerical ways out, such as Quantum Trajectory Method (QTM) have been proposed to circumvent this problem. The solutions obtained so, however are often unstable.

In this work, we present an answer to the question: whether there exists an analytical method of obtaining the Quantum Potential without solving the Schrodinger Equation. For this purpose, we resort to Feynman Path Integrals (PI). Empowered with its integral equations,

we logically derive an analytic form of the Quantum Potential, as a functional of the classical path and using it obtain the Quantum Trajectories. The work formally bridges the Path Integral approach with Quantum Fluid Dynamics. As a model application to illustrate the method, we work out a toy model viz. the double-well potential, where the boundary value problem for the classical path has been computed perturbatively. We, then, delve into seeking insight in one of the long standing debates with regard to Quantum Tunneling.

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Chapter 1

Introduction

In Classical theories of Dynamics, the dynamical state of a system at a particular instance is determined completely by specifying the co-ordinates, x_i and the momenta, p_i of each of its constituent particles (point-mass). The whole programme of dynamics then reduces to study the time evolution of this system, the governing laws being the equations of motion. Given a potential $V(\mathbf{x})$, these can be obtained, for example by Newton's law. There, however, exists several other formulations of classical dynamics, each with their own programme of obtaining the equations of motions, and all can be shown to be equivalent in the sharing domain of their applicability. Each of these formulations has their own advantages and disadvantages when it comes to computation of various quantities.

The Lagrangian formulation of Classical Mechanics allows one to obtain the equations motion by optimising a scalar quantity, which is often a simpler method than the component-wise force balance, as is prescribed by Newton. [1] We define the scalar quantity Lagrangian $\mathcal{L} = T - V$, where T is the kinetic energy of the system and V is the potential. The action integral, or the Hamilton's principle function is then defined as, $S = \int_{t_i}^{t_f} \mathcal{L}(x, \dot{x}, t')dt'$. The equations of motion, namely the Euler-Lagrange is then obtained by optimising the integral, $\delta S = 0$ using variational calculus. The resulting equations are,

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt}\Big(\frac{\partial \mathcal{L}}{\partial \dot{x}}\Big) = 0 \tag{1.1}$$

These equation is equivalent to Newton's Laws for the same system [2, 3].

The Hamiltonian is constructed from the Lagrangian using a Legendre Transformation,

$$H(\mathbf{x}, \mathbf{p}) = \mathbf{p}.\dot{\mathbf{x}} - \mathcal{L}(\mathbf{x}, \dot{\mathbf{x}}) \tag{1.2}$$

[1] The equations of motions for Hamiltonian formulation are first order and 2-n many.

[1] the boldface letters denote a vector.

$$\dot{x_i} = \frac{\partial H}{\partial p_i} \;\; ; \;\; \dot{p_i} = -\frac{\partial H}{\partial x_i} \tag{1.3}$$

Based on this governing equations, the theory of Classical Mechanics forms one of the most developed mathematical formulations among physical theories. It offers robust and well-founded tools to physicists to study a wide range of diverse phenomena. The theory of Quantum Dynamics, hence, in general has been formulated in parallelism to it, such that once the basic equations and quantities of the two formulations are identified, all the machinery of classical mechanics can be put into use in the exact same way. This construction of this map between quantities and dynamical equations of two theories, or, defining the quantum analogues of observables in classical mechanics is called the process of *Quantization.*

The orthodox interpretations of non-relativistic quantum theory is fulcrumed upon representation of dynamical states of a system with wave functions $|\psi\rangle$. These wave functions are elements of a Hilbert space with a complex field. One of the two equivalent ways of computing these wave functions is given by the Heisenberg matrices. The Hiesenberg formulation of quantum mechanics had been developed in close analogy with the Hamiltonian formulation of Classical Mechanics, with an one-to-one relation between the operators and the observables, and between Commutators and Poisson Brackets respectively, which yields equations of motion of exactly the same form in both the formulations.

$$(p, q) \to (\hat{P}, \hat{Q})$$
$$\frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q} = \{A, B\} \to [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

and

$$\frac{dA(t)}{dt} = \{H(t), A(t)\} \to \frac{d\hat{A(t)}}{dt} = \frac{i}{\hbar}[\hat{H(t)}, \hat{A(t)}] \tag{1.4}$$

where the last set are the equations of motion of the respective formulations. This is termed as *Canonical Quantization.*

The other theory is a based on differential equation. The vectors that are allowed to represent physical states of a system are given by square integrable solutions of the equation of Schrodinger [4]

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{1.5}$$

It can be shown that eq (1.4) and (1.5) are related by a change of basis in the Hilbert Space (an *Unitary Transformation*, to be specific), and hence are similar. Without

loss of generality, through out the discourse we refer to the second formulation as the *usual* formulation of Quantum Theory.

The orthodox theory stands on a set of axioms (postulates). It turns out that the internal consistency of the formulation demands us to define the wave function to be the most complete description of the system, even though it provides us only with the statistical moments of various observables. The measurements in this formulation also requires us to divide the world into quantum system and classical observers.[5] To be consistent with experimental results the orthodox theory takes resort to the axiom of irreversible wave function collapse. *Measurement* in Quantum Theory is usually modelled as an interaction between a classical (like a needle) and quantum (like a atom) system using a single photon. The quantum system under this interaction can in general be any of the multiple possible *eigen-states* of the operator corresponding to classical apparatus. Quantum theory allows the quantum system to be in a superposition of the aforementioned eigenstates. In that case, under the measurement, the wave funtion will at random to any of the eigen states, and the device records the corresponding eigenvalue. This process is assumed to be inherently unpredictable, uncontrollable and unanalyzable.[6] The experimental measurements in quantum theory is supposed to be sampled over many many instances of identical set-up. The orthodox interpretation then successfully predicts the average and other moments of the distribution.

Due to the famous inequality due to John Bell[5, 7], the property of non-locality is incircumventedly attributed to any valid formulation of quantum theory. This inherent non-local nature allows one to analyze the quantum phenomena in parallelism to the theory of complex systems. A *complex system* usually has a large numbers of coupled degrees of freedom. This often makes the overall dynamics to decipher by keeping track of all the dynamical details of degrees of freedoms. The rules governing the complex systems, hence, depend upon the level at which it is studied. The models at different level can be very distinct and often it is impossible to reduce the rules at a higher level, in terms of combination of lower ones, a property named as *emergence*. A classic example for same is Biological systems. It is understood that the basic governing laws for dynamics of individual atoms is given by the theory of Quantum Mechanics. In principle one could write down a wave-function of a human body and deduce in principle every aspect of its dynamics from the same. However such a task is ridiculously impractical. There however exists sound understanding of the chemical reactions in our physiology, how they combine with each other to dictate the overall mechanism e.t.c. which in most cases are not drawn from a theoretical quantum foundation. Similarly chances are, that the mathematics of the orthodox formulation with its statistical nature studies the system at a level underlying to which an entirely deterministic theory is hiding.

Various enquirers have been driven forward in various routes in search of such an underlying structure to the wave function dynamics. The Madelung transformation [8, 9] had opened a possibility of looking at the quantum systems as probability fluids, a philosophy later theorized and interpreted by works of David Bohm.[10, 11].[2]. It is

[2]Later more general derivation has been carried out by Takabyashi[12]

this hydrodynamic interpretation of Quantum Mechanics, that we deal with during this work.

The Bohmian formulation is essentially looking at the solution of Schrodinger equation decoupled in two polar components. The primary advantage it provides is that the quantities being dealt with here are reals, (namely the probability density $\rho(x,t)$ and action, $S(x,t)$), both of which has straightforward classical analogues. Historically, hence, it has been used significantly to usher lights on problems of Quantum-Classical transitions e.t.c. [13]. Owing to its *classical-like* formulation it has also found wide application studying dynamics of systems, especially in the context of chemical systems.[14–16]. Especially in this context various numerical methods have been developed to solve for time evolution of the two aforementioned quantities [17].

On the other hand, people have also looked for the foundation of the wave-function formalism starting from Classical principles. This quest in particular started from the question of what is the role of Lagrangian in Quantum Mechanics [18]. Developing on these ideas of Dirac, Feynman formulated the Path Integrals formalism, which can be shown to be an integral equation formulation for non-relativistic quantum theory. In this work, we primarily attempt to bridge the gap between the Path Integral formulation with Bohmian equations.

The rest of the report is organised as follows. In the remaining of this chapter we briefly introduce both the theories and layout the known results that we need. Chapter 2 deals with our formulation of Quantum Fluid Dynamics from the Path Integrals. In Chapter 3 we study the anaharmonic oscillator as model to illustrate our methodology. Chapter 4 deals with an incomplete attempt for a relativistic generalisation of our work.

1.1 Quantum Fluid Dynamics

Consider the Schrodinger equation for a body with mass m, traversing under the action of a potential $V(x)$ (in 1 dimension).

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \frac{(-i\hbar\nabla)^2}{2m}\left|\psi(t)\right\rangle + V(x)\left|\psi(t)\right\rangle \tag{1.6}$$

where, without loss of generality we substitute,

$$\left|\psi(x,t)\right\rangle = R(x,t)e^{iS(x,t)/\hbar} \tag{1.7}$$

Here both R(x,t), the amplitude and S(x,t), the phase function are real and always, $R(x,t) \geq 0$. The probability density associated with $\Psi(x,t)$ is defined as

$$\rho(x,t) = R(x,t)^2 \tag{1.8}$$

and the local mean flow velocity[19] as

$$v(x,t) = \nabla \frac{S(x,t)}{m} \tag{1.9}$$

Acting on this, the resultant equation can be decoupled into the real and imaginary components,

$$\begin{aligned} -\hbar \frac{\partial R(x,t)}{\partial t} &= \frac{2\hbar}{2m} \nabla R(x,t) \nabla S(x,t) + \frac{\hbar}{2m} R(x,t) \nabla^2 S(x,t) \\ -R(x,t) \frac{\partial S(x,t)}{\partial t} &= \frac{1}{2m} R(x,t) (\nabla S(x,t))^2 + V(x) R(x,t) - \frac{\hbar^2}{2m} \nabla^2 R(x,t) \end{aligned}$$

which can be reduced to

$$\frac{\partial \rho}{\partial t} + \nabla(\rho v) = 0 \tag{1.10}$$

$$-\frac{\partial S}{\partial t} = \frac{1}{2} m v^2 + V(x,t) + Q(x,t) \tag{1.11}$$

using $\rho(x,t) = R(x,t)^2$ and the definition of velocity. Here $Q(x,t)$ denotes the quantum potential and is given by,

$$Q(x,t) = -\frac{\hbar^2}{2m} \frac{\nabla^2 R(x,t)}{R(x,t)} \tag{1.12}$$

Equation (1.10), is a continuity equation which states that the probability is conserved. (1.11), on the other hand gives a dynamical equation of the Hamilton-Jacobi form, with the *quantum correction* term $Q(x,t)$. Interpreted in this way, Quantum Dynamics can be thought of as a dynamics of probability fluids.

The only explicit dependence on $\hbar$ comes in this set of equation via the Quantum Potential. At the classical limit, $\hbar \to 0$, this term vanishes and we retrieve governing equation for a Hamiltonian fluid. $Q(x,t)$ hence is thought of as the origin of all Quantum effects. It is inherently non-local in nature, bringing in the consistency required by Bell.

The measurement problem is addressed in this formulation by introducing an extra variable, the particle position, that exists, according to this theory irrespective of it is measured or not. In par with the concepts classical physics, measurements of all other variables are reduced to measurement of positions. [3]

[3]How measurement is to be treated from this angle of looking at quantum systems is discussed in detail by Bohm in his second paper [11]

The dynamical problem under Quantum Fluid Dynamics, is formulated as solving for the *Quantum Trajectories* which satisfies a *Quantum* equation of motion, viz.

$$\frac{d^2x(t)}{dt^2} = -\nabla(V + Q) \tag{1.13}$$

These trajectories are interpreted as streamlines of probability fluid element. The structure of this equation illustrates the deterministic nature of the time evolution. However the fundamental drawback of this formulation is the difficulties that it poses in finding the solutions of Quantum Trajectory. If the wave-function is not known, then it is fairly hard to iterate this equations in a self-consistent manner, and it is impossible to do so analytically.

Bohm [10] had suggested that the easiest way to obtain the Quantum Potential is to first solve for the solution of Schrodinger Equation, $\psi(x,t)$, then obtain the Quantum Potential via a Madelung Transformation. But question arises about the practicality of doing such extra calculation, when the physically relevant quantities can already be obtained directly from $\psi(x,t)$ itself by the Orthodox interpretation. Numerical attempts has been made to circumvent this issue, by forming a self consistent set of coupled dynamical equations. [17] There are several ways of combining the available informations to form such a set. One of them is the *force version*,

$$\frac{d\rho}{dt} = -\rho\nabla.v \tag{1.14}$$
$$m\frac{dv}{dt} = -\nabla(V + Q) \tag{1.15}$$
$$\frac{dS}{dt} = \mathcal{L}(t) = \frac{1}{2}mv^2 - (V + Q) \tag{1.16}$$

A disadvantage of this method is the spatial derivatives of Quantum Potential is required for the same, which brings additional sources of errors. Another version is the *Potential Energy Method*, where the force is not explictly calculated,

$$\frac{d\rho}{dt} = -\rho\nabla.v \tag{1.17}$$
$$\frac{dS}{dt} = \mathcal{L}(t) = \frac{1}{2}mv^2 - (V + Q) \tag{1.18}$$
$$\frac{dx}{dt} = v = \frac{\nabla S}{m} \tag{1.19}$$

In absence of the terms which involves spatial derivatives, these equations would have been easier to solve for. This because we know the value Hydrodynamic fields only in the positions of the fluid elements. This positions are in turn to be dictated by the equation we solve for. So, even if one starts from a regular grid, under time

evolution it usually becomes non-structured very fast. This error can be rectified to some extent by using algorithms like moving-least-square methods[15], or adaptive grids, making the iteration fairly complex.

The main question that we wish to address is whether there is an analytical way out to this problem. That is, given the information of an initial distribution and an applied potential, whether it is possible to write down the Quantum Potential as a functional of them.

To that end we start with reformulating the formulation from the theory of Path Integrals, the basic principles of which is illustrated bellow.

1.2 Path Integral Formulation

The main idea behind the formulation of Path Integrals was engraved in the search for an *Lagrangian Formulation* of Quantum Mechanics.[18] In the classical case, these equation of motions could as well be obtained by varying the action function in the Lagrangian Formulation. However it is not feasible to do an analogous thing in quantum mechanics, as over there the derivatives w.r.t. coordinates and momenta can only enter in the equation of motion through the commutators.

The analogous quantity to the classical mechanical Lagrangian was thus constructed in a different route by Dirac [20], from the study of quantum mechanical contact transformations. Form the theory of functions of non-commutative observables, it can be shown that the analogue of Lagrangian can be achieved, if the quantum mechanical contact transformation is postulated to have a form $\exp\left(\frac{iS}{\hbar}\right)$. This forms the foundations of the theory of Path Integrals in Quantum Mechanics.

Definition 1 (Observables)**.** *Observables in quantum mechanics are defined as Hermitian quantities (in general non-commutating) with a complete eigenbasis.*

In Hiesenberg formulation the observables are represented as matrices, whereas in Schrodinger formulation these are represented as operators acting on functions of positional (and other relevant) variables. A function of such non-comutative observables can be defined as follows,

Definition 2 (Functions of non-commuting variables)**.** *Let A, B be two operators, and*

$$A\left|a\right\rangle = a\left|a\right\rangle, B\left|b\right\rangle = b\left|b\right\rangle$$

where $\left|a\right\rangle, \left|b\right\rangle$ is sampled from the respective complete basis sets. Let $f(ab)$ be a function having (a,b) as its domain, a,b being eigenvalues of A,B respectively. A function of a single observable is then defined treating the other eigenvalue as a parameter such that,

$$f(Ab)\left|a\right\rangle = f(ab)\left|a\right\rangle \tag{1.20}$$

holds for every eigenvector $|a\rangle$ of A. The function of two non-commuting observable $f(AB)$ is then defined as,

$$f(AB)\,|b\rangle = f(Ab)\,|b\rangle \tag{1.21}$$

Note, since A, B do not commute in general, the definition is dependent on order, and in general the result will be different if they are exchanged. The same can be extended to accommodate functions of any finite number of non-commuting operators. In non-relativistic quantum mechanics, this ordering is given naturally by the ordering of time and can accommodate any number of variables as long as the variables defined at same time are not non-commuting.

Definition 3 (Probability)**.** *A probability theory can be set up, using the indicator function, $I(abc\cdots)$, such that it is unity when, a,b,c e.t.c are eigen values of the operators A,B,C. For any state $|\psi\rangle$, the probability of a being an eigen-value of A, b being an eigen-value of B e.t.c is then given by,*

$$P(abc\cdots) = \langle\psi|\, I(abc\cdots)\,|\psi\rangle \tag{1.22}$$

So the average of any other function can be obtained as,

$$\langle f(ABC\cdots)\rangle = \sum_{a,b,c} f(abc\cdots)P(abc\cdots) \tag{1.23}$$

for any state. Now, using suitable basis changes, it can be shown that for any state $|\psi\rangle$,

$$\begin{aligned}&\langle\psi|\, f(Q_1Q_2\cdots Q_n)\,|\psi\rangle \\ &\qquad = \int\int\cdots\int dq_1' dq_2'\cdots dq_n' f(q_1'q_2'\cdots q_n')\,\langle\psi|\,|q_1'\rangle\,\langle q_1'|\,|q_2'\rangle\cdots\langle q_n'|\,|\psi\rangle\end{aligned}$$

The propagator, $\langle\psi(t)|\,|\psi(0)\rangle$ can be obtained from the same, if we substitute $f(q_1'q_2'\cdots q_n') = 1$. Now, consider the particular form of $\langle q|\,|Q\rangle$,

$$\langle q|\,|Q\rangle = \exp(\frac{iS(qQ)}{\hbar}) \tag{1.24}$$

then,

$$\langle q|\, p_r\,|Q\rangle = -i\hbar\frac{\partial}{\partial q_r}\,\langle q|\,|Q\rangle = \langle q|\,\frac{\partial S(qQ)}{\partial q_r}\,|Q\rangle \tag{1.25}$$

$$\langle q|\, P_r\,|Q\rangle = -i\hbar\frac{\partial}{\partial Q_r}\,\langle q|\,|Q\rangle = -\,\langle q|\,\frac{\partial S(qQ)}{\partial q_r}\,|Q\rangle \tag{1.26}$$

which in the operator language translates to,

$$p_r = \frac{\partial S(qQ)}{\partial q_r} \; ; \; P_r = -\frac{\partial S(qQ)}{\partial Q_r} \tag{1.27}$$

which have the exact same form as of the classical equations of transformation, where S denotes the action. This then paves out the way for constructing an *Lagrangian* formulation of Quantum Mechanics.

The propagator then becomes,

$$\begin{aligned} K(x, x_0; t, 0) &= \langle \psi(t) | \, | \psi(0) \rangle \\ &= \int \int \cdots \int dq_1' dq_2' \cdots dq_n' \exp\Big(\frac{i \sum_i S(q_i, q_{i-1})}{\hbar}\Big) \end{aligned}$$

Which forms the basis of the path integral formulation.

Leaping from this suggestion of Dirac, Richard Feynman postulated[21, 22] that, starting from a given point, the dynamics of a particle to a final point in a given time interval, according to this formulation is contributed by all the possible paths, the particle can take. Their contribution to the dynamics is weighed by $\exp(iS[x(t)]/\hbar)$, where S[x(t)] is the action or Hamilton's principle function associated with that particular path. Equipped with this, the path integral formulation is able to tell us the probability of finding a particle at a final point after a finite time interval, starting from a given point. The initial wave-function and the final wave-function after time t is related by a propagator. The integral,

$$\psi(x_b, t) = \int_{-\infty}^{\infty} K(x_b, t; x_a, 0) \psi_0(x_a) dx_a \tag{1.28}$$

gives the time evolution.

The propagator can be identified as the Green's function to Schrodinger equation.

In spite of its remarkable internal consistency and aesthetics. the path integral formulation suffers from two folds of problems. The action of a path is not a function of the path variables but its a functional of the path itself, which makes it difficult to integrate over. To find a propagator we need to have in principle an weighted summation of contribution of continuum amount of possible paths. This makes general computations for Path Integrals extremely hard.

In some cases this can be by-passed by discretizing the path variables in time, evaluate the integrals at each of them and finally obtain the limit from discrete to continuum, in a manner analogous to the Riemann Integrals. By this method we can obtain the propagator for free particle and Simple Harmonic Oscillators. But in most cases the integrals are hard to do and in some cases, impossible.

As is illustrated earlier, we start our analytical quest by first a closed form solution for the propagator. Then we use the same to obtain the Quantum Trajectories.

1.3 Problem Statement

As was mentioned in section 1.2, Bohmian formulation suffers from a practical question of applicability. Even as various numerical methods have been suggested [15, 17, 23] as a remedy, those usually suffer from the problems of unstructred grids and unstable solutions. In this project we attempt to answer the question whether there exists an analytical solution for the same.

The path integral formulation in principle calculates the time evolution of the wave function of a system, just from the knowledge the of classical Lagrangian (which requires us to specify the applied potential term only) and a given initial distribution. This property is inevitable to any governing equation of quantum mechanics as the Hamiltonian is undetermined over an applied potential and the Schrodinger's equation is first order in time.

The Bohmian formulation, on the other hand, starts from these solution and then picturizes a dynamics which is very analogous to the classical philosophy, and in principle produces all the results as that of the orthodox formulation. Here we delve into the possibility of obtaining the Madelung's Equations and the Quantum Trajectories directly from the Path Integrals, bypassing the solution to Schrodinger's equation entirely.

As we illustrate in the next sections, it is entirely possible to give a functional form to the Madelung Potential, in terms of the classical path and the initial wave function and thereby obtain the Quantum trajectories directly, just by specifying the two. We first construct a general solution for the propagator, and then use it to develop the Quantum Trajectories. For any system, for which the classical boundary value problem can be solved exactly, we can obtain the propagator analytically. Otherwise the complexity of the problem is formally reduced to the solution of this BVP, numerically.

Chapter 2

Formulation

In this section we present an exact analytical series form for the propagator (two-point correlator) for a quantum particle in a general applied potential $V(x)$. In Path Integral formalism, the correlator gives the amplitude at a point x, after a time of flight t, given that it has started from an initial point y. This propagator serves as a Green's function to the Schrodinger equation [21], which renders Path Integrals its formal equivalence with the usual formulations. Equipped with this, we pose the solution to quantum trajectories, in an integral equation framework.

2.1 The Theory

Consider a particle with mass M, moving in one dimension under the action of a conservative force generated by potential $V(x)$. We first treat the one dimensional system and then extend it to higher dimensions.

Let's $x^{cl}(t)$ denote the classical path of the system, from the initial position x_a, to a final point x_b after a time of flight t. Being solution to a second order Boundary Value Problem, it parametrically depends on x_a, x_b.

A general path, $x(t)$ of the system is any continuous function of t that satisfies the constraint, $x(0) = x_a$ & $x(t) = x_b$.

Any such general path can be decomposed as

$$x(t) = x^{cl}(t) + y(t) \tag{2.1}$$

Varying $y(t)$ to span the space of continuous functions on $[t_0, t]$ subjected to the boundary conditions, $y(t_0) = y(t) = 0$ is tantamount to spanning the space of allowed paths of Path Integral formulation, over which we need to integrate in order to obtain the propagator.[22]

One way to compute the path integral is to first discretise the time axis into n moments, separated by ϵ units.

$$t_j = j\epsilon,$$
$$t_0 = 0\ ,\ \ t_n = t$$

The path integral can then be recovered by finally taking the limit $n \to 0, \epsilon \to \infty$, such that the product remains constant, $n\epsilon = t$, after the n-dimensional integral is carried out. Equation (2.1) then becomes,

$$x(t_j) = x_j = x_j^{cl} + y_j. \tag{2.2}$$

at each of these moments. By definition $y_0 = y_n = 0$.

The propagator is defined as,

$$K(x_b, t; x_a, 0) = \int \exp\big[\ \frac{i}{\hbar}\int_0^t \mathcal{L}(x, \dot{x}, t')\ dt'\big]\ \ \mathcal{D}x \tag{2.3}$$

where $\mathcal{L}(x, \dot{x}, t')$ is the classical Lagrangian of the system. Eq (2.3) can be rewritten, in the discretised version as,

$$\lim_{n\to\infty}\ \frac{1}{A}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\Big(\frac{i\epsilon}{\hbar}\sum_{j=1}^{n}\Big[\frac{M}{2\epsilon^2}(x_j - x_{j-1})^2 - V(x_j)\Big]\Big)dx_1\cdots dx_n \tag{2.4}$$

Here A is the normalization constant, which is the product of the respective normalization constants of the individual y_j integrals. In general, it depends on n.

Throughout this report, the limit is understood to be taken as $n \to \infty$ and $\epsilon \to 0$ simultaneously, with $n\epsilon = t$ remaining constant.

The potential over the general path can be Taylor expanded the around the classical position at each of this moments, as [1]

$$V(x_j) = V(x_j^{cl} + y_j) = V(x_j^{cl}) + \sum_{m=1}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}} \tag{2.5}$$

Substituting (2.2),(2.5) into (2.4) we obtain,

[1]The radius of convergence depends on the V(x), its higher derivatives and the convergence is not guaranteed in general.

$$\lim_{n\to\infty} \frac{1}{A}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\Big(\frac{i\epsilon}{\hbar}\sum_{j=1}^{n}\Big[\frac{M}{2\epsilon^2}(x_j^{cl}-x_{j-1}^{cl})^2+\frac{M}{2\epsilon^2}(x_j^{cl}-x_{j-1}^{cl})(y_j-y_{j-1}) + \frac{M}{2\epsilon^2}(y_j-y_{j-1})^2 - V(x_j^{cl}) - \sum_{m=1}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}}\Big]\Big)dy_1\cdots dy_n \quad (2.6)$$

The terms in (2.6), those are independent of y_j, can be taken out of the integrals and they would add upto $\exp\big[iS_{cl}(x,t;x_0,0)/\hbar\big]$, where $S_{cl}(x,t;x_0,0)$ is the Classical Action. It can be shown that, the linear terms in y_j do not contribute, using a change of variables having Jacobian determinant 1.[22] [2]

For the Harmonic Oscillator, the rest of the integral is independent of $x^{cl}(t)$, since the second derivative of $V(x)$ is a constant and higher derivatives vanish. After all y_j are integrated out, it leaves out only a time dependent factor.

The primary difference as well as the complication in the generalization from the corresponding case of Harmonic Oscillator, that forms the thesis of this work, stems form the fact that the higher derivatives of the potential ($m = 3$ and higher) do not go to zero and, in general, depends on the positional variables x_j^{cl}. These, in turn, show up in the pre-factor, and, in general, makes it dependent on position.

The rest of the general integral, that denotes the pure quantum part, is

$$\lim_{n\to\infty} \frac{1}{A}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\Big(\frac{i\epsilon}{\hbar}\sum_{j=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_j-y_{j-1})^2-\frac{y_j^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_j^{cl}} - \sum_{m=3}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}}\Big]\Big)dy_1\cdots dy_n \quad (2.7)$$

The main sketch of our construction derives from the fact that this n dimensional integral can be reduced to combination of simpler integrals which can be computed in closed form formulae. First we systematically expand the integral, substitute for the simpler integrals, and then wind it up back. Convergence conditions are not discussed.

We do a series of rearrangements.

[2] Feynman and Hibbs , offered a different *physical* proof. The linear terms in y_j essentially consolidates the contribution of the first variation of the action functional over the classical path. By the principle of Least Action, that is zero and hence its exponential is unity.

$$\lim_{n\to\infty}\prod_{j=1}^{n}\frac{1}{A_j}\iint_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\frac{i\epsilon}{\hbar}\sum_{j=1}^{n}\Big[\frac{m}{2\epsilon^2}(y_j-y_{j-1})^2-\frac{y_j^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_j^{cl}} - \sum_{m=3}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}}\Big]dy_1\cdots dy_n$$

$$= \lim_{n\to\infty}\prod_{j=1}^{n}\frac{1}{A_j}\iint_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\frac{i\epsilon}{\hbar}\sum_{j=1}^{n}\Big[\frac{m}{2\epsilon^2}(y_j-y_{j-1})^2-\frac{y_j^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_j^{cl}}\Big] \times\exp\frac{-i\epsilon}{\hbar}\sum_{j=1}^{n}\Big[\sum_{m=3}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}}\Big]dy_1\cdots dy_n$$

$$= \lim_{n\to\infty}\prod_{j=1}^{n}\frac{1}{A_j}\iint_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\frac{i\epsilon}{\hbar}\sum_{j=1}^{n}\Big[\frac{m}{2\epsilon^2}(y_j-y_{j-1})^2-\frac{y_j^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_j^{cl}}\Big] \times\sum_{j=1}^{n}\Big[1+\frac{-i\epsilon}{\hbar}\sum_{m=3}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}} +\frac{1}{2!}\left(\frac{-i\epsilon}{\hbar}\sum_{m=3}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}}\right)^2 +\frac{1}{3!}\left(\frac{-i\epsilon}{\hbar}\sum_{m=3}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}}\right)^3 +\cdots\Big]dy_1\cdots dy_n$$

$$= \lim_{n\to\infty}\prod_{j=1}^{n}\frac{1}{A_j}\iint_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\frac{i\epsilon}{\hbar}\sum_{j=1}^{n}\Big[\frac{m}{2\epsilon^2}(y_j-y_{j-1})^2-\frac{y_j^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_j^{cl}}\Big] \times\sum_{j=1}^{n}\Big[\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{-i\epsilon}{\hbar}\sum_{m=3}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}}\right)^k\Big] dy_1\cdots dy_n$$

Since the limit does not depend on k, we can take the k sum out. This step tells us, that we can deal separately with the various orders of k and carry out the path integral for them individually.

$$\sum_{k=0}^{\infty}\lim_{n\to\infty}\frac{1}{A}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\Big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{y_{j'}^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_{j'}^{cl}}\Big]\Big) \times\Big[\frac{1}{k!}\left(\frac{-i\epsilon}{\hbar}\sum_{j=1}^{n}\sum_{m=3}^{\infty}\frac{y_j^m}{m!}\frac{\partial^m}{\partial x^m}V(x)|_{x=x_j^{cl}}\right)^k\Big]dy_1\cdots dy_n \quad (2.8)$$

Which can be re-expressed as,

$$\sum_{k=0}^{\infty}\frac{1}{k!}\lim_{n\to\infty}\frac{1}{A}\Big(\frac{-i\epsilon}{\hbar}\Big)^k\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{y_{j'}^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_{j'}^{cl}}\Big]\big)$$
$$\times\sum_{m_1=3}^{\infty}\sum_{m_2=3}^{\infty}\cdots\sum_{m_k=3}^{\infty}\sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\cdots\sum_{j_k=1}^{n}\Big[\prod_{\alpha=1}^{k}\frac{1}{m_\alpha!}\frac{\partial^{m_\alpha}}{\partial x^{m_\alpha}}V(x)|_{x=x_{j_\alpha}^{cl}}\;\;y_{j_\alpha}^{m_\alpha}\Big]dy_1\cdots dy_n \quad (2.9)$$

Since the limit does not depend on m, the multi-dimensional sum over m can be taken out.

$$\sum_{k=0}^{\infty}\frac{1}{k!}\Big(\frac{-i}{\hbar}\Big)^k\sum_{m_1=3}^{\infty}\cdots\sum_{m_k=3}^{\infty}\lim_{n\to\infty}\frac{1}{A}\epsilon^k\sum_{j_1=1}^{n}\cdots\sum_{j_k=1}^{n}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\Big[\prod_{\alpha=1}^{k}\frac{1}{m_\alpha!}\frac{\partial^{m_\alpha}}{\partial x^{m_\alpha}}V(x)|_{x=x_{j_\alpha}^{cl}}y_{j_\alpha}^{m_\alpha}\Big]$$
$$\times\exp\big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{y_{j'}^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_{j'}^{cl}}\Big]\big)dy_1\cdots dy_n \quad (2.10)$$

The same can not be done with the j sums, as they depend on n. However, at each order of k there are exactly k of y_j, which can be converted to time integrals with the help of the k ϵ-s at our disposal.

But, before that we concentrate on the y integrals. They have the general form,

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{y_{j'}^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_{j'}^{cl}}\Big]\big)\Big[\prod_{\alpha=1}^{k}y_{j_\alpha}^{m_\alpha}\Big]dy_1\cdots dy_n \quad (2.11)$$

Computing this integral for various combinations of m_αs is tantamount to solving the complete Path Integral.

Before we delve into the actual computation, we notice the following properties of (2.11).

Theorem 1. *The integral (2.11), converges for all choices of m_α and for all n. For the choices where all m_α are even, the integral can be expressed as partial derivatives of,*

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{y_{j'}^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_{j'}^{cl}}\Big]\big)dy_1\cdots dy_n \quad (2.12)$$

For odd m_α the integral vanishes.

Theorem 2. *The form of the integral is independent of the particular choice and order of j_α. It only depends on the combination of the powers m_αs. Thus, it suffices to substitute a particular combination of j_α with various powers m_α and compute the integral.*

That is, for example,

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{y_{j'}^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_{j'}^{cl}}\Big]\big)\Big[y_1^{m_\alpha}\Big]dy_1\cdots dy_n \tag{2.13}$$

represents the whole family of integrals

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{y_{j'}^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_{j'}^{cl}}\Big]\big)\Big[y_{j_\alpha}^{m_\alpha}\Big]dy_1\cdots dy_n \tag{2.14}$$

for various m_α and the integrals corresponding to $\Big[y_1^3y_2\Big]$, $\Big[y_2y_1^3\Big]$, $\Big[y_1y_2^3\Big]$ all have the exact same form.

The integral in (2.12) is an multidimensional Gaussian Integral. In the next two sections we compute these in closed form. And then we would substitute them in (2.7) to complete the derivation.

2.2 Gaussian Integrals

The general integral we will be concentrating to evaluate is,

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{y_{j'}^2}{2!}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_{j'}^{cl}}\Big]\big)dy_1\cdots dy_n \tag{2.15}$$

We will first rearrange the kinetic term using *lattice derivatives*. Consider the partition of time interval, on which the integral is defined. The lattice derivatives at an instant j is defined as,

$$\nabla_+ y_j = \frac{1}{\epsilon}(y_{j+1} - y_j) \tag{2.16}$$

$$\nabla_- y_j = \frac{1}{\epsilon}(y_j - y_{j-1}) \tag{2.17}$$

Then,

$$\begin{aligned}\sum_{j=0}^{n}(\nabla_+ y_j)^2 &= y_j \nabla_+ y_j|_{j=0}^{j=n} - \sum_{j=0}^{n} y_j \nabla_- \nabla_+ y_j \\ &= -\sum_{j=0}^{n} y_j \nabla_- \nabla_+ y_j\end{aligned}$$

In terms of the lattice derivatives the integral (2.12) looks like,

$$\Big(\frac{M}{2\pi i\hbar\epsilon}\Big)^{\frac{n+1}{2}} \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp\frac{-i\epsilon}{\hbar}\sum_{j,j'=1}^{n}\Big[\frac{M}{2}y_j[\nabla_-\nabla_+ + \omega_j^2\delta_{j,j'}]y_{j'}\Big]\, dy_1\cdots dy_n \tag{2.18}$$

where we have defined the local frequency,

$$\omega_j^2 = \frac{1}{M}\frac{\partial^2}{\partial x^2}V(x)|_{x=x_j^{cl}}$$

and the normalisation constant is chosen as,

$$A = \sqrt{\frac{2\pi i\hbar\epsilon}{M}}^{n+1} \tag{2.19}$$

The multivariate Gaussian integral problem is then solved using the following results,

Theorem 3. *Let* $\mathbf{y} = \{y_j\}$ *be a* $n \times 1$ *vector, and let* $\mathbf{M}$ *be a* $n \times n$ *matrix, with real or complex entries. Then the integral,*

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{-\mathbf{yMy^T}}\, dy_1\cdots dy_n = \sqrt{\frac{\pi^n}{\mathbf{det\ M}}}$$

The proof is straight forward for reals, and is done by weak rotation for complex entries in $\mathbf{M}$. This reduces the integral (2.18) to,

$$\Big(\frac{M}{2\pi i\hbar\epsilon}\Big)^{\frac{n+1}{2}}\Big(\frac{2\pi i\hbar}{M\epsilon}\Big)^{\frac{n}{2}}\mathbf{det}[\nabla_-\nabla_+ + \omega_j^2\delta_{j,j'}]^{\frac{-1}{2}} \tag{2.20}$$

The problem hence reduces to computation of the determinant. Now from the definition of the lattice derivatives, the matrix has the form

$$\mathbf{M} = \frac{1}{\epsilon^2}\begin{pmatrix} 2+\epsilon^2\omega_1^2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2+\epsilon^2\omega_2^2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2+\epsilon^2\omega_3^2 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & 2+\epsilon^2\omega_{n-2}^2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2+\epsilon^2\omega_{n-1}^2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2+\epsilon^2\omega_n^2 \end{pmatrix} \tag{2.21}$$

A determinant of an invertible matrix is given by product of its eigenvalues. The following section deals with determining the eigenvalues of the tri-diagonal matrices.

2.3 Spectral theory of tri-diagonal matrices

The general algorithm for determining the eigenvalues of a square matrix $\mathbf{A}$, is done by solving the roots of the characteristic polynomial defined by

$$f(x) = \mathbf{det}[\mathbf{A} - x\mathbf{I}] \tag{2.22}$$

where $\mathbf{I}$ is the identity matrix of the same dimension.

First we consider the constant diagonal or toeplitz special case, where each descending diagonal from left to right has identical entries. The general form of the tri-diagonal toeplitz matrix is,

$$\begin{pmatrix} a & b & 0 & \cdots & 0 & 0 & 0 \\ c & a & b & \cdots & 0 & 0 & 0 \\ 0 & c & a & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & a & b & 0 \\ 0 & 0 & 0 & \cdots & c & a & b \\ 0 & 0 & 0 & \cdots & 0 & c & a \end{pmatrix} \tag{2.23}$$

The roots of the characteristic polynomial or the eigenvalues of this matrix can be expressed in a closed form as [24, 25],

$$\lambda_k = a - 2\sqrt{bc}\cos\big(\frac{k\pi}{n+1}\big) \tag{2.24}$$

Both the free particle and simple harmonic oscillator problem falls in this category. We first solve the propagator for them and then move on to develop the spectral theory for non-toeplitz tri-diagonal matrices.

For the free particle problem the matrix looks like,

$$\mathbf{M} = \frac{1}{\epsilon^2}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ . & . & . & \cdots & . & . & . \\ . & . & . & \cdots & . & . & . \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix} \tag{2.25}$$

So the determinant is given by,

$$\prod_{k=1}^{n} \lambda_k = \prod_{k=1}^{n} 2 - 2\cos\big(\frac{k\pi}{n+1}\big) \tag{2.26}$$

This free particle determinant is easier evaluated using the following recursion relation,

$$\mathbf{det}_n[-\epsilon^2\mathbf{M}] = 2\mathbf{det}_{n-1}[-\epsilon^2\mathbf{M}] - \mathbf{det}_{n-2}[-\epsilon^2\mathbf{M}] \tag{2.27}$$

$$\mathbf{det}_1[-\epsilon^2\mathbf{M}] = 2;\ \mathbf{det}_2[-\epsilon^2\mathbf{M}] = 3; \tag{2.28}$$

and evaluates to,

$$\mathbf{det}_n[\mathbf{M}] = (\frac{1}{\epsilon^2})^n(n+1) = (\frac{1}{\epsilon^2})^n \prod_{k=1}^{n} 2 - 2\cos\big(\frac{k\pi}{n+1}\big) \tag{2.29}$$

The same can obtained by taking the limit $x \to 1$ [3], in the following asymptotic formula,

$$\prod_{k=1}^{n} 1 + x^2 - 2x\cos\Big[\frac{\pi k}{n+1}\Big] = \frac{x^{2(n+1)} - 1}{x^2 - 1} \tag{2.30}$$

We will use this identity in the later calculations.

[3] using L'-Hospital rule

For the Harmonic Oscillator, the matrix is,

$$\mathbf{M} = \frac{1}{\epsilon^2}\begin{pmatrix} 2+\epsilon^2\omega_0^2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2+\epsilon^2\omega_0^2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2+\epsilon^2\omega_0^2 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & 2+\epsilon^2\omega_0^2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2+\epsilon^2\omega_0^2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2+\epsilon^2\omega_0^2 \end{pmatrix} \tag{2.31}$$

Where, w_0 denotes the natural angular frequency of the oscillation. [4] The determinant is given by,

$$\begin{aligned} &(\frac{1}{\epsilon^2})^n \prod_{k=1}^{n} 2+\epsilon^2\omega_0^2 - 2\cos\left(\frac{k\pi}{n+1}\right) \\ &= (\frac{1}{\epsilon^2})^n (n+1) \frac{\prod_{k=1}^{n} 2+\epsilon^2\omega_0^2 - 2\cos\left(\frac{k\pi}{n+1}\right)}{\prod_{k=1}^{n} 2-2\cos\left(\frac{k\pi}{n+1}\right)} \\ &= (\frac{1}{\epsilon^2})^n (n+1) \prod_{k=1}^{n} \frac{2+\epsilon^2\omega_0^2 - 2\cos\left(\frac{k\pi}{n+1}\right)}{2-2\cos\left(\frac{k\pi}{n+1}\right)} \end{aligned}$$

We are interested only in the limit where ϵ is small. In that regime we can always define,

$$\epsilon\omega_0 = \sin(x) \tag{2.32}$$

for which the formula simplifes to,

$$(\frac{1}{\epsilon^2})^n (n+1) \prod_{k=1}^{n} 1 - \frac{\sin(x)^2}{\sin(\frac{\pi k}{2(n+1)})^2}$$

which in the asymptotic limit reduces to,

$$\prod_{k=1}^{n} 1 - \frac{\sin(x)^2}{\sin(\frac{\pi k}{2(n+1)})^2} = \frac{\sin((n+1)x)}{(n+1)\sin(x)} = \frac{\sin((n+1)\epsilon\omega_0)}{(n+1)\epsilon\omega_0} = \frac{\sin(\omega_0 t)}{\omega_0 t} \tag{2.33}$$

So that the coefficient for the Harmonic Oscillator path integral finally evaluates to,

[4] note that it is index independent

$$\Big(\frac{M}{2\pi i\hbar\epsilon}\Big)^{\frac{n+1}{2}}\Big(\frac{2\pi i\hbar}{M\epsilon}\Big)^{\frac{n}{2}}\frac{\epsilon^n}{\sqrt{(n+1)}}\sqrt{\frac{\omega_0 t}{\sin(\omega_0 t)}} \tag{2.34}$$

$$=\sqrt{\frac{M\omega_0}{2\pi i\hbar\sin(\omega_0 t)}} \tag{2.35}$$

And the complete Path Integral is,

$$\sqrt{\frac{M\omega_0}{2\pi i\hbar\sin(\omega_0 t)}}\exp\Big(\frac{iS^{cl}[x^{cl}(t)]}{\hbar}\Big) \tag{2.36}$$

$$=\sqrt{\frac{M\omega_0}{2\pi i\hbar\sin(\omega_0 t)}}\exp\Big(\frac{iM\omega_0}{2\hbar\sin(\omega_0 t)}[(x_b^2+x_a^2)\cos(\omega_0 t)+2x_b x_a]\Big) \tag{2.37}$$

The first point of difference in the general calculation is that the tri-diagonal matrix (2.21) is no more toeptliz, and hence the closed form eigenvalue expression of Eqn (2.24) is no more valid. It turns out there is actually no general closed form formula available for the eigen-values of such aperiodic [5] and non-toeptliz tridiagnoal matrices, for the finite dimensional cases.

We postulate an approximate closed from expression for the spectrum of the eigenvalues of (2.21),

$$\lambda_k=\frac{1}{\epsilon^2}\Big[2+\epsilon^2\omega_k^2-2\cos\big(\frac{k\pi}{n+1}\big)\Big] \tag{2.38}$$

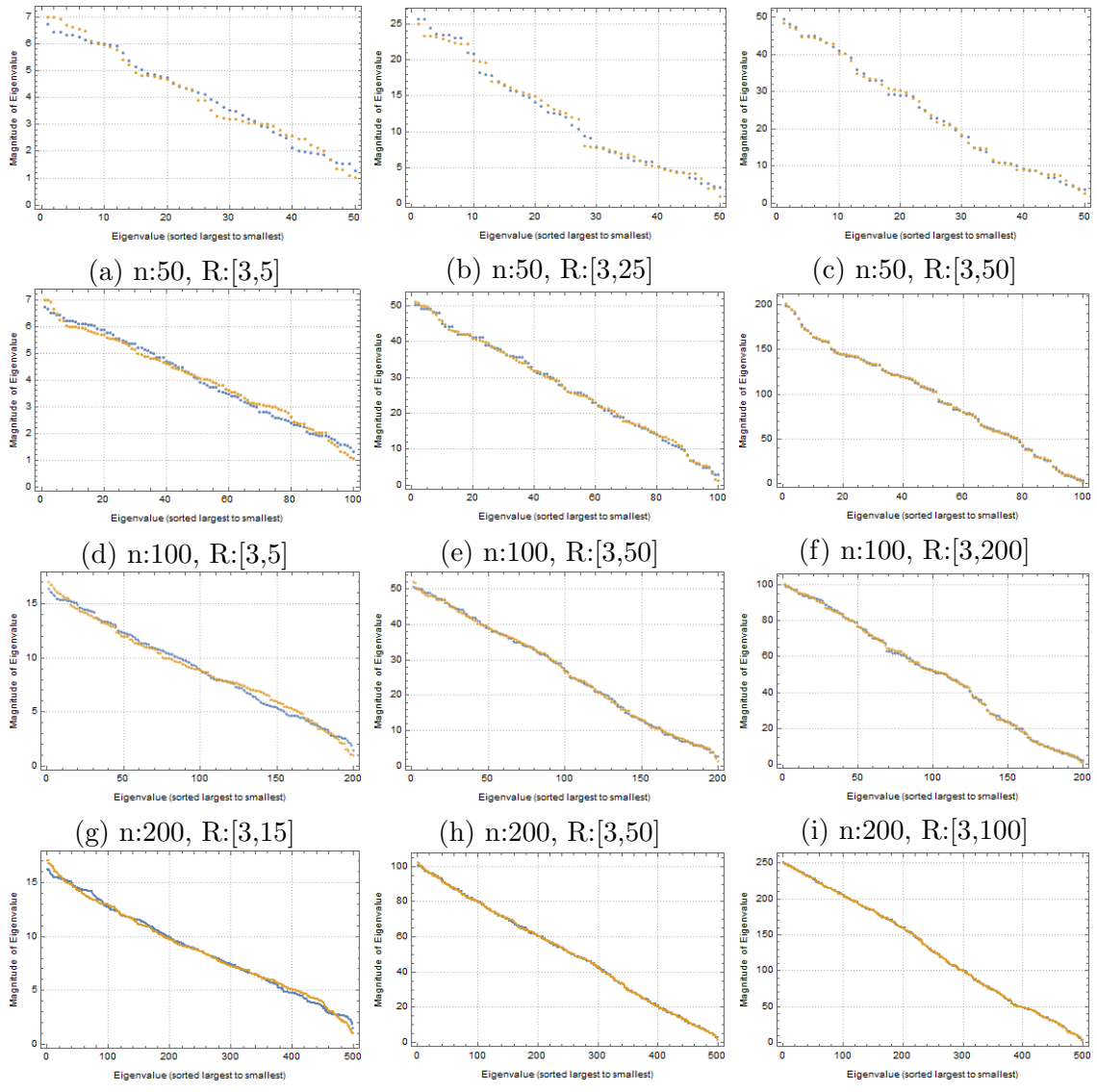
This expression is approximate in any finite dimensions n, but becomes exact at the infinite dimensional limit, as long as the local frequency ω_k is bounded from both below and above, which is the case for all physical phenomena.

The figure (2.1) compares the actual eigenvalue spectrum (in blue) which are compared numerically vs the approximate eigenvalue spectrum (in orange) that are postulated by the formula (2.38) for tri-diagonal matrices of the form (2.21). We have sampled the values of various ω_k here using a random number generator between the ranges specified.

We can see the following trends. The formula (2.38) approximates the eigen spectrum of the matrix of a given dimension better as the range from which the values of ω_k is sampled is broadened. For a given range, the variation (percentage error) decreases with the increase of dimension of the matrix. The formula for eigen spectrum becomes asymptotically exact, with increasing matrix dimension, n.

So the determinant is given by,

[5] For Periodic cases there is a closed form formula [25], under some restricted conditions



(a) n:50, R:[3,5] (b) n:50, R:[3,25] (c) n:50, R:[3,50]

(d) n:100, R:[3,5] (e) n:100, R:[3,50] (f) n:100, R:[3,200]

(g) n:200, R:[3,15] (h) n:200, R:[3,50] (i) n:200, R:[3,100]

(j) n:500, R:[3,15] (k) n:500, R:[3,100] (l) n:500, R:[3,250]

Figure 2.1: Comparison of actual (blue) and predicted (orange) spectra as postulated in formula (2.38) for various matrix dimensions (n) and randomly sampled diagonal entry for tri-diagonal matrices of the form (2.21). The Diagonal entries are integers sampled using a random number generator from the range specified by (R).

$$(\frac{1}{\epsilon^2})^n \prod_{k=1}^{n} 2 + \epsilon^2\omega_k^2 - 2\cos\left(\frac{k\pi}{n+1}\right) \tag{2.39}$$

Multiplying both the denominator and numerator by the free particle determinant,

$$\begin{aligned}
&(\frac{1}{\epsilon^2})^n (n+1) \frac{\prod_{k=1}^{n} 2 + \epsilon^2\omega_k^2 - 2\cos\left(\frac{k\pi}{n+1}\right)}{\prod_{k=1}^{n} 2 - 2\cos\left(\frac{k\pi}{n+1}\right)} \\
&= (\frac{1}{\epsilon^2})^n (n+1) \prod_{k=1}^{n} \frac{2 + \epsilon^2\omega_k^2 - 2\cos\left(\frac{k\pi}{n+1}\right)}{2 - 2\cos\left(\frac{k\pi}{n+1}\right)}
\end{aligned}$$

Just like the Harmonic Oscillator, we are interested only in the limit where ϵ is small. Likewise, in that regime we define,

$$\epsilon\omega_k = \sin(x_k) \tag{2.40}$$

for each k. Since ω_k is finite for all k, we can choose the largest among them. The ϵ is chosen in such that (2.40) holds for the largest ω_k. It then automatically holds for all k. This simplifies the determinant to,

$$(\frac{1}{\epsilon^2})^n (n+1) \prod_{k=1}^{n} 1 - \frac{\sin(x_k)^2}{\sin(\frac{\pi k}{2(n+1)})^2}$$

In the asymptotic limit, the product reduces to,

$$\prod_{k=1}^{n} 1 - \frac{\sin(x_k)^2}{\sin(\frac{\pi k}{2(n+1)})^2} = \frac{\sin(\sum_{k=1}^{n} x_k)}{\sum_{k=1}^{n} \sin(x_k)} = \frac{\sin(\epsilon \sum_{k=1}^{n} \omega_k)}{\epsilon \sum_{k=1}^{n} \omega_k} = \frac{\sin\phi}{\phi} \tag{2.41}$$

where,

$$\phi = \int_0^t \omega(t')dt' \tag{2.42}$$

The pre-factor gives rise to an overall normalization just like the Harmonic Oscillator case.

2.4 The Final Expression

From (2.41), the integrals classified in Theorem 2 can be obtained by taking corresponding partial derivatives with respect to coefficients of y_j^2. This is facilitated by the fact that all y_j^2 have different coefficients, $\beta_j = \frac{-iM\omega_j^2\epsilon}{2\hbar}$. Therefore the individual integrals are,

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\big(\frac{i\epsilon}{\hbar}\sum_{j'=1}^{n}\Big[\frac{M}{2\epsilon^2}(y_{j'}-y_{j'-1})^2-\frac{M\omega_{j'}^2y_{j'}^2}{2}\Big]\big)\Big[\prod_{\alpha=1}^{k}y_{j_\alpha}^{m'_\alpha}\Big]dy_1\cdots dy_n \tag{2.43}$$

$$=\sqrt{\frac{M}{2\pi i\hbar t}}\prod_{\alpha=1}^{k}\Big[\frac{\partial}{\partial\beta_{j_\alpha}}\Big]^{m'_\alpha}\sqrt{\frac{\epsilon\sum_{j=1}^{n}\omega_j}{\sin\left(\epsilon\sum_{j=1}^{n}\omega_j\right)}} \tag{2.44}$$

$$=\sqrt{\frac{M}{2\pi i\hbar t}}\prod_{\alpha=1}^{k}\Big[\frac{\hbar}{-iM\epsilon\omega_j}\frac{\partial}{\partial\omega_{j_\alpha}}\Big]^{m'_\alpha}\sqrt{\frac{\epsilon\sum_{j=1}^{n}\omega_j}{\sin\left(\epsilon\sum_{j=1}^{n}\omega_j\right)}} \tag{2.45}$$

$$=\sqrt{\frac{M}{2\pi i\hbar t}}\prod_{\alpha=1}^{k}\Big[\frac{\hbar}{-iM\omega_j}\frac{\partial}{\partial\phi}\Big]^{m'_\alpha}\sqrt{\frac{\phi}{\sin\left(\phi\right)}} \tag{2.46}$$

where $m' = m/2$ for all α, the jacobian of transformation is,

$$\frac{\partial}{\partial\beta_{j_\alpha}}=\frac{\hbar}{-iM\epsilon\omega_j}\frac{\partial}{\partial\omega_{j_\alpha}} \tag{2.47}$$

And the last statement follows from the fact that ϕ in the discrete version is sum over ω_j. Substituting this back to (2.10),

$$\sqrt{\frac{M}{2\pi i\hbar t}}\sum_{k=0}^{\infty}\frac{1}{k!}\Big(\frac{-i}{\hbar}\Big)^k\sum_{m_1=3}^{\infty}\cdots\sum_{m_k=3}^{\infty}\frac{\partial}{\partial\phi}^{\sum_\alpha m'_\alpha}\sqrt{\frac{\phi}{\sin\left(\phi\right)}}\lim_{n\to\infty}\epsilon^k\times$$
$$\sum_{j_1=1}^{n}\cdots\sum_{j_k=1}^{n}\Big[\prod_{\alpha=1}^{k}\frac{1}{m_\alpha!}\Big(\frac{\hbar}{-iM\omega_{j_\alpha}}\Big)^{m'_\alpha}\frac{\partial^{m_\alpha}}{\partial x^{m_\alpha}}V(x)|_{x=x_{j_\alpha}^{cl}}\Big] \tag{2.48}$$

At the limit the j sums becomes integrals,

$$\sqrt{\frac{M}{2\pi i\hbar t}}\sum_{k=0}^{\infty}\frac{1}{k!}\Big(\frac{-i}{\hbar}\Big)^k\sum_{m_1=3}^{\infty}\cdots\sum_{m_k=3}^{\infty}\prod_{\alpha=1}^{k}\frac{1}{m_\alpha!}\Big(\frac{\hbar}{-iM}\Big)^N\frac{\partial}{\partial\phi}^N\sqrt{\frac{\phi}{\sin\left(\phi\right)}}$$
$$\Big[\prod_{\alpha=1}^{k}\int_0^t\frac{1}{\omega(t_\alpha)^{m'_\alpha}}\frac{\partial^{m_\alpha}}{\partial x^{m_\alpha}}V(x)|_{x=x^{cl}(t_\alpha)}dt_\alpha\Big] \tag{2.49}$$

where we have defined, $N = \sum_\alpha m'_\alpha$. This series expresses the complete path integral as a functional of the classical path. The complete expression of the Kernel is,

$$K(x_b, x_a; t, 0) = \sqrt{\frac{M}{2\pi i\hbar t}} \exp \frac{iS^{cl}(x_b, x_a; t)}{\hbar} \sum_{k=0}^{\infty} \frac{1}{k!} \Big(\frac{-i}{\hbar}\Big)^k \sum_{m_1=3}^{\infty} \cdots \sum_{m_k=3}^{\infty} \prod_{\alpha=1}^{k} \frac{1}{m_\alpha!} \Big(\frac{\hbar}{-iM}\Big)^N \frac{\partial}{\partial\phi}^N \sqrt{\frac{\phi}{\sin(\phi)}} \Big[\prod_{\alpha=1}^{k} \int_0^t \frac{1}{\omega(t_\alpha)^{m'_\alpha}} \frac{\partial^{m_\alpha}}{\partial x^{m_\alpha}} V(x)|_{x=x^{cl}(t_\alpha)} dt_\alpha\Big] \quad (2.50)$$

Equipped with this we can obtain the Dynamics of an initial wavefunction as,

$$\psi(x_b, t) = \int_{-\infty}^{\infty} K(x_b, t; x_a, 0)\psi_0(x_a)dx_a \quad (2.51)$$

which then, after a Madelung transformation, can be used to obtain the Quantum Potential as,

$$Q(x, t) = -\frac{\hbar^2}{2M} \frac{\nabla^2 R(x, t)}{R(x, t)} \quad (2.52)$$

which then can be used to obtain the quantum Trajectories. Expression (2.50) extends the domain of analytically solvable path integrals to any system whose classical action (and the path) can be computed in a closed form. In cases where the trajectories cannot be obtained in closed form, we have argued that the problem can be reduced to numerically computing the classical path as a BVP.

In the following chapter, we solve for a toy model of Anharmonic Oscilator to illustrate the computation of trajectories using expression (2.50). In this case the classical action can be obtained in a closed form only perturbatively. We, use the perturbative expression for classical action and leave the Quantum Part of the calculation exact.

2.5 Multidimensional Generalisation

Most of the derivation goes through while further generalising it to higher dimensions. Only change is brought about through the Taylor Expansion of the potential, which becomes multidimensional.

The generalisation to multidimensional (as well as multi-particle) case is done easiest in the generalised coordinates. Consider a three dimensional space with,

$\mathbf{x} = (x_1, x_2, x_3)$. The potential is still a scalar $V(\mathbf{x})$. $\mathbf{x}(t)$ defines a path in this three dimensional space. We can split such a general path similar to (2.1)

$$\mathbf{x}(t) = \mathbf{x}^{cl}(t) + \mathbf{y}(t). \tag{2.53}$$

This brings in changes in the Taylor expansion (2.5)

$$V(\mathbf{x}_j) = V(\mathbf{x}_j^{cl} + \mathbf{y}_j) = V(\mathbf{x}_j^{cl}) + \sum_{m=1}^{\infty} \frac{\mathbf{y}_j^m}{m!} \mathbf{D}^m V(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_j^{cl}} \tag{2.54}$$

where,

$$\mathbf{D}^m V(\mathbf{x}) = \frac{\partial^m V(\mathbf{x})}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \partial x_3^{\alpha_3}} \tag{2.55}$$

$$\alpha_1 + \alpha_2 + \alpha_3 = m \tag{2.56}$$

Accordingly the integrals over each dy_j in (2.6) is replaced by the corresponding volume integral $\mathbf{dy}_j$. In essence the higher dimensional case is like a foliation of space in the one dimensional case, where each one dimensional line integral foliates into a higher dimensional volume. For the multi-particle case the one-dimensional case foliates into a $3n$ dimensional space. The rest of the derivation goes through exactly. The $\mathbf{y}$ independent parts generate the exponentiation of classical action, and the prefactor is written as a series, of various moments of k, only in this case the partial derivatives are more diverse.

Chapter 3

Tunneling

In this chapter we turn to applications of the theory developed in chapter 2. The Anharmonic Oscilator is one of the non-trivial case which has been studied in gory details, both classically [26–29] and Quantum Mechanically [30], owing to its applicability in various fields of of physics. Although for the initial value problem of the equation of motion, the Classical Path [26, 27] and the Classical Action [29] are available in closed form, same is not true for the Boundary Value Problem. The solution for classical path for the BVP is not even unique.

Hence to illustrate the closed form calculation of trajectories, we resort to derive the Classical Action perturbatively and leave the Quantum Part of the calculation exact. It is shown that, even in this *mixed* treatment, the model reproduces properties of Barrier Tunneling.

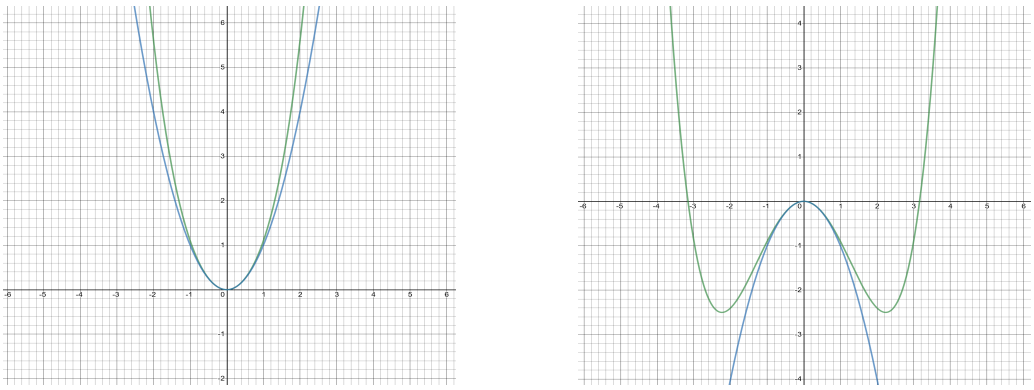
3.1 The Anharmonic Oscillator

In general an Anharmonic potential (in one dimension) is any oscillator of the form,

$$V(x) = \frac{1}{2}MK_2x^2 + \sum_{n=3}^{\infty}\frac{1}{n}MK_nx^n$$

Where M is the mass of the particle, and the factors $\frac{1}{n}$ has been added as they simplify the form of the equations of motion. The even powers, are even functions of x, and hence their presence produce symmetric anharmonicity (e.g. symmetric wells). Whereas the odd powers can be tuned to render asymmetry and hence bias. The K_ns specifies the relative strengths of various anharmonicities.

For most cases of physical concerns the sum does not run to infinity. As long as the highest power is positive, any motion under the action of the potential have closed orbits, if the motion is Hamiltonian (i.e the total energy is a constant of motion.) Presence of forcing/ damping term can complicate the dynamics (e.g the Duffing Oscillator). The positivity of the highest power of position is also a necessary



(a) $a > 0$ (b) $a < 0$

Figure 3.1: Graphic comparison of Anharmonic Potential (Green) with the corresponding Harmonic analouge (blue), for positive and negative a respectively. The $a < 0$ case generates a double well. As is shown, positivity of K_4 ensures Bound State solutions unlike the corresponding Harmonic problem in this case. for $a > 0$ bound state periodic solutions always exist for Hamiltonian systems.

condition for existence of bound states in Quantum Mechanics, which is necessary requirement for most of the models having physical interest.

Although, in these cases, the classical treatments always gives rise to closed orbits, the topology of the closed orbits, depends on relative signs of various K_ns, which decides how many wells are there, and how many of them are equivalent. The physical significance this toy problem renders is listed in [26, 27, 30].

The potential hence reduces to,

$$V(x) = \frac{1}{2}Max^2 + \frac{1}{4}M\lambda Kx^4 \tag{3.1}$$

where K is positive. As is shown in Fig. (3.1b), the double well is realised for $a < 0$. That is the case we will be concerned hereafter. Here λ is the perturbation parameter. The positional derivatives of this potential, which appears as a function of classical path in (2.50) are,

$$\begin{aligned}
\frac{\partial}{\partial x}V(x) &= Max + M\lambda Kx^3 \\
\frac{\partial^2}{\partial x^2}V(x) &= Ma + 3M\lambda Kx^2 \\
\frac{\partial^3}{\partial x^3}V(x) &= 6M\lambda Kx \\
\frac{\partial^4}{\partial x^4}V(x) &= 6M\lambda K
\end{aligned}$$

and all the higher derivatives vanish. Since the odd values m drops out in the sum, the only non vanishing contribution in the sum comes from $m = 4$. This reduces (2.50) to,

$$K(x_b, x_a; t, 0) =$$
$$\sqrt{\frac{M}{2\pi i\hbar t}} \exp \frac{iS^{cl}(x_b, x_a; t)}{\hbar} \sum_{k=0}^{\infty} \frac{1}{k!} \Big(\frac{-i}{\hbar}\Big)^k (\frac{1}{4!})^k \Big(\frac{\hbar}{-iM}\Big)^{2k} \Big(\frac{\partial}{\partial \phi}\Big)^{2k} \sqrt{\frac{\phi}{\sin(\phi)}}$$
$$\Big[\int_0^t \frac{1}{\omega(t)^2} \frac{\partial^4}{\partial x^4} V(x)|_{x=x^{cl}(t)} dt\Big]^k$$
$$= \sqrt{\frac{M}{2\pi i\hbar t}} \exp \frac{iS^{cl}(x_b, x_a; t)}{\hbar} \sum_{k=0}^{\infty} \frac{1}{k!} \Big(\frac{-i}{\hbar}\Big)^k (\frac{1}{4!})^k \Big(\frac{\hbar}{-iM}\Big)^{2k} \Big(\frac{\partial}{\partial \phi}\Big)^{2k} \sqrt{\frac{\phi}{\sin(\phi)}}$$
$$\Big[\int_0^t \frac{1}{a + 3\lambda K x^{cl}(t)^2} 6M\lambda K dt\Big]^k \quad (3.2)$$

which is reduced to,

$$K(x_b, x_a; t, 0) =$$
$$\sqrt{\frac{M}{2\pi i\hbar t}} \exp \frac{iS^{cl}(x_b, x_a; t)}{\hbar} \sum_{k=0}^{\infty} \frac{1}{k!} \Big(\frac{i\hbar\lambda K}{4M}\Big)^k \Big[\int_0^t \frac{1}{a + 3\lambda K x^{cl}(t')^2} dt'\Big]^k$$
$$\Big(\frac{\partial}{\partial \phi}\Big)^{2k} \sqrt{\frac{\phi}{\sin(\phi)}} \quad (3.3)$$

Few observations are obvious at once from the expression (3.3). As λ goes to zero, the series reproduces the Harmonic Oscillator Kernel. More importantly, at the classical limit, as $\hbar$ goes to zero, the position dependent terms in the expansion vanish. So the only contribution comes from the very first term (corresponding to $k = 0$), which goes as $\exp\left(\frac{iS^{cl}}{\hbar}\right)$. This term, in the same limit, reduces to a Dirac Delta around the classical path, and recovers the Classical Dynamics. At this limit, the contribution from all other path vanishes.

In the next sections, we go on to compute the functional forms of the remaining unknowns of (3.3), namely the classical path and the action perturbatively.

3.2 The Classical Problem

Perturbative Analysis

In regime of perturbation theory the potential is replaced by,

$$V(x) = \frac{m}{2}\omega_0^2 x^2 + \lambda \frac{mK}{4} x^4 \quad (3.4)$$

where lambda is the perturbation parameter.

We present here a perturbative analysis of the boundary value problem. The analogous treatment for the initial value problem is a standard text book example, E.g. [1]. The standard perturbative ansatz is done on the amplitude,

$$x(t) = x_0(t) + \lambda x_1(t) + \lambda^2 x_2(t) + \lambda^3 x_3(t) + \cdots \tag{3.5}$$

Substituting this in the Euler-Lagrnage Equation, we can obtain the equation of motion order by order by collecting the powers of λ.

$$\begin{aligned}
&\omega_0^2 x_0(t) + x_0''(t) = 0 \\
&x_0(t)^3 + \omega_0^2 x_1(t) + x_1''(t) = 0 \\
&3x_0(t)^2 x_1(t) + \omega_0^2 x_2(t) + x_2''(t) = 0 \\
&3x_0(t) x_1(t)^2 + 3x_0(t)^2 x_2(t) + \omega_0^2 x_3(t) + x_3''(t) = 0 \\
&\vdots
\end{aligned}$$

The zeroth order equation for the classical path corresponds to the free simple harmonic oscillator problem. Once we have the solution to $x_0(t)$, it can be used to solve for the first order correction, treated as a forcing. Similarly, solving for the n-th order correction requires knowledge of all the lower orders, and can be solved recursively.

The boundary value problem for the zeroth order is given by,

$$\omega_0^2 x_0(t) + x_0''(t) = 0, x_0(0) = x_i, x_0(t_f) = x_f \tag{3.6}$$

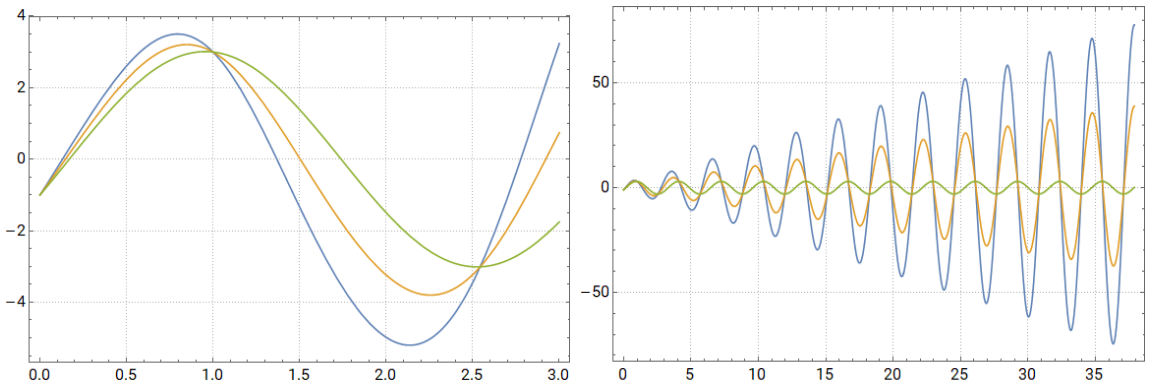
and the solution is evaluated as,

$$x_0(t) = \frac{x_f \sin[\omega_0 t] + x_i \sin[\omega_0 (t_f - t)]}{\sin[\omega_0 t_f]} \tag{3.7}$$

The first order equation then becomes,

$$x_0(t)^3 + \omega_0^2 x_1(t) + x_1''(t) = 0, x_1(0) = 0, x_1(t_f) = 0 \tag{3.8}$$

Now, $\sin(\omega_0 t)^3$ has two dominant frequencies, $\omega_0, 3\omega_0$. The presence of the ω_0 term, makes the forced oscillator resonant and hence the amplitude grows unboundedly. This invariably after sometime crosses the perturbative regime breaking the ansatz. The total solution upto first order, obtained by this method is plotted in figure (3.2a.) This difficulty can be rectified by changing the perturbative ansatz using Linsted-Poincare method.



(a) close-up view (b) long time behaviour

Figure 3.2: The total solution for the classical boundary value problem upto first order obtained for various values of ω_0. The close-up view shows that indeed the solutions satisfy boundary conditions. The long term behaviour shows its diverging nature irrespective of the value of ω_0

Linsted-Poincare Method

The secular terms can be avoided, as in the initial value problem, by choosing an ansatz that also allows for changing frequency as a result of the perturbation besides the path.

$$x(t) = x_0(t) + \lambda x_1(t) + \lambda^2 x_2(t) + \lambda^3 x_3(t) + \cdots \tag{3.9}$$
$$\omega = \omega_0 + \lambda\omega_1 + \lambda^2\omega_2 + \lambda^3\omega_3 + \cdots \tag{3.10}$$

To obtain the equations of motion we first change the dynamical variable to $\phi = \omega t$, and note that the Jacobian of the transformation is given by $\frac{d}{dt} = \frac{1}{\omega}\frac{d}{d\phi}$. Now substituting the ansatz in the Euler-Lagrnage Equation, one can obtain the equations of motion order by order by collecting the powers of λ. We denote $\frac{d}{d\phi}$ with $'$.

$$\omega_0^2 x_0(\phi) + \omega_0^2 x_0''(\phi) = 0$$
$$K x_0(\phi)^3 + \omega_0^2 x_1(\phi) + 2\omega_0\omega_1 x_0''(\phi) + \omega_0^2 x_1''(\phi) = 0$$
$$3K x_0(\phi)^2 x_1(\phi) + \omega_0^2 x_2(\phi) + \omega_1^2 x_0''(\phi) + 2\omega_0\omega_2 x_0''(\phi) + 2\omega_0\omega_1 x_1''(\phi) + \omega_0^2 x_2''(\phi) = 0$$
$$\vdots$$

The general solution upto the first order for classical path is given by,

$$x_0(\phi) = A\cos[\theta + \phi] \tag{3.11}$$
$$x_1(\phi) = -\frac{A^3 K \cos[3\theta + \phi]\sin[\phi]^2}{8w_0^2} \tag{3.12}$$

with A, θ being the undetermined constants, and,

$$w_1 = \frac{3A^2K}{8w_0} \; ; \; w_2 = \frac{9A^4K^2}{128w_0^3} \; ; \; w_3 = \frac{27A^6K^3}{1024w_0^5} \; ; \; \cdots \tag{3.13}$$

Given this solution to the classical boundary value problem, the Classical Action or the Hamilton's Principal function can be obtained as follows,

$$\begin{aligned}
S[x_{cl}(t)] =& \int_{t_i}^{t_f} dt \; \mathcal{L}(x_{cl}, \dot{x}_{cl}, t) \\
=& \frac{m}{2} \int_{t_i}^{t_f} dt \; [\dot{x}_{cl}(t)^2 - \omega^2 x_{cl}^2(t) - \frac{K}{2} x_{cl}(t)^4] \\
=& \frac{m}{2} x_{cl}(t)\dot{x}_{cl}(t)|_{t_i}^{t_f} - \frac{m}{2} \int_{t_i}^{t_f} dt \; x_{cl}[\ddot{x}_{cl}(t) + \omega^2 x_{cl}(t) + K x_{cl}(t)^3] + \frac{mK}{4} \int_{t_i}^{t_f} dt \; x_{cl}(t)^4 \\
=& \frac{m}{2} x_{cl}(t)\dot{x}_{cl}(t)|_{t_i}^{t_f} + \frac{mK}{4} \int_{t_i}^{t_f} dt \; x_{cl}(t)^4
\end{aligned}$$

where we have obtained the third step from the second by an integration by parts on the kinetic term and the second term of the third step evaluates to zero as its integrand satisfies the Euler-Lagrange Equation.

3.3 Results

The classical action of the system is obtained , by substituting the classical path, into the Lagrangian, integrating out time, and neglecting the terms of higher orders in λ. The obtained action is denoted by $S_{cl}(x_f, t; x_i, 0)$ for the rest of the discussion. The integration constants, A and ϕ , can be solved for the boundary conditions $x(0) = x_i$, $x(t) = x_f$ and substituted in expression of the classical action. The inverse solution is not unique, and we choose the solution in which both A,ϕ are both real and positive.

$$A = \sqrt{x_f^2 + x_i^2 - 2x_f x_i \cos[t\omega_0]} \csc[t\omega_0] \tag{3.14}$$

$$\phi = \arccos\left[\frac{x_i \sin[t\omega_0]}{\sqrt{x_f^2 + x_i^2 - 2x_f x_i \cos[t\omega_0]}}\right] \tag{3.15}$$

The perturbative proagator till the first order of λ, then is given by,

$$\begin{aligned}
&K(x_b, x_a; t, 0) = \\
&\sqrt{\frac{M}{2\pi i\hbar t}} \exp \frac{iS^{cl}(x_b, x_a; t)}{\hbar} \left[\sqrt{\frac{\phi}{\sin(\phi)}} + \Big(\frac{i\hbar\lambda K}{4M}\Big)\Big[\int_0^t \frac{1}{\omega(t')^2} dt'\Big]\Big(\frac{\partial}{\partial\phi}\Big)^2 \sqrt{\frac{\phi}{\sin(\phi)}}\right]
\end{aligned}$$

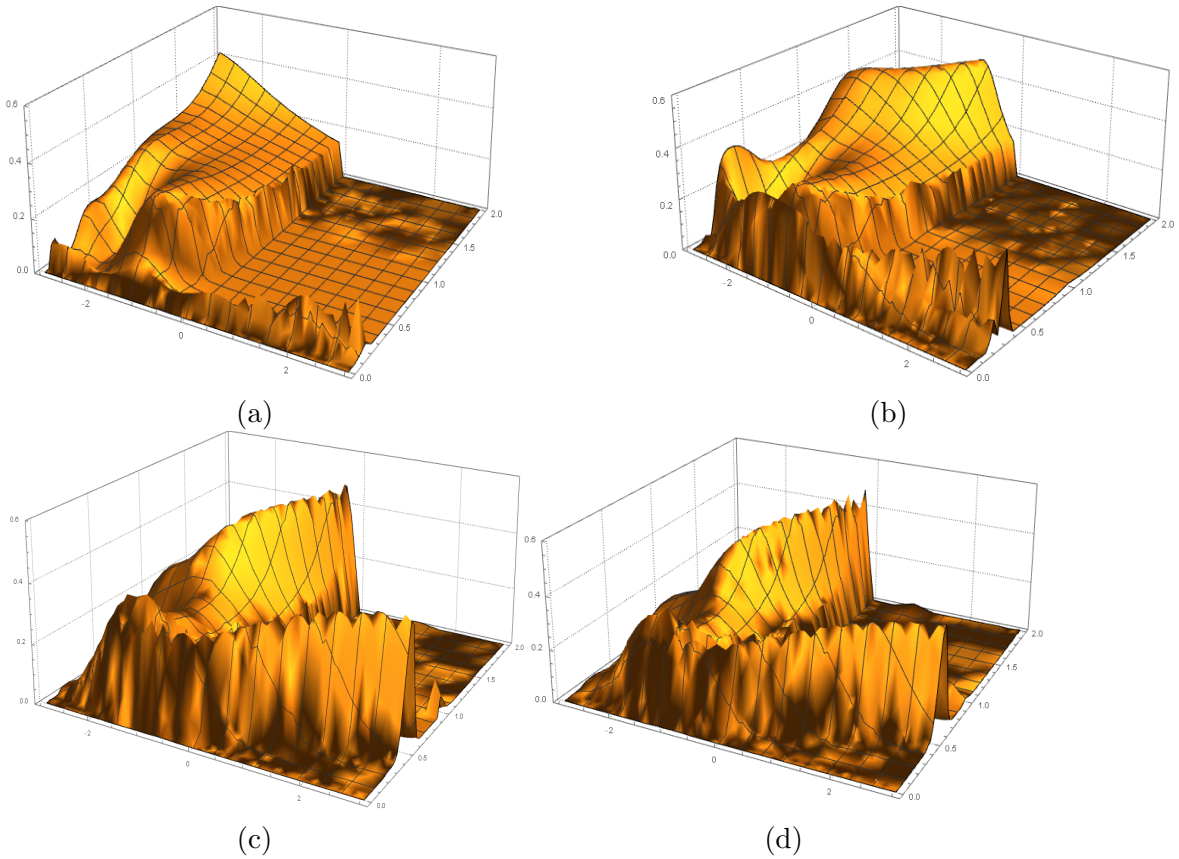


Figure 3.3: Plots for the Probability Density for evolution of a Gaussian Wavelet under a perturbative Quartic Anharmonic potential till first order with $m = 1, k = -2, \lambda = 10^{-4}, \hbar = 1$, with (a) $\lambda = 0.01$, (b) $\lambda = 0.05$ and (c) $\lambda = 0.2$ respectively

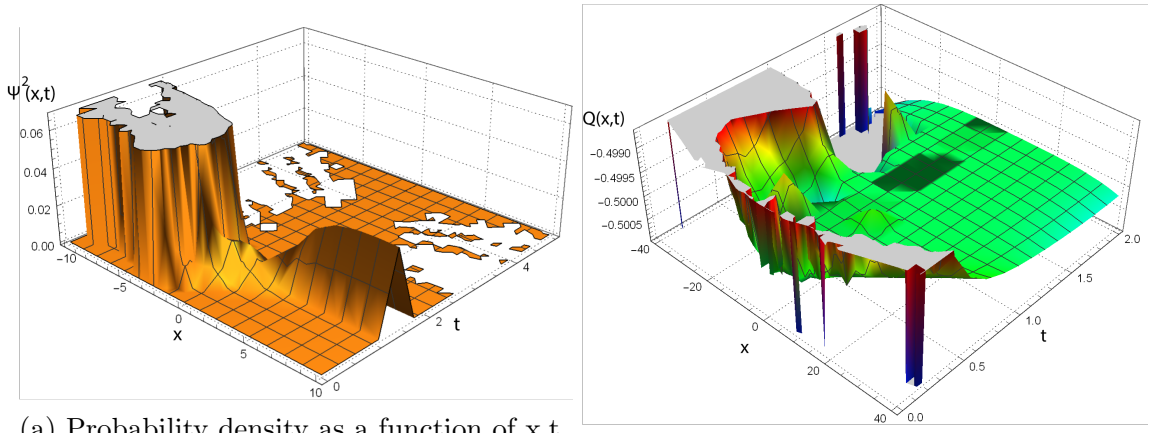
The Angular frequency is defined as,

$$\omega(t) = \sqrt{\frac{1}{m}\frac{\partial^2 V(x)}{\partial x^2}|_{x=x^{cl}(t)}} \tag{3.16}$$

Substituting (3.4), neglecting higher order terms and using the formula of double-angles, the angular frequency becomes,

$$\omega(t) = \sqrt{a + \frac{3K\lambda A^2}{2} + \frac{3K\lambda A^2}{2}\cos[2(\omega_0 + \frac{3\lambda A^2}{8\omega_0})t + 2\phi]} \tag{3.17}$$

The integrals involving $\omega(t)$ can be computed analytically by expressing them as elliptic integrals and using standard forms,[31, 32]



(a) Probability density as a function of x,t

(b) Quantum potential as a function of x,t

Figure 3.4: Plots for the Probability Density and Quantum Potential for the double-well with $M = 1, a = -2, \lambda = 10^{-4}, K = 1, \hbar = 1$. As is shown, the quantum potential is negative in the right well, after certain an initial time. This can be interpreted as lowering of the classical barrier.

$$\int_0^t \omega(t')^{-2}\, dt' = \frac{\arctan\left[\frac{w_0^2 \tan\left[\frac{1}{2}t\left(\frac{3A^2K\lambda}{8w_0}+w_0\right)\right]}{\sqrt{-\frac{9}{4}A^4K^2\lambda^2+\left(\frac{3}{2}A^2K\lambda+w_0^2\right)^2}}\right]}{\left(\frac{3A^2K\lambda}{8w_0}+w_0\right)\sqrt{-\frac{9}{4}A^4K^2\lambda^2+\left(\frac{3}{2}A^2K\lambda+w_0^2\right)^2}} \tag{3.18}$$

The figure reports the probability density and the Quantum Potential as function of space and time, computed numerically using equations (1.13), for the parameter values $m = 1, a = -4, K = 3.2, \hbar = 1$ and various values of λ and the initial Gaussian wavelet,

$$\Psi_0(x_0) = 0.997356 e^{-3.125(1.1+x_i)^2} \tag{3.19}$$

The parameters of the initial wave function is chosen such that the probability of finding the particle in the left well is ~ 1, as well as it is centered very close to the barrier wall to show some interesting dynamics, even in its initial time of flight.

As is expected from earlier studies, a part of the probability density is clearly observed to cross the classically forbidden barrier, which is situated at $x = 0$, and the tunneling probability increases as the anharmonicity is increased, by tuning the value of λ.

In a double well potential the Probability amplitude is expected to oscillate between two wells, which is not evident in our plots, and probably is rendered due to higher order corrections. The higher order effects were not incorporated as our main interest was in tunneling, which is well studied even within first order. However, as is suggested by the formulation the incorporation should be straight forward. We reserve this material for further study and discourse.

Another set of study was done to probe the nature of Quantum Potential, as the barrier penetration happens. The figure (3.4b) reports the probability density and

the Quantum Potential as function of space and time, computed numerically using equations (1.13), for the parameter values $M = 1, a = -2, \lambda = 10^{-4}, K = 1, \hbar = 1$ and the initial Gaussian wave packet,

$$\Psi_0(x_i) = \frac{1}{\sqrt{2\pi\alpha^2}} e^{\frac{-(x_i-l)^2}{2\alpha^2}} \tag{3.20}$$

where for the purpose of the plot we have chosen $\alpha = 0.4$ and $l = -3.126$.

Bohm had interpreted the mechanism of tunneling by proposing that the Quantum Potential creates channels, by lowering the applied potential. If the QP is negative then the effective total potential is lower than the actual applied potential. Then the whole dynamics can be seen as a blob of fluid traversing through the lowered potential.[10] On the other hand according to Wyatt [15] et al, it is the initial position dependent acceleration, during initial period of flight, that causes certain fluid elements to fly over the classical barrier. That is, whether a particle will be tunneled or not, is encoded in its initial position in the wave-packet which determines the acceleration for initial moments. This in turn would dictate whether the particle will finally gather enough momentum to cross the barrier.

Our results indicate a reconciliation of the two seemingly contradicting views. The fact that Bohm's interpretation is validated is obvious from the flat groove travelling towards the right well in the Quantum Potential, as well as, the fact that, initially the QP is steep, and thus its gradient is large. Depending on the initial position of the fluid element, the force directs it to either the left or the right well. However, with time the QP becomes flat and thus its gradient becomes zero. Thus, it is only the initial time of flight that decides the fate of the fluid element in crossing the barrier, and to a good approximation the QP can be neglected for further dynamics, as was conceived by Wyatt. Both the interpretations are thus found to be completely consistent with each other as far as the toy model is concerned.[1]. Exploration in this direction using more complicated and general models forms material for further study and discourse.

[1]Other studies on tunneling using quantum trajectories can be found in [33]

Chapter 4

Conclusions

To summarize, in this paper we have bridged the Quantum Fluid Dynamics with the Path Integral formulation and presented a general derivation of the Quantum Potential of QFD from the principles of Path Integrals, expressing it analytically as a functional of the classical path and the initial wave-function of a system. These analytical expressions are valid for any general well-behaved potential, and can be provided to computers directly as inputs, completely bypassing the task of solving the Schrodinger's equation, to compute the QP and trajectories. For any given initial wave-function the computation requires to solve the boundary value problem for the classical path, which has linear time complexity, thus making it faster than any preceding algorithm.

QP is regarded as the origin of non-locality in QFD[10, 15]. Invoking Feynman's idea of contribution from all possible paths in governing the dynamics, and quantifying their overall effect in the Dynamics, the formulation presented in this paper, unravels a new arena of possibilities in the understanding of the processes quantum nonlocality and entanglement, which are of utmost importance in the fields of Quantum Meteorology, Condensed Matter systems and most importantly in developing Quantum Computers. The various terms in the series in (2.50), quantify different kind of correlations. This is best explained in an analogy with Quantum Circuits.

Consider the space to be a discrete lattice. In the circuit model of quantum computation a finite dimensional Hilbert space (usually qubits) lives at every lattice points, and the time evolution is given by unitary gates connecting qubits of an instant with qubits of the next. the number of qubits one gate mixes by its action, is the number of legs that the gate has. And different number of gates gives generate different type of correlations. Now consider a discrete version of (2.50). The integrals are changed into sums, and various order of k generates correlations between various modes of m, which in turn generates spatial and temporal correlations through the various partial derivatives of the potential. Likewise the different n-legged gates in a quantum circuit, the series allows one to study separate orders of correlation for continuum systems individually.

It might be worthwhile to note, we have not used any extra assumptions than the original quantum theories and have merely mathematically connected results of two preexisting seemingly disconnected nodes. Recently, Quantum Fluids have found re-

cent applications in the non-linear framework of Gross-Pitaevski equations[34], which governs the dynamics of BEC, soliton-polariton semiconductor systems etc. There are several straight-forward scopes of generalizing our work to these domains, to generate analytical solutions. From a mathematical perspective, this problem is interesting, as the integral formulation corresponding to a non-linear PDE is not well understood. Enquiry in this direction can open up an opportunity to study at least a special class of those.

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