PATH INTEGRALS IN NON-RELATIVISTIC QUANTUM MECHANICS

by

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ABSTRACT

PATH INTEGRALS IN NON-RELATIVISTIC QUANTUM MECHANICS

This thesis starts with a brief review of local and global approaches to classical mechanics. Path integral formalism, which constitutes a global approach to quantum mechanics, is introduced. A brief history of non-relativistic applications is given.

The Lagrangian and the Hamiltonian forms of the path integral are derived. The path integral solutions of the simple problems of the free particle and the harmonic oscillator are given.

The path integral solution of the fundamental problem of the hydrogen atom is reviewed. The Kustaanheimo-Stiefel transformation and the Duru-Kleinert time transformation are exhibited. It is shown that the Kustaanheimo-Stiefel transformation can be expressed in a simple form in terms of quaternions. A similar approach is applied to five dimensional hydrogen using octonions. A transformation between nine dimensional hydrogen and sixteen dimensional oscillator is derived as an example of higher dimensional generalizations.

The path integral solutions to some problems that either have conceptual importance or demonstrate transformation techniques are given. These include: the free particle on a circle, the delta function potential, the Pöschl-Teller potential, the Wood-Saxon potential, Rosen-Morse and Hulthen potentials, and the rigidly moving potential. The condition for the validity of the semi-classical approximation for the propagator in one dimension is derived.

ÖZET

RELATİVİSTİK OLMAYAN KUANTUM MEKANİĞİNDE İZ İNTEGRALLERİ

Bu tezde, önce klasik mekaniğe lokal ve global yaklaşımlar kısaca gözden geçirildi. Kuantum mekaniğine global bir yaklaşım getiren İz İntegrali formalizmi tanıtıldı. Relativistik olmayan uygulamaların kısa bir tarihçesi verildi.

İz İntegralinin Lagranjiyen ve Hamiltoniyen formları elde edildi. İki basit problemin, yani serbest parçacık ve harmonik salınıcının iz integrali çözümleri verildi.

Temel bir problem olan hidrojen atomunun iz integrali çözümü gözden geçirildi. Kustaanheimo-Stiefel ve Duru-Kleinert dönüşümleri gösterildi. Kustaanheimo-Stiefel dönüşümünün kuaterniyonlar cinsinden basitçe ifade edilebileceği gösterildi. Benzer bir yaklaşım beş boyutlu hidrojene, oktoniyonlar kullanılarak uygulandı. Daha yüksek boyutlara genelleştirmenin bir örneği olarak, dokuz boyutlu hidrojen ile on altı boyutlu salınıcı arasında bir dönüşüm türetildi.

Kavramsal önemi olan veya dönüşüm tekniklerini gösteren bazı problemlerin iz integrali çözümleri verildi. Bu problemler şunları içerir: çember üzerinde serbest parçacık, Pöschl-Teller potansiyeli, Wood-Saxon potansiyeli, Rosen-Morse ve Hulthen potansiyelleri, ve katı olarak hareket eden potansiyel. Bir boyutta yayıcı(propagatör) için yarı-klasik yaklaştırmanın geçerliliğinin şartı türetildi.

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LIST OF SYMBOLS/ABBREVIATIONS

$\mathcal{D}$	The infinite dimensional differential of the path integral
e	Electron's charge
E_n	Energy eigenvalues
G	Green's function
H	Hamiltonian
$\hbar$	Planck's constant
$\mathcal{H}^E$	Energy dependent pseudo Hamiltonian
H_n	Hermite polynpmials
i, j, k	Units of quaternions
K	The propagator
K_0	Free particle propagator
k_{B}	Boltzmann constant
$\mathcal{K}^E$	The propagator for an energy dependent pseudo Hamiltonian
L	Lagrangian
l, li, lj, lk	Units of octonions
L_n	Laguerre Polynomials
m	mass
$N, N+1$	Number of steps
$O(\ )$	Order of
P	Momentum
$P_c^{(a,b)}$	Jacobi Polynomials
$P_{\alpha\beta}^l$	Associated Legendre polynomials
P_u	Momentum conjugate to u coordinate
s	Pseudo-time
S	Action
t	Time
T	Kinetic energy
u	Energy eigenfunction
$\bar{u}$	Conjugate of a quaternion or octonion u

u^*	Star conjugate of a quaternion or octonion u
$\|u\|$	Modulus of a quaternion or octonion u
u_i	Coordinates in a transformed space
V	Potential
w	Frequency of the harmonic oscillator
α	Angle associated with the fourth dimension
ϵ	Length of the time step
μ	Effective mass
τ	Time difference between end points
ϕ	Phase of a path
Ψ	Wave–function
D-K	Duru Kleinert
K-S	Kustaanheimo Stiefel
O	Orthogonal
QED	Quantum Electrodynamics
SU	Special Unitary

1. INTRODUCTION

1.1. Local and Global Approaches to Classical Mechanics

In classical mechanics, a system is described by equations of motion. These are differential equations for n generalized coordinates $q_1 \dots q_n$, evolving in time. The n coordinates and their ranges determine the *configuration space*, a space each point of which corresponds to the way the system can look at a point in time[1] . For example, for N particles without internal structure, moving in real (3-D) space, the configuration space would be 3N dimensional.

This approach is *local*, in the sense that the equations of motion refer to *here* and *now,* to determine the near future. More precisely, the behavior of the point representing the system, moving in configuration space, depends on values of some functions –which appear in the equations of motion– and/or their derivatives *at that point* and *at the present time* to determine where the point will be in the infinitesimal future. The *path* in configuration-time space of the representative point is then composed of a succession of such positions with their attached time values.

The equations of motion could be derived by applying Newton's 2nd and 3rd laws to point masses and rigid objects in the system[2] , first in cartesian coordinates where they are simple, then transforming to generalized coordinates. However, this may be impractical in dealing with more complicated problems or in cases where the configuration space is a subspace of the space in which Newton's laws in cartesian form can be applied; for example those which involve forces of constraints maintaining the particle in contact with a specified surface.

To get the equations of motion directly in generalized coordinates, the *Lagrangian Formalism* was developed: One only needs to specify a scalar function, the *Lagrangian*

[1] i.e. a possible "snapshot" of the system

[2] Any non-rigid objects can be treated as an infinite number of point particles.

L, then express it in terms of the desired generalized coordinates and their time derivatives, and the equations of motion follow by a standard prescription, the *Euler-Lagrange equations*. In other words, one can say equally well that a system is described by its Lagrangian.

The Euler-Lagrange prescription can also be formulated as an extremum principle: For any path $x(t)$, a functional S is defined as the line integral of the Lagrangian, $S = \int L dt$. Then, among all possible paths accessible to a system, the system chooses the unique path for which S is an extremum, usually a minimum, which means that the value of S remains unchanged in the first order if the path $x(t)$ is modified slightly. The functional S is called the *action* and this way of describing the system is called *Hamilton's Principle* or *Principle of Least Action*. In contrast to the equations of motion, the Hamilton's principle is a *global* approach, in the sense that it is a statement about the whole history of the system between given initial and final points in the configuration space and given initial and final times.

Although the global approach is mathematically equivalent to the local approach, it does not give any results by itself in practice: To solve for the evolution of a system, one has to resort to the equations of motion again. Therefore, in a sense, this approach is a *posteriori*; or one may think of the Lagrangian as a convenient way to summarize –sometimes guess– the equations of motion.

1.2. Local Approach to Quantum Mechanics

In the Schrödinger form of Quantum Mechanics, the wave-function of the particle (or the point in configuration space) evolves, rather than its position. In fact, owing to the Heisenberg principle, the position is inherently uncertain.

The Schrödinger equation(s) are the quantum analog of the equations of motion in classical mechanics; in fact, they are usually derived from the classical equations of motion by giving operator status to the generalized coordinates and their conjugate canonical momenta which are defined in the Lagrangian formalism.

Let us recall that the square of the wave function in the Schrödinger form of quantum mechanics gives the probability density, and the "inner product" of two normalized wavefunctions gives the transition amplitude between the states described by the respective wavefunctions. For example the amplitude of the probability that a particle inially at the position x_a at time t_a, to be found later at the position x_b at time t_b, in Dirac's notation is given by

$$< x_b|x_a > \tag{1.1}$$

where $|x_i >$ are the position eigenkets. This expression is valid in the Heisenberg picture, where state kets are stationary and operators move. In Schrödinger picture it must be written as:

$$< x_b, t_b| \exp\left(\frac{-iH(t_b - t_a)}{\hbar}\right) |x_a, t_a > \tag{1.2}$$

Note that (1.1) is also the propagator or the Green's function for Schrödinger's time-dependent wave equation, satisfying

$$\left[-\left(\frac{\hbar^2}{2m}\right)\nabla^{"2} + V(x'') - i\hbar\frac{\partial}{\partial t}\right] G(x'', t; x', t_0) = -i\hbar\delta^3(x'' - x')\delta(t - t_0) \tag{1.3}$$

This can be seen explicitly by expanding the wave-function $\Psi(x'', t)$ in terms of the base kets $|x', t_0 >$

$$< x'', t|\alpha, t_0 >= \int d^3x' < x'', t|x', t_0 >< x', t_0|\alpha, t_0 > \tag{1.4}$$

where $|\alpha, t_0 >$ is the Heisenberg-picture state ket which is fixed in time; $< x'', t|\alpha, t_0 >$ is the wavefunction $\Psi(x'', t)$, and $< x', t_0|\alpha, t_0 >$ is the wavefunction $\Psi(x', t_0)$, while $\int d^3x'|x', t_0 >< x', t_0|$ is the identity.

For time independent potentials the propagator, written in the Schrödinger pic-

ture, can be expanded in terms of energy eigenstates and eigenvalues:

$$\begin{aligned} K(x_b,t;x_a,t_0) &= < x_b| \exp\left(\frac{-iH(t_b-t_a)}{\hbar}\right)|x_a> \\ &= \sum_{a'} < x_b| \exp\left(\frac{-iH(t_b-t_a)}{\hbar}\right)|a'><a'|x_a> \end{aligned} \tag{1.5}$$

since $\sum |a'><a'|$ is the identity. Now we make use of the fact that $|a'>$'s are the eigenstates of the Hamiltonian.

$$\begin{aligned} K(x_b,t;x_a,t_0) &= < x_b|a'><a'|x_a> \exp\left(\frac{-iE_{a'}(t_b-t_a)}{\hbar}\right) \\ &= \sum_{a'} u_a(x_b)u_a^*(x_a) \exp\left(\frac{-iE_{a'}(t_b-t_a)}{\hbar}\right) \end{aligned} \tag{1.6}$$

where $< x_b|a' >= u_a(x_b)$ is the energy eigenstate with eigenvalue E_a.

1.3. Path Integral: Global Approach to Quantum Mechanics

There was no quantum analog –or extension– of the least action principle until R.P.Feynman derived the *Path Integral Formalism* in 1942 [1, 2]. In this thesis we will explain this formalism and present various applications.

The path integral recipe –to be derived in Chapter 2– states that the propagator is given by

$$K(x_b,t_b;x_a,t_a) =< x_b|x_a >= \int \mathcal{D}x \exp\frac{i}{\hbar}\int_{t_a}^{t_b} L\ dt \tag{1.7}$$

where $\mathcal{D}x$ denotes $dx_1dx_2\ldots dx_N$, up to a normalization. Here $x_1, x_2 \ldots x_N$ are the positions of the particle at intermediate times $t_1, \ldots t_N$. Therefore the sequence $x_1, x_2 \ldots x_N$ corresponds to a path in the configuration-time space, just like in classical mechanics.

Since we integrate over $x_1, x_2 \ldots x_N$ (1.7) is a "sum over all paths". The quantity

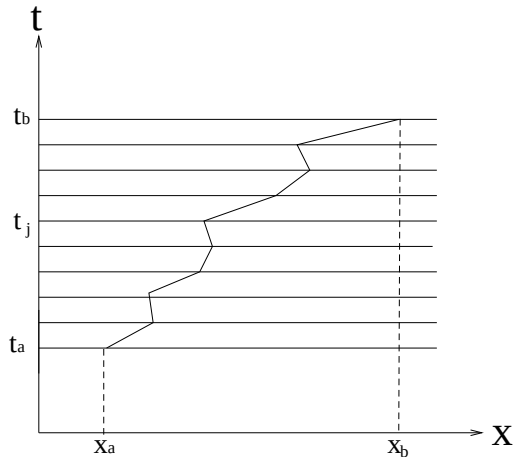

Figure 1.1. A representative path

being summed is a pure phase:

$$K(b,a) \simeq \sum_{\text{all paths}} \phi[x,t]$$

So the amplitude of the contribution of each path is the same, while the phase is the action S for that path in units of the quantum of action $\hbar$:

$$\phi[x(t)] = \mathrm{C}e^{\frac{i}{\hbar}S[x(t)]}$$

The probability to go from point x_a at time t_a to the point x_b at t_b is the absolute square of $K(b,a)$,

$$P(b,a) = |K(b,a)|^2$$

and the constant C is chosen to normalize K properly.

In the path integral formalism it is apparent that Quantum Mechanics differs from classical mechanics fundamentally in the sense all paths to play a role, through superposition. This characteristic is not explicit in the usual Schrödinger formalism.

For time independent potentials, the expansion (1.6) can in principle be used

to find the energy eigenfunctions u_a, and the energy eigenvalues E_a directly, that is, without solving the Schrödinger equation; once the propagator has been calculated in closed form using the path integral method. From that point of view one can conclude that path integration is more useful than the "Least Action Principle" in classical mechanics: One can –at least theoretically– calculate the global quantity and then solve the system completely without resorting to the local approach; whereas the least action principle just takes one back to the equations of motion.

1.4. From the double-slit to the Path Integral

Path integral approach can be made clearer to the less familiar by the following example [3]. Consider a particle, emitted from a source S at time $t = 0$, passes through one of the holes A_1 & A_2 drilled in a screen and is detected at $t = \tau$ by a detector at O.

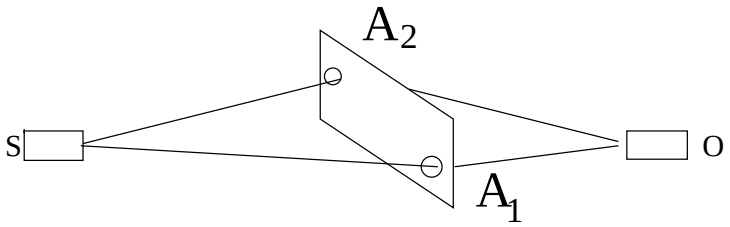

Figure 1.2. Two holes; $K_0 = K_1 + K_2$

The amplitude for the detection is given by the sum of the amplitude for the particle to propagate from S to A_1 and to O, and the amplitude to propagate from S to A_2 and to O. The two dimensional version of this is the well-known double-slit experiment and gives rise to interference fringes as a result of addition of complex amplitudes (rather than probabilities).

If we drill third, fourth holes ... etc. in the screen, of course we will have to sum over all holes.

If we add another screen we just take the amplitude from S to the hole A_i then B_j and O, then sum over $i\&j$. If we put in a third, fourth ... screen, we must sum over

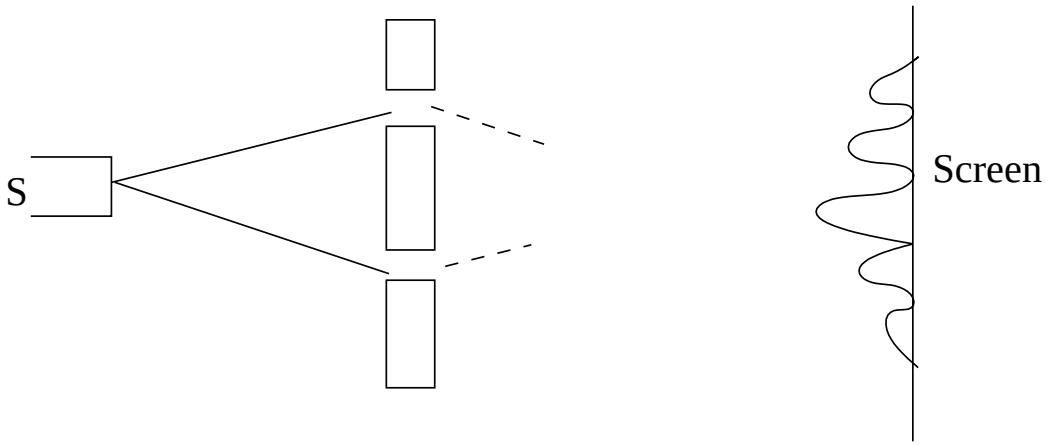

Figure 1.3. Double-Slit

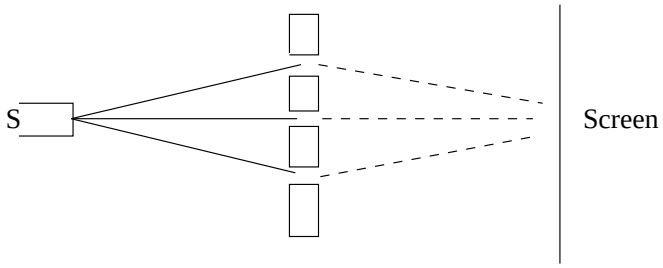

Figure 1.4. More holes; $K_s = \sum K_i$

three, four... indices.

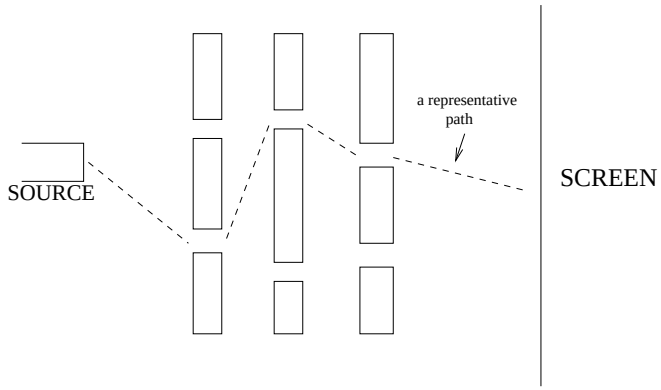

Figure 1.5. Third, fourth screen etc. $K_s = \sum K_{ij}$

Now imagine in every screen we drill infinite number holes in a way that the screen is no longer there. Then, a path is merely height x as a particular function of distance y; $x(y)$. We may continue to apply superposition until we arrive at the

integral over all paths of the amplitude for each path.

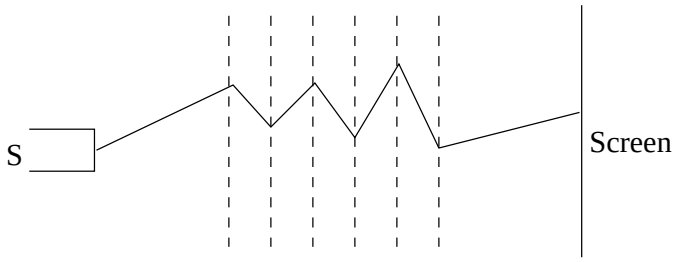

Figure 1.6. Empty space ≡ Infinite number of infinitely drilled screens

A finer description of the motion will be obtained if we specify the time, the path $x(y)$ passes each point in space. In that case a path will be given if $x(t)$, $y(t)$ are given. The total amplitude is again the sum over all possible paths. Our only remaining problem is to define this concept mathematically.

1.5. The Classical Limit

We have mentioned that, in quantum mechanics all paths contribute equal amounts to the total amplitude, but at different phases. Yet, we must be able to reproduce classical mechanics in the limit $\hbar$ goes to zero. In other words, how does some particular path become most important in the classical limit when all paths are –in some sense– on equal footing? The key lies in the oscillatory nature of the imaginary exponential.

The classical approximation corresponds to the case where S is large in relation to $\hbar$. If we moved the path by a small amount δx, the change in S would be small on the classical scale but not in the tiny unit $\hbar$. These small changes is S would lead to enormous changes in phase due to the factor $S/\hbar$ and cosine and sine would oscillate extremely rapidly. The total contribution would then add to zero. Therefore no paths really need to be considered if the neighboring paths have different actions. For the special path $\bar{x}$, for which S is an extremum, a small change in path produces no change in S, at least in the first order. All the contributions from the paths in this region are nearly in phase at $S_{\rm cl}$, and *interfere constructively.* Only for paths in the vicinity of $\bar{x}$ we can get non-vanishing contributions and in the classical limit we need only to consider this particular trajectory. From this point of view one can conclude that

classical laws of motion arise from quantum laws.

Note that according to the discussion above the trajectories which differ from $\bar{x}$ also contribute as long as the action is still within $\hbar$ of $S_{\rm cl}$. The classical trajectory is indefinite to this slight extent, and this rule serves as a measure of the limitations of the precision of the classically defined trajectory.

1.6. History

In early forties, while Feynman was a young graduate student at Princeton University and working on QED a least action principle had been found dealing with the infinite energy of the electron in classical electrodynamics [4], and he intended to use a similar procedure in dealing with the infinities in QED. He had to formulate QED using *Least Action* and *Hamilton's Principal Function* in such a way as to reproduce Classical Mechanics in the limit $\hbar$ goes to zero. He was inspired by a mysterious remark in a paper of Dirac [5], to develop a global approach to quantum mechanics analogous to Hamilton's principle of least action.

$$< x_2, t_2 | x_1, t_1 > \sim \exp\left(\frac{i}{\hbar}\int_{t_1}^{t_2} L_{\rm classical}(x, \dot{x})\, dt\right) \tag{1.8}$$

Here we have to emphasize that Dirac uses the term the *analogous to* for the relation above which refers to a loose connection. Dirac made many assumptions in arriving at (1.8) and didn't bother to justify them.

Feynman's primary aim in developing the "Path Integration" technique was to apply it in Quantum Electrodynamics, but the attempt to use Path Integration in developing a satisfactory method of avoiding the divergence difficulties in QED failed. He only managed to derive an expression for QED laws in a form that relativistic invariance is obvious [6].

The earliest application yielding a proper result was achieved shortly after the discovery of Lamb Shift and subsequent theoretical difficulties in explaining this shift

without obviously artificial means of getting rid of divergent integrals. Path Integration provided a decent way of handling these awkward infinities in a consistent manner [6].

Feynman taught Path Integration as a method of Quantum Mechanics in his courses in California Institute of Technology for a few years. Meanwhile one of his students, Hibbs, collected a set of notes from Feynman's lectures and prepared a book called 'Quantum Mechanics and Path Integrals' [7]. In his book Feynman explains the reason of the failure of path integration in QED as: 'For a relativistic particle with spin the amplitude can not be described by a simple path integral based on any reasonable action', however Duru & Barut would find a reasonable action and develop QED by integrating classical trajectories in 1989 [8].

In addition to inability in dealing with the infinities in QED, the solution of Hydrogen atom –which is one of the fundamental problems of Quantum mechanics– was not accomplished using path integration. (though it was to be solved in 1982 by Duru & Kleinert) These factors led Feynman to conclude that the operator method of Quantum Mechanics is both deeper and more powerful, and path integration lost its popularity until 1970's when Gauge Field theories appeared in particle physics. Path integration formalism was used to fix these gauges since, in this formalism, constraints can be employed much more properly than operator formalism. However, path integral formalism wouldn't gain the reputation that it deserves until the solution of the hydrogen atom was achieved.

In 1972 R.P.Feynman suggested a German physicist, Hagen Kleinert, who was spending his sabbatical year at Caltech, that he should work on the problem of the path integral of the hydrogen atom. Kleinert had demonstrated that all dynamical questions on the hydrogen atom could be answered using only operations within a dynamical group $O(4,2)$, in his Ph.D thesis in 1967. In that work the four dimensional oscillator was playing a crucial role. In fact the duality between $1/r$ potential in three dimensions and the four dimensional oscillator was known since Robert Hooke drew attention to the analogy in an attempt to understand the elliptic orbit of planets. The relationship between the Kepler problem and the harmonic oscillator was remarked

upon by Bertrand in 1875, who showed that a particle moving under the influence of a central force would move in closed and non-precessing orbits only for force laws which are inverse square or linear.

Hydrogen problem came up again in 1978 when Kleinert was teaching a course on quantum mechanics, in the Institute of Theoretical Physics in Berlin. At the same time a post-doc from Turkey, İsmail Hakkı Duru joined his group as a Humboldt fellow. In 1979 Duru and Kleinert found that the most important ingredient to solution was to work with a generalized pseudo time sliced path integral, which allows the motion to take place in pseudo time with the hamiltonian H', the operator conjugate in that basis, generating translation in pseudo time. Since all dynamical variables are classical in path integration, point canonical transformations can be employed leaving the volume element invariant. Duru and Kleinert manipulated this property to apply appropriate coordinate transformations and the path integral became harmonic and solvable [9]. Though these applications led to the correct result the procedure was criticized for its sloppy time treatment [10, 11]. The first consistent solution was presented in Kleinert's book 'Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets' [12]. Many other problems can be solved with Duru-Kleinert time transformation. For example, the Pöschl-Teller potential in nuclear physics is transformed to exactly solvable $H_{SU(2)}$ hamiltonian which describes motion over group manifolds [13]. Wood-Saxon, Rosen-Morse, and Hulthen potentials can be treated with the same procedure [14].

2. LAGRANGIAN AND HAMILTONIAN FORMS OF THE PATH INTEGRAL

2.1. Hamiltonian Form

The Hamiltonian form of path integration was put in use historically much later than the Lagrangian form, though it is much more advantageous. It is normalized and it enables canonical transformations to be employed which is a very important advantage if we consider the fact that only few problems –like free particle, harmonic oscillator (at most quadratic potential)– have been solved using the Lagrangian form of path integration.

We deduce the hamiltonian form from the knowledge of quantum mechanics. The state ket of a non-relativistic spinless particle in one dimension evolves according to Schrödinger's equation

$$H\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

We are interested in the propagator or the Green's function G which satisfies the equation

$$\left(H_x - i\hbar\partial_t\right) G(x_b, t; x_a, t_0) = -i\hbar\delta(x_b - x_a)\delta(t - t_0)$$

The function G is related to the operator G by

$$G(x_b, t; x_a, t_0) = < x_b|G(t, t_0)|x_a >$$

For time independent H, the operator solution can immediately be written down

$$G(t, t_0) = \theta(t, t_0)\exp\left[-\frac{iH(t - t_0)}{\hbar}\right] \tag{2.1}$$

where θ is the step function. Since H is assumed to be time independent we can take $t_0 = 0$ without loss of generality. Then for $t > 0$ we have

$$G(x_b, t; x_a) =< x_b|e^{-iHt/\hbar}|x_a > \tag{2.2}$$

where the argument 0 has been deleted. Though (2.2) is not valid in cases where the potential explicitly depends on time, it is always valid as far as the infinitesimal propagator $< x_n|x_{n-1} >$ is concerned.

The path integral arises from the fact that

$$e^A = (e^{A/N})^N$$

Applying this to (2.2) and letting $\lambda = it/\hbar$ and assuming $H = T + V(x)$ yields

$$G(x_b, t; x_a) =< x_b|e^{-\lambda(T+V)/N}e^{-\lambda(T+V)/N} \cdots e^{-\lambda(T+V)/N}|x_a > \tag{2.3}$$

with the product in the brackets taken N times. In other words, we have broken the time interval into N pieces. Now we make use of a fundamental property of the exponential of two operators, namely

$$e^{-\lambda(T+V)/N} = e^{-\lambda T/N}e^{-\lambda V/N} + O\left(\frac{\lambda^2}{N^2}\right) \tag{2.4}$$

This is proved easily[3] , and in a power series expansion the coefficient of the λ^2/N^2 term is

$$A = \frac{1}{2}[V, T]$$

In the subsequent manipulations we assume that the $O(1/N^2)$ term is well behaved, that it stays bounded when applied to states. For reasonable potentials this assumption

[3]An expansion is generated with the derivatives of $\exp(\lambda T/N)\exp(-\lambda(T+V)/N)\exp(\lambda V/N)$.

is justified. Next, we attempt to replace the term

$$[\exp(-\lambda(T+V)/N)]^N = \left[\exp(-\lambda T/N)\exp(-\lambda V/N) + O(1/N^2)\right]^N \tag{2.5}$$

by the term

$$\left[e^{-\lambda T/N}e^{-\lambda V/N}\right]^N \tag{2.6}$$

For real numbers (rather than operators) this substitution is a reflection of a fundamental fact about exponentials. The expression

$$\left(1+\frac{(x+y_n)}{n}\right)^n$$

converges to e^x despite the presence of y_n so long as $y_n \to 0$ as $n \to \infty$.

For operators more care is required, and the trick is to express the difference of (2.5) and (2.6) in a peculiar way:

$$\begin{aligned}
[e^{-\lambda T/N}e^{-\lambda V/N}]^N \;-\; & [e^{-\lambda(T+V)/N}]^N = \\
+\; & [e^{-\lambda T/N}e^{-\lambda V/N} - e^{-\lambda(T+V)/N}]e^{\frac{-\lambda(T+V)(N-1)}{N}} \\
+\; & e^{-\lambda T/N}e^{-\lambda V/N}[e^{-\lambda T/N}e^{-\lambda V/N} - e^{-\lambda(T+V)/N}]e^{\frac{-\lambda(T+V)(N-2)}{N}} \\
+\; & (e^{-\lambda T/N}e^{-\lambda V/N})^2[e^{-\lambda T/N}e^{-\lambda V/N} - e^{-\lambda(T+V)/N}]e^{\frac{-\lambda(T+V)(N-3)}{N}} \\
+\; & \cdots \\
+\; & (e^{-\lambda T/N}e^{-\lambda V/N})^{N-1}[e^{-\lambda T/N}e^{-\lambda V/N} - e^{-\lambda(T+V)/N}]
\end{aligned} \tag{2.7}$$

Equation (2.7) is an identity. It contains N terms each of which has the factor $e^{-\lambda T/N}e^{-\lambda V/N} - e^{-\lambda(T+V)/N}$ which is of first order $1/N^2$ by virtue of (2.4). Hence in the limit the difference is zero.

We have therefore justified the replacement of (2.3) by

$$G(x_b,t;x_a)=\lim_{N\to\infty}<x_b|(e^{-\lambda T/N}e^{-\lambda V/N})^N|x_a> \tag{2.8}$$

This can also be called an application of the Trotter product formula [15]. Let us proceed with inserting the identity operator in the form

$$\int dx_j|x_j><x_j|, j=1,\ldots,N-1 \tag{2.9}$$

between $(e^{-\lambda T/N}e^{-\lambda V/N})$ terms in the product (2.8), yielding

$$G(x_b,t;x_a)=\lim_{N\to\infty}\int dx_1\ldots dx_{N-1}\prod_{j=0}^{N-1}<x_{j+1}|e^{-\lambda T/N}e^{-\lambda V/N}|x_j> \tag{2.10}$$

(we have taken $x_b=x_N$ and $x_a=x_0$) The multiplication operator V is diagonal in the coordinate space so that

$$e^{-\lambda V/N}|x_j>=|x_j>e^{-\lambda V/N} \tag{2.11}$$

To obtain the coordinate space matrix elements of $e^{-\lambda T/N}$ we insert a complete set of momentum states. This gives

$$\begin{aligned}G(x_b,t;x_a) &= \lim_{N\to\infty}\int dx_1\ldots dx_{N-1}dp_1\ldots dp_N\\ &<x_N|p_N><p_N|x_{N-1}>\ldots<x_1|p_1><p_1|x_0>\\ &\times\exp\left(\sum_{j=1}^{N}\frac{\lambda p_j^2}{2mN}-\frac{\lambda V(x_j)}{N}\right)\end{aligned} \tag{2.12}$$

If we now use

$$<x|p>=(2\pi\hbar)^{-1/2}\exp\left(\frac{ipx}{\hbar}\right)$$

and call the time step ϵ, then $\tau=N\epsilon$, the ratio λ/N becomes $i\epsilon/\hbar$. Using this, we

arrive at the expanded form of the path integral. Before writing the final form we let $N \to N+1$:

$$G(x_b,t;x_a) = \lim_{N\to\infty} \int \prod_{j=1}^{N} dx_j \int \prod_{j=1}^{N+1} \frac{dp_j}{2\pi\hbar} \exp\left\{ \frac{i}{\hbar} \sum_{j=1}^{N+1} \left(p_j(x_j - x_{j-1}) - \frac{\epsilon p_j^2}{2m} - \epsilon V(x_j) \right) \right\} \tag{2.13}$$

where $\epsilon = \tau/(N+1)$

Let us concentrate on the exponential in (2.13),

$$\frac{i}{\hbar} \sum_{j=1}^{N+1} \left(p_j(x_j - x_{j-1}) - \frac{\epsilon p_j^2}{2m} - \epsilon V(x_j) \right)$$

which is the sum of a certain quantity at points (x_j, p_j), $j = 1 \ldots N$. Each j corresponds to a time later than that of $j-1$, therefore these points constitute a time labeled path in phase space, and in the limit $N \to \infty$, the sum can be written formally as a time integral over that path.

$$\sum_{j=1}^{N+1} \left(p_j(x_j - x_{j-1}) - \frac{\epsilon p_j^2}{2m} - \epsilon V(x_j) \right) \sim \int_0^\tau dt \left(p\dot{x} - \frac{p^2}{2m} - V(x) \right) \tag{2.14}$$

Integrating over x_j and p_k means varying over all of phase space at a given time, therefore the multiple integral in (2.13) can be called an integral over all possible paths in phase space, subject to the condition $x_0 = x_a$, $x_{N+1} = x_b$. We can write the Green's function more formally as:

$$G(x_b,t;x_a) = \int \mathcal{D}p\mathcal{D}x \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt(p\dot{x} - H) \right\} \tag{2.15}$$

This equation, (2.15), is what one remembers first, and writes down for the Hamiltonian form of the non-relativistic path integral, but what one really means is the expanded

form (2.13).

2.2. Lagrangian Form

The Lagrangian form of path integrals is obtained from the Hamiltonian form. Note that if we integrate over the momentum variables in (2.13) using

$$\int_{-\infty}^{\infty} e^{-ay^2+by} dy = \sqrt{\frac{\pi}{a}} e^{b^2/4a} \tag{2.16}$$

We get

$$G(x_b, t; x_a) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{(N+1)/2} \prod_{j=1}^{N} dx_N \exp\left[\frac{i\epsilon}{\hbar} \sum_{j=0}^{N} \left[\frac{m}{2}\left(\frac{(x_{j+1}-x_j)}{\epsilon}\right)^2 - V(x_j)\right]\right] \tag{2.17}$$

Equation (2.17) is the path integral expression in lagrangian form. Once again the points x_j, $j = 1 \ldots N$ constitute a broken time labeled path, this time in configuration space. Therefore in the limit $N \to \infty$ the exponential can be written as:

$$\sum_{j=0}^{N} \epsilon \left[\frac{m}{2}\left(\frac{(x_{j+1}-x_j)}{\epsilon}\right)^2 - V(x_j)\right] \sim \int_0^{\tau} dt \left[\frac{1}{2}m\dot{x}^2 - V(x)\right] \tag{2.18}$$

We can recognize the integral in (2.18) as the lagrangian in classical mechanics.

The integrals over the quantities $x_1 \ldots x_N$ $(N \to \infty)$ can be interpreted as integrating over all possible paths connecting the end points. Lagrangian form is not normalized like the Hamiltonian form, i.e. a normalization constant

$$C = \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{(N+1)/2} \tag{2.19}$$

appears in front of $e^{iS/\hbar}$ in (2.17). Though C is infinite in the limit $N \to \infty$ it serves to assure that K is a unitary operator. It is also required to make the sum (the integral)

converge, and for dimensional considerations. The Lagrangian form of the path integral is written more formally as

$$\int \mathcal{D}x \; e^{i \int L dt} \tag{2.20}$$

but what is really meant is (2.17). The infinite dimensional differential operator $\mathcal{D}$ includes the normalization constant.

Note that these derivations can also be interpreted as the proof of the equivalence of the path integration and operator formalisms of quantum mechanics.

2.3. Path Integral Evaluation of the Free-Particle Propagator in Lagrangian Form

Though the evaluation of the free particle propagator is a little messier using the Lagrangian form of path integration, the calculation is worth a check for practical purposes. The free particle Lagrangian is well-known.

$$L_{\text{free}} = \frac{1}{2} m \dot{x}^2$$

We wish to evaluate the propagator, that is, to integrate $e^{iS/\hbar}$ over all paths connecting (x_b, t_b) and(x_a, t_a). A path is described by a function $x(t)$. We split the time interval $\tau = t_b - t_a$ into $N + 1$ intervals of width ϵ such that $(N + 1)\epsilon = \tau$ and approximate the function $x(t)$ by its values at the end points and N points $t_n = t_0 + n\epsilon$, $n = 1 \ldots N$. The points are connected by straight lines, giving us a broken path, as discussed in sections 1.3, 2.1, 2.2 and shown in Figure1.1.

The result should be insensitive to these approximations in the limit $N \to \infty$. The abrupt changes in velocity at the points $t_0 + n\epsilon$ that arise due to our approximation may be ignored because the Lagrangian does not depend on the acceleration or higher derivatives. We may proceed our calculation with applying the same procedure to the

action integral. We replace the continuous path definition

$$S = \int_{t_0}^{t_b} L(t)\, dt = \int_{t_0}^{t_b} \frac{1}{2} m\dot{x}^2\, dt$$

by

$$S = \sum_{i=0}^{N} \frac{m}{2} \left(\frac{x_{i+1} - x_i}{\epsilon} \right)^2 \epsilon \tag{2.21}$$

We wish to calculate

$$\begin{aligned} K(x_b, t_b; x_a, t_a) &= \int_{x_a}^{x_b} \exp\{iS[x(t), \dot{x}(t)]/\hbar\} \mathcal{D}[x(t)] \\ &= \lim_{N\to\infty} C \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left[\frac{im}{2\hbar} \sum_{i=0}^{N} \frac{(x_{i+1} - x_i)^2}{\epsilon} \right] \\ &\quad \times dx_1 \ldots dx_N \end{aligned} \tag{2.22}$$

Let us switch to the variables

$$y_i = \left(\frac{m}{2\hbar\epsilon} \right)^{\frac{1}{2}} x_i$$

K becomes

$$\lim_{N\to\infty} C' \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left[-\sum_{i=0}^{N} \frac{(y_{i+1} - y_i)^2}{i} \right] dy_1 \ldots dy_N \tag{2.23}$$

where

$$C' = C \left(\frac{2\hbar\epsilon}{m} \right)^{N/2}$$

Although the multiple integral looks formidable it can be evaluated. Considering just

the part of the integration that involves y_1, we get

$$\begin{aligned}\int_{-\infty}^{\infty} e^{-\frac{1}{i}[(y_2-y_1)^2+(y_1-y_0)^2]}\,dy_1 &= \int e^{\left\{\frac{-2}{i}\left(y_1-\frac{y_0+y_2}{2}\right)^2-\frac{1}{2i}(y_o^2+y_2^2-2y_0y_2)\right\}} \\ &= \left(\frac{i\pi}{2}\right)^{\frac{1}{2}} e^{-(y_2-y_0)^2/2i} \end{aligned} \tag{2.24}$$

Consider next the integration over y_2. Bringing in the part of the integrand involving y_2 and combining it with the result above we compute next

$$\begin{aligned}\left(\frac{i\pi}{2}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty} e^{\frac{-(y_3-y_2)^2}{i}}.e^{\frac{-(y_2-y_0)^2}{2i}}\,dy_2 &= \left(\frac{i\pi}{2}\right)^{1/2}\int e^{-\frac{3}{2i}\left(y_2-\frac{2y_3+y_0}{3}\right)^2}e^{-\frac{(y_3-y_0)^2}{3i}} \\ &= \frac{(i\pi)}{\sqrt{3}}e^{-(y_3-y_0)^2/3i} \end{aligned} \tag{2.25}$$

By comparing this result to the one from the y_1 integration, we deduce the pattern: If we carry out this process N times so as to evaluate the integral in (2.23), the result will be

$$\frac{(i\pi)^{\frac{N}{2}}}{(N+1)^{\frac{1}{2}}}e^{-(y_n-y_0)^2/(N+1)i}$$

or

$$\frac{(i\pi)^{\frac{N}{2}}}{(N+1)^{\frac{1}{2}}}e^{-m(x_b-x_a)^2/2\hbar\epsilon(N+1)i}$$

Bringing in the factor $C\left(\frac{2\hbar\epsilon}{m}\right)^{\frac{N}{2}}$ from up front, we get

$$K = C\left(\frac{2\pi\hbar\epsilon i}{m}\right)^{\frac{N}{2}}\sqrt{\frac{1}{(N+1)}}\exp\left[\frac{im(x_b-x_0)^2}{2\hbar(N+1)\epsilon}\right] \tag{2.26}$$

giving

$$K(x_b, t_b; x_a, t_0) = \sqrt{\frac{m}{2\pi i\hbar\tau}} \exp\left[\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)}\right] \tag{2.27}$$

We notice that all the x dependence is in the exponential, the pre-factor depending only on the time difference.

We would also like to compare the argument of the exponential with $iS_{\rm cl}/\hbar$. The classical path satisfies

$$\dot{x}_{\rm cl} = \frac{x_b - x_a}{\tau} = \text{Const}$$

hence the lagrangian is also constant and its time integral is trivial:

$$S_{\rm cl} = \int \frac{1}{2} m\dot{x}^2 dt = \frac{1}{2} m \left(\frac{x_b - x_a}{\tau}\right)^2 \tau = \frac{m(x_b - x_a)^2}{2\tau}$$

So we realize that the propagator in the case of the free particle is of the form

$$K_{\rm free} = f(\tau) e^{iS_{\rm cl}/\hbar} \tag{2.28}$$

We will comment more on this feature in section 4.7.

2.4. Free Particle Propagator in Hamiltonian Form

To evaluate the free particle propagator in Hamiltonian formalism we start from (2.13) with $V = 0$:

$$\begin{aligned} K(x_a, x_b; \tau) &= \lim_{N\to\infty} \int \prod_{j=1}^{N} dx_j \int \prod_{j=1}^{N+1} \frac{dp_j}{2\pi} \exp\left\{ i \sum_{j=1}^{N+1} \left(p_j(x_j - x_{j-1}) - \frac{\epsilon p_j^2}{2m} \right) \right\} \\ &= \lim_{N\to\infty} \int \prod_{j=1}^{N} dx_j \int \prod_{j=1}^{N+1} \frac{dp_j}{2\pi} \\ &\qquad \times \left(\prod_{j=1}^{N} e^{i x_j (p_j - p_{j+1})} \right) e^{i(p_{N+1} x_b - p_1 x_a)} \prod_{j=1}^{N+1} e^{-\frac{i\epsilon}{2m} p_j^2} \end{aligned} \tag{2.29}$$

In units where $\hbar = 1$. Note here $x_{N+1} \equiv x_b$ and $x_0 \equiv x_a$. Proceed with dx_j integrations giving N δ functions

$$\left(\prod_{j=1}^{N+1} \frac{dp_j}{2\pi} e^{-\frac{i\epsilon}{2m} p_j^2} \right) \left(\prod_{j=1}^{N} 2\pi \delta(p_j - p_{j+1}) \right) e^{i(p_{n+1} x_b - p_1 x_a)}$$

next we perform $dp_1 \ldots dp_n$ integrations using N δ functions.

$$K = \int \frac{dp_{N+1}}{2\pi} e^{-i\frac{\tau}{2m} p_{N+1}^2} e^{i p_{N+1}(x_b - x_a)} \tag{2.30}$$

where we have used $(N+1)\epsilon = \tau$; $\tau \equiv t_b - t_a$. Now drop subscript $N+1$ and use

$$\int_{-\infty}^{\infty} e^{-ay^2 + by} dy = \sqrt{\frac{\pi}{a}} e^{b^2/4a}$$

which yields

$$K(x_b, x_a; \tau) = \sqrt{\frac{m}{2\pi i(\hbar)\tau}} e^{\frac{im}{2\tau}(x_b - x_a)^2} \tag{2.31}$$

We see that in the Hamiltonian form, the free-particle propagator is a little more straightforward than in the lagrangian form since there is only one Gaussian integral.

2.5. Harmonic Oscillator

In path integral formalism, harmonic oscillator is solved by brute force, without any clever manipulations. Its solution enables us to solve many other problems the potentials of which can be transformed to oscillator potential with appropriate canonical and time transformations, hydrogen atom being an example. We consider the simple one dimensional case with the Lagrangian

$$L(x,\dot{x}) = \frac{m}{2}\dot{x}^2 - \frac{c(t)}{2}x^2 + b(t)x\dot{x} - e(t)x \tag{2.32}$$

For the time being we assume that the various coefficients are time dependent. The path integral has the form

$$K(x_b,x_a;t_b,t_a) = \int_{x_a}^{x_b} \mathcal{D}x(t) \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\left[\frac{m}{2}\dot{x}^2 - \frac{c(t)}{2}x^2 + b(t)x\dot{x} - e(t)x\right]\right\} \tag{2.33}$$

Let us expand the path $x(t)$ around the classical path $\bar{x}(t)$, ie:

$$x(t) = \bar{x}(t) + y(t)$$

where $y(t)$ denotes a quantum fluctuation. Expanding the action around the classical solution

$$\begin{aligned} S[x,\dot{x}] &= S[\bar{x}(t)] + \left.\frac{\delta S}{\delta x}\right|_{\bar{x}(t)} y + \left.\frac{\delta S}{\delta \dot{x}}\right|_{\bar{x}(t)} \dot{y} \\ &\quad + \frac{1}{2}\left.\frac{\delta^2 S}{\delta x^2}\right|_{\bar{x}(t)} y^2 + \frac{1}{2}\left.\frac{\delta^2 S}{\delta \dot{x}^2}\right|_{\bar{x}(t)} \dot{y}^2 + \frac{1}{2}\left.\frac{\delta^2 S}{\delta x \delta \dot{x}}\right|_{\bar{x}(t)} y\dot{y} + 0 \end{aligned} \tag{2.34}$$

The classical path minimizes the action by definition so its first variation is zero. Thus, the action reduces to

$$S[x,\dot{x}] = S_{\mathrm{cl}}(x_b,t_b;x_a,t_a) + \int_{t_a}^{t_b}\left[\frac{m}{2}\dot{y}^2 - \frac{c}{2}y^2 + by\dot{y}\right]dt \tag{2.35}$$

Note that

$$\prod_{j=1}^{n} dx_j = \prod_{j=1}^{n} dy_j$$

since the Jacobian of the linear transformation is 1. We can write the $by\dot{y}$ term as $(b/2)(\dot{y^2})$ and integrate by parts. The surface term vanishes because y goes from 0 to 0 as x goes from x_a to x_b. Then K becomes:

$$K(x_b, x_a; t_b, t_a) = \exp\left\{\frac{i}{\hbar} S[\bar{x}(t_b), \bar{x}(t_a)]\right\} F(t_b, t_a) \tag{2.36}$$

where

$$F(t_b, t_a) = \int_{y(t_a)=0}^{y(t_b)=0} \mathcal{D}y(t) \exp\left[\frac{im}{2\hbar} \int_{t_a}^{t_b} (\dot{y}^2 - w^2(t) y^2) dt\right]$$

Here we have used the abbreviation $mw^2(t) = c(t) + \dot{b}(t)$. Now

$$\begin{aligned} F(t_b, t_a) &= \lim_{N\to\infty} F_N \\ &= \lim_{N\to\infty} C \int_{-\infty}^{\infty} dy^1 \dots dy^N \\ &\quad \times \exp\left\{-\frac{m}{2i\epsilon\hbar} \sum_{j=0}^{N} \left[(y_{j+1} - y_j)^2 - \epsilon^2 w_j^2 y_j^2\right]\right\} \end{aligned} \tag{2.37}$$

Let us introduce N dimensional vector $\eta = (y_1 \dots y_N)^T$ and the $N \times N$ matrix B:

$$B = \begin{pmatrix} 2-\epsilon^2 w_1^2 & -1 & 0 & \dots & 0 \\ -1 & 2-\epsilon^2 w_2^2 & -1 & \dots & 0 \\ 0 & -1 & 2-\epsilon^2 w_3^2 & -1 & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & -1 & 2-\epsilon^2 w_{N-1}^2 & -1 \\ 0 & 0 & \cdots & -1 & 2-\epsilon^2 w_N^2 \end{pmatrix} \tag{2.38}$$

Thus we get

$$F_N = \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{N+1}{2}} \int d^N\eta \exp\left(-\frac{m}{2i\epsilon\hbar}\eta^T B\eta\right) \tag{2.39}$$

It would be much simpler to work with the diagonal form of B. In that case

$$\eta^T B\eta \to (\eta^T U)U^{-1}BU(U^{-1}\eta)$$

Note that B is hermitian therefore it is diagonalized by a unitary matrix. If we call $z = (U^{-1}\eta)$, $d^N(z) = d^N\eta$ since the jacobian of the unitary transformation is 1. Next using solving the gaussian integral we get:

$$F_N = \left(\frac{m}{2\pi i\epsilon\hbar}\right)^{\frac{N+1}{2}} \left(\frac{2\pi i\epsilon\hbar}{m}\right)^{\frac{N}{2}} \frac{1}{\sqrt{\det B}} = \left(\frac{m}{2\pi i\epsilon\hbar\ \det B}\right)^{1/2} \tag{2.40}$$

Our final task is to determine $\det B$. Consider the $j \times j$ matrix B in (2.38). If we expand the determinant with respect to the last row and let j to $j+1$, we easily see that the following recursion relation holds:

$$\det B^{(j+1)} = (2 - \epsilon^2 w^{(j+1)2})\ \det B^{(j)} \text{-} \det B^{(j-1)} \tag{2.41}$$

Let us define $g^{(j)} = \epsilon\ \det B$ then we have

$$g^{(j+1)} - 2g^{(j)} + g^{(j-1)} = -\epsilon^2 w^{(j+1)2} g^{(j)}$$

Turning to continuous notation and using $\dot{g} \sim (g^{(j+1)} - g^{(j)})/\epsilon$ we find a differential equation for the function $g(t)$:

$$\ddot{g}(t) + w^2(t)g(t) = 0$$

Finally we have to insert the $g(t)$ into the expression for F_N. The case of usual harmonic

oscillator with $w(t) = w$ (time independent) is given by $g(t) = Acos(wt) + Bsin(wt)$. We have to impose the initial conditions to obtain our particular solution. Using the recursion relation (2.41) we may find $\det B_1 = 2 - \epsilon^2 w^2$ and $\det B_0 = 1$ which yields

$$g^{(0)} = \epsilon \to 0 \ , \ g^{(1)} = \epsilon(2 - \epsilon^2 w^2) \to 0$$

as $\epsilon \to 0$. Using $g^{(1)}$ and $g^{(0)}$ we get $\dot{g}(0) = 1$ as ϵ goes to 0. Initial conditions $g(0) = 0$ and $\dot{g}(0) = 1$ lead to the particular solution

$$g(t) = \frac{1}{w} \sin wt$$

To get the path integral solution for the harmonic oscillator we must calculate its classical action.

$$S_{cl} = \int_{t_a}^{t_b} dt \left(\frac{m}{2} \dot{x}^2 - \frac{m}{2} w^2 x^2 \right) \tag{2.42}$$

Using the classical solution $x(t) = A\cos(wt) + B\sin(wt)$ with $x(t_a) = x_a$ and $x(t_b) = x_b$ we find

$$S_{cl} = \frac{mw}{2 \sin w\tau} [(x_b^2 + x_a^2) \cos w\tau - 2x_b x_a] \tag{2.43}$$

and we have for the Feynman Kernel

$$K(x_b, x_a; \tau) = \left(\frac{mw}{2\pi i\hbar \sin w\tau} \right)^{\frac{1}{2}} \exp \left\{ -\frac{mw}{2i\hbar} \left[(x_b^2 + x_a^2) \cot w\tau - \frac{2x_b x_a}{\sin w\tau} \right] \right\} \tag{2.44}$$

To find the energy eigenstates and eigenvalues we have to express the propagator

in the form (1.6). For that purpose we use Mehler's formula [16]:

$$e^{-(x^2+y^2)/2}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{z}{2}\right)^n H_n(x)H_n(y)=\frac{1}{\sqrt{1-z^2}}\exp\left[\frac{4xyz-(x^2+y^2)(1+z^2)}{2(1-z^2)}\right] \tag{2.45}$$

where H_n denote the Hermite polynomials. We can expand the Feynman Kernel according to (identify $x\equiv\sqrt{mw/\hbar}x_a$, $y\equiv\sqrt{mw/\hbar}x_b$ and $z=e^{-iw\tau}$)

$$K(x_b,x_a,\tau)=\sum_{n=0}^{\infty}e^{-i\tau E_n/\hbar}\Psi_n^*(x_a)\Psi_n(x_b) \tag{2.46}$$

and determine the energy spectrum and the wave functions (energy eigen-functions)

$$E_n=\hbar w(n+\frac{1}{2}) \tag{2.47}$$

$$\Psi_n(x)=(2^n n!)^{-1/2}\left(\frac{mw}{\pi\hbar}\right)^{\frac{1}{4}}\exp\left(-\frac{mw}{2\hbar}x^2\right)H_n\left(\sqrt{\frac{mw}{\hbar}}x\right) \tag{2.48}$$

3. HYDROGEN ATOM

In order to lay the groundwork for an alternative treatment of quantum mechanics from the point of view of fluctuating paths one has to solve the well known quantum mechanical problems via path integrals. I.H.Duru and Hagen Kleinert were motivated by this fact to present a complete treatment of one of the most important quantum mechanical systems, the hydrogen atom [9].

Though the inverse square law of force and linear dependence have been linked from time to time in history, it was Kustaanheimo and Stiefel who brought out a more direct relationship, transforming one problem to the other [17]. Duru and Kleinert also gained the correct results mapping three dimensional Coulomb problem to four dimensional oscillator.

Since the basic technical procedure can most easily be explained in two dimensions it is appropriate to start our discussion in this reduced space.

3.1. The Two-Dimensional H-Atom

Consider the Hamiltonian of the hydrogen atom in two dimensions

$$H = \frac{\vec{p}^2}{2m} - \frac{e^2}{r}, r \equiv \sqrt{x_1^2 + x_2^2}$$

where m is the mass of the electron and e is its charge. In that case the propagator is

$$K = \int \mathcal{D}^2 x \mathcal{D}^2 P \exp\left\{ i \int_{t_a}^{t_b} dt \left(\vec{p} \cdot \dot{\vec{x}} - \frac{\vec{p}^2}{2m} + \frac{e^2}{r} \right) \right\} \tag{3.1}$$

in units $\hbar = 1$. We first employ a point canonical transformation

$$\begin{array}{ll} x_1 = u_1^2 - u_2^2 & p_1 = \frac{1}{2u^2}(u_1 p_{u_1} - u_2 p_{u_2}) \\ x_2 = 2u_1 u_2 & p_2 = \frac{1}{2u^2}(u_2 p_{u_1} + u_1 p_{u_2}) \end{array} \tag{3.2}$$

where $u^2 \equiv u_1^2 + u_2^2$ and we have derived the dependence of p_1 and p_2 on u_i, p_{u_i} using Poisson brackets which are canonical invariants

$$[x_i, p_j]_{x,p} = [x_i, p_j]_{u,p_u} = \delta_{ij}$$

The volume element $d^2x d^2p$ is invariant under a canonical transformation. An extra term in the path integral comes from the d^2p_{n+1} integration which is not accompanied by a d^2x_{n+1} since $x_{n+1} = x_b$ is the fixed coordinate of the end point.

$$d^2p_{n+1} = \begin{vmatrix} \frac{\partial p_1}{\partial p_{u_1}} & \frac{\partial p_1}{\partial p_{u_2}} \\ \frac{\partial p_2}{\partial p_{u_1}} & \frac{\partial p_2}{\partial p_{u_2}} \end{vmatrix} d^2p_{u_{n+1}} = \frac{1}{4u_{n+1}^2} \equiv \frac{1}{4u_b^2}$$

$$r \to u^2 = u_1^2 + u_2^2 \; ; \; p^2 = p_1^2 + p_2^2 = \frac{p_u^2}{4u^2}$$

After these transformations the propagator takes the form

$$K = \frac{1}{4u_b^2} \int \mathcal{D}^2 u \mathcal{D}^2 P_u \exp\left\{ i \int_{t_a}^{t_b} dt \left(\vec{P}_u \cdot \dot{\vec{u}} - \frac{P_u^2}{8mu^2} + \frac{e^2}{u^2} \right) \right\} \tag{3.3}$$

This form of the propagator suggests applying the time transformation $t \to s$ such that $dt = u^2 ds$, so we get rid of the u^2 terms in the denominators. Notice that only the initial and final times of the path (t_a and t_b) are fixed and the parameters s_b and s_a satisfy

$$t_b - t_a = \int_{s_a}^{s_b} u^2 ds$$

We have to incorporate this constraint into the path integral:

$$\begin{aligned} K(x_a, t_a; x_b, t_b) \;\; = \;\; & \frac{1}{4u_b^2} \int_{s_a}^{\infty} ds_b u_b^2 \delta \left(t_b - t_a - \int_{s_a}^{s_b} u^2 ds \right) \int \mathcal{D}^2 u \mathcal{D}^2 P_u \\ & \exp\left\{ i \int_{s_a}^{s_b} ds \left(\vec{P}_u \cdot \vec{u}' - \frac{P_u^2}{8m} + e^2 \right) \right\} \end{aligned} \tag{3.4}$$

Upon a Fourier representation of the delta function this becomes

$$\begin{aligned} K(x_a,t_a;x_b,t_b) &= \frac{1}{4}\int_{s_a}^{\infty} ds_b \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{-iE(t_b-t_a)} \int \mathcal{D}^2 u \mathcal{D}^2 P_u \\ &\quad \exp\left\{ i\int_{s_a}^{s_b} ds \left(\vec{P}_u \cdot \vec{u}' - \frac{P_u^2}{8m} + e^2 - Eu^2 \right) \right\} \end{aligned} \tag{3.5}$$

carrying out the integration of the constant term in the exponential

$$\begin{aligned} K(x_a,t_a;x_b,t_b) &= \frac{1}{4}\int_{s_a}^{\infty} ds_b e^{ie^2(s_b-s_a)} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{-iE(t_b-t_a)} \int \mathcal{D}^2 u \mathcal{D}^2 P_u \\ &\quad \exp\left\{ i\int_{s_a}^{s_b} ds \left(\vec{P}_u \cdot \vec{u}' - \frac{P_u^2}{8m} - Eu^2 \right) \right\} \end{aligned} \tag{3.6}$$

or

$$K(x_a,t_a;x_b,t_b) = \frac{1}{4}\int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{-iE(t_b-t_a)} \int_{s_a}^{\infty} ds_b \mathcal{K}^E(u_b,s_b;u_a,s_a) \tag{3.7}$$

where $\mathcal{K}^E$ is the propagator of an auxiliary quantum problem which is governed by an E dependent pseudo Hamiltonian

$$\mathcal{H}^E(p,x) = \frac{dt}{ds}(H(p,x) - E) \tag{3.8}$$

with motion taking place along pseudo time s. Note that

$$\mathcal{K}^E(u_b,s_b;u_a,s_a) = \frac{1}{4} e^{ie^2(s_b-s_a)} K(u_b,s_b;u_a,s_a) \tag{3.9}$$

where $K(u_b, s_b; u_a, s_a)$ is the usual oscillator Green's function in $u(s)$ space with mass $\mu = 4m$ and frequency $w^2 = -2E/\mu$.

Since the mapping (3.2) is of square root type, u^2 and $(-u)^2$ can not be distinguished. If one considers all paths in the complex $x = x_1 + ix_2$ plane from x_a to x_b, they will be mapped into two different classes of paths in the u plane, going from u_a to u_b and from u_a to $-u_b$. There is a branch cut in x plane which lies in $x = 0$ to $x = -\infty$. If we choose the u_a corresponding to the initial x_a to lie in the right half of u plane, paths in the x plane –starting from x_a ending in x_b– that pass through the branch cut an even number of times are mapped to paths from u_a to u_b, and those that pass through the branh cut an odd number of times are mapped to paths from u_a to $-u_b$; i.e. the final u_b can be in the right as well as the left half plane. Thus the propagator should be expressed as

$$K(x_a, t_a; x_b, t_b) = \frac{1}{4}\int_{s_a}^{\infty} ds_b e^{ie^2(s_b - s_a)} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{-iE(t_b - t_a)} \left(K(u_b, s_b; u_a, s_a) + K(-u_b, s_b; u_a, s_a)\right) \tag{3.10}$$

inserting the solutions of the oscillator we get

$$K(u_b, s_b; u_a, s_a) = \sum_{n_1, n_2 = 0}^{\infty} \Psi_{n_1 n_2}(u_b) \Psi^*_{n_1 n_2}(u_a) \exp\left\{iw(n_1 + n_2 + 1)(s_b - s_a)\right\} \tag{3.11}$$

where $\Psi_{n_1 n_2}(u)$ involves Hermite polynomials:

$$\Psi_{n_1 n_2}(u) = \sqrt{\frac{\mu\omega}{\pi}} \frac{1}{2^{(n_1+n_2)/2}\sqrt{n_1! n_2!}} e^{-\mu\omega u^2/2} H_{n_1}(\sqrt{\mu\omega}u_1) H_{n_2}(\sqrt{\mu\omega}u_2) \tag{3.12}$$

$H_n(x)$ is odd when n is odd, and even when n is even. Apparently $\Psi_{n_1 n_2}(u)$ will be odd if one of n_1 and n_2 is odd, the other is even; and will be even if both n_1 and n_2 are

odd or even. Therefore in the summation of $K(u_b, s_b; u_a, s_a)$ with $K(-u_b, s_b; u_a, s_a)$, only the even values of $n_1 + n_2$ survive.

$$n_1 + n_2 = 2n \ ; \ n = 0, 1, 2, \ldots$$

The energy equations in (3.5) and (3.6) suggest introducing in addition the Fourier transformed Green's function

$$K(x_b, x_a|E) = \int_{t_a}^{\infty} dt_b e^{iE(t_b - t_a)} K(x_b, t_b; x_a, t_a) \tag{3.13}$$

Performing the ds_b integration in (3.10) $K(x_b, x_a|E)$ becomes

$$\begin{aligned} K(x_b, x_a|E) &= \frac{1}{2} \sum_{n_1, n_2}^{\infty} \frac{i}{e^2 + (2n+1)\sqrt{\frac{-2E}{\mu}}} \Psi_{n_1 n_2}(u_b) \Psi^*_{n_1 n_2}(u_a) \\ &= \frac{-m}{p_0^2} \sum_{n=0}^{\infty} \frac{i}{1 - \frac{\nu}{n+\frac{1}{2}}} \frac{p_0}{2n+1} \sum \Psi_{n_1 n_2}(u_b) \Psi^*_{n_1 n_2}(u_a) \end{aligned} \tag{3.14}$$

where we have used

$$p_0 \equiv \sqrt{-2mE} = 2m\omega = \frac{\mu\omega}{2}$$

and

$$\nu \equiv \frac{e^2}{2\omega} = \sqrt{-\frac{me^4}{2E}}$$

The poles of the Green's function (3.14) display the energy spectrum of the two dimensional hydrogen atom.

$$E = E_n = -\frac{me^4}{2\left(n + \frac{1}{2}\right)^2} \tag{3.15}$$

In the neighborhood of these poles, the factor

$$-i\frac{m}{p_0^2}\left(\frac{\nu}{n+\frac{1}{2}}\right)^{-1}$$

behaves as $i/E - E_n$such that the factorized residues:

$$\Psi^H_{n_1n_2}(x) = \sqrt{\frac{p_0}{2n+1}}\Psi_{n_1n_2}(u) \tag{3.16}$$

represent the properly normalized wave functions of the Hydrogen atom.

To put these solutions in the form of the results obtained using the Schrödinger equation for the bound two dimensional Hydrogen atom, we will use an identity between Hermite and Languerre polynomials.

$$\begin{aligned}
&\frac{e^{-\varrho}}{2^n\sqrt{(n+l)!(n-l)!}}H_{n+l}\left(\sqrt{\varrho}\cos\frac{\theta}{2}\right)H_{n-l}\left(\sqrt{\varrho}\sin\frac{\theta}{2}\right)\\
= &\sum_{M=-n}^{n} e^{iM\pi}d^n_{Ml}\left(-\frac{\pi}{2}\right)\sqrt{\frac{(n-|M|)!}{(n+|M|)!}}e^{-\varrho}e^{iM\theta}(2\varrho)^{|M|}L^{2|M|}_{n-|M|}(\varrho)\\
= &\sqrt{\frac{(n-|M|)!}{(n+|M|)!}}e^{-\varrho}e^{iM\theta}(2\varrho)^{|M|}L^{2|M|}_{n-|M|}(2\varrho)\\
= &\sum_{l=0}^{n} e^{iM\pi}d^n_{Ml}\left(\frac{-\pi}{2}\right)\frac{e^{-\varrho}}{2^n\sqrt{(n+l)!(n-l)!}}H_{n+l}\left(\sqrt{\varrho}\cos\frac{\theta}{2}\right)H_{n-l}\left(\sqrt{\varrho}\sin\frac{\theta}{2}\right)
\end{aligned} \tag{3.17}$$

where $l \equiv (n_1 - n_2)/2$ and d^n_{Ml} are the usual representation functions of rotations. Thus we can express the residue in the form:

$$\sum_{n_1+n_2=2n}\Psi_{n_1n_2}(u_b)\Psi^*_{n_1n_2}(u_a) = \sum_{M=-n}^{n}\Psi_{nM}(x_b)\Psi^*_{nM}(x_a) \tag{3.18}$$

with spherical wave functions

$$\begin{aligned}
\Psi_{nM}(x) &= \frac{e^{iM\phi}}{\sqrt{2\pi}}R_{nM}(r)\\
&= \frac{p_0}{\sqrt{n+1/2}}\sqrt{\frac{(n-|M|)!}{(n+|M|)!}}e^{-p_0r}(2p_0r)^{|M|}\frac{e^{iM\phi}}{\sqrt{2\pi}}L^{2|M|}_{n-|M|}(2p_0r)
\end{aligned} \tag{3.19}$$

3.2. The Three Dimensional H-Atom

In the case of three dimensions the propagator is

$$K(\vec{x}_a, t_a; \vec{x}_b, t_b) = \int \mathcal{D}^3 x \mathcal{D}^3 P \exp\left\{ i \int dt \left(\vec{p} \cdot \dot{\vec{x}} - \frac{\vec{p}^2}{2m} + \frac{e^2}{r} \right) \right\} \tag{3.20}$$

First we shall employ a coordinate transformation to square root type coordinates, which requires a generalization of the transformation (3.2). A transformation of this type was used in astronomy by Kustaanheimo and Stiefel for the purpose of regularizing the Kepler problem [17].

3.2.1. Kustaanheimo-Stiefel Transformation

Kustaanheimo and Stiefel have shown that the three dimensional Kepler problem may be reduced to a four dimensional harmonic oscillator by using a transformation given by

$$\begin{aligned} x_1 &= 2(u_1 u_3 + u_2 u_4) \\ x_2 &= -2(u_1 u_2 - u_3 u_4) \\ x_3 &= -u_1^2 + u_2^2 + u_3^2 - u_4^2 \end{aligned} \tag{3.21}$$

so that

$$r = (x_1^2 + x_2^2 + x_3^2)^{1/2} \equiv u^2 = u_1^2 + u_2^2 + u_3^2 + u_4^2 \tag{3.22}$$

where x_1, x_2, x_3 are the cartesian components of the position vector $\vec{x}$. The time t is replaced by s defined by

$$\frac{dt}{ds} = r = u^2 \tag{3.23}$$

Then the equation of motion

$$m\ddot{x} = -\kappa^2 |x|^{-3} x \tag{3.24}$$

is shown to be equivalent in u space to the equations

$$\frac{d^2 u_\alpha}{ds^2} \equiv u_\alpha^{''} = (E/2m) u_\alpha,\ \alpha = 1, 2, 3, 4 \tag{3.25}$$

where E is the total energy of the Kepler orbit provided that the variables u_α satisfy the condition

$$u_4 u_1' - u_3 u_2' + u_2 u_3' - u_1 u_4' = 0 \tag{3.26}$$

Therefore Kustaanheimo-Stiefel transformation has the property of "linearizing" the equations of motion of the two body Kepler problem.

3.2.2. Evaluation of the Propagator

So we have embedded the three dimensional physical space into a four dimensional auxiliary space. In the case of two dimensions, the mapping of points in x space into those in u space was ambiguous only up to the sign of the $u = \pm\sqrt{|x|}$. Here we have continuous set of possible image points. The freedom in this mapping can be parametrized by introducing a dummy fourth component x_4 in addition to three space components $\vec{x}$. Due to the four component nature of u there exists quite a natural choice for such a fourth component x_4.

Consider the differential change of x as u proceeds along an arbitrary path.From

(3.21) we find

$$\begin{pmatrix} dx_1 \\ dx_2 \\ dx_3 \end{pmatrix} = 2 \begin{pmatrix} u_3 & u_4 & u_1 & u_2 \\ -u_2 & -u_1 & u_4 & u_3 \\ -u_1 & u_2 & u_3 & -u_4 \end{pmatrix} \begin{pmatrix} du_1 \\ du_2 \\ du_3 \\ du_4 \end{pmatrix} \tag{3.27}$$

For symmetry reasons the fourth row is introduced as

$$dx_4 = 2(u_4 - u_3 + u_2 - u_1) \begin{pmatrix} du_1 \\ du_2 \\ du_3 \\ du_4 \end{pmatrix} \tag{3.28}$$

The extra coordinate x_4 is uniquely defined as

$$x_4 = 2 \int dt(u_4 \dot{u}_1 - u_3 \dot{u}_2 + u_2 \dot{u}_3 - u_1 \dot{u}_4) \tag{3.29}$$

In this way we have established a one to one correspondence between paths in x space and those in u space. Notice that dx_4 classically equals zero referring to (3.26).

We now have to search for some trivial dynamics for the motion along x_4 in such a way that the path integral remains unchanged and becomes soluble. Since we work in the phase space formulation, we shall search for convenient path integrals involving also a momentum variable p_4 associated with x_4. If there is no dynamics at all, the basic canonical relation is expressed by

$$\int_{x_4(t_a)}^{x_4(t_b)} \mathcal{D}x_4 \frac{\mathcal{D}P_4}{2\pi} \exp\left(i \int_{t_a}^{t_b} dt(p_4 \dot{x}_4) \right) = \delta\left(x_4(t_b) - x_4(t_a)\right) \tag{3.30}$$

This corresponds to the propagator of a particle moving in the dummy phase space x_4,

p_4 with vanishing Hamiltonian. One may integrate in $x_4(t_b)$ and obtain the identity

$$\int_{-\infty}^{\infty} dx_4(t_b) \int_{x_4(t_a)}^{x_4(t_b)} \mathcal{D}x_4 \frac{\mathcal{D}P_4}{2\pi} \exp\left(i \int_{t_a}^{t_b} dt (p_4 \dot{x}_4) \right) = 1 \tag{3.31}$$

Such a factor can be multiplied with the propagator expressing the original dynamical problem in the extended x_μ, p_μ space. Actually, there exists a great variety of such extensions. For example we may use a free particle Hamiltonian. In this case

$$\int_{x_4(t_a)}^{x_4(t_b)} \mathcal{D}x_4 \frac{\mathcal{D}P_4}{2\pi} \exp\left(i \int_{t_a}^{t_b} dt (p_4 \dot{x}_4 - {p_4}^2/2\mu) \right) = \frac{1}{\sqrt{2\pi i (t_b - t_a)/m}} e^{(im/2(t_b - t_a))(x_{4b} - x_{4a})^2} \tag{3.32}$$

the right hand side being the free particle propagator. Then the integral in (3.31) is gaussian in $x_4(t_b)$ and the identity still holds with $p_4 \dot{x}_4 - H_{\text{free}}$ in the exponent. Moreover we can multiply with H_{free} an arbitrary t dependent factor $\varrho(t)$ and still find

$$\int_{-\infty}^{\infty} dx_4(t_b) \int_{x_4(t_a)}^{x_4(t_b)} \mathcal{D}x_4 \frac{\mathcal{D}P_4}{2\pi} \exp\left\{ i \int_{t_a}^{t_b} dt \left(p_4 \dot{x}_4 - \varrho(t) \frac{{p_4}^2}{2\mu} \right) \right\} = 1 \tag{3.33}$$

This can be seen easily in the grated version. Dropping the subscript 4 and using $(N+1)\epsilon = t_b - t_a$:

$$\int_{-\infty}^{\infty} dx_{N+1} \prod_{n=1}^{N} dx_n \prod_{n=1}^{N+1} \frac{dp_n}{2\pi} \exp\left\{ i \sum_{n=1}^{N+1} \left(p_n (x_n - x_{n-1}) - \epsilon \varrho(t_n) \frac{{p_n}^2}{2m} \right) \right\} \tag{3.34}$$

The integrals over dx_n give δ functions. Performing the integrals over $dp_n/2\pi$ we get

$$\begin{aligned} & \int_{-\infty}^{\infty} dx_{N+1} \prod_{n=1}^{N+1} \frac{dp_n}{2\pi} \prod_{n=1}^{N} \delta(p_{n+1} - p_n) e^{i(p_{n+1} x_{n+1} - p_1 x_0)} \exp\left\{ i \sum_{n=1}^{N+1} \epsilon \varrho(t_n) \frac{{p_n}^2}{2m} \right\} \\ = & \int_{-\infty}^{\infty} dx_{N+1} \int_{-\infty}^{\infty} \frac{dp_{n+1}}{2\pi} e^{i p_{n+1}(x_{n+1} - x_0)} \exp\left\{ -i \left(\sum_{n=1}^{N+1} \epsilon \varrho(t_n) \right) \frac{p_{N+1}^2}{2m} \right\} = 1 \end{aligned} \tag{3.35}$$

We can rewrite the propagator for three dimensional H-atom with a free-particle motion

in the dummy coordinate x_4 as

$$\begin{aligned} K &= \int_{-\infty}^{\infty} d(x_4)_b \int \mathcal{D}x_4 \mathcal{D}p_4 \mathcal{D}^3 x \mathcal{D}^3 P \exp\left\{ i \int dt \left(p_4 \dot{x}_4 + \vec{p}\cdot\dot{\vec{x}} - \frac{p^2}{2m} - \frac{{p_4}^2}{2m} + \frac{e^2}{r} \right) \right\} \\ &= \int_{-\infty}^{\infty} d(x_4)_b \int \mathcal{D}^4 x \mathcal{D}^4 P \exp\left\{ i \int dt \left((\vec{p}\cdot\dot{\vec{x}})_{[4]} - \frac{p_{[4]}^2}{2m} + \frac{e^2}{r} \right) \right\} \end{aligned} \tag{3.36}$$

Having extended the propagator to four dimensions we are ready to employ a canonical transformation from the phase space of x, p_x to u, p_u. Consider the matrix of (3.27) and (3.28)

$$\begin{pmatrix} dx_1 \\ dx_2 \\ dx_3 \\ dx_4 \end{pmatrix} = 2 \begin{pmatrix} u_3 & u_4 & u_1 & u_2 \\ -u_2 & -u_1 & u_4 & u_3 \\ -u_1 & u_2 & u_3 & -u_4 \\ u_4 & -u_3 & u_2 & -u_1 \end{pmatrix} \begin{pmatrix} du_1 \\ du_2 \\ du_3 \\ du_4 \end{pmatrix} = A \begin{pmatrix} du_1 \\ du_2 \\ du_3 \\ du_4 \end{pmatrix} \tag{3.37}$$

A is orthogonal up to a factor

$$A^{-1} = \frac{1}{4u^2} A^T = \frac{1}{4r} A^T$$

and $\det A = 16r^2$ So the volume elements are related by

$$d^4x = \det A d^4u = 16r^2 d^4u \tag{3.38}$$

We now introduce the relation between p and p_u by

$$p = \frac{1}{4r} A p_u$$

Using Poisson brackets or else it can be verified that the transformation $x \to u$ $p \to p_u$ is canonical, with the volume elements in momentum space related as

$$d^4p = \frac{1}{16r^2} d^4p_u \tag{3.39}$$

which verifies the invariance of the phase space volume element.

$$d^4x d^4p = d^4u d^4p_u$$

For the $(N+1)^{th}$ momentum integration in the path integral we have

$$d^4p_{N+1} = \frac{1}{16{r_b}^2} d^4p_u$$

Applying the transformation the propagator takes the form

$$K(\vec{x}_a, t_a; \vec{x}_b, t_b) = \frac{1}{16r_b^2} \int_{-\infty}^{\infty} d(x_4)_b \int \mathcal{D}^4u \mathcal{D}^4P_u \exp\left\{ i \int dt \left(\vec{p}_u \cdot \dot{\vec{u}} - \frac{{p_u}^2}{8u^2 m} + \frac{e^2}{u^2} \right) \right\} \tag{3.40}$$

Again time parameter change $dt = u^2 ds$

$$\begin{aligned} K(x_a, t_a; x_b, t_b) &= \frac{1}{16r_b^2} \int_{-\infty}^{\infty} d(x_4)_b \int_{s_a}^{\infty} ds_b r_b e^{ie^2(s_b - s_a)} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{-iE(t_b - t_a)} \int \mathcal{D}^4u \mathcal{D}^4P_u \\ &\quad \exp\left\{ i \int_{s_a}^{s_b} ds \left(\vec{P}_u \cdot \vec{u}' - \frac{P_u^2}{8m} - Eu^2 \right) \right\} \end{aligned} \tag{3.41}$$

whose Fourier transform is

$$K(x_b, x_a|E) = \frac{1}{16r_b} \int_{s_a}^{\infty} ds_b e^{ie^2(s_b - s_a)} \int_{-\infty}^{\infty} d(x_4)_b K(u_b, s_b; u_a, s_a) \tag{3.42}$$

where

$$K(u_b, s_b; u_a, s_a) = \int \mathcal{D}^4u \frac{\mathcal{D}^4p_u}{2\pi} \exp\left\{ i \int_{s_a}^{s_b} ds \left(\vec{p}_u \cdot \vec{u}' - \frac{p_u^2}{2\mu} + \frac{1}{2}\omega^2 \mu u^2 \right) \right\} \tag{3.43}$$

where μ and ω^2 are defined as before: $\mu = 4m$, $\omega^2 = \sqrt{-E/2m}$

To bring the energy dependent propagator (3.42) to a form similar to the two dimensional case, we introduce a parametrization of the u coordinates in terms of r, θ, ϕ

of three-space, and an extra angle $\alpha \in [0, 4\pi)$:

$$\begin{aligned} u_1 &= \sqrt{r}\sin\tfrac{\theta}{2}\cos\tfrac{\alpha+\varphi}{2} \\ u_2 &= \sqrt{r}\cos\tfrac{\theta}{2}\sin\tfrac{\alpha-\varphi}{2} \\ u_3 &= \sqrt{r}\cos\tfrac{\theta}{2}\cos\tfrac{\alpha-\varphi}{2} \\ u_4 &= \sqrt{r}\sin\tfrac{\theta}{2}\sin\tfrac{\alpha+\varphi}{2} \end{aligned} \tag{3.44}$$

For a given final point $u_b(x_b, \alpha_b)$ there are infinitely many final angles α_b, with any number of jumps, going from u_a to u_b, which have to be summed in order to account for all paths, just like the addition of $\pm u$ contributions in the two dimensional case. Consequently, when we express the Green's function in terms of the angular variable α, it consists of an infinite sum of amplitudes.

$$K(u_b, s_b; u_a, s_a) \to \sum_{n=-\infty}^{\infty} K(u_b(x_b, \alpha_b + 4\pi n), s_b; u_a(x_a, \alpha_a), s_a) \tag{3.45}$$

Substituting (3.44) in (3.29) we see that

$$x_4 = -\int dt(\dot{\alpha} - \cos\theta\dot{\varphi})r \tag{3.46}$$

and the $dx_4(s_b)$ integration in (3.42) can be rewritten as an integral over α_b:

$$\int_{-\infty}^{\infty} \frac{dx_4(s_b)}{r}\bigg|_{x=fixed} = \int_{-\infty}^{\infty} d\alpha_b \tag{3.47}$$

If we split this according to

$$\int_{-\infty}^{\infty} d\alpha_b = \int_0^{4\pi} \alpha_b \sum_{\alpha_b \to \alpha_b + 2\pi n} \tag{3.48}$$

the final result follows

$$K(x_b, x_a|E) = \int_0^\infty ds_b e^{ie^2(s_b-s_a)} \left(\frac{1}{4}\int_{s_a}^{2\pi} d\alpha_b\right) \frac{1}{4}\left(K(u_b, s_b; u_a, s_a) + K(-u_b, s_b; u_a, s_a)\right) \tag{3.49}$$

where we have manipulated the fact that the shift $\alpha_b \to \alpha_b + 2\pi$ amounts to a reflection in u_b. This enables us to present the propagator in a symmetrized form in the closest possible relation with the procedure applied in solving the two dimensional problem.

For the explicit determination of the wave functions we shall again resort to the direct expansion of the oscillator Green's function which reads for $\omega^2 > 0$, $E < 0$;

$$K^E(u_b, s_b; u_a, s_a) = \frac{e^{ie^2(s_b-s_a)^2}}{8} \int_0^{2\pi} d\alpha_b \sum_{n_1 n_2 n_3 n_4} \psi_{n_1 n_2 n_3 n_4}(u_b)\psi^*_{n_1 n_2 n_3 n_4}(u_a) e^{-i\omega(n_1+n_2+n_3+n_4+2)S} \tag{3.50}$$

where $\psi_{n_1 n_2 n_3 n_4}$ are oscillator wave functions

$$\psi_{n_1 n_2 n_3 n_4}(u) = \frac{\mu\omega}{\pi} \frac{e^{-\mu\omega u^2/2}}{2^{(\Sigma n_i)/2}} \prod_{i=1}^{4} \frac{1}{\sqrt{n_i!}} H_{n_1}(\sqrt{\mu\omega} u_i) \tag{3.51}$$

Due to the final symmetrization in u_b only the states with an even number of oscillator quanta contribute. We may therefore introduce a principal quantum number $n = 1, 2, 3, \ldots$ as

$$n_1 + n_2 + n_3 + n_4 = 2(n-1)$$

Such that (3.49) becomes

$$\begin{aligned} K(x_b, x_a|E) &= \sum_{n=0}^{\infty} \frac{1}{8(e^2 - 2n\omega)} \sum_{\substack{\Sigma n_i = 2(n-1) \\ n = 1,2,3,\ldots}} \\ &\quad s \int_0^{2\pi} d\alpha_b \psi_{n_1 n_2 n_3 n_4}(u_b) \psi^*_{n_1 n_2 n_3 n_4}(u_a) \qquad (3.52) \\ &= \sum_{n=1}^{\infty} \frac{-im}{{p_0}^2 \left(1 - \frac{\nu}{n}\right)} \sum_{\substack{\Sigma n_i = 2(n-1) \\ n = 1,2,3,\ldots}} \frac{p_0}{8n} \\ &\quad \times \int_0^{2\pi} d\alpha_b \psi_{n_1 n_2 n_3 n_4}(u_b) \psi^*_{n_1 n_2 n_3 n_4}(u_a) \qquad (3.53) \end{aligned}$$

This form displays poles at E_n of the form

$$\frac{i}{E - E_n} \sum_{\Sigma n_i = 2(n-1)} \int_0^{2\pi} d\alpha_b \sqrt{\frac{p_0}{8n}} \psi_{n_1 n_2 n_3 n_4}(u_b) \sqrt{\frac{p_0}{8n}} \psi^*_{n_1 n_2 n_3 n_4}(u_a) \qquad (3.54)$$

where

$$E_n = \frac{-me^4}{2n^2} \qquad (3.55)$$

The residues are the atomic bound state wave functions with unconventional quantum numbers.In order to establish contact with standard form we use $p_0|_{pole} = me^2/n$ to rewrite the residue as

$$\sum_{m=0}^{n-1} \sum_{\substack{n_1' = 0 \\ n_2' = n - n_1' - |m| - 1}} \psi_{n_1' n_2' m}(x_b) \psi^*_{n_1' n_2' m}(x_a) \qquad (3.56)$$

where

$$\begin{aligned}\psi_{n_1' n_2' m}(x_b) &= \frac{1}{\pi n}\sqrt{{p_0}^3}\sqrt{\frac{n_1'!n_2'!}{(n_1'+|m|)!-(n_2'-|m|)!}}e^{im\varphi}(p_o r\sin\theta)^{|m|} \\ & e^{-p_0 r}L_{n_1'}^{|m|}\left(2p_0 r\cos^2\frac{\theta}{2}\right)L_{n_2'}^{|m|}\left(2p_0 r\sin^2\frac{\theta}{2}\right) \end{aligned} \tag{3.57}$$

are the parabolic wave functions used describing the Stark effect. For fixed m the quantum numbers n_1',n_2' take all integers from 0 to $|m|$ subject to the condition

$$n_1' + n_2' + |m| + 1 = n$$

These wave functions in parabolic coordinates are related to the Clebsch-Gordon coefficients.

$$\begin{aligned}\psi_{n_1' n_2' m}(x) &= \sum_{l=m}^{n-1}(-1)^{n_1'}\sqrt{2l+1}\begin{pmatrix} \frac{n-1}{2} & \frac{n-1}{2} & l \\ \frac{2m-n+2n_1'+1}{2} & \frac{n-2n_1'-1}{2} & -m \end{pmatrix} \\ & \times\psi_{nlm}(r,\theta,\varphi)\end{aligned} \tag{3.58}$$

Then the residue (3.56) can be written as

$$\sum_{\pm m=1}^{n-1}\sum_{n_1'=0}^{n-|m|}\psi_{n_1' n_2' m}(x_b)\psi^*_{n_1' n_2' m}(x_a) = \sum_{l=m}^{n-1}\sum_{m=-l}^{l}\psi_{nlm}(x_b)\psi^*_{nlm}(x_a) \tag{3.59}$$

where $\psi_{nlm}(x)$ are the usual spherical wave functions of the hydrogen atom.

$$\begin{aligned}\psi_{nlm}(x) &= \sqrt{\frac{{p_o}^3}{\pi n}}\sqrt{\frac{(2l+1)(l-|m|)!(n-l-1)!}{(l+|m|)!(n+l)!}}e^{im\varphi}{P_l}^m(\cos\theta) \\ & \times(2p_0 r)^l e^{-p_0 r}L_{n-l-1}^{2l+1}(2p_0 r)\end{aligned} \tag{3.60}$$

3.3. Kustaanheimo–Stiefel Transformation and Quaternions

It turns out that the Kustaanheimo–Stiefel transformation (3.21) can be expressed very naturally in terms of quaternions [18, 19, 20].

3.3.1. Quaternions

Quaternion algebra, introduced by W.R.Hamilton in 1856, is a generalization of the algebra of complex numbers obtained by using three independent imaginary units i, j, k. The rules

$$i^2 = j^2 = k^2 = -1$$

are postulated with the non-commutative multiplication rules

$$ij = -ji = k,\ jk = -kj = i,\ ki = -ik = j$$

Given real numbers u_l, $l = 0, 1, 2, 3$, the object

$$\mathbf{u} = u_0 + iu_1 + ju_2 + ku_3$$

is called a *quaternion* $\mathbf{u} \in U$. The sum $iu_1 + ju_2 + ku_3$ is called the *quaternion part* of $\mathbf{u}$, whereas u_0 is naturally referred to as its real part.

The *conjugate* $\bar{\mathbf{u}}$ of the quaternion $\mathbf{u}$ is defined as

$$\bar{\mathbf{u}} = u_0 - iu_1 - ju_2 - ku_3$$

then the *modulus* $|\mathbf{u}|$ is obtained by

$$|\mathbf{u}|^2 = \mathbf{u}\bar{\mathbf{u}} = \bar{\mathbf{u}}\mathbf{u} = \sum_{l=0}^{3} u_l^2$$

3.3.2. Derivation of the Kustaanheimo–Stiefel Transformation

KS regularization can be derived using quaternion algebra. For that purpose one has to present the unconventional conjugate $\mathbf{u}^*$ referred to as the *star conjugate* of the quaternion $\mathbf{u} = u_0 + iu_1 + ju_2 + ku_3$:

$$\mathbf{u}^* = u_0 + iu_1 + ju_2 - ku_3 \tag{3.61}$$

The star conjugate of $\mathbf{u}$ may be expressed in terms of the conventional conjugate $\bar{\mathbf{u}}$ as

$$\mathbf{u}^* = -k\bar{\mathbf{u}}k$$

The definition 3.61 leads to an elegant treatment of the KS regularization. The following elementary properties are easy to verify

$$\begin{aligned} (\mathbf{u}^*)^* &= \mathbf{u} \\ |\mathbf{u}^*|^2 &= |\mathbf{u}|^2 \\ (\mathbf{uv})^* &= \mathbf{v}^*\mathbf{u}^* \end{aligned} \tag{3.62}$$

Now consider the mapping

$$\mathbf{u} \rightarrow \mathbf{x} = \mathbf{u}\mathbf{u}^* \tag{3.63}$$

Star conjugation immediately yields $\mathbf{x}^* = (\mathbf{u}^*)^*\mathbf{u}^* = \mathbf{x}$; hence $\mathbf{x}$ is a quaternion of the form $x_0 + x_1 i + x_2 j$ (i.e. no k part) which may be associated with the vector $\vec{x} = (x_o, x_1, x_2) \in R^3$. Using the definition of $\mathbf{u}$ as $\mathbf{u} = u_0 + u_1 i + u_2 j + u_3 k$ and (3.63) we obtain

$$\begin{aligned} x_0 &= u_0^2 - u_1^2 - u_2^2 + u_3^2 \\ x_1 &= 2(u_0 u_1 - u_2 u_3) \\ x_2 &= 2(u_0 u_2 + u_1 u_3) \end{aligned} \tag{3.64}$$

which is the KS transformation in its classical form. So up to a permutation of the indices the KS transformation is given by the quaternion relation $\mathbf{x} = \mathbf{u}\mathbf{u}^*$. The norms of the vectors $\vec{x}$ and $\vec{u}$ satisfy

$$r = \|x\| = \|u\|^2 = \mathbf{u}\bar{\mathbf{u}} \tag{3.65}$$

which follows from

$$\|x\|^2 = \mathbf{x}\bar{\mathbf{x}} = \mathbf{u}(\mathbf{u}^*\bar{\mathbf{u}}^*)\bar{\mathbf{u}} = |\mathbf{u}^*|^2|\mathbf{u}|^2 = |\mathbf{u}|^4 = \|u\|^4$$

In order to regularize the three dimensional Kepler problem by means of the KS transformation it is necessary to look at the properties of the map (3.63) under differentiation. The transformation (3.63) or (3.64) is a mapping from R^4 to R^3; therefore it leaves one degree of freedom in the parametric space undetermined. By imposing the bilinear relation which is equivalent to (3.26)

$$2(u_3du_0 - u_2du_1 + u_1du_2 - u_0du_3) = \mathbf{u}d\mathbf{u}^* - d\mathbf{u}\mathbf{u}^* = 0 \tag{3.66}$$

between the vector $\vec{u} = (u_0, u_1, u_2, u_3)$ and its differential du on orbits, the tangential map of (3.64) becomes a linear map with an orthogonal but non-normalized matrix.

This property has a simple consequence on the differentiation of the quaternion representation (3.63) of the KS transformation.

$$d\mathbf{x} = d\mathbf{u}\mathbf{u}^* + \mathbf{u}d\mathbf{u}^*$$

Imposing (3.66) yields the elegant result

$$d\mathbf{x} = 2\mathbf{u}d\mathbf{u}^*$$

Then dx is given by

$$dx = 2 \begin{pmatrix} u_0 & -u_1 & -u_2 & u_3 \\ u_1 & u_0 & -u_3 & -u_2 \\ u_2 & u_3 & u_0 & u_1 \\ u_3 & -u_2 & u_1 & -u_0 \end{pmatrix} du \tag{3.67}$$

where $dx_3 = 0$ by (3.26) and (3.66). Note that (3.67) is equal to (3.37).

3.3.3. Inverse map

Since the mapping (3.63) does not preserve the dimension, its inverse does not exist in the usual sense. However the quaternion formalism yields an elegant way of finding the corresponding *fibration* of the space R^4. Given a quaternion $\mathbf{x} = x_0 + ix_1 + jx_2$ with vanishing k component so that $\mathbf{x} = \mathbf{x}^*$, we want to find all quaternions $\mathbf{u}$ such that $\mathbf{u}\mathbf{u}^* = \mathbf{x}$. This may be done in two steps: First we find a particular solution $\mathbf{u} = \mathbf{v} = \mathbf{v}^* = v_0 + iv_1 + jv_2$ which also has a vanishing k component. Since $\mathbf{v}\mathbf{v}^* = \mathbf{v}^2$ we may use the expression below for the square root of a quaternion

$$\mathbf{v} = \frac{\mathbf{x} + |\mathbf{x}|}{\sqrt{2(|\mathbf{x}| + x_0)}}$$

Clearly, $\mathbf{v}$ has a vanishing k component and it is a straightforward calculation to show that $|\mathbf{v}|^2 = |\mathbf{x}|$. The entire family of solutions (the fibre corresponding to $\mathbf{x}$, geometrically a circle in R^4 parametrized by the angle α), is given by

$$\mathbf{u} = \mathbf{v}.e^{k\alpha} = \mathbf{v}(\cos\alpha + k\sin\alpha)$$

$$\mathbf{u}\mathbf{u}^* = \mathbf{v}e^{k\alpha}e^{-k\alpha}\mathbf{v}^* = \mathbf{v}\mathbf{v}^* = \mathbf{x}$$

So the KS map has a freedom parametrized by the angle $\alpha \in [0, 4\pi)$, which corresponds to the angle α introduced in (3.44).

3.4. Higher Dimensional Generalizations

3.4.1. Octonions

The octonions were discovered in 1843 by John T. Graves, a friend of William Hamilton, who called them octaves. They were discovered independently by Arthur Cayley, who published the first paper on them in 1845. They are sometimes referred to as Cayley numbers or the Cayley algebra.

3.4.1.1. Octonion Algebra. The octonions can be thought of as octets of real numbers. Every octonion is a real linear combination of the unit octonions $\{1, i, j, k, l, li, lj, lk\}$. That is, every octonion x can be written in the form

$$x = x_0 + x_1 i + x_2 j + x_3 k + x_4 l + x_5 li + x_6 lj + x_7 lk$$

with real coefficients x_a.

Addition of octonions is accomplished by adding corresponding coefficients, as with the complex numbers and quaternions. By linearity, multiplication of octonions is completely determined by the multiplication table for the unit octonions given in table 3.1.

The basis for the octonions given here is not nearly as universal as the standard basis for the quaternions, however, nearly all other choices differ from this one only in order and sign.

3.4.1.2. Cayley-Dickson Construction. A more systematic way of defining the octonions is via the Cayley-Dickson construction. Just as quaternions can be defined as pairs of complex numbers, the octonions can be defined as pairs of quaternions. Ad-

1	i	j	k	l	li	lj	lk
i	-1	k	-j	-li	l	-lk	lj
j	-k	-1	i	-lj	lk	l	-li
k	j	-i	-1	-lk	-lj	li	l
l	li	lj	lk	-1	-i	-j	-k
li	-l	-lk	lj	i	-1	-k	j
lj	lk	-l	-li	j	k	-1	-i
lk	-lj	li	-l	k	-j	i	-1

Table 3.1. Octonion Multiplication

dition is defined pairwise. The product of two pairs of quaternions (a, b) and (c, d) is defined by

$$(a, b)(c, d) = (ac - d\bar{b}, \bar{a}d + cb)$$

where $\bar{z}$ denotes the conjugate of the quaternion z. This definition is equivalent to the one given above when the eight unit octonions are identified with the pairs

$$(1, 0), (i, 0), (j, 0), (k, 0), (0, 1), (0, i), (0, j), (0, k)$$

3.4.1.3. Conjugate and Norm. The conjugate of an octonion

$$x = x_0 + x_1 i + x_2 j + x_3 k + x_4 l + x_5 li + x_6 lj + x_7 lk$$

is given by

$$\bar{x} = x_0 - x_1 i - x_2 j - x_3 k - x_4 l - x_5 li - x_6 lj - x_7 lk$$

Conjugation is an involution of O and satisfies $\bar{(xy)} = \bar{y}\bar{x}$ (note the change in order).

The real part of x is defined as $1/2(x + \bar{x}) = x_0$ and the imaginary part as $1/2(x - \bar{x})$. The set of all purely imaginary octonions span a 7 dimension subspace of O, denoted $\mathrm{Im}(O)$.

The norm of the octonion x is defined as

$$|x| = \left(x_0^2 + x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 + x_6^2 + x_7^2\right)^{1/2}$$

This norm agrees with the standard Euclidean norm on R^8 and satisfies

$$|xy| = |x||y|$$

as in R, C, and Q.

3.4.1.4. Properties Octonionic Multiplication. Octonionic Multiplication is neither commutative:

$$ij = -ji \neq ji$$

nor associative:

$$(ij)l = -i(jl) \neq i(jl)$$

They do satisfy a weaker form of associativity. Namely the subalgebra generated by any two elements is associative. Actually, one can show that the subalgebra generated by any two elements of O is isomorphic to R, C, or Q, all of which are associative.

This implies that the octonions form a non-associative normed division algebra. The higher-dimensional algebras defined by the Cayley-Dickson construction (e.g. the sedenions) all fail to satisfy this property. They all have zero divisors.

It turns out that the only normed division algebras over the reals are R, C, Q, and O. These four algebras also form the only alternative, finite-dimensional division algebra over the reals (up to isomorphism).

3.4.2. Transforming 5-D Hydrogen

Just like using quaternions to transfer 3-d hydrogen atom to 4-d oscillator, one can manipulate octonion algebra to transfer 5-d hydrogen atom to 8-d oscillator. Such a transformation was given by Davtyan [21], but it is derived in a much simpler way using octonions. Defining an unconventional conjugate

$$o^* = o_0 - o_1 i - o_2 j - o_3 k + o_4 l + o_5 li + o_6 lj + o_7 lk \tag{3.68}$$

The transformation is completely described by the octonion equation:

$$\mathbf{x} = \mathbf{o}\mathbf{o}^* \tag{3.69}$$

which implies:

$$|x| = |o|^2 \tag{3.70}$$

Transformation equation (3.69) may be written explicitly as

$$\begin{aligned}
x_0 &= o_0^2 + o_1^2 + o_2^2 + o_3^2 - o_4^2 - o_5^2 - o_6^2 - o_7^2 \\
x_1 &= 0 \\
x_2 &= 0 \\
x_3 &= 0 \\
x_4 &= 2(o_0 o_4 + o_1 o_5 + o_2 o_6 + o_3 o_7) \\
x_5 &= 2(o_0 o_5 - o_1 o_4 - o_2 o_7 + o_3 o_6) \\
x_6 &= 2(o_0 o_6 + o_1 o_7 - o_2 o_4 - o_3 o_5) \\
x_7 &= 2(o_0 o_7 - o_1 o_6 + o_2 o_5 - o_3 o_4)
\end{aligned} \tag{3.71}$$

Imposing the bilinear condition $dx = 2odo^*$ as in the case of quaternions we find

$$\begin{aligned}
2(o_1 do_0 - o_0 do_1 + o_3 do_2 - o_2 do_3 + o_5 do_4 - o_4 do_5 + o_7 do_6 - o_6 do_7) &= 0 \\
2(o_2 do_0 - o_3 do_1 - o_0 do_2 + o_1 do_3 + o_6 do_4 - o_7 do_5 - o_4 do_6 + o_5 do_7) &= 0 \\
2(o_3 do_0 + o_2 do_1 - o_1 do_2 - o_0 do_3 + o_7 do_4 + o_6 do_5 - o_5 do_6 - o_4 do_7) &= 0
\end{aligned} \tag{3.72}$$

The differential change of x is given by

$$dx = 2Ado \tag{3.73}$$

where

$$A = \begin{pmatrix}
o_0 & o_1 & o_2 & o_3 & -o_4 & -o_5 & -o_6 & -o_7 \\
o_1 & -o_0 & o_3 & -o_2 & o_5 & -o_4 & o_7 & -o_6 \\
o_2 & -o_3 & -o_0 & o_1 & o_6 & -o_7 & -o_4 & o_5 \\
o_3 & o_2 & -o_1 & -o_0 & o_7 & o_6 & -o_5 & -o_4 \\
o_4 & o_5 & o_6 & o_7 & o_0 & o_1 & o_2 & o_3 \\
o_5 & -o_4 & -o_7 & o_6 & -o_1 & o_0 & o_3 & -o_2 \\
o_6 & o_7 & -o_4 & -o_5 & -o_2 & -o_3 & o_0 & o_1 \\
o_7 & -o_6 & o_5 & -o_4 & -o_3 & o_2 & -o_1 & o_0
\end{pmatrix} \tag{3.74}$$

Note that A is orthogonal up to the factor $|o|^2$.

In order to evaluate the path integral, we have to introduce the momenta canonical to the coordinate o:

$$p = \frac{1}{2r} A p_o \tag{3.75}$$

It can be verified that the transformation (3.69) with (3.75) is really canonical with

$$[x_i, p_j]_{o,p_o} = \delta_{i,j}$$

The volume in phase space remains invariant under canonical transformations:

$$d^8x d^8p = d^8o d^8p_o$$

p^2 and p_o^2 are related by

$$p^2 = p^T p = \frac{1}{4r^2} p_o^T A^T A p_o = \frac{1}{4r} p_o^2$$

The propagator for 5-d hydrogen is

$$K = \int \mathcal{D}^5 x \mathcal{D}^5 p \exp\left\{ i \int_{t_a}^{t_b} dt \left(\vec{p}.\dot{\vec{x}} - \frac{p^2}{2\mu} + \frac{e^2}{r} \right) \right\} \tag{3.76}$$

We have to introduce three dummy coordinates to the propagator so that it is transformed to a solvable form. Using the techniques of section 3.1 and 3.2:

$$K = \int_{-\infty}^{\infty} dx_b^6 \int_{-\infty}^{\infty} dx_b^7 \int_{-\infty}^{\infty} dx_b^8 \int \mathcal{D}^8 x \mathcal{D}^8 p \exp\left\{ i \int_{t_a}^{t_b} dt \left(\vec{p}.\dot{\vec{x}} - \frac{p^2}{2\mu} + \frac{e^2}{r} \right) \right\} \tag{3.77}$$

Now, apply transformation (3.69)-(3.75)

$$K = \frac{1}{256r_b^4}\int_{-\infty}^{\infty}dx_b^6\int_{-\infty}^{\infty}dx_b^7\int_{-\infty}^{\infty}dx_b^8 \tag{3.78}$$

$$\times \int \mathcal{D}^8 o\mathcal{D}^8 p_o \exp\left\{i\int_{t_a}^{t_b}dt\left(\vec{p_o}.\dot{o} - \frac{p_o^2}{8\mu o^2} + \frac{e^2}{o^2}\right)\right\} \tag{3.79}$$

This form suggests applying Duru-Kleinert time transformation $dt = |o|^2 ds$:

$$K = \frac{1}{256r_b^3}\int_{-\infty}^{\infty}\frac{dE}{2\pi}e^{-iE(s_b-s_a)}\int_{s_a}^{\infty}ds_b e^{ie^2(s_b-s_a)}\int_{-\infty}^{\infty}dx_b^6\int_{-\infty}^{\infty}dx_b^7\int_{-\infty}^{\infty}dx_b^8 \tag{3.80}$$

$$\times \int \mathcal{D}^8 o\mathcal{D}^8 p_o \exp\left\{i\int_{s_a}^{s_b}ds\left(p_o.o' - \frac{p_o^2}{8\mu} + o^2 E\right)\right\} \tag{3.81}$$

where prime denotes derivative with respect to s. We have the hamiltonian of an 8-d radial oscillator in the exponential with $\mu = 4m$ and $w^2 = \sqrt{-E/2m}$

3.4.3. 9 and Higher Dimensions

It turns out that n dimensional hydrogen can be transformed to $2(n-1)$ dimensional oscillator provided that $2(n-1) = 2^m$ where $m = 0, 1, 2, \ldots$. Since numbers including sixteen units do not exist, we have to find the transformations in higher

dimensions using elementary algebra. For example a 9-16 transformation is given by:

$$\begin{aligned}
x_1 &= u_1^2 - u_2^2 - u_3^2 - u_4^2 - u_5^2 - u_6^2 - u_7^2 - u_8^2 - u_9^2 \\
&\quad + u_{10}^2 + u_{11}^2 + u_{12}^2 + u_{13}^2 + u_{14}^2 + u_{15}^2 + u_{16}^2 \\
x_2 &= 2(u_1u_2 + u_3u_{10} + u_4u_{11} + u_5u_{12} + u_6u_{13} + u_7u_{14} + u_8u_{15} + u_9u_{16}) \\
x_3 &= 2(u_1u_3 - u_2u_{10} + u_4u_{12} - u_5u_{11} + u_6u_{14} - u_7u_{13} - u_8u_{16} + u_9u_{15}) \\
x_4 &= 2(u_1u_4 - u_2u_{11} - u_3u_{12} + u_5u_{10} + u_6u_{15} + u_7u_{16} - u_8u_{13} - u_9u_{14}) \\
x_5 &= 2(u_1u_5 - u_2u_{12} + u_3u_{11} - u_4u_{10} + u_6u_{16} - u_7u_{15} + u_8u_{14} - u_9u_{13}) \\
x_6 &= 2(u_1u_6 - u_2u_{13} - u_3u_{14} - u_4u_{15} - u_5u_{16} + u_7u_{10} + u_8u_{11} + u_9u_{12}) \\
x_7 &= 2(u_1u_7 - u_2u_{14} + u_3u_{13} - u_4u_{16} + u_5u_{15} - u_6u_{10} - u_8u_{12} + u_9u_{11}) \\
x_8 &= 2(u_1u_8 - u_2u_{15} + u_3u_{16} + u_4u_{13} - u_5u_{14} - u_6u_{11} + u_7u_{12} - u_9u_{10}) \\
x_9 &= 2(u_1u_9 - u_2u_{16} - u_3u_{15} + u_4u_{14} + u_5u_{13} - u_6u_{12} - u_7u_{11} + u_8u_{10}) \quad (3.82)
\end{aligned}$$

Next we construct the matrix A that represents the differential change of x with rewspect to u, in the form:

$$dx = 2Adu$$

We find the differential change of the dummy coordinates –dx_{10} to dx_{16}– considering the orthoganality condition of A; that is A has to be orthogonal up to the factor $|u|^2$

$$A = \begin{pmatrix}
u_1 & -u_2 & -u_3 & -u_4 & -u_5 & -u_6 & -u_7 & -u_8 & -u_9 & u_{10} \\
u_2 & u_1 & u_{10} & u_{11} & u_{12} & u_{13} & u_{14} & u_{15} & u_{16} & u_3 \\
u_3 & -u_{10} & u_1 & u_{12} & -u_{11} & u_{14} & -u_{13} & -u_{16} & u_{15} & -u_2 \\
u_4 & -u_{11} & -u_{12} & u_1 & u_{10} & u_{15} & u_{16} & -u_{13} & -u_{14} & u_5 \\
u_5 & -u_{12} & u_{11} & -u_{10} & u_1 & u_{16} & -u_{15} & u_{14} & -u_{13} & -u_4 \\
u_6 & -u_{13} & -u_{14} & -u_{15} & -u_{16} & u_1 & u_{10} & u_{11} & u_{12} & u_7 \\
u_7 & -u_{14} & u_{13} & -u_{16} & u_{15} & -u_{10} & u_1 & -u_{12} & u_{11} & -u_6 \\
u_8 & -u_{15} & u_{16} & u_{13} & -u_{14} & -u_{11} & u_{12} & u_1 & -u_{10} & -u_9 \\
u_9 & -u_{16} & -u_{15} & u_{14} & u_{13} & -u_{12} & -u_{11} & u_{10} & u_1 & u_8 \\
u_{10} & u_3 & -u_2 & u_{15} & -u_4 & u_7 & -u_6 & -u_9 & u_8 & -u_1 \\
u_{11} & u_4 & -u_5 & -u_2 & u_3 & u_8 & u_9 & -u_6 & -u_7 & -u_{12} \\
u_{12} & u_5 & u_4 & -u_3 & -u_2 & u_9 & -u_8 & u_7 & -u_6 & u_{11} \\
u_{13} & u_6 & -u_7 & -u_8 & -u_9 & -u_2 & u_3 & u_4 & u_5 & -u_{14} \\
u_{14} & u_7 & u_6 & -u_9 & u_8 & -u_3 & -u_2 & -u_5 & u_4 & u_{13} \\
u_{15} & u_8 & u_9 & u_6 & -u_7 & -u_4 & u_5 & -u_2 & -u_3 & -u_{16} \\
u_{16} & u_9 & -u_8 & u_7 & u_6 & -u_5 & -u_4 & u_3 & -u_2 & u_{15}
\end{pmatrix}$$

$$\begin{pmatrix}
u_{11} & u_{12} & u_{13} & u_{14} & u_{15} & u_{16} \\
u_4 & u_5 & u_6 & u_7 & u_8 & u_9 \\
-u_5 & u_4 & -u_7 & u_6 & u_9 & -u_8 \\
-u_2 & -u_3 & -u_8 & -u_9 & u_6 & u_7 \\
u_3 & -u_2 & -u_9 & u_8 & -u_7 & u_6 \\
u_8 & u_9 & -u_2 & -u_3 & -u_4 & -u_5 \\
u_9 & -u_8 & u_3 & -u_2 & u_5 & -u_4 \\
-u_6 & u_7 & u_4 & -u_5 & -u_2 & u_3 \\
-u_7 & -u_6 & u_5 & u_4 & -u_3 & -u_2 \\
u_{12} & -u_{11} & u_{14} & -u_{13} & u_{16} & -u_{15} \\
-u_1 & u_{10} & u_{15} & -u_{16} & -u_{13} & u_{14} \\
-u_{10} & -u_1 & -u_{16} & -u_{15} & u_{14} & u_{13} \\
-u_{15} & u_{16} & -u_1 & u_{10} & u_{11} & -u_{12} \\
u_{16} & u_{15} & -u_{10} & -u_1 & -u_{12} & -u_{11} \\
u_{13} & -u_{14} & -u_{11} & u_{12} & -u_1 & u_{10} \\
-u_{14} & -u_{13} & u_{12} & u_{11} & -u_{10} & -u_1
\end{pmatrix} \tag{3.83}$$

As usual, momenta canonical to coordinate u is transferred by

$$p = \frac{1}{2r} A p_u \tag{3.84}$$

We may proceed from here to make a time transformation $dt = u^2 ds$ and evaluate the path integral, despite mathematical rigor.

4. FURTHER APPLICATIONS OF PATH INTEGRALS

4.1. Free Particle on a Circle

In order to develop the path integral evaluation of a point particle on a circle we start with the following transition amplitude:

$$< \varphi_b, t_b|\varphi_a t_a >=< \varphi_b| \prod_{n=1}^{N+1} \exp\left(\frac{-i}{\hbar}\epsilon H\right) |\varphi_a > \tag{4.1}$$

We start with $H = 0$. The restricted geometry of the circle reveals itself in the completeness relations to be inserted in (4.1)

$$\int_0^{2\pi} |\varphi_n >< \varphi_n| = 1 \tag{4.2}$$

We insert N completeness relations and get $N+1$ δ functions since:

$$< \varphi_n|\varphi_{n-1} >= \delta(\varphi_n - \varphi_{n-1}) \ , \ \varphi_n \in [0, 2\pi)$$

2π is not included to avoid double counting. δ function can be expanded into a complete set of periodic functions on the circle as below:

$$\delta(\varphi_n - \varphi_{n-1}) = \sum_{m_n=-\infty}^{\infty} \frac{1}{2\pi} \exp[im_n(\varphi_n - \varphi_{n-1})] \tag{4.3}$$

To get a proper continuous path integral first recall Poisson's summation formula:

$$\sum_{l=-\infty}^{\infty} e^{2\pi ikl} = \sum_{m=-\infty}^{\infty} \delta(k-m) \tag{4.4}$$

The function $S(k) = \sum_m \delta(k-m)$ is periodic in k with period 1, so it can be expanded as a Fourier series of the form

$$S(k) = \sum_{l=\infty}^{\infty} S_l e^{2\pi i k l}$$

The Fourier coefficients, S_l, are given by

$$S_l = \int_{-1/2}^{1/2} dk S(k) e^{-2\pi i k l} \equiv 1$$

Therefore the Fourier expansion of $S(k)$ is exactly the left hand side of (4.4). Using (4.4) (4.1) becomes

$$< \varphi_n | \varphi_{n-1} >= \sum_{l=-\infty}^{\infty} \frac{1}{2\pi} \delta(\varphi_n - \varphi_{n-1} + 2\pi l) \tag{4.5}$$

We have made the right hand side of (4.3) periodic. Now fourier decompose with respect to momentum variables:

$$< \varphi_n | \varphi_{n-1} >= \sum_{l=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dp_n}{\pi} \exp[i p_n(\varphi_n - \varphi_{n-1}) + 2\pi i p_n l] \tag{4.6}$$

Using this expansion the amplitude with no Hamiltonian takes the form:

$$\begin{aligned} K(\varphi_b, t_b; \varphi_a, t_a) \;=\; & \prod_{n=1}^{N} \left[\int_0^{2\pi} d\varphi_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi} \sum_{l_n=-\infty}^{\infty} \right] \\ & \exp\left\{ i \sum_{n=1}^{N+1} [p_n(\varphi_n - \varphi_{n-1}) + 2\pi p_n l_n] \right\} \end{aligned} \tag{4.7}$$

Sums over l_n can be absorbed into the variables φ_n by extending their range of integration from $[0, 2\pi)$ to $-\infty$, ∞. Only in the last sum l_{N+1} this is impossible.

$$\begin{aligned} K(\varphi_b, t_b; \varphi_a, t_a) &= \sum_{l=-\infty}^{\infty} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} d\varphi_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi} \right] \\ &\quad \exp\left\{ i \sum_{n=1}^{N+1} [p_n(\varphi_n - \varphi_{n-1}) + 2\pi l p_{N+1}] \right\} \end{aligned} \tag{4.8}$$

The Hamiltonian can be inserted as usual

$$\begin{aligned} K(\varphi_b, t_b; \varphi_a, t_a) &= \sum_{l=-\infty}^{\infty} \prod_{n=1}^{N} \left[\int_{-\infty}^{\infty} d\varphi_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{dp_n}{2\pi} \right] \\ &\quad \exp\left\{ i \sum_{n=1}^{N+1} [p_n(\varphi_n - \varphi_{n-1}) + 2\pi l p_{N+1} - \epsilon H] \right\} \end{aligned} \tag{4.9}$$

In the continuum limit the expression for cyclic path integral tends to:

$$K \to \sum_{l=-\infty}^{\infty} \int_{\varphi_a \to \varphi_b + 2\pi l} \mathcal{D}\varphi \int \frac{\mathcal{D}p}{2\pi} \exp\left\{ i \int_{t_a}^{t_b} dt (p\dot{\varphi} - H) \right\} \tag{4.10}$$

Now we can use (4.9) to evaluate the propagator for a free particle on a unit circle

$$\begin{aligned} K &= \sum_{l=-\infty}^{\infty} \prod_{j=1}^{N} d\varphi_j \prod_{n=1}^{N+1} \frac{dp_j}{2\pi} \\ &\quad \exp\left\{ i \sum_{j=1}^{N+1} [p_{\varphi_j}(\varphi_j - \varphi_{j-1}) + \frac{\epsilon p_{\varphi_j}^2}{2\mu} + 2\pi l p_{\varphi_{N+1}} \right\} \end{aligned} \tag{4.11}$$

We proceed just like the free particle propagator:

$$\begin{aligned} K(\varphi_b, t_b; \varphi_a, t_a) &= \sum_{l=-\infty}^{\infty} \int \frac{dp_{n+1}}{2\pi} \exp\left\{ -i \frac{\tau p_{n+1}^2}{2\mu} + i(\varphi_b - \varphi_a + 2\pi l) p_{n+1} \right\} \\ &= \frac{1}{2\pi i \tau/\mu} \sum_{l=-\infty}^{\infty} \exp\left[\frac{i\mu}{2} \frac{(\varphi_b - \varphi_a + 2\pi l)^2}{\tau} \right] \end{aligned} \tag{4.12}$$

4.2. The Delta Function Potential

The exact propagator for δ function potential was first derived by Gaveau and Schulman [23], using path integral formalism. These authors derive the propagator using a functional integral approach. Lawande and Bhagwat presented a derivation which is directly based on Feynman's definition of path integrals [22].

Consider the Lagrangian

$$L = \frac{1}{2}m\dot{x}^2 - a\delta(x)$$

where a is a positive real constant. The propagator is defined by

$$K(x_b, t_b; x_a, t_a) = \int \mathcal{D}x \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} L dt\right) \tag{4.13}$$

Now, we split the action and let $t_a = 0$ without loss of generality.

$$S = \int_0^\tau L dt = S_0 + S_1 \tag{4.14}$$

where S_0 is the free particle action and

$$S_1 = -a\int_0^\tau \delta x(t) dt \tag{4.15}$$

To carry the δ functions out of the exponential, it would be legitimate to expand $\exp[(i/\hbar)S_1]$, which yields

$$K = \int \mathcal{D}x \exp[(i/\hbar)S_0]\left(1 + \sum_{n=1}^{\infty}\frac{(i/\hbar)^n}{n!}S_1^n\right) = K_0(x_b, \tau; x_a, 0) + K_1(x_b, \tau; x_a, 0) \tag{4.16}$$

where K_0 is the free particle propagator and K_1 is given by:

$$K_1(x_b, \tau; x_a, 0) = \sum_{n=1}^{\infty}(i/\hbar)^n G_n(x_b, \tau; x_a, 0) \tag{4.17}$$

where

$$G_n(x_b,\tau;x_a,0)=\frac{1}{n!}\int \mathcal{D}x\exp[(i/\hbar)S_0]S_1^n \tag{4.18}$$

Note that

$$\begin{aligned} S_1^n &= (-a)^n\int_0^\tau dt_n\int_0^\tau dt_{n-1}\ldots\int_0^\tau dt_1\prod_{k=1}^n\delta(x(t_k)) \\ &= (-a)^n n!\int_0^\tau dt_n\int_0^{t_n} dt_{n-1}\ldots\int_0^{t_2} dt_1\prod_{k=1}^n\delta(x_k) \end{aligned} \tag{4.19}$$

In the second step we have ordered the time as $t_1<t_2<\ldots<t_n<\tau$ and denoted $x(t_k)$ by x_k. Now we substitute the time ordered expression for S_1^n in (4.18) and take path integrals from 0 to x_1, x_1 to x_2, ..., x_n to x_b, leaving $dx_1\ldots dx_n$ integrals unevaluated.

$$\begin{aligned} G_n(x_b,\tau;x_a,0) &= (-a)^n\int_0^\tau dt_n\ldots\int_0^{t_2} dt_1\int_{-\infty}^{\infty} dx_n\ldots\int_{-\infty}^{\infty} dx_1 K_0(x_b,\tau;x_n,t_n) \\ &\quad\times K_0(x_n,t_n;x_{n-1},t_{n-1})\ldots K_0(x_1,t_1;x_a,0)\prod_{k=1}^n\delta(x_k) \end{aligned} \tag{4.20}$$

Integration over x_k variables can be performed using δ functions.

$$G_n(x_b,\tau;x_a,0)=(-a)^n\int_0^\tau dt_n\ldots\int_0^{t_2} dt_1 K_0(x_b,\tau;0,t_n)\prod_{k=2}^n K_0(0,t_n;0,t_{n-1})K_0(0,t_1;x_a,0) \tag{4.21}$$

Next we take the Laplace transform of $G_n(x_b,\tau;x_a,0)$ with respect to τ.

$$\widetilde{G}_n(x_b,s;x_a,0)=\int_o^\infty d\tau\exp(-s\tau)G_n(x_b,\tau;x_a,0) \tag{4.22}$$

Using the convolution theorem we can write

$$\begin{aligned} \widetilde{G}_n(x_b,s;x_a,0) &= (-a)^n\widetilde{K}_0(x_b,s)\widetilde{K}_0(x_a,s)[\widetilde{K}_0(0,s)]^{n-1} \\ &= (-a)^n(\alpha/is)^{\frac{n+1}{2}}\exp[-2(\alpha s/i)^{\frac{1}{2}}\xi] \end{aligned} \tag{4.23}$$

where $\xi = |x_b| + |x_a|$ and we have used the formula:

$$\widetilde{K}_0(x,s) \equiv (\alpha/i\pi)^{1/2} = \int_o^\infty d\tau \exp(-s\tau + i\alpha x^2/\tau) = (\alpha/i\pi)^{1/2} \exp[-2|x|(\alpha s/i)^{1/2}] \tag{4.24}$$

It is now convenient to carry out the sum.

$$\begin{aligned} K_1 &= \sum_{n=1}^{\infty} (i/\hbar)^n G_n(x_b, s; x_a, 0) \\ &= \sum_{n=1}^{\infty} (-i\alpha/\hbar)^n (\alpha/is)^{(n+1)/2} \exp[-2(\alpha s/i)^{1/2}\xi] \\ &= \frac{(-a\alpha/\hbar)\exp[-2(\alpha s/i)^{1/2}\xi]}{\sqrt{s}[\sqrt{s} + (a/\hbar)(i\alpha)^{1/2}]} \end{aligned} \tag{4.25}$$

Taking the inverse Laplace transform we get

$$K_1(x_b, \tau; x_a, 0) = -\frac{a\alpha}{2\pi i\hbar} \int_{x_a - i\infty}^{x_a + i\infty} ds \frac{\exp[-2(-i\alpha s)^{1/2}\xi + s\tau]}{\sqrt{s}[\sqrt{s} + (a/\hbar)(i\alpha)^{1/2}]} \tag{4.26}$$

Let $s = w^2$, $(w = u + iv)$, so that the line of integration in the w plane is defined by the set of points satisfying $u^2 + v^2 = \gamma$ where γ is a suitable path parallel to the imaginary axis, and $uv = \eta$ with $-\infty < \eta < \infty$, which shall be denoted by C. Hence,

$$K_1(x_b, \tau; x_a, 0) = -\frac{a\alpha}{\pi i\hbar} \int_C dw \frac{\exp[-2(-i\alpha)^{1/2} w\xi + w^2\tau]}{w + (a/\hbar)(i\alpha)^{1/2}} \tag{4.27}$$

Using an integral representation of $1/z$ with z having positive real part we get

$$\begin{aligned} K_1(x_b, \tau; x_a, 0) = -\frac{a\alpha}{\pi i\hbar} \int_C dw \int_0^\infty \quad & d\zeta \quad \exp[-2(-i\alpha)^{1/2} w\xi + w^2\tau] \\ & \times \quad \exp\left\{[w + (a/\hbar)(i\alpha)^{1/2}]\zeta\right\} \end{aligned} \tag{4.28}$$

This allows us to deform the arc C to coincide with the imaginary axis. The gaussian integral in (4.28) may be evaluated to give:

$$\begin{aligned} K_1(x_b, \tau; x_a, 0) = -\frac{a\alpha}{(\pi\tau)^{1/2}\hbar} \int_0^\infty \quad & d\zeta \quad \exp\left\{[-2(-i\alpha)^{1/2}\xi + \zeta/2]^2/\tau\right\} \\ & \times \quad \exp[-\zeta + (a/\hbar)(i\alpha)^{1/2}] \end{aligned} \tag{4.29}$$

Letting $\zeta = 2(-i\alpha)^{1/2}z$ yields:

$$\begin{aligned} K_1(x_b,\tau;x_a,0) &= -\frac{2a\alpha(-i\alpha)^{1/2}}{(\pi\tau)^{1/2}\hbar}\int_0^\infty dz\exp[-i\alpha(\xi+z)^2/\tau]\exp(2a\alpha z/\hbar) \\ &= -\frac{ma}{\hbar^2}\int_0^\infty dz\exp(maz/\hbar^2)K_0(\xi+z,\tau;0,0) \end{aligned} \tag{4.30}$$

Hence the exact propagator for the δ function is given by:

$$K_1(x_b,\tau;x_a,0) = K_0(x_b,\tau;x_a,0) - \frac{ma}{\hbar^2}\int_0^\infty dz\exp(-maz/\hbar^2)K_0(\xi+z,\tau;0,0) \tag{4.31}$$

which agrees with the result obtained by Gaveau and Schulman. A similar approach can be used for δ function perturbation to other potentials the propagators of which are known in advance, though the process can involve some mathematical rigor.

4.3. Pöschl-Teller Potential

The path integral for a particle moving on the SU(2) manifold S^3, is solvable [13]. The resulting Green function can be used directly in solving the path integral for the Pöschl-Teller potential:

$$V(x) = \frac{1}{2\mu}\left(\frac{\kappa(\kappa-1)}{\sin^2 x} + \frac{\lambda(\lambda-1)}{\cos^2 x}\right)\ ;\ \kappa,\lambda > 1 \tag{4.32}$$

With a simple change of variable $\theta = 2x$, $0 \le x \le \pi/2$

$$K(x_a,x_b;\tau) = 2\int_{[0]}^{\pi}\mathcal{D}\theta\mathcal{D}P_\theta e^{i\int_0^\tau dt\ \ P_\theta\dot{\theta} - \frac{P_\theta^2}{2I} - \frac{\alpha^2+\beta^2-2\alpha\beta\cos\theta-1/4}{2I\sin^2\theta}} \tag{4.33}$$

This propagator has the same form as the propagator for the $H_{SU(2)}$ Hamiltonian:

$$H_{SU(2)} = \frac{1}{2I}\left(P_{\theta^2} + \frac{P_{\varphi^2} + P_{\psi^2} - 2P_\phi P_\psi\cos\theta}{\sin^2\theta}\right) \tag{4.34}$$

imposing

$$\begin{aligned} \alpha &\equiv (\lambda + \kappa - 1) \\ \beta &\equiv (\lambda - \kappa)/2 \\ I &= \mu/4 \end{aligned} \tag{4.35}$$

The propagator for the Pöschl-Teller potential corresponds to free motion over SU(2) manifold with angular momenta P_φ, P_ψ fixed to be α, β respectively. We can incorporate this relation into the path integral as

$$\begin{aligned} &\exp\left[i\int_0^\tau dt\left(\frac{-\alpha^2+\beta^2-2\alpha\beta\cos\theta}{2I\sin^2\theta}\right)\right] = \int_0^{2\pi} d\varphi_b e^{i\alpha(\varphi_b-\varphi_a)}\int_{-2\pi}^{2\pi} d\psi_b e^{-i\beta(\psi_b-\psi_a)} \\ &\int \mathcal{D}\varphi\mathcal{D}\psi\mathcal{D}P_\varphi\mathcal{D}P_\psi \exp\left(i\int_0^\tau P_\varphi\dot{\varphi}+P_\psi\dot{\psi}-\frac{P_\varphi^2+P_\psi^2-2P_\varphi P_\psi\cos\theta}{2I\sin^2\theta}\right) \end{aligned} \tag{4.36}$$

Then the Green function for the Pöschl-Teller potential is

$$\begin{aligned} K(x_a,x_b;\tau) &= \frac{2}{16\pi^2}\int_0^{2\pi} d\varphi_b \int_{-2\pi}^{2\pi} d\psi_b e^{-i\beta(\psi_b-\psi_a)}\sqrt{\sin\theta_a\sin\theta_b} \\ &\times \sum_{l=0}^{\infty}(2l+1)e^{\frac{-i\pi}{2I}(l(l+1)+1/4)}\sum_{m,n=-l}^{l} e^{im(\varphi_b-\varphi_a)}e^{in(\psi_b-\psi_a)}P^l_{mn}(\cos\theta_a)P^l_{nm}(\cos\theta_b) \end{aligned}$$

where P^l_{mn} are associated Legendre polynomials. After integrating over $d\varphi_b$, $d\psi_b$

$$K(x_a,x_b;\tau) = \sqrt{\sin\theta_a\sin\theta_b}\sum_{l=max(|\alpha|,|\beta|)}^{\infty}(2l+1)e^{\frac{-i\pi}{2I}(l+1/2)^2}P^l_{\alpha\beta}(\cos\theta_a)P^l_{\beta\alpha}(\cos\theta_b) \tag{4.37}$$

The energy eigen-functions and eigen-values can be obtained

$$\begin{aligned} &E_n = \tfrac{1}{2\mu}(\kappa+\lambda+2n)\ ;\ n=0,1,2,\ldots \\ &\Psi_n(x) = \sqrt{2(\kappa+\lambda+2n)(\sin 2x)(\cos 2x)}P^{\frac{(\kappa+\lambda-1)}{2}+n}_{\frac{(\kappa+\lambda-1)}{2},\frac{\lambda-\kappa}{2}}(1-2\sin^2 x) \end{aligned} \tag{4.38}$$

4.4. Wood-Saxon Potential

Wood-Saxon potential describes the interaction of a neutron with a heavy nucleus.

$$V(x) = \frac{-V_0}{1+e^{x/a}} \; ; \; -\infty < x < \infty \tag{4.39}$$

The path integral is solvable [14]. We start with

$$K(x_a, x_b; \tau) = \int \mathcal{D}x\mathcal{D}p \exp\left[i\int_0^\tau dt \left(p\dot{x} - \frac{p^2}{2\mu} + \frac{V_0}{1+e^{x/a}}\right)\right] \tag{4.40}$$

We employ a point transformation of the form

$$\frac{1}{1+e^{x/a}} = \cos^2\theta \; , \; p = \frac{1}{2a}\sin(\theta)\cos(\theta)p_\theta \; , \; 0 \le \theta \le \pi/2 \tag{4.41}$$

The propagator transforms as

$$K(x_a, x_b; \tau) = \frac{\sin\theta_b \cos\theta_b}{2a}\int \mathcal{D}\theta\mathcal{D}p_\theta \exp\left[i\int_0^\tau dt \left(p_\theta\dot{\theta} - \frac{\sin^2\theta\cos^2\theta}{4a^2}\frac{p_\theta^2}{2\mu} + V_0\cos^2\theta\right)\right] \tag{4.42}$$

Next we employ D-K time transformation s

$$dt = \frac{4a^2}{\sin^2\theta\cos^2\theta}ds \tag{4.43}$$

Incorporating the constraint

$$\tau = \int_0^S ds \frac{4a^2}{\sin^2\theta\cos^2\theta}$$

Equation (4.42) can be written as

$$\begin{aligned} K(x_a, x_b; \tau) &= \int_0^\infty ds \int_{-\infty}^\infty \frac{dE}{2\pi} e^{iE\tau} \frac{2a}{\sin\theta_b\cos\theta_b} \\ \times \quad &\int \mathcal{D}\theta\mathcal{D}p_\theta \exp\left[i\int_0^S ds \left(p_\theta\theta' - \frac{p_\theta^2}{2\mu} - \frac{4a^2(E-V_0)}{\sin^2\theta} - \frac{4a^2E}{\cos^2\theta}\right)\right] \end{aligned} \tag{4.44}$$

To have a symmetric expression for the amplitude in terms of the points a and b, we write the factor in front of the path integral as

$$\begin{aligned}\frac{1}{\sin\theta_b\cos\theta_b} &= \frac{2}{\sqrt{\sin 2\theta_a \sin 2\theta_b}}\exp\left(-\frac{1}{2}ln\frac{\sin 2\theta_a}{\sin 2\theta_b}\right) \\ &= \frac{2}{\sqrt{\sin 2\theta_a \sin 2\theta_b}}\exp\left(i\int_0^S ds(-i)\frac{\cos 2\theta}{\sin 2\theta}\theta'\right) \end{aligned} \tag{4.45}$$

After inserting this formula into (4.44) and shifting p_θ by $i\cos 2\theta/\sin 2\theta$ we obtain

$$K(x_a, x_b; \tau) = \int_0^\infty ds e^{iS/2\mu}\int_{-\infty}^\infty \frac{dE}{2\pi}e^{iE\tau}\frac{4a}{\sqrt{\sin 2\theta_a \sin 2\theta_b}}\mathcal{K}(\theta_b, \theta_a; S) \tag{4.46}$$

where

$$\mathcal{K}(\theta_b, \theta_a; S) = \int \mathcal{D}\theta\mathcal{D}p_\theta \exp\left\{i\int_0^S ds\left[p_\theta\theta' - \frac{p_\theta^2}{2\mu} - \frac{1}{2\mu}\left(\frac{\kappa(\kappa-1)}{\sin^\theta} + \frac{\lambda(\lambda-1)}{\cos\theta^2}\right)\right]\right\} \tag{4.47}$$

which is the path integral for the Pöschl-Teller potential with

$$\kappa = \frac{1}{2}[1 + \sqrt{32\mu a^2(E - V_0)}]\ ,\ \lambda = \frac{1}{2}[1 + \sqrt{32\mu a^2 E}]$$

In that case we can directly write the result

$$\mathcal{K}(\theta_b, \theta_a; S) = \sum_{n=0}^\infty \exp[-i(S/2\mu)(\kappa + \lambda + 2n)^2]\Psi^n(\theta_a)\bar{\Psi}^n(\theta_b) \tag{4.48}$$

where

$$\begin{aligned}\Psi^n(\theta) &= \sqrt{2(\kappa+\lambda+2n)}\sqrt{\frac{\Gamma(n+1)\Gamma(\kappa+\lambda+n)}{\Gamma(\kappa+n+1/2)\Gamma(\lambda+n+1/2)}} \\ &\times \ (\cos\theta)^\lambda(\sin\theta)^\kappa P_n^{(\kappa-1/2,\lambda-1/2)}(1-2\sin^2\theta)\end{aligned} \tag{4.49}$$

where $P_n^{(\kappa-1/2,\lambda-1/2)}$ is the Jacobi polynomial. Inserting (4.48) into (4.46)and integrating over ds we obtain

$$K(x_a, x_b; \tau) = \frac{-8i\mu a}{\sqrt{\sin 2\theta_a \cos 2\theta_b}} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \frac{dE}{2\pi} \frac{e^{iE\tau}}{(\kappa + \lambda + 2n)^2 - 1} \Psi^n(\theta_a) \bar{\Psi}^n(\theta_b) \quad (4.50)$$

then we introduce the expressions for κ and λ, and perform the dE integration to obtain the propagator in the form

$$K(x_a, x_b; \tau) = \sum_{n=0}^{\infty} e^{-iE_n\tau} \varphi_n(x_a) \bar{\varphi}_n(x_b) \quad (4.51)$$

where the energy eigenvalues and wave-functions are given by

$$E_n = -\frac{1}{8\mu a^2 (n+1)^2} [(n+1)^2 + 2\mu a^2 V_0] \quad (4.52)$$

and

$$\begin{aligned} \varphi(x) &= \frac{i}{2\sqrt{2(n+1)}} \sqrt{4(n+1)^2 - (\lambda_n - \kappa_n)^2} \sqrt{\frac{\Gamma(n+1)\Gamma(-n-1)}{\Gamma(\kappa_n + n + 1/2)\Gamma(\lambda_n + n + 1/2)}} \\ &\times \frac{\exp[(\kappa_n - 1/2)x/2a]}{(1+e^{x/a})^{(\kappa_n + \lambda_n - 1)/2}} P_n^{(\kappa_n - 1/2, \lambda_n - 1/2)}(1 + e^{x/a})(1 - e^{x/a}) \end{aligned} \quad (4.53)$$

with

$$\kappa_n = \frac{1}{2} + \frac{1}{n+1}[(n+1)^2 - 2\mu a^2 V_0],\ \lambda_n = \frac{1}{2} + \frac{1}{n+1}[(n+1)^2 + 2\mu a^2 V_0] \quad (4.54)$$

4.5. Rosen-Morse and Hulthen Potentials

The Rosen-Morse potential describes the interatomic interaction of linear molecules.

$$V(x) = B_0 \tanh ax - U_0 \cosh^{-2} ax \ , \ -\infty < x < \infty \tag{4.55}$$

The path integral can be solved for the symmetric potential [14], which is obtained by letting either $B_0 = 0$ or $U_0 = 0$, or $B_0 = U_0$. We introduce the point transformation

$$\tanh(ax) = \cos(2y) \ , \ p = \frac{-1}{2} \sin(2y) p_y \ , \ 0 \leq y \leq \pi/2 \tag{4.56}$$

The new time variable s is given by

$$dt = \frac{ds}{1/4a^2 \sin^2(2y)}$$

Then the problem takes the form of the Pöschl-Teller Green function with

$$\kappa = \frac{1}{2}\sqrt{(2\mu/a^2)(E + B_0)} \text{ and } \lambda = \frac{1}{2}\sqrt{(2\mu/a^2)(E - B_0)}$$

The Hulthen potential is given by

$$V(r) = -V_0 \frac{e^{-r/a}}{1 - e^{-r/a}} \ , \ 0 \leq r < \infty \tag{4.57}$$

Its Schrödinger equation is exactly solvable for s-waves. It behaves like the Coulomb potential for $r \to 0$. The path integral for the Hulthen potential is solved by introducing the point transformation and the D-K time transformation in the form:

$$r = -2a \ln(\sin(\theta)) \ , \ p_r = \frac{\sin\theta}{2\cos\theta} p_\theta$$

and

$$dt = -4a^2 \frac{\cos^2\theta}{\sin^2\theta} dx$$

With these transformations the problem is converted to the Green function for the Pöschl-Teller potential with

$$\kappa = \frac{1}{2} + 2\sqrt{-\mu a^2 E} \text{ and } \lambda = \frac{-1}{4}$$

4.6. "Rigidly" Moving Potentials

In this section we will present a general solution for a time dependent potential that can be expressed in the form:

$$V(x,t) = V[x - f(t)]$$

that is, a potential of shape $V(x)$, moving with velocity $f(t)$. This was first studied by Duru [24]. The propagator for that potential is

$$K(x_a, x_b; t_a, t_b) = \int \mathcal{D}x\mathcal{D}p \exp\left\{ i \int_{t_a}^{t_b} dt \left(p_x \dot{x} - \frac{p_x^2}{2\mu} - V[x - f(t)] \right) \right\} \tag{4.58}$$

First we employ a point canonical transformation from x, p_x to Q, P.

$$\begin{aligned} Q &= x - f(t) \\ P &= p_x - \mu \dot{f}(t) \end{aligned} \tag{4.59}$$

The generating function for transformation (4.59) is

$$F_2(x,P,t) = (P + \mu\dot{f}(t))(x - f(t)) \tag{4.60}$$

Remember $dF_2 = p_i dq_i + Q_i dP_i + (K - H)dt$. The new Hamiltonian is

$$\begin{aligned} K &= H + \frac{\partial F_2}{\partial t} \\ &= \frac{1}{2\mu}\left(P + \mu\dot{f}(t)\right)^2 + V(Q) + (P + \mu\dot{f})(-\dot{f}) + \mu\ddot{f}(x - f) \qquad (4.61) \\ &= \frac{P^2}{2\mu} + V(Q) + \mu\ddot{f}Q - \frac{1}{2}\mu\dot{f}^2 \qquad (4.62) \end{aligned}$$

Using the definition of dF_2 we deduce that

$$p_x\dot{x} - H = \frac{dF_2}{dt} - Q_i dP_i - K$$

So the action transforms as

$$I = \int_{t_a}^{t_b} dt(p_x\dot{x} - H) \rightarrow \int_{t_a}^{t_b} dt\left(-Q_i dP_i - K + \frac{dF_2}{dt}\right) \tag{4.63}$$

Note that we are now concerned with the total time derivative of F_2, which equals

$$\frac{dF_2}{dt} = \dot{P}Q + \dot{Q}P + \frac{d}{dt}(\mu\dot{f}Q)$$

Then (4.63) becomes

$$I = \mu\left[\dot{f}(t_b)Q_b - \dot{f}(t_a)Q_a\right] + \int_{t_a}^{t_b} dt[P\dot{Q} - K] \tag{4.64}$$

The propagator of the time dependent potential takes the form

$$\begin{aligned} K(x_a, x_b; t_a, t_b) &= e^{i\mu\left[\dot{f}(t_b)Q_b - \dot{f}(t_a)Q_a\right]} e^{\frac{i\mu}{2}\int_{t_a}^{t_b} dt\dot{f}^2(t)} \\ &\times \int \mathcal{D}Q\mathcal{D}P \exp\left\{i\int_{t_a}^{t_b} dt\left(P\dot{Q} - \tfrac{P^2}{2\mu} - V(Q) - \mu\ddot{f}Q\right)\right\} \end{aligned} \tag{4.65}$$

We may now consider specific examples:

$f(t) = \frac{1}{2}\gamma t^2$ describes the case of a source moving with constant acceleration where γ has dimensions of acceleration. Accelerating oscillator is an exactly solvable case with

$$v(x,t) = \frac{\mu}{2}w^2\left(x - \frac{1}{2}\gamma t^2\right)^2$$

The potential in Q space is

$$U(Q) = \frac{\mu}{2}w^2Q^2 - \mu\gamma Q = \frac{\mu}{2}w^2(Q - \gamma/w^2)^2 - \frac{\mu}{2}(\gamma/w^2)^2$$

$U(Q)$ describes an oscillator with $Q \to Q - \gamma/w^2$, as required by the *equivalence principle* which states that constant acceleration is equivalent to constant force $F = m\gamma$, and the effect of the constant force is merely to displace the equilibrium point by

$$F/\kappa = \frac{m\gamma}{\kappa} = \frac{m\gamma}{mw^2} = \gamma/w^2$$

Another solvable case is $f(t) = vt$ with v =constant.

$$\begin{aligned} K(x_a, x_b; t_a, t_b) &= e^{i\mu/2v^2(t_b - t_a) - i\mu v(x_b - x_a)} \\ &\times \int \mathcal{D}Q\mathcal{D}P \exp\left\{ i\int_{t_a}^{t_b} dt \left(P\dot{Q} - \frac{P^2}{2\mu} - V(Q)\right)\right\} \end{aligned} \tag{4.66}$$

Wave function is that of the static potential case, as seen in a frame moving with speed v to the left

$$\Psi_\nu(x,t) = e^{-i\left(E - \frac{\mu}{2}v^2\right)t} e^{i\mu v x}\phi(x - vt)$$

4.7. Exactness of the Semi-Classical Approximation

In some problems such as the free particle and the harmonic oscillator we found that the propagator has the form:

$$K(x,t;x_a) = f(t)e^{iS_{\rm cl}(x,t,x_a)/\hbar} \tag{4.67}$$

where $S_{\rm cl}$ is the action of the classical path.

We would like to investigate under what conditions this holds. We will assume that the Hamiltonian is of the form $\frac{p^2}{2m} + V(x,t)$, i.e. limit ourselves to the case of a potential independent velocity, but which may depend on time. Then, the propagator satisfies the corresponding Schrödinger equation for $x > x_a$, as argued in (1.3):

$$-i\hbar\partial_t\left[f(t)e^{iS_{\rm cl}(x,t;x_a)/\hbar}\right] - f(t)\frac{\hbar^2}{2m}\partial_x^2\left[e^{iS_{\rm cl}(x,t;x_a)/\hbar}\right] + V(x,t)f(t)e^{iS_{\rm cl}(x,t;x_a)/\hbar} = 0 \tag{4.68}$$

Upon expanding the derivatives and cancellation of the common exponential factor, we get:

$$\begin{aligned} -i\hbar\dot{f}(t) + f(t)\frac{\partial S_{\rm cl}}{\partial t} + V(x,t)f(t) \quad &- \quad \frac{i\hbar}{2m}f(t)\frac{\partial^2 S_{\rm cl}}{\partial x^2} \\ &+ \quad \frac{1}{2m}f(t)\left(\frac{\partial S_{\rm cl}}{\partial x}\right)^2 = 0 \end{aligned} \tag{4.69}$$

dividing by $f(t)$,

$$-i\hbar\frac{\dot{f}(t)}{f(t)} + \frac{\partial S_{\rm cl}}{\partial t} + V(x,t) - \frac{-i\hbar}{2m}\frac{\partial^2 S_{\rm cl}}{\partial x^2} + \frac{1}{2m}\left(\frac{\partial S_{\rm cl}}{\partial x}\right)^2 = 0 \tag{4.70}$$

Since $S_{\rm cl}$ and $V(x,t)$ are real, the real part of the equation (4.70) is

$$\frac{\partial S_{\rm cl}}{\partial t} + V(x,t) + \frac{1}{2m}\left(\frac{\partial S_{\rm cl}}{\partial x}\right)^2 + {\rm Re}\left[-i\hbar\frac{\dot{f}(t)}{f(t)}\right] = 0 \tag{4.71}$$

and the imaginary part is:

$$\frac{-\hbar}{2m}\frac{\partial^2 S_{\rm cl}}{\partial x^2} + \mathrm{Im}\left[-i\hbar\frac{\dot{f}(t)}{f(t)}\right] = 0 \tag{4.72}$$

from which it follows that $\partial^2 S_{\rm cl}/\partial x^2$ is a function of t only:

$$\frac{\partial^2 S_{\rm cl}}{\partial x^2} = F(t) \Rightarrow S_{\rm cl} = F(t)x^2 + G(t)x + H(t)$$

Putting this equation for $S_{\rm cl}$ and its derivatives into (4.71)

$$\dot{F}(t)x^2 + \dot{G}(t)x + \dot{H}(t) + V(x,t) + \frac{1}{2m}(2F(t)x + G(t))^2 + I(t) = 0 \tag{4.73}$$

rearranging

$$\left(\dot{F} + \frac{2F^2}{m}\right)x^2 + \left(\dot{G} + \frac{2FG}{m}\right)x + \left(\dot{H} + \frac{G^2}{2m} + I\right) + V(x,t) = 0 \tag{4.74}$$

The expressions in parantheses have no x dependence. Therefore the potential can be written as

$$V(x,t) = F_1(t)x^2 + G_1(t)x + H_1(t) \tag{4.75}$$

i.e. the only velocity independent potentials for which the propagator can be written in the form (4.67) are quadratic in x, although the time dependence is arbitrary.

5. CONCLUSIONS

In this thesis we have reviewed the Feynman Path Integral Formalism for non-relativistic quantum mechanics. We exhibited some applications and discussed some aspects such as the validity of the so called semi-classical approximation.

The path integral approach is mathematically more complicated than the operator formalism: The hydrogen atom could only be solved 37 years after the introduction of the method. The attraction of the global method lies not in its computational utility, but in its quite different conceptional outlook. In some sense it can be said that the path integral approach enables a smoother connection between classical and quantum mechanics: The concepts of operators and the Schrödinger wave-functions are totally alien to classical mechanics and the path integral formalism avoids their use. Of course, there is the concept of probability amplitude and probability, but without these we would not have quantum mechanics. The key concepts in path integral formalism are the sum over histories and the contribution of each path as a phase proportional to its action, which enables a smooth transition to classical mechanics in the limit $\hbar \to 0$.

The generalization of path integral to the case of N particles with the hamiltonian

$$H = \sum_a \frac{1}{2m_a} p_a^2 + v(q_1, q_2, \ldots, q_N)$$

leads to the quantum field theory which combines special relativity and quantum physics. In the field theory the trajectory $x(t)$'s replaced by a field function $\Phi(x,t)$. The degrees of freedom are labelled by the continuous index x; and the number of degrees of freedom is infinite. The quantum field theory is formulated in terms of the vacuum expectation values of the Green functions.

$$G^{(n)}(x_1, \ldots, x_n) \sim \int \mathcal{D}\Phi \ \Phi(x_1) \ldots \Phi(x_n) \exp\left[(i/\hbar) \int d^4x \mathcal{L}\right] \tag{5.1}$$

where $\mathcal{D}\Phi$ denotes integration over all functions $\Phi(x,t)$, $\mathcal{L}$'s the Lagrangian density. In Quantum Field Theory, the concept of Path Integrals is indispensable today.

Path integrals are the most ideal tool to describe fluctuating line-like structures; whether the origin of fluctuation is quantum mechanical, statistical or thermodynamic. This leads to a unified understanding of many different physical phenomena.

In statistical mechanics the partition function is a sum or integral of $e^{-E/k_{\mathrm{B}}T}$, which formally looks like the expression for the path integral. Therefore with the substitution $(t_b - t_a) \rightarrow -i\hbar/k_{\mathrm{B}}T$ the partition function and the density matrix can be calculated from analytic continuation of quantum mechanical time evolution amplitudes to an imaginary time. The propagator in Statistical Mechanics corresponds to probability itself, not to a probability amplitude as in Quantum Mechanics.

Path integrals can be used in polymer physics to evaluate the statistical fluctuations of line-like physical objects.

In financial markets the prices of assets fluctuate as a function of time. If the number of participants in the market is large the fluctuation is pretty random and the t dependence can modelled by fluctuating paths.

To summarize, it is seen that the Path Integral method is a conceptually attractive tool with a very wide range of potential applicability, but the practical application can be very tedious.

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