Path Integral for the Hydrogen Atom

Solutions in two and three dimensions

Vägintegral för Väteatomen
Lösningar i två och tre dimensioner

Anders Svensson

Faculty of Health, Science and Technology

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Supervisor: Jürgen Fuchs

Examiner: Marcus Berg

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Abstract

The path integral formulation of quantum mechanics generalizes the action principle of classical mechanics. The *Feynman path integral* is, roughly speaking, a sum over all possible paths that a particle can take between fixed endpoints, where each path contributes to the sum by a phase factor involving the action for the path. The resulting sum gives the probability amplitude of propagation between the two endpoints, a quantity called the *propagator*. Solutions of the Feynman path integral formula exist, however, only for a small number of simple systems, and modifications need to be made when dealing with more complicated systems involving singular potentials, including the Coulomb potential. We derive a generalized path integral formula, that can be used in these cases, for a quantity called the *pseudo-propagator* from which we obtain the *fixed-energy amplitude*, related to the propagator by a Fourier transform. The new path integral formula is then successfully solved for the Hydrogen atom in two and three dimensions, and we obtain integral representations for the fixed-energy amplitude.

Sammanfattning

Vägintegral-formuleringen av kvantmekanik generaliserar minsta-verkanprincipen från klassisk mekanik. Feynmans vägintegral kan ses som en summa över alla möjliga vägar en partikel kan ta mellan två givna ändpunkter A och B, där varje väg bidrar till summan med en fasfaktor innehållande den klassiska verkan för vägen. Den resulterande summan ger *propagatorn*, sannolikhetsamplituden att partikeln går från A till B. Feynmans vägintegral är dock bara lösbar för ett fåtal simpla system, och modifikationer behöver göras när det gäller mer komplexa system vars potentialer innehåller singulariteter, såsom Coulomb–potentialen. Vi härleder en generaliserad vägintegral-formel som kan användas i dessa fall, för en *pseudo-propagator*, från vilken vi erhåller *fix-energi-amplituden* som är relaterad till propagatorn via en Fourier-transform. Den nya vägintegral-formeln löses sedan med framgång för väteatomen i två och tre dimensioner, och vi erhåller integral-representationer för fix-energi-amplituden.

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Contents

1 Introduction

Developed by Richard Feynman in the 1940s, the path integral formulation of quantum mechanics generalizes the action principle of classical mechanics. In classical mechanics, extremizing the action functional $\mathcal{S}[\mathbf{x}(t)]$ determines the unique path $\mathbf{x}(t)$ taken by a particle between two endpoints $\mathbf{x}_a, \mathbf{x}_b$. In quantum mechanics there is no such path describing the motion of the particle. Instead, the quantum particle has a *probability amplitude* for going from $\mathbf{x}_a$ to $\mathbf{x}_b$. Feynman showed that this probability amplitude is obtained by summing up phase factors $\exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}(t)]\right]$ over each and every path connecting $\mathbf{x}_a$ and $\mathbf{x}_b$. This sum is called the *Feynman path integral*, written as

$$\int_{\mathbf{x}_a}^{\mathbf{x}_b} \mathscr{D}[\mathbf{x}(t)] \exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}(t)]\right]. \tag{1.1}$$

This expression is to be viewed as a *functional integral*. While an ordinary integral $\int_{x_a}^{x_b} \mathrm{d}x\, f(x)$ sums up values of a *function* $f(x)$ over all *numbers* x from x_a to x_b, a functional integral $\int_{x_a}^{x_b} \mathscr{D}[x(t)]\, F[x(t)]$ sums up values of a *functional* $F[x(t)]$ over all *functions* $x(t)$ with endpoints $x(t_a) = x_a$ and $x(t_b) = x_b$. More explicitly, the Feynman path integral may be expressed in D dimensions as

$$\int_{\mathbf{x}_a}^{\mathbf{x}_b} \mathscr{D}[\mathbf{x}(t)] \exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}(t)]\right] = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\delta t}\right)^{DN/2} \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}_{\{\mathbf{x}_i\}}(t)]\right] \tag{1.2}$$

where m is the particle's mass, $\delta t = (t_b - t_a)/N$ and $\mathbf{x}_{\{\mathbf{x}_1,\ldots,\mathbf{x}_{N-1}\}}(t)$ is a piecewise linear path with values $\mathbf{x}_k$ at the times $t_k = t_a + k\delta t$ $(k = 1, \ldots, N-1)$ as well as the endpoints $\mathbf{x}_a$ and $\mathbf{x}_b$ at the times t_a and t_b, respectively. The integrals on the right hand side of (1.2) are understood to go over the whole of $\mathbb{R}^D$. It is important to understand that the resulting "sum" is over *all possible* paths $\mathbf{x}_{\{\mathbf{x}_i\}}(t)$ taking the values $\{\mathbf{x}_a, \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_b\}$ at the times $\{t_a, t_1, t_2, \ldots, t_b\}$ – even those that are absurd from a classical viewpoint. In the limit $N \to \infty$ we have $t_k - t_{k-1} \to 0$, but $|\mathbf{x}_k - \mathbf{x}_{k-1}|$ will in general be large for an arbitrary such path, resulting in a highly discontinuous path. Only a small subset of paths will be continuous and differentiable.

In general, it is hard to give the functional integral (1.1) a precise mathematical meaning. Accordingly, (1.1) should be viewed as a formal expression that needs to be supplemented by a proper prescription on how to evaluate it. In particular, it is possible to define (1.1) as a sum over the subset of continuous paths (see Glimm and Jaffe [5], chapter 3). For a standard form of the action, one can then show that the path integral resulting from this definition coincides with the right-hand side of (1.2) [5]. This means that the discontinuous paths do not contribute to the overall sum in the continuum limit. Consequently, when evaluating the path integral (1.2) one can make approximations such as $|\mathbf{x}_{k+1}|/|\mathbf{x}_k| \to 1$ to first order in δt.

In mathematics, the basic idea of the path integral can be traced back to the Wiener integral, introduced by Norbert Wiener for solving problems dealing with Brownian motion and diffusion. In physics, the idea was further developed by Paul Dirac in his 1933 paper [1], for the use of the Lagrangian in quantum mechanics. Inspired by Dirac's idea, Feynman worked out the preliminaries in his 1942 doctoral thesis, before developing the complete formulation in 1948 [1]. The Feynman path integral has since become one of the most prominent tools in quantum mechanics and quantum field theory. Other areas of application include

- quantum statistics, where the quantum mechanical partition function can be written as, or obtained from, a path integral in imaginary time;
- polymer physics, where path integrals are useful for studying the statistical fluctuations of chains of molecules, modelled as random chains consisting of N links; and
- financial markets, where the time dependence of prices of assets can be modelled by fluctuating paths.

In physics, path integrals have found their main application in perturbative quantum field theory. In elementary quantum mechanics, however, the formulation has not had as much impact due to the difficulties in dealing with the resulting path integrals, with only a few standard problems having been solved analytically.

In particular, the path integral for the Hydrogen atom remained unsolved until Duru and Kleinert published their solution in 1979 [2].

The goal of this thesis is to provide an exact solution of the path integral for the Hydrogen atom, following the steps of Duru–Kleinert. Before doing so, we shall develop the necessary preliminaries, including a derivation of the path integral formalism. Moreover, due to the singular nature of the Coulomb potential, the corresponding path integral can be shown to diverge when written down in the original form [4], and hence a new, modified, path integral must be constructed.

In the following Section we begin by reviewing some basic concepts from classical mechanics and quantum mechanics. In Section 3 we continue by studying the propagator and its related quantities, including the *fixed-energy amplitude*, which is related to the propagator by a Fourier transform. We then derive the basic path integral formulas in phase space and configuration space in Section 4, before deriving more flexible versions of these in Section 5 that can be applied to problems involving singular potentials. These new path integral formulas yield an auxiliary quantity known as the *pseudo-propagator*, from which the fixed-energy amplitude can be obtained. This modified formalism is then finally applied in Section 6 to the two- and three-dimensional Hydrogen atoms, for which we solve the corresponding modified path integral formulas in configuration space, thus obtaining integral representations for the fixed-energy amplitude.

2 Basic Concepts

This Section will serve as a review of the key ingredients from classical mechanics and quantum mechanics that are relevant to the subsequent sections.

2.1 Classical Mechanics

Throughout this thesis we will restrict our attention to a physical system consisting of a single spinless particle of mass m subjected to a time-independent potential $V(\mathbf{x})$ in D dimensions. In the Lagrangian formulation of classical mechanics, the **Lagrangian** for this system is defined by

$$\mathscr{L}\big(\mathbf{x}, \dot{\mathbf{x}}\big) := \frac{1}{2} m \dot{\mathbf{x}}^2 - V(\mathbf{x}) \tag{2.1}$$

and the **action** functional by

$$\mathcal{S}\big[\mathbf{x}(t); t_a, t_b\big] := \int_{t_a}^{t_b} \mathrm{d}t\, \mathscr{L}\big(\mathbf{x}(t), \dot{\mathbf{x}}(t)\big), \tag{2.2}$$

with $\mathbf{x}(t)$ an arbitrary differentiable path in **configuration space**, the D-dimensional space of points $\mathbf{x}$. Let $\mathbf{x}_{\mathrm{cl}}(t)$ be the true classical path taken by the particle from the point $\mathbf{x}_a$ at time t_a, to the point $\mathbf{x}_b$ at time t_b. The **principle of stationary action** then states that the action functional for this path has a stationary value with respect to all infinitesimally neighbouring paths having the same endpoints. By extremizing the action with respect to all such neighbouring paths, we obtain the **Euler-Lagrange equations of motion**,

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathscr{L}}{\partial \dot{x}^i} - \frac{\partial \mathscr{L}}{\partial x^i} = 0. \tag{2.3}$$

For the Lagrangian (2.1), these are nothing but Newton's equation of motion

$$m\ddot{\mathbf{x}} = -\nabla V(\mathbf{x}). \tag{2.4}$$

The **canonical momentum** conjugate to the coordinate x^i is generally defined by

$$p_i := \frac{\partial \mathscr{L}}{\partial \dot{x}^i}, \tag{2.5}$$

which for the Lagrangian (2.1) is nothing but the ordinary classical momentum $\mathbf{p} = m\dot{\mathbf{x}}$. In the Hamiltonian formulation of classical mechanics, the **Hamiltonian** is generally defined by

$$H\big(\mathbf{x}, \mathbf{p}\big) := \sum_i p_i \dot{x}^i - \mathscr{L}\big(\mathbf{x}, \dot{\mathbf{x}}\big) \tag{2.6}$$

and for the single particle,

$$H\big(\mathbf{x}, \mathbf{p}\big) = \mathbf{p} \cdot \dot{\mathbf{x}} - \mathscr{L}\big(\mathbf{x}, \dot{\mathbf{x}}\big) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}), \tag{2.7}$$

i.e. the total energy of the particle. The motion of the particle is in the Hamiltonian formulation described by a path $(\mathbf{x}(t), \mathbf{p}(t))$ in **phase space**, the $2D$-dimensional space of points $(\mathbf{x}, \mathbf{p})$. We can write the action (2.2) in terms of the Hamiltonian (2.7) as

$$\mathcal{S}\big[\mathbf{x}(t); t_a, t_b\big] = \int_{t_a}^{t_b} \mathrm{d}t\, \Big[\mathbf{p}(t) \cdot \dot{\mathbf{x}}(t) - H\big(\mathbf{x}(t), \mathbf{p}(t)\big)\Big] \tag{2.8}$$

where we have to remember that $\mathbf{p}(t) = m\dot{\mathbf{x}}(t)$. We can also define a **canonical action** functional by

$$\mathcal{S}\big[\mathbf{x}(t), \mathbf{p}(t); t_a, t_b\big] := \int_{t_a}^{t_b} \mathrm{d}t \,\Big[\mathbf{p}(t) \cdot \dot{\mathbf{x}}(t) - H\big(\mathbf{x}(t), \mathbf{p}(t)\big)\Big] \tag{2.9}$$

defined for arbitrary paths in phase space. Thus in this expression we let $\mathbf{x}(t)$ and $\mathbf{p}(t)$ be completely independent, with no relation between $\mathbf{p}$ and $\dot{\mathbf{x}}$. The Lagrangian action (2.2) and the canonical action (2.9) are related by

$$\mathcal{S}\big[\mathbf{x}(t), \mathbf{p}(t); t_a, t_b\big] = \mathcal{S}\big[\mathbf{x}(t); t_a, t_b\big] - \int_{t_a}^{t_b} \mathrm{d}t \,\frac{\big(\mathbf{p}(t) - m\dot{\mathbf{x}}(t)\big)^2}{2m}. \tag{2.10}$$

The principle of stationary action also holds for the canonical action (2.9), except that there is no restriction on the endpoints of $\mathbf{p}(t)$. This leads to the **Hamilton's equations motion**

$$\dot{p}_i = -\frac{\partial H}{\partial \dot{x}^i}, \quad \dot{x}^i = \frac{\partial H}{\partial p_i}, \tag{2.11}$$

which are equivalent with the Euler-Lagrange equations (2.3) via (2.5) and (2.6).

2.2 Quantum Mechanics

Classical mechanics is deterministic, meaning that by knowing the position $\mathbf{x}_a$ and momentum $\mathbf{p}_a$ of the particle at some initial time t_a, we can with certainty predict the position $\mathbf{x}_b$ and momentum $\mathbf{p}_b$ at any later time t_b. We now turn to quantum mechanics. The motion of a quantum particle cannot be described by some classical path $\mathbf{x}(t)$. If by a measurement the particle is determined to be at a point $\mathbf{x}_a$ at time t_a, we can only know the **probability** of the particle to found at $\mathbf{x}_b$ at time t_b. Moreover, the position and momentum cannot be known simultaneously due to the **Heisenberg uncertainty principle**, which states that the product of the uncertainties in position and momentum is always greater than, or the order of, Planck's constant $\hbar$.

Any general state of the particle is represented by a **ket vector** $|\psi\rangle$ in a Hilbert space over the complex numbers. Conversely, each non-zero vector of the Hilbert space corresponds to some state of the particle. Two nonzero vectors that are proportional to each other represent the same physical state, and thus we always assume state vectors to be of unit norm. For each ket-vector $|\psi\rangle$, there exists a **bra-vector** $\langle\psi|$ in the dual vector space, such that $\langle\psi|$ acting on a ket $|\psi'\rangle$ gives the inner product $\langle\psi|\psi'\rangle$ of the kets $|\psi\rangle$ and $|\psi'\rangle$.

The state vector corresponding to the particle being at position $\mathbf{x}$ is denoted by $|\mathbf{x}\rangle$. A general state $|\psi\rangle$ is a superposition of such position-states:

$$|\psi\rangle = \int \mathrm{d}^D\mathbf{x}\, \psi(\mathbf{x})\, |\mathbf{x}\rangle. \tag{2.12}$$

Here

$$\psi(\mathbf{x}) \equiv \langle\mathbf{x}|\psi\rangle \tag{2.13}$$

is called the **wave function** of the system, or the **probability amplitude** for finding the particle at $\mathbf{x}$. The **probability** of finding the particle in a volume element $\mathrm{d}^3\mathbf{x}$ about $\mathbf{x}$ is given by $|\psi(\mathbf{x})|^2\,\mathrm{d}^3\mathbf{x} = \psi^*(\mathbf{x})\psi(\mathbf{x})\,\mathrm{d}^3\mathbf{x}$.

Observables such as position, momentum and energy are in quantum mechanics represented by **Hermitian operators** on the Hilbert space. It is postulated that every such operator possesses a complete set of eigenvectors (or **eigenkets**), complete in the sense that any general state may be expressed as a superposition of these. The eigenvalues constitute all possible outcomes for a measurement of the observable. For example, the position-kets $|\mathbf{x}\rangle$ are eigenkets of the position operator $\hat{\mathbf{x}}$ with eigenvalues $\mathbf{x}$.

Similarly, the momentum operator $\hat{\mathbf{p}}$ has eigenkets $|\mathbf{p}\rangle$ with eigenvalues $\mathbf{p}$. The state $|\mathbf{p}\rangle$ describes the particle having a well-defined momentum given by the corresponding eigenvalue $\mathbf{p}$. The momentum operator may be defined in the position representation by

$$\langle\mathbf{x}|\hat{\mathbf{p}}|\psi\rangle = -i\hbar\nabla\,\langle\mathbf{x}|\psi\rangle \tag{2.14}$$

where ∇ is the gradient differential operator acting on the wave function. By writing down the eigenvalue equation

$$\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle \tag{2.15}$$

and acting from the left with $\langle\mathbf{x}|$, we get the differential equation

$$-i\hbar\nabla\,\langle\mathbf{x}|\mathbf{p}\rangle = \mathbf{p}\langle\mathbf{x}|\mathbf{p}\rangle \tag{2.16}$$

for which the solutions are the momentum eigenfunctions

$$\langle\mathbf{x}|\mathbf{p}\rangle = \frac{\exp\left[\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}\right]}{(2\pi\hbar)^{D/2}}, \tag{2.17}$$

up to normalisation. The position- and momentum eigenkets $|\mathbf{x}\rangle$ and $|\mathbf{p}\rangle$ are not strictly members of the Hilbert space, and cannot be normalized to unity. Instead, they satisfy the normalisations

$$\langle\mathbf{x}|\mathbf{x}'\rangle = \delta^D(\mathbf{x}-\mathbf{x}') \tag{2.18}$$

and

$$\langle\mathbf{p}|\mathbf{p}'\rangle = \delta^D(\mathbf{p}-\mathbf{p}') \tag{2.19}$$

where $\delta^D(\mathbf{x}-\mathbf{x}_0) \equiv \prod_{i=1}^D \delta(x^i - x_0^i)$ and $\delta(x-x_0)$ is the Dirac delta function.

The **Hamilton operator** $\hat{H}$ is obtained by replacing $\mathbf{x}$ and $\mathbf{p}$ in (2.7) by the corresponding operators:

$$\hat{H} := H(\hat{\mathbf{x}},\hat{\mathbf{p}}). \tag{2.20}$$

To find the energy eigenkets and the energy eigenvalues, we write down the eigenvalue equation

$$\hat{H}|E\rangle = E|E\rangle. \tag{2.21}$$

where $|E\rangle$ denotes an eigenket of $\hat{H}$ with eigenvalue E. This is known as the **time-independent Schrödinger equation**. In the position representation, it becomes

$$H(\mathbf{x},-i\hbar\nabla)\langle\mathbf{x}|E\rangle = E\,\langle\mathbf{x}|E\rangle \tag{2.22}$$

or, using (2.7) and writing $\psi_E(\mathbf{x}) \equiv \langle\mathbf{x}|E\rangle$, we obtain

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right]\psi_E(\mathbf{x}) = E\,\psi_E(\mathbf{x}), \tag{2.23}$$

for which the solutions are the energy eigenfunctions with energy eigenvalues E. In general the space of eigenkets corresponding to a particular eigenvalue has a dimensionality greater than one, in which case the eigenvalue is said to be **degenerate**. The number $\alpha(E)$ of linearly independent eigenkets having eigenvalue E is called the **degeneracy** of the eigenvalue. An eigenvalue E is said to be non-degenerate if $\alpha(E)=1$. If an eigenvalue E is degenerate, we may label its eigenkets by $|E,k\rangle$ with $k=1,\ldots,\alpha(E)$. Once a complete set of orthonormal eigenkets of $\hat{H}$ has been found, we can expand any general state $|\psi\rangle$ as

$$|\psi\rangle = \sum_E \sum_{k=1}^{\alpha(E)} |E,k\rangle \langle E,k|\psi\rangle. \tag{2.24}$$

The expansion coefficient $\langle E,k|\psi\rangle$ is the probability amplitude for finding the particle in the state $|E,k\rangle$. The probability that an energy measurement yields the value E is given by $\sum_{k=1}^{\alpha(E)} |\langle E,k|\psi\rangle|^2$.

If we make an ordered list of all eigenkets $|E,k\rangle$ and relabel them by $|n\rangle$ with $n=1,2,\ldots$, then $|n\rangle$ is an eigenket of $\hat{H}$ with eigenvalue E_n. Note that, if there is degeneracy, then there will be n,n' ($n\neq n'$) such that $E_n = E_{n'}$. With this notation, we can write (2.24) as

$$|\psi\rangle = \sum_n |n\rangle \langle n|\psi\rangle. \tag{2.25}$$

Quantum mechanics is deterministic in the sense that by knowing the state vector $|\psi,t_0\rangle$ at some time t_0, the state of the system $|\psi,t\rangle$ at any later time can be determined with certainty (provided we have not disturbed the system in any way, as happens e.g. in a measurement). The time evolution of the system is governed by the **time-dependent Schrödinger equation**

$$\hat{H}|\psi,t\rangle = i\hbar\frac{\partial}{\partial t}|\psi,t\rangle. \tag{2.26}$$

In the position representation this becomes

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right]\psi(\mathbf{x},t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t). \tag{2.27}$$

If we know the state $|\psi,t_0\rangle$ at time t_0, the time evolution can also be described by the equation

$$|\psi,t\rangle = \hat{U}(t,t_0)|\psi,t_0\rangle, \tag{2.28}$$

where the operator $\hat{U}(t,t_0)$ is known as the **time-evolution operator**. For the time-independent Hamiltonian (2.20) it is given by

$$\hat{U}(t,t_0) = \exp\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right]. \tag{2.29}$$

3 Propagators

3.1 The Propagator and its Properties

Throughout this thesis, we will restrict our attention to quantum systems consisting of a single spinless particle of mass m, subjected to a time-independent potential $V(\mathbf{x})$ in D dimensions. Thus we shall assume the Hamiltonian to be of the form

$$H(\mathbf{x},\mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \tag{3.1}$$

with the corresponding operator (2.20). The time evolution operator is then given by

$$\hat{U}(t,t_0) = \exp\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right]. \tag{3.2}$$

We define the **propagator** or **time evolution amplitude** of such a system by

$$K(\mathbf{x},t;\mathbf{x}_0,t_0) := \langle \mathbf{x}|\hat{U}(t,t_0)|\mathbf{x}_0\rangle. \tag{3.3}$$

We interpret this quantity as the probability amplitude for the particle to be found at the point $\mathbf{x}$ at time t, given that it was known to be at the point $\mathbf{x}_0$ at time t_0. By fixing $\mathbf{x}_0, t_0$ and viewing $\mathbf{x}, t$ as variables, the propagator is simply the wave function $\psi(\mathbf{x},t)$ of the particle, valid for times $t \geq t_0$, given that the particle was in the state $|\mathbf{x}_0\rangle$ at time t_0.

We now show that the propagator not only determines the wave function for a particle starting in a state $|\mathbf{x}_0\rangle$, but for *any* general state $|\psi, t_0\rangle$. For $t \geq t_0$, the state of the particle is determined by applying the time-evolution operator:

$$|\psi;t\rangle = \hat{U}(t,t_0)|\psi,t_0\rangle. \tag{3.4}$$

The wave function corresponding to the state $|\psi;t\rangle$ may then be written as

$$\begin{aligned}\psi(\mathbf{x},t) = \langle\mathbf{x}|\psi;t\rangle = \langle\mathbf{x}|\hat{U}(t,t_0)|\psi,t_0\rangle &= \langle\mathbf{x}|\hat{U}(t,t_0)\int \mathrm{d}^D\mathbf{x}'\,|\mathbf{x}'\rangle\,\langle\mathbf{x}'|\psi,t_0\rangle \\ &= \int \mathrm{d}^D\mathbf{x}'\,\langle\mathbf{x}|\hat{U}(t,t_0)|\mathbf{x}'\rangle\,\psi(\mathbf{x}',t_0).\end{aligned} \tag{3.5}$$

This shows that by knowing the propagator $K(\mathbf{x},t;\mathbf{x}',t_0)$ and the wave function $\psi(\mathbf{x},t_0)$ at time t_0, the wave function for times $t \geq t_0$ is determined from

$$\psi(\mathbf{x},t) = \int \mathrm{d}^D\mathbf{x}'\,K(\mathbf{x},t;\mathbf{x}',t_0)\,\psi(\mathbf{x}',t_0). \tag{3.6}$$

Setting $t = t_0$ in this equation suggests that the propagator for $t = t_0$ serves as a Dirac delta function:

$$K(\mathbf{x},t_0;\mathbf{x}',t_0) = \delta^D(\mathbf{x}-\mathbf{x}'). \tag{3.7}$$

Indeed, since $\hat{U}(t_0,t_0) = 1$ it follows that

$$K(\mathbf{x},t_0;\mathbf{x}',t_0) = \langle\mathbf{x}|\hat{U}(t_0,t_0)|\mathbf{x}'\rangle = \langle\mathbf{x}|\mathbf{x}'\rangle = \delta^D(\mathbf{x}-\mathbf{x}'). \tag{3.8}$$

Furthermore, using the basic property of the Dirac delta function as well as the unitarity of the time evolution operator, the calculation

$$\begin{aligned}1 &= \int \mathrm{d}^D\mathbf{x}'_0\,\delta^D(\mathbf{x}'_0-\mathbf{x}_0) = \int \mathrm{d}^D\mathbf{x}'_0\,\langle\mathbf{x}'_0|\mathbf{x}_0\rangle = \int \mathrm{d}^D\mathbf{x}'_0\,\langle\mathbf{x}'_0|\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)|\mathbf{x}_0\rangle \\ &= \int \mathrm{d}^D\mathbf{x}'_0 \int \mathrm{d}^D\mathbf{x}\,\langle\mathbf{x}'_0|\hat{U}^\dagger(t,t_0)|\mathbf{x}\rangle\langle\mathbf{x}|\hat{U}(t,t_0)|\mathbf{x}_0\rangle \\ &= \int \mathrm{d}^D\mathbf{x}'_0 \int \mathrm{d}^D\mathbf{x}\,\langle\mathbf{x}|\hat{U}(t,t_0)|\mathbf{x}'_0\rangle^*\langle\mathbf{x}|\hat{U}(t,t_0)|\mathbf{x}_0\rangle\end{aligned} \tag{3.9}$$

shows that the propagator satisfies the normalisation condition

$$\int \mathrm{d}^D\mathbf{x}_0' \int \mathrm{d}^D\mathbf{x}\, K^*(\mathbf{x},t;\mathbf{x}_0',t_0)\, K(\mathbf{x},t;\mathbf{x}_0,t_0) = 1 \quad \forall\, \mathbf{x}_0, \tag{3.10}$$

valid for each starting point $\mathbf{x}_0$, with K^* denoting the complex conjugate of K.

For a general quantum state $|\psi,t\rangle$, the wave function $\psi(\mathbf{x},t)$ satisfies the Schrödinger equation (2.27). Since the propagator itself is a perfectly good wave function, it must satisfy this equation also:

$$\left[-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}} + V(\mathbf{x})\right] K(\mathbf{x},t;\mathbf{x}_0,t_0) = i\hbar\frac{\partial}{\partial t}K(\mathbf{x},t;\mathbf{x}_0,t_0). \tag{3.11}$$

Suppose we have a complete set of orthonormal energy eigenkets $|n\rangle$ $(n = 1, 2, \ldots)$ with corresponding energy eigenvalues E_n, where we allow for degeneracy. Using the completeness of this set, the propagator can be expanded as

$$\begin{aligned} K(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a) = \langle \mathbf{x}_b|\hat{U}(t_b,t_a)|\mathbf{x}_a\rangle &= \sum_n \langle \mathbf{x}_b|\exp\left[-\frac{i}{\hbar}\hat{H}(t_b-t_a)\right]|n\rangle\,\langle n|\mathbf{x}_a\rangle \\ &= \sum_n \langle \mathbf{x}_b|n\rangle\langle n|\mathbf{x}_a\rangle\, \exp\left[-\frac{i}{\hbar}E_n(t_b-t_a)\right]. \end{aligned} \tag{3.12}$$

Thus, by knowing a complete set of normalised energy eigenfunctions $\psi_n(\mathbf{x}) \equiv \langle \mathbf{x}|n\rangle$ with energy eigenvalues E_n, the propagator can be determined from

$$K(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a) = \sum_n \psi_n(\mathbf{x}_b)\psi_n^*(\mathbf{x}_a)\, \exp\left[-\frac{i}{\hbar}E_n(t_b-t_a)\right], \tag{3.13}$$

called the **spectral representation** of the propagator. Conversely, if we know the propagator and can write it in the form (3.13), we can extract the energy eigenfunctions and the energy eigenvalues [4].

Since the trace of the time evolution operator is given by

$$\mathrm{Tr}\,\hat{U}(t,t_0) = \int \mathrm{d}^D\mathbf{x}\, \langle \mathbf{x}|\hat{U}(t,t_0)|\mathbf{x}\rangle \tag{3.14}$$

it can be obtained from the propagator by setting $\mathbf{x}_a = \mathbf{x}_b$ and integrating:

$$\mathrm{Tr}\,\hat{U}(t,t_0) = \int \mathrm{d}^D\mathbf{x}\, K(\mathbf{x},t;\mathbf{x},t_0). \tag{3.15}$$

Using the expansion (3.13), the trace can be expressed as

$$\begin{aligned} \mathrm{Tr}\,\hat{U}(t,t_0) &= \int \mathrm{d}^D\mathbf{x}\, K(\mathbf{x},t;\mathbf{x},t_0) = \int \mathrm{d}^D\mathbf{x} \sum_n \psi_n(\mathbf{x})\psi_n^*(\mathbf{x})\, \exp\left[-\frac{i}{\hbar}E_n(t-t_0)\right] \\ &= \sum_n \exp\left[-\frac{i}{\hbar}E_n(t-t_0)\right] \int \mathrm{d}^D\mathbf{x}\, \psi_n(\mathbf{x})\psi_n^*(\mathbf{x}) = \sum_n \exp\left[-\frac{i}{\hbar}E_n(t-t_0)\right], \end{aligned} \tag{3.16}$$

which is simply the sum of eigenvalues of $\hat{U}(t,t_0)$, in agreement with a basic fact from linear algebra.

The Fourier transform of $\mathrm{Tr}\,\hat{U}(t,t_0)$ with respect to $\Delta t \equiv t - t_0$ is given by

$$\begin{aligned} \mathscr{F}\{\,\mathrm{Tr}\,\hat{U}(\Delta t,0)\,\}(E) &= \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right]\, \mathrm{Tr}\,\hat{U}(\Delta t,0) \\ &= \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] \sum_n \exp\left[-\frac{i}{\hbar}E_n\Delta t\right] \\ &= \hbar \sum_n \int_{-\infty}^{+\infty} \mathrm{d}\Delta t\, \exp\left[i(E-E_n)\Delta t\right]. \end{aligned} \tag{3.17}$$

Using the formula

$$\int_{-\infty}^{+\infty} \mathrm{d}t' \, \exp\left[i(E - E_n)t'\right] = 2\pi\delta(E - E_n) \tag{3.18}$$

we then have

$$\mathscr{F}\left\{ \operatorname{Tr} \hat{U}(\Delta t, 0) \right\}(E) = 2\pi\hbar \sum_n \delta(E - E_n). \tag{3.19}$$

However, due to the delta functions, this result is not that useful. In the following subsection we will find an improved version of this formula.

3.2 The Retarded Propagator and Fixed-Energy Amplitude

In calculations involving the propagator (3.3), we will always consider $t \geq t_0$. In what follows, it will be convenient to take the propagator to be zero for times $t < t_0$. By making use of the Heaviside step function, defined as

$$\Theta(t) := \begin{cases} 0 & t < 0 \\ 1 & t \geq 0 \end{cases} \tag{3.20}$$

we first define a **retarded time evolution operator** by

$$\hat{U}_R(t, t_0) := \Theta(t - t_0)\hat{U}(t, t_0), \tag{3.21}$$

as well as a **retarded Hamiltonian** by

$$H_R(\mathbf{x}, \mathbf{p}; t) := \Theta(t - t_0)H(\mathbf{x}, \mathbf{p}), \tag{3.22}$$

with the corresponding operator

$$\hat{H}_R := H_R(\hat{\mathbf{x}}, \hat{\mathbf{p}}; t) = \Theta(t - t_0)\hat{H}. \tag{3.23}$$

We then define a **retarded propagator** by

$$K_R(\mathbf{x}, t; \mathbf{x}_0, t_0) := \left\langle \mathbf{x} \middle| \hat{U}_R(t, t_0) \middle| \mathbf{x}_0 \right\rangle = \Theta(t - t_0)K(\mathbf{x}, t; \mathbf{x}_0, t_0). \tag{3.24}$$

Recalling that the propagator satisfies the Schrödinger equation (3.11), we can derive an analogous Schrödinger equation satisfied by the retarded propagator. By taking the standard viewpoint of the Dirac delta function as the "derivative" of the Heaviside step function, we have

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}K_R(\mathbf{x}, t; \mathbf{x}_0, t_0) &= i\hbar\frac{\partial}{\partial t}\Theta(t - t_0)K(\mathbf{x}, t; \mathbf{x}_0, t_0) \\
&= i\hbar\left(\frac{\mathrm{d}}{\mathrm{d}t}\Theta(t - t_0)\right)K(\mathbf{x}, t; \mathbf{x}_0, t_0) + i\hbar\Theta(t - t_0)\frac{\partial}{\partial t}K(\mathbf{x}, t; \mathbf{x}_0, t_0) \\
&= i\hbar\delta(t - t_0)K(\mathbf{x}, t; \mathbf{x}_0, t_0) + \Theta(t - t_0)H(-i\hbar\nabla, \mathbf{x})K(\mathbf{x}, t; \mathbf{x}_0, t_0) \\
&= i\hbar\delta(t - t_0)K(\mathbf{x}, t_0; \mathbf{x}_0, t_0) + \Theta(t - t_0)H(-i\hbar\nabla, \mathbf{x})\Theta(t - t_0)K(\mathbf{x}, t; \mathbf{x}_0, t_0) \\
&= i\hbar\delta(t - t_0)\delta^D(\mathbf{x} - \mathbf{x}_0) + H_R(-i\hbar\nabla, \mathbf{x}; t)K_R(\mathbf{x}, t; \mathbf{x}_0, t_0).
\end{aligned} \tag{3.25}$$

In the third line we have used (3.11), in the fourth line the fact that $\Theta(t - t_0) = \Theta(t - t_0)\Theta(t - t_0)$, and in the fifth line the result (3.7). Thus the retarded propagator satisfies the Schrödinger equation

$$H_R(-i\hbar\nabla, \mathbf{x}; t)K_R(\mathbf{x}, t; \mathbf{x}_0, t_0) = i\hbar\frac{\partial}{\partial t}K_R(\mathbf{x}, t; \mathbf{x}_0, t_0) - i\hbar\delta(t - t_0)\delta^D(\mathbf{x} - \mathbf{x}_0). \tag{3.26}$$

We now make use of the result [4] that for a function $f(t)$ that vanishes for $t < 0$, the Fourier transform

$$\tilde{f}(E) = \int_{-\infty}^{+\infty} \mathrm{d}t \, \exp\left[\frac{i}{\hbar}Et\right] f(t) \tag{3.27}$$

is an analytic function in the upper half of the complex plane, and the inverse transform correctly gives

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} \mathrm{d}E \, \exp\left[-\frac{i}{\hbar}Et\right] \tilde{f}(E) = f(t) \quad \forall\, t. \tag{3.28}$$

In particular, the retarded propagator (3.24),

$$K_R(\mathbf{x},t;\mathbf{x}_0,t_0) = \Theta(t-t_0)\big\langle\mathbf{x}\big| \exp\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right]\big|\mathbf{x}_0\big\rangle = K_R(\mathbf{x},\Delta t;\mathbf{x}_0,0), \tag{3.29}$$

depends only on $\Delta t \equiv t - t_0$ (for given $\mathbf{x}_b, \mathbf{x}_a$) and vanishes for $\Delta t < 0$.

We then define the **fixed energy amplitude** $\tilde{K}(\mathbf{x},\mathbf{x}_0;E)$ as the Fourier transform of $K_R(\mathbf{x},\Delta t;\mathbf{x}_0,0)$ with respect to Δt, i.e.

$$\tilde{K}(\mathbf{x},\mathbf{x}_0;E) := \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] K_R(\mathbf{x},\Delta t;\mathbf{x}_0,0) = \int_0^{\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] K(\mathbf{x},\Delta t;\mathbf{x}_0,0). \tag{3.30}$$

The inverse transform is given by

$$K_R(\mathbf{x},t;\mathbf{x}_0,t_0) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} \mathrm{d}E\, \exp\left[-\frac{i}{\hbar}E(t-t_0)\right] \tilde{K}(\mathbf{x}_b,\mathbf{x}_a;E). \tag{3.31}$$

Obviously, the fixed energy amplitude contains as much information as the retarded propagator.

Analogously, we define a **resolvent operator** $\hat{R}(E)$ as the Fourier transform of $\hat{U}_R(t,t_0) = \hat{U}_R(\Delta t, 0)$ with respect to Δt:

$$\hat{R}(E) := \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] \hat{U}_R(\Delta t,0) = \int_0^{\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] \hat{U}(\Delta t,0). \tag{3.32}$$

Then its matrix elements in the position basis are

$$\begin{aligned}\big\langle\mathbf{x}'\big|\hat{R}(E)\big|\mathbf{x}\big\rangle &= \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] \big\langle\mathbf{x}'\big|\hat{U}_R(\Delta t,0)\big|\mathbf{x}\big\rangle \\ &= \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] K_R(\mathbf{x}',\Delta t;\mathbf{x},0),\end{aligned} \tag{3.33}$$

which is nothing but the fixed energy amplitude:

$$\tilde{K}(\mathbf{x}',\mathbf{x};E) = \big\langle\mathbf{x}'\big|\hat{R}(E)\big|\mathbf{x}\big\rangle. \tag{3.34}$$

Using the expansion (3.13) of the propagator in the energy eigenfunctions, we have

$$\begin{aligned}\big\langle\mathbf{x}'\big|\hat{R}(E)\big|\mathbf{x}\big\rangle = \tilde{K}(\mathbf{x}',\mathbf{x};E) &= \int_0^{\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] K(\mathbf{x}',\Delta t;\mathbf{x},0) \\ &= \int_0^{\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] \sum_n \psi_n(\mathbf{x}')\psi_n^*(\mathbf{x}) \exp\left[-\frac{i}{\hbar}E_n\Delta t\right] \\ &= \sum_n \big\langle\mathbf{x}'\big|n\big\rangle\big\langle n\big|\mathbf{x}\big\rangle \int_0^{\infty} \mathrm{d}t\, \exp\left[\frac{i}{\hbar}(E-E_n)t\right].\end{aligned} \tag{3.35}$$

The integral over t in this expression is not convergent as it stands. To make it convergent, we instead evaluate it by replacing E with $E + i\eta$ where $\eta > 0$ is infinitesimal, eventually to be set to zero in all expressions for which this makes sense. Then

$$\int_0^\infty \mathrm{d}t\, \exp\left[\frac{i}{\hbar}(E + i\eta - E_n)t\right] = \left[\frac{\exp\left[\frac{i}{\hbar}(E + i\eta - E_n)t\right]}{\frac{i}{\hbar}(E + i\eta - E_n)}\right]_0^\infty = \frac{i\hbar}{E - E_n + i\eta}, \tag{3.36}$$

and (3.35) becomes

$$\langle \mathbf{x}'|\hat{R}(E)|\mathbf{x}\rangle = \sum_n \langle \mathbf{x}'|n\rangle\langle n|\mathbf{x}\rangle \frac{i\hbar}{E - E_n + i\eta} = \sum_n \langle \mathbf{x}'|\frac{i\hbar}{E - \hat{H} + i\eta}|n\rangle\langle n|\mathbf{x}\rangle = \langle \mathbf{x}'|\frac{i\hbar}{E - \hat{H} + i\eta}|\mathbf{x}\rangle. \tag{3.37}$$

Since this holds for all $\mathbf{x}', \mathbf{x}$ we conclude that the resolvent operator is given by

$$\hat{R}(E) = \frac{i\hbar}{E - \hat{H} + i\eta} \qquad (\eta \text{ infinitesimal}). \tag{3.38}$$

This shows in particular that the expression on the right-hand side, with $\hat{H}$ in the denominator, makes sense.

The calculation (3.37) also shows that

$$\tilde{K}(\mathbf{x}', \mathbf{x}; E) = \langle \mathbf{x}'|\hat{R}(E)|\mathbf{x}\rangle = \sum_n \langle \mathbf{x}'|n\rangle\langle n|\mathbf{x}\rangle \frac{i\hbar}{E - E_n + i\eta} \tag{3.39}$$

and thus the fixed energy amplitude can be expanded in the energy eigenfunctions as

$$\tilde{K}(\mathbf{x}', \mathbf{x}; E) = \sum_n \psi_n(\mathbf{x}')\psi_n^*(\mathbf{x}) \frac{i\hbar}{E - E_n + i\eta} \qquad (\eta \text{ infinitesimal}). \tag{3.40}$$

This is called the **spectral representation** of the fixed energy amplitude. Knowing the fixed-energy amplitude, we can extract the energy eigenfunctions and energy eigenvalues from spectral analysis [4].

Since the trace of $\hat{U}_R$ is given by

$$\mathrm{Tr}\, \hat{U}_R(t, t_0) = \int \mathrm{d}^D\mathbf{x}\, \langle \mathbf{x}|\hat{U}_R(t, t_0)|\mathbf{x}\rangle \tag{3.41}$$

it is also obtained from the retarded propagator as

$$\mathrm{Tr}\, \hat{U}_R(t, t_0) = \int \mathrm{d}^D\mathbf{x}\, K_R(\mathbf{x}, t; \mathbf{x}, t_0) = \Theta(t - t_0)\, \mathrm{Tr}\, \hat{U}(t, t_0). \tag{3.42}$$

Using this result, the Fourier transform of $\mathrm{Tr}\, \hat{U}_R(t, t_0)$ with respect to $\Delta t \equiv t - t_0$ gives

$$\begin{aligned}
\mathscr{F}\{\, \mathrm{Tr}\, \hat{U}_R(\Delta t, 0)\,\}(E) &= \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right]\, \mathrm{Tr}\, \hat{U}_R(\Delta t, 0) \\
&= \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] \int \mathrm{d}^D\mathbf{x}\, K_R(\mathbf{x}, \Delta t; \mathbf{x}, 0) \\
&= \int \mathrm{d}^D\mathbf{x} \int_{-\infty}^{+\infty} \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] K_R(\mathbf{x}, \Delta t; \mathbf{x}, 0).
\end{aligned} \tag{3.43}$$

From the definition (3.30) this in turn becomes

$$\mathscr{F}\{\, \mathrm{Tr}\, \hat{U}_R(\Delta t, 0)\,\}(E) = \int \mathrm{d}^D\mathbf{x}\, \tilde{K}(\mathbf{x}, \mathbf{x}; E). \tag{3.44}$$

Then using the expansion (3.40) of $\tilde{K}$ in the energy eigenfunctions, this becomes

$$\begin{aligned}\mathscr{F}\{\,\mathrm{Tr}\,\hat{U}_R(\Delta t,0)\,\}(E) &= \int \mathrm{d}^D\mathbf{x}\,\tilde{K}(\mathbf{x},\mathbf{x};E) = \int \mathrm{d}^D\mathbf{x}\,\sum_n \psi_n(\mathbf{x})\psi_n^*(\mathbf{x})\frac{i\hbar}{E-E_n+i\eta}\\ &= \sum_n \frac{i\hbar}{E-E_n+i\eta}\int \mathrm{d}^D\mathbf{x}\,\psi_n(\mathbf{x})\psi_n^*(\mathbf{x}). \end{aligned} \tag{3.45}$$

Here the integral is unity due to the normalisation of the eigenfunctions. Thus

$$\mathscr{F}\{\,\mathrm{Tr}\,\hat{U}_R(\Delta t,0)\,\}(E) = \sum_n \frac{i\hbar}{E-E_n+i\eta} \quad (\eta \text{ infinitesimal}) \tag{3.46}$$

(compare with the result (3.19)).

4 Path Integrals

4.1 The Short-time Propagator

In this section we will derive expressions for the propagator corresponding to the time evolution during an infinitesimal time interval δt. To start off, we note the following fact. For arbitrary operators $\hat{A}$, $\hat{B}$ and infinitesimal ϵ, we have

$$\exp\left[\epsilon\hat{A}\right]\exp\left[\epsilon\hat{B}\right] = \left(1+\epsilon\hat{A}+O(\epsilon^2)\right)\left(1+\epsilon\hat{B}+O(\epsilon^2)\right) = 1+\epsilon\hat{A}+\epsilon\hat{B}+O(\epsilon^2) = \exp\left[\epsilon\hat{A}+\epsilon\hat{B}\right] \quad (4.1)$$

to first order in ϵ, even if $\hat{A}$ and $\hat{B}$ do not commute. Thus for infinitesimal time evolution δt the time evolution operator may be written as

$$U(t+\delta t,t) = \exp\left[-\frac{i}{\hbar}\hat{H}\delta t\right] = \exp\left[-\frac{i}{\hbar}\left(V(\hat{\mathbf{x}})+\frac{\hat{\mathbf{p}}^2}{2m}\right)\delta t\right] = \exp\left[-\frac{i}{\hbar}V(\hat{\mathbf{x}})\delta t\right]\exp\left[-\frac{i}{\hbar}\frac{\hat{\mathbf{p}}^2}{2m}\delta t\right]. \quad (4.2)$$

The corresponding short-time propagator then becomes

$$\begin{aligned} K(\mathbf{x}',t+\delta t;\mathbf{x},t) &= \langle\mathbf{x}'|U(t+\delta t,t)|\mathbf{x}\rangle = \langle\mathbf{x}'|\exp\left[-\frac{i}{\hbar}V(\hat{\mathbf{x}})\delta t\right]\exp\left[-\frac{i}{\hbar}\frac{\hat{\mathbf{p}}^2}{2m}\delta t\right]|\mathbf{x}\rangle \\ &= \int \mathrm{d}^D\mathbf{p}\,\langle\mathbf{x}'|\exp\left[-\frac{i}{\hbar}V(\hat{\mathbf{x}})\delta t\right]\exp\left[-\frac{i}{\hbar}\frac{\hat{\mathbf{p}}^2}{2m}\delta t\right]|\mathbf{p}\rangle\langle\mathbf{p}|\mathbf{x}\rangle \\ &= \int \mathrm{d}^D\mathbf{p}\,\exp\left[-\frac{i}{\hbar}V(\mathbf{x}')\delta t\right]\exp\left[-\frac{i}{\hbar}\frac{\mathbf{p}^2}{2m}\delta t\right]\langle\mathbf{x}'|\mathbf{p}\rangle\langle\mathbf{p}|\mathbf{x}\rangle, \end{aligned} \quad (4.3)$$

where we have inserted the identity operator $\int \mathrm{d}^D\mathbf{p}\,|\mathbf{p}\rangle\langle\mathbf{p}|$ on the second line. Using the momentum eigenfunction (2.5), this becomes

$$\begin{aligned} K(\mathbf{x}',t+\delta t;\mathbf{x},t) &= \int \mathrm{d}^D\mathbf{p}\,\exp\left[-\frac{i}{\hbar}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x}')\right)\delta t\right]\frac{\exp\left[\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}'\right]}{(2\pi\hbar)^{D/2}}\frac{\exp\left[-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}\right]}{(2\pi\hbar)^{D/2}} \\ &= \int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D}\exp\left[\frac{i}{\hbar}\left[\mathbf{p}\cdot(\mathbf{x}'-\mathbf{x})-\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x}')\right)\delta t\right]\right] \end{aligned} \quad (4.4)$$

or

$$K(\mathbf{x}',t+\delta t;\mathbf{x},t) = \int \frac{\mathrm{d}^D\mathbf{p}'}{(2\pi\hbar)^D}\exp\left[\frac{i}{\hbar}\left(\mathbf{p}'\cdot\frac{\mathbf{x}'-\mathbf{x}}{\delta t}-H(\mathbf{x}',\mathbf{p}')\right)\delta t\right]. \quad (4.5)$$

We recognise the exponent as the short-time canonical action for a path connecting the points $\mathbf{x}$ and $\mathbf{x}'$.

Setting $\Delta\mathbf{x}' \equiv \mathbf{x}'-\mathbf{x}$ for notational convenience, we now proceed to integrate out the momentum variable:

$$\begin{aligned} K(\mathbf{x}',t+\delta t;\mathbf{x},t) &= \int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D}\exp\left[\frac{i}{\hbar}\left(\mathbf{p}\cdot\frac{\Delta\mathbf{x}'}{\delta t}-\frac{\mathbf{p}^2}{2m}-V(\mathbf{x}')\right)\delta t\right] \\ &= \frac{\exp\left[-\frac{i}{\hbar}V(\mathbf{x}')\delta t\right]}{(2\pi\hbar)^D}\int \mathrm{d}^D\mathbf{p}\,\exp\left[\frac{i}{\hbar}\left(-\frac{\delta t}{2m}\mathbf{p}^2+\Delta\mathbf{x}'\cdot\mathbf{p}\right)\right] \end{aligned} \quad (4.6)$$

Using (A.23), the integral on the right evaluates to

$$\int \mathrm{d}^D\mathbf{p}\,\exp\left[\frac{i}{\hbar}\left(-\frac{\delta t}{2m}\mathbf{p}^2+\Delta\mathbf{x}'\cdot\mathbf{p}\right)\right] = \left(\frac{2\pi\hbar m}{i\delta t}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{1}{2}m\left(\frac{\Delta\mathbf{x}'}{\delta t}\right)^2\delta t\right] \quad (4.7)$$

and the short-time propagator (4.6) becomes

$$K(\mathbf{x}',t+\delta t;\mathbf{x},t) = \left(\frac{m}{2\pi i\hbar\delta t}\right)^{D/2}\exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\left(\frac{\mathbf{x}'-\mathbf{x}}{\delta t}\right)^2-V(\mathbf{x}')\right)\delta t\right]. \quad (4.8)$$

Here we recognise the exponent as the short-time *Lagrangian* action for a path connecting $\mathbf{x}$ and $\mathbf{x}'$.

4.2 The Finite-time Propagator From the Short-time Propagator

The propagator $K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)$ corresponding to the time evolution during a finite time interval $\Delta t \equiv t_b - t_a$ may be obtained from the short-time propagator as follows. We first note that the time-evolution operator (3.2) may be written as

$$\hat{U}(t_b, t_a) = \exp\left[-\frac{i}{\hbar}\hat{H}\Delta t\right] = \left(\exp\left[-\frac{i}{\hbar}\hat{H}\Delta t/N\right]\right)^N = \hat{U}^N(\delta t, 0) \tag{4.9}$$

with $\delta t \equiv \frac{t_b - t_a}{N}$ and $N \geq 1$ an integer. Consequently, we can write the propagator as

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \langle \mathbf{x}_b | \hat{U}(t_b, t_a) | \mathbf{x}_a \rangle = \langle \mathbf{x}_b | \hat{U}^N(\delta t, 0) | \mathbf{x}_a \rangle. \tag{4.10}$$

By expressing the operator $\hat{U}^N(\delta t, 0)$ as a product of N operators $\hat{U}(\delta t, 0)$ and inserting $N-1$ copies of the identity operator $\int \mathrm{d}^D\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|$ between these, this becomes

$$\begin{aligned} K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) &= \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1\, \langle \mathbf{x}_b | \hat{U}(\delta t, 0) | \mathbf{x}_{N-1} \rangle \langle \mathbf{x}_{N-1} | \hat{U}(\delta t, 0) \cdots | \mathbf{x}_1 \rangle \langle \mathbf{x}_1 | \hat{U}(\delta t, 0) | \mathbf{x}_a \rangle \\ &= \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \prod_{k=1}^{N} K(\mathbf{x}_k, \delta t; \mathbf{x}_{k-1}, 0), \end{aligned} \tag{4.11}$$

with $\mathbf{x}_0 \equiv \mathbf{x}_a$ and $\mathbf{x}_N \equiv \mathbf{x}_b$. This equation holds for any integer $N \geq 1$. By taking $N \to \infty$, we can write

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \lim_{N\to\infty} K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) \tag{4.12}$$

with

$$K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) := \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \prod_{k=1}^{N} K(\mathbf{x}_k, \delta t; \mathbf{x}_{k-1}, 0). \tag{4.13}$$

where $\delta t \equiv \frac{t_b - t_a}{N}$ is now small enough so that $K(\mathbf{x}_k, \delta t; \mathbf{x}_{k-1}, 0)$ becomes the short-time propagator given by (4.5) or (4.8).

4.3 The Phase Space Path Integral

We now make use of the result (4.5) for the short-time propagator without the momentum integrated out, and plug it into (4.13). We then find

$$K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \prod_{k=1}^{N} \int \frac{\mathrm{d}^D\mathbf{p}_k}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\left(\mathbf{p}_k \cdot \frac{\Delta\mathbf{x}_k}{\delta t} - H(\mathbf{x}_k, \mathbf{p}_k)\right)\delta t\right], \tag{4.14}$$

where $\Delta\mathbf{x}_k \equiv \mathbf{x}_k - \mathbf{x}_{k-1}$ and $\delta t \equiv \frac{t_b - t_a}{N}$. After expanding the product, this becomes

$$\begin{aligned} K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \int \frac{\mathrm{d}^D\mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D\mathbf{p}_1}{(2\pi\hbar)^D} \times \\ \exp\left[\frac{i}{\hbar}\sum_{k=1}^{N}\left(\mathbf{p}_k \cdot \frac{\Delta\mathbf{x}_k}{\delta t} - H(\mathbf{x}_k, \mathbf{p}_k)\right)\delta t\right]. \end{aligned} \tag{4.15}$$

We now introduce a **time-slicing** of the interval $t_b - t_a$ as

$$t_k = t_a + k\delta t \quad (k = 0, \ldots, N) \quad \text{with} \quad t_0 \equiv t_a \quad \text{and} \quad t_N \equiv t_b, \tag{4.16}$$

and for each of the ordered sets $\{\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}\}$ and $\{\mathbf{p}_1, \ldots, \mathbf{p}_N\}$, we define piecewise linear paths

$$\mathbf{x}_{\{\mathbf{x}_i\}}(t) := \mathbf{x}_{k-1} + \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{t_k - t_{k-1}}(t - t_{k-1}) \qquad (t_{k-1} \leq t \leq t_k) \qquad (k = 1, \ldots, N) \tag{4.17}$$

and

$$\mathbf{p}_{\{\mathbf{p}_i\}}(t) := \mathbf{p}_{k-1} + \frac{\mathbf{p}_k - \mathbf{p}_{k-1}}{t_k - t_{k-1}}(t - t_{k-1}) \qquad (t_{k-1} \leq t \leq t_k) \qquad (k = 2, \ldots, N). \tag{4.18}$$

That way we have $\mathbf{x}_{\{\mathbf{x}_i\}}(t_k) = \mathbf{x}_k$ and $\mathbf{p}_{\{\mathbf{p}_i\}}(t_k) = \mathbf{p}_k$ and in the limit of large N the sum in the exponential of (4.15) becomes

$$\begin{aligned}
\sum_{k=1}^{N} \left[\mathbf{p}_k \cdot \frac{\Delta \mathbf{x}_k}{\delta t} - H(\mathbf{x}_k, \mathbf{p}_k)\right] \delta t &= \sum_{k=1}^{N} \Big[\mathbf{p}_{\{\mathbf{p}_i\}}(t_k) \cdot \dot{\mathbf{x}}_{\{\mathbf{x}_i\}}(t_k) - H\big(\mathbf{x}_{\{\mathbf{x}_i\}}(t_k), \mathbf{p}_{\{\mathbf{p}_i\}}(t_k)\big)\Big](t_k - t_{k-1}) \\
&\longrightarrow \int_{t_a}^{t_b} \mathrm{d}t \Big[\mathbf{p}_{\{\mathbf{p}_i\}}(t) \cdot \dot{\mathbf{x}}_{\{\mathbf{x}_i\}}(t) - H\big(\mathbf{x}_{\{\mathbf{x}_i\}}(t), \mathbf{p}_{\{\mathbf{p}_i\}}(t)\big)\Big] \\
&= \mathcal{S}\big[\mathbf{x}_{\{\mathbf{x}_i\}}(t), \mathbf{p}_{\{\mathbf{p}_i\}}(t); t_a, t_b\big]
\end{aligned} \tag{4.19}$$

where $\mathcal{S}[\mathbf{x}(t), \mathbf{p}(t); t_a, t_b]$ is the classical canonical action (2.9) for the Hamiltonian. The propagator, being the limit of (4.15), then becomes

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \lim_{N \to \infty} \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \int \frac{\mathrm{d}^D \mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D \mathbf{p}_1}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar} \mathcal{S}\big[\mathbf{x}_{\{\mathbf{x}_i\}}(t), \mathbf{p}_{\{\mathbf{p}_i\}}(t); t_a, t_b\big]\right]. \tag{4.20}$$

We interpret this as a sum over all paths in phase space connecting the configuration space endpoints $\mathbf{x}_a$ and $\mathbf{x}_b$. The following definition will give us a simpler way of writing this beast.

Definition:
Let $\mathcal{Q}$ denote the space of functions $\mathbf{q}(t) : \mathbb{R} \to \mathbb{R}^D$ and let $\mathcal{F}$ denote the space of functionals $F : \mathcal{Q} \times \mathcal{Q} \to \mathbb{C}$. Define a **functional integral** on $\mathcal{F}$,

$$\int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathcal{D}\big[\mathbf{x}(t)\big] \int \frac{\mathcal{D}\big[\mathbf{p}(t)\big]}{2\pi\hbar} \quad : \quad \mathcal{F} \to \mathbb{C}$$

by

$$\begin{aligned}
&\int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathcal{D}\big[\mathbf{x}(t)\big] \int \frac{\mathcal{D}\big[\mathbf{p}(t)\big]}{2\pi\hbar} F\big[\mathbf{x}(t), \mathbf{p}(t)\big] := \\
&\qquad \lim_{N \to \infty} \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \int \frac{\mathrm{d}^D \mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D \mathbf{p}_1}{(2\pi\hbar)^D} F\big[\mathbf{x}_{\mathbf{x}_1 \ldots \mathbf{x}_{N-1}}(t), \mathbf{p}_{\mathbf{p}_1 \ldots \mathbf{p}_N}(t)\big]
\end{aligned} \tag{4.21}$$

with

$$\mathbf{x}_{\mathbf{x}_1 \ldots \mathbf{x}_{N-1}}(t) := \mathbf{x}_{k-1} + \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{t_k - t_{k-1}}(t - t_{k-1}) \qquad (t_{k-1} \leq t \leq t_k) \qquad (k = 1, \ldots, N)$$

and

$$\mathbf{p}_{\mathbf{p}_1 \ldots \mathbf{p}_N}(t) := \mathbf{p}_{k-1} + \frac{\mathbf{p}_k - \mathbf{p}_{k-1}}{t_k - t_{k-1}}(t - t_{k-1}) \qquad (t_{k-1} \leq t \leq t_k) \qquad (k = 2, \ldots, N)$$

where $\mathbf{x}_0 \equiv \mathbf{x}_a$, $\mathbf{x}_N \equiv \mathbf{x}_b$ and $t_k = t_a + k\delta t$ $(k = 0, \ldots, N)$ with $t_0 \equiv t_a$, $t_N \equiv t_b$ and $\delta t \equiv \frac{t_b - t_a}{N}$.

We can then write the propagator (4.20) as

$$K(\mathbf{x}_a, t_a; \mathbf{x}_b, t_b) = \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathcal{D}\big[\mathbf{x}(t)\big] \int \frac{\mathcal{D}\big[\mathbf{p}(t)\big]}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}(t), \mathbf{p}(t); t_a, t_b]\right]. \tag{4.22}$$

The expression on the right is called the **phase space path integral**.

The definition above is not really mathematically rigorous, and it is hard to give (4.21) a precise mathematical meaning. Accordingly, (4.22) should be regarded as a formal expression that must be supplemented by a proper prescription to evaluate it. For our purposes, to calculate a phase space path integral we write it in the finite-N time-sliced form (4.15) as

$$K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \int \frac{\mathrm{d}^D\mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D\mathbf{p}_1}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\mathcal{S}^{(N)}[\mathbf{x}, \mathbf{p}]\right] \tag{4.23}$$

with the **time-sliced canonical action**

$$\mathcal{S}^{(N)}[\mathbf{x}, \mathbf{p}] := \sum_{k=1}^{N} \left[\mathbf{p}_k \cdot \frac{\Delta\mathbf{x}_k}{\delta t} - H(\mathbf{x}_k, \mathbf{p}_k)\right] \delta t, \tag{4.24}$$

where $\Delta\mathbf{x}_k \equiv \mathbf{x}_k - \mathbf{x}_{k-1}$, and then we take the limit $N \to \infty$.

4.4 The Configuration Space Path Integral

We can derive an analogous path integral in configuration space by integrating out all momentum variables in (4.23). Equivalently, we can make use of the result (4.8) for the short-time propagator where the momentum has been integrated out, and plug it into formula (4.12). We then find

$$K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \prod_{k=1}^{N} \left(\frac{m}{2\pi i\hbar\delta t}\right)^{D/2} \exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\left(\frac{\Delta\mathbf{x}_k}{\delta t}\right)^2 - V(\mathbf{x}_k)\right)\delta t\right], \tag{4.25}$$

where $\Delta\mathbf{x}_k \equiv \mathbf{x}_k - \mathbf{x}_{k-1}$ and $\delta t \equiv \frac{t_b - t_a}{N}$. After expanding the product, this becomes

$$K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \left(\frac{m}{2\pi i\hbar\delta t}\right)^{DN/2} \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \exp\left[\frac{i}{\hbar}\sum_{k=1}^{N}\left(\frac{1}{2}m\left(\frac{\Delta\mathbf{x}_k}{\delta t}\right)^2 - V(\mathbf{x}_k)\right)\delta t\right]. \tag{4.26}$$

As in the previous subsection, we introduce a time-slicing of the interval $t_b - t_a$ as

$$t_k = t_a + k\delta t \quad (k = 0, \ldots, N) \quad \text{with} \quad t_0 \equiv t_a \quad \text{and} \quad t_N \equiv t_b, \tag{4.27}$$

and for each ordered set $\{\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}\} \equiv \{\mathbf{x}_i\}$, we define a piecewise linear path

$$\mathbf{x}_{\{\mathbf{x}_i\}}(t) := \mathbf{x}_{k-1} + \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{t_k - t_{k-1}}(t - t_{k-1}) \qquad (t_{k-1} \le t \le t_k) \qquad (k = 1, \ldots, N). \tag{4.28}$$

That way we have $\mathbf{x}_{\{\mathbf{x}_i\}}(t_k) = \mathbf{x}_k$ and the summand in the exponential of (4.26) becomes

$$\frac{1}{2}m\left(\frac{\Delta\mathbf{x}_k}{\delta t}\right)^2 - V(\mathbf{x}_k) = \frac{1}{2}m\left(\dot{\mathbf{x}}_{\{\mathbf{x}_i\}}(t_k)\right)^2 - V\big(\mathbf{x}_{\{\mathbf{x}_i\}}(t_k)\big) = \mathscr{L}\Big(\mathbf{x}_{\{\mathbf{x}_i\}}(t_k)\ ,\ \dot{\mathbf{x}}_{\{\mathbf{x}_i\}}(t_k)\Big) \tag{4.29}$$

where $\mathscr{L}$ is the classical Lagrangian (2.1). The sum in (4.26) becomes, in the limit of large N,

$$\begin{aligned}\sum_{k=1}^{N}\left[\frac{1}{2}m\left(\frac{\Delta\mathbf{x}_k}{\delta t}\right)^2 - V(\mathbf{x}_k)\right]\delta t &= \sum_{k=1}^{N}\mathscr{L}\Big(\mathbf{x}_{\{\mathbf{x}_i\}}(t_k)\ ,\ \dot{\mathbf{x}}_{\{\mathbf{x}_i\}}(t_k)\Big)(t_k - t_{k-1}) \\ &\longrightarrow \int_{t_a}^{t_b}\mathrm{d}t\,\mathscr{L}\Big(\mathbf{x}_{\{\mathbf{x}_i\}}(t)\ ,\ \dot{\mathbf{x}}_{\{\mathbf{x}_i\}}(t)\Big) = \mathcal{S}\big[\mathbf{x}_{\{\mathbf{x}_i\}}(t); t_a, t_b\big]\end{aligned} \tag{4.30}$$

where $\mathcal{S}[\mathbf{x}(t); t_a, t_b]$ is the classical action (2.2). The propagator, being the limit of (4.26), then becomes

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\delta t}\right)^{DN/2} \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \; \exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}_{\{\mathbf{x}_i\}}(t); t_a, t_b]\right]. \tag{4.31}$$

This is to be interpreted as a sum of the action-exponentials over all possible paths $\mathbf{x}(t)$ connecting the endpoints $\mathbf{x}_a$ and $\mathbf{x}_b$. As in the previous subsection, we now give a more compact way of writing this result.

Definition:
Let $\mathcal{X}$ denote the space of functions $\mathbf{x}(t) : \mathbb{R} \to \mathbb{R}^D$ and let $\mathcal{F}$ denote the space of functionals $F : \mathcal{X} \to \mathbb{C}$. Define a **functional integral**

$$\int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathscr{D}\big[\mathbf{x}(t)\big] \;:\; \mathcal{F} \to \mathbb{C}$$

by

$$\int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathscr{D}\big[\mathbf{x}(t)\big]\, F\big[\mathbf{x}(t)\big] := \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\delta t}\right)^{DN/2} \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \, F[\mathbf{x}_{\mathbf{x}_1\ldots\mathbf{x}_{N-1}}(t)] \tag{4.32}$$

with

$$\mathbf{x}_{\mathbf{x}_1\ldots\mathbf{x}_{N-1}}(t) := \mathbf{x}_{k-1} + \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{t_k - t_{k-1}}(t - t_{k-1}) \qquad (t_{k-1} \le t \le t_k) \qquad (k = 1, \ldots, N)$$

where $\mathbf{x}_0 \equiv \mathbf{x}_a$, $\mathbf{x}_N \equiv \mathbf{x}_b$ and $t_k = t_a + k\delta t$ $(k = 0, \ldots, N)$ with $t_0 \equiv t_a$, $t_N \equiv t_b$ and $\delta t \equiv \frac{t_b - t_a}{N}$.

We can then write the propagator (4.31) as

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathscr{D}\big[\mathbf{x}(t)\big] \; \exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}(t); t_a, t_b]\right]. \tag{4.33}$$

The expression on the right is called the **configuration space path integral**.

As in the previous subsection, the definition above is not really mathematically rigorous, and it is hard to give (4.32) a precise mathematical meaning. Accordingly, (4.33) should be regarded as a formal expression that must be supplemented by a proper prescription to evaluate it. For our purposes, to calculate a configuration space path integral we write it in the finite-N time-sliced form (4.26) as

$$K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \left(\frac{m}{2\pi i\hbar\delta t}\right)^{DN/2} \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \; \exp\left[\frac{i}{\hbar}\mathcal{S}^{(N)}[\mathbf{x}]\right] \tag{4.34}$$

with the **time-sliced Lagrangian action**

$$\mathcal{S}^{(N)}[\mathbf{x}] := \sum_{k=1}^{N} \left[\frac{1}{2}m\left(\frac{\Delta\mathbf{x}_k}{\delta t}\right)^2 - V(\mathbf{x}_k)\right]\delta t, \tag{4.35}$$

where $\Delta\mathbf{x}_k \equiv \mathbf{x}_k - \mathbf{x}_{k-1}$, and then we take the limit $N \to \infty$.

5 Finding a More Flexible Path Integral Formula

In Appendix B we solve the path integrals for the most simple physical systems – the free particle and the harmonic oscillator. The solutions are straightforward and without difficulties. For more complicated systems, however, this is not the case. In particular, for systems with a centrifugal barrier the path integrals (4.15) and (4.26) can be shown to diverge [4]. This also happens for the Coulomb potential and hence any atomic system, i.e. systems which are of much interest. The goal of this Section is therefore to find new, modified, path integral formulas that are free of this problem for singular potentials.

5.1 The Pseudo-propagator

The starting point in the search for new path integral formulas is to consider the fixed-energy amplitude rather than the propagator itself, i.e.

$$\tilde{K}(\mathbf{x},\mathbf{x}_0;E) = \int_0^\infty \mathrm{d}(\Delta t)\, \exp\left[\frac{i}{\hbar}E\Delta t\right] K(\mathbf{x},\Delta t;\mathbf{x}_0,0) = \big\langle \mathbf{x}_b \big| \hat{R}(E) \big| \mathbf{x}_a \big\rangle \tag{5.1}$$

with the resolvent operator

$$\hat{R}(E) = \frac{i\hbar}{E-\hat{H}+i\eta} \quad (\eta \text{ infinitesimal}). \tag{5.2}$$

Since the propagator and the fixed-energy amplitude are obtained from one another through Fourier transforms, no information is lost. Now, if the system has a path integral formula for the propagator, it does also for the fixed-energy amplitude. To see this, we introduce a modified propagator and corresponding path integral by shifting the energy scale. For some fixed energy E, we first define an energy-shifted potential

$$V_E(\mathbf{x}) := V(\mathbf{x}) - E. \tag{5.3}$$

The classical Hamiltonian and canonical action functional corresponding to this potential are

$$H_E(\mathbf{x},\mathbf{p}) := \frac{\hat{\mathbf{p}}^2}{2m} + V_E(\mathbf{x}) = H(\mathbf{x},\mathbf{p}) - E \tag{5.4}$$

and

$$\mathcal{S}_E[\mathbf{x}(t),\mathbf{p}(t);t_a,t_b] := \int_{t_a}^{t_b} \mathrm{d}t\ [\mathbf{p}\cdot\dot{\mathbf{x}} - H_E(\mathbf{x},\mathbf{p})] = \mathcal{S}[\mathbf{x}(t),\mathbf{p}(t);t_a,t_b] + E(t_b-t_a) \tag{5.5}$$

while the classical Lagrangian and Lagrangian action functional for the potential (5.3) are

$$\mathscr{L}_E\big(\mathbf{x},\dot{\mathbf{x}}\big) := \frac{1}{2}m\dot{\mathbf{x}}^2 - V_E(\mathbf{x}) = \mathscr{L}\big(\mathbf{x},\dot{\mathbf{x}}\big) + E \tag{5.6}$$

and

$$\mathcal{S}_E[\mathbf{x}(t);t_a,t_b] := \int_{t_a}^{t_b} \mathrm{d}t\, \mathscr{L}_E\big(\mathbf{x}(t),\dot{\mathbf{x}}(t)\big) = \mathcal{S}[\mathbf{x}(t);t_a,t_b] + E(t_b-t_a). \tag{5.7}$$

The energy-shifted Hamiltonian operator, time-evolution operator, and propagator are then

$$\hat{H}_E := H_E(\hat{\mathbf{x}},\hat{\mathbf{p}}) = \hat{H} - E \tag{5.8}$$

and

$$\hat{U}_E(t_b,t_a) := \exp\left[-\frac{i}{\hbar}\hat{H}_E(t_b-t_a)\right] = \exp\left[\frac{i}{\hbar}E(t_b-t_a)\right]\hat{U}(t_b,t_a) \tag{5.9}$$

and

$$K_E(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) := \big\langle \mathbf{x}_b \big| \hat{U}_E(t_b, t_a) \big| \mathbf{x}_a \big\rangle = \exp\left[\frac{i}{\hbar} E(t_b - t_a)\right] K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a), \tag{5.10}$$

respectively.

All quantities and operators above merely correspond to a shift in the energy scale by E. In Section 4 we derived the path integral formalism for a general Hamiltonian of the form (3.1). Since H_E has this form, all results from Section 4 also hold for $K_E(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)$. Thus the short-time propagator K_E is given by

$$K_E(\mathbf{x}', t + \delta t; \mathbf{x}, t) = \int \frac{\mathrm{d}^D \mathbf{p}'}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\Big(\mathbf{p}' \cdot \frac{\mathbf{x}' - \mathbf{x}}{\delta t} - H_E(\mathbf{x}', \mathbf{p}')\Big)\delta t\right] \tag{5.11}$$

$$= \Big(\frac{m}{2\pi i \hbar \delta t}\Big)^{D/2} \exp\left[\frac{i}{\hbar}\left(\frac{1}{2} m \Big(\frac{\mathbf{x}' - \mathbf{x}}{\delta t}\Big)^2 - V_E(\mathbf{x}')\right)\delta t\right]. \tag{5.12}$$

For a finite time-difference, K_E can be written as the phase- and configuration-space path integrals

$$K_E(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathcal{D}\big[\mathbf{x}(t)\big] \int \frac{\mathcal{D}\big[\mathbf{p}(t)\big]}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\mathcal{S}_E[\mathbf{x}(t), \mathbf{p}(t); t_a, t_b]\right] \tag{5.13}$$

$$= \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathscr{D}\big[\mathbf{x}(t)\big] \exp\left[\frac{i}{\hbar}\mathcal{S}_E[\mathbf{x}(t); t_a, t_b]\right] \tag{5.14}$$

$$= \lim_{N\to\infty} K_E^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a), \tag{5.15}$$

where the finite-N time-sliced versions are (with $\delta t \equiv \frac{t_b - t_a}{N}$)

$$K_E^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \int \frac{\mathrm{d}^D \mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D \mathbf{p}_1}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\mathcal{S}_E^{(N)}[\mathbf{x}, \mathbf{p}]\right] \tag{5.16}$$

$$= \Big(\frac{m}{2\pi i \hbar \delta t}\Big)^{DN/2} \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \exp\left[\frac{i}{\hbar}\mathcal{S}_E^{(N)}[\mathbf{x}]\right] \tag{5.17}$$

with time-sliced canonical and Lagrangian actions ($\Delta\mathbf{x}_k \equiv \mathbf{x}_k - \mathbf{x}_{k-1}$, $\mathbf{x}_0 \equiv \mathbf{x}_a$, $\mathbf{x}_b \equiv \mathbf{x}_N$)

$$\mathcal{S}_E^{(N)}[\mathbf{x}, \mathbf{p}] := \sum_{k=1}^{N} \left[\mathbf{p}_k \cdot \frac{\Delta \mathbf{x}_k}{\delta t} - H_E(\mathbf{x}_k, \mathbf{p}_k)\right] \delta t \tag{5.18}$$

and

$$\mathcal{S}_E^{(N)}[\mathbf{x}] := \sum_{k=1}^{N} \left[\frac{1}{2} m \left(\frac{\Delta \mathbf{x}_k}{\delta t}\right)^2 - V_E(\mathbf{x}_k)\right] \delta t, \tag{5.19}$$

respectively.

The fixed-energy amplitude (5.1) may now be written in terms of the energy-shifted propagator (5.10) as

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_0^\infty \mathrm{d}(\Delta t)\, K_E(\mathbf{x}_b, \Delta t; \mathbf{x}_a, 0). \tag{5.20}$$

A finite-N version of this can be obtained by writing

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_0^\infty \mathrm{d}(\Delta t) \lim_{N\to\infty} K_E^{(N)}(\mathbf{x}_b, \Delta t; \mathbf{x}_a, 0) = \lim_{N\to\infty} \int_0^\infty \mathrm{d}(\Delta t)\, K_E^{(N)}(\mathbf{x}_b, \Delta t; \mathbf{x}_a, 0), \tag{5.21}$$

implying that

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \lim_{N\to\infty} \tilde{K}^{(N)}(\mathbf{x}_b, \mathbf{x}_a; E), \tag{5.22}$$

where

$$\tilde{K}^{(N)}(\mathbf{x}_b, \mathbf{x}_a; E) := \int_0^\infty \mathrm{d}(\Delta t)\, K_E^{(N)}(\mathbf{x}_b, \Delta t; \mathbf{x}_a, 0) = N \int_0^\infty \mathrm{d}\epsilon\, K_E^{(N)}(\mathbf{x}_b, N\epsilon; \mathbf{x}_a, 0). \tag{5.23}$$

In terms of the energy-shifted Hamiltonian $\hat{H}_E$, the resolvent operator (5.2) may be written

$$\hat{R}(E) = \frac{i\hbar}{-\hat{H}_E + i\eta}. \tag{5.24}$$

For the new yet-to-found path integral formulas, we would like to incorporate a functional degree of freedom through some arbitrary function of $\mathbf{x}$ that we can choose to our liking without changing the physical results. To proceed, it will be convenient with the following definition.

Definition:
For a given function $f : \mathbb{R}^D \to \mathbb{C}$, depending on $\mathbf{x}$, and for $\lambda \in \mathbb{R}$, define functions

$$f_l := f^{1-\lambda} \quad \text{and} \quad f_r := f^\lambda.$$

These are called **regulating functions**, satisfying $f_l(\mathbf{x}) f_r(\mathbf{x}) = f(\mathbf{x})$, and the parameter λ is called the **splitting parameter**.

Given a choice of f, we can incorporate the regulating functions into the resolvent operator using the operator identity

$$\hat{R}(E) = \frac{i\hbar}{-\hat{H}_E + i\eta} = f_r(\hat{\mathbf{x}}) \frac{i\hbar}{f_l(\hat{\mathbf{x}})(-\hat{H}_E + i\eta) f_r(\hat{\mathbf{x}})} f_l(\hat{\mathbf{x}}). \tag{5.25}$$

We then define a **pseudo-Hamiltonian**

$$\hat{\mathcal{H}}_E := f_l(\hat{\mathbf{x}}) \hat{H}_E f_r(\hat{\mathbf{x}}). \tag{5.26}$$

and a corresponding **pseudo-time evolution operator**

$$\hat{\mathcal{U}}_E(s_b, s_a) := f_r(\hat{\mathbf{x}}) \exp\left[-\frac{i}{\hbar} \hat{\mathcal{H}}_E (s_b - s_a)\right] f_l(\hat{\mathbf{x}}), \tag{5.27}$$

and a **pseudo-propagator**

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) := \big\langle \mathbf{x}_b \big| \hat{\mathcal{U}}_E(s_b, s_a) \big| \mathbf{x}_a \big\rangle. \tag{5.28}$$

In terms of this pseudo-propagator, the generalization of the formula (5.20) then reads [4].

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_0^\infty \mathrm{d}(\Delta s)\, \mathcal{K}_E(\mathbf{x}_b, \Delta s; \mathbf{x}_a, 0) \tag{5.29}$$

which is independent of the choice of f.

Classically, the splitting of f into f_l and f_r through the splitting parameter λ is of no specific interest, but quantum mechanically the factor ordering involving the corresponding operators is nontrivial. However, the pseudo-time evolution operator is in fact independent of λ. By expanding the pseudo-time evolution operator (5.27) in its Taylor series and using $f_r f_l = f$, it can be rewritten as

$$\hat{\mathcal{U}}_E(s_b, s_a) = \exp\left[-\frac{i}{\hbar} f(\hat{\mathbf{x}}) \hat{H}_E (s_b - s_a)\right] f(\hat{\mathbf{x}}). \tag{5.30}$$

Consequently the pseudo-propagator (5.28) is independent of the choice of λ, too.

Proceeding the same way as in Section 4.2, the operator $\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E(s_b - s_a)\right]$ in (5.27) is written as

$$\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E(s_b - s_a)\right] = \lim_{N\to\infty}\left(\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right]\right)^N \quad \text{with} \quad \delta s \equiv \frac{s_b - s_a}{N}. \tag{5.31}$$

Consequently, the pseudo-time evolution operator (5.27) can be expressed as

$$\hat{\mathcal{U}}_E(s_b, s_a) = f_r(\hat{\mathbf{x}}) \exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E(s_b - s_a)\right] f_l(\hat{\mathbf{x}}) = \lim_{N\to\infty} f_r(\hat{\mathbf{x}}) \left(\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right]\right)^N f_l(\hat{\mathbf{x}}), \tag{5.32}$$

and the pesudo-propagator (5.28) then becomes

$$\begin{aligned}\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) &= \langle \mathbf{x}_b | \hat{\mathcal{U}}_E(s_b, s_a) | \mathbf{x}_a \rangle = \lim_{N\to\infty} \langle \mathbf{x}_b | f_r(\hat{\mathbf{x}}) \left(\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right]\right)^N f_l(\hat{\mathbf{x}}) | \mathbf{x}_a \rangle \\ &= \lim_{N\to\infty} f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \langle \mathbf{x}_b | \left(\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right]\right)^N | \mathbf{x}_a \rangle. \end{aligned} \tag{5.33}$$

By writing the operator $\left(\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right]\right)^N$ as a product of N operators $\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right]$ and inserting $N-1$ copies of the identity operator $\int \mathrm{d}^D\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|$ between these, this becomes

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \lim_{N\to\infty} f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \prod_{k=1}^{N} \langle \mathbf{x}_k | \exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right] | \mathbf{x}_{k-1} \rangle. \tag{5.34}$$

In the limit of large N (i.e. small δs) we can write

$$\exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right] = 1 - \frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s = 1 - \frac{i}{\hbar} f_l(\hat{\mathbf{x}}) \hat{H}_E f_r(\hat{\mathbf{x}}) \delta s, \tag{5.35}$$

so that

$$\begin{aligned}\langle \mathbf{x}_k | \exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right] | \mathbf{x}_{k-1} \rangle &= \langle \mathbf{x}_k | \left(1 - \frac{i}{\hbar} f_l(\hat{\mathbf{x}}) \hat{H}_E f_r(\hat{\mathbf{x}}) \delta s\right) | \mathbf{x}_{k-1} \rangle \\ &= \langle \mathbf{x}_k | \left(1 - \frac{i}{\hbar} f_l(\mathbf{x}_k) \hat{H}_E f_r(\mathbf{x}_{k-1}) \delta s\right) | \mathbf{x}_{k-1} \rangle. \end{aligned} \tag{5.36}$$

By letting

$$\delta t_k := f_l(\mathbf{x}_k) f_r(\mathbf{x}_{k-1}) \delta s \tag{5.37}$$

we then have, for small enough δs,

$$\begin{aligned}\langle \mathbf{x}_k | \exp\left[-\frac{i}{\hbar}\hat{\mathcal{H}}_E \delta s\right] | \mathbf{x}_{k-1} \rangle &= \langle \mathbf{x}_k | \left(1 - \frac{i}{\hbar} \hat{H}_E \delta t_k\right) | \mathbf{x}_{k-1} \rangle = \langle \mathbf{x}_k | \exp\left[-\frac{i}{\hbar}\hat{H}_E \delta t_k\right] | \mathbf{x}_{k-1} \rangle \\ &= K_E(\mathbf{x}_k, \delta t_k; \mathbf{x}_{k-1}, 0), \end{aligned} \tag{5.38}$$

giving

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \lim_{N\to\infty} f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \prod_{k=1}^{N} K_E(\mathbf{x}_k, \delta t_k; \mathbf{x}_{k-1}, 0), \tag{5.39}$$

or

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \lim_{N\to\infty} \mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a), \tag{5.40}$$

where

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) := f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \prod_{k=1}^{N} K_E(\mathbf{x}_k, \delta t_k; \mathbf{x}_{k-1}, 0) \tag{5.41}$$

with $\delta t_k \equiv f_l(\mathbf{x}_k) f_r(\mathbf{x}_{k-1}) \delta s$ and $\delta s \equiv \frac{s_b - s_a}{N}$.

5.2 New Path Integral Formula: Phase Space

We now derive a phase space path integral formula for the pseudo-propagator using the result (5.41). For large enough N (i.e. small δs), δt_k is small enough so that, using (5.11),

$$\begin{aligned} K_E(\mathbf{x}_k, \delta t_k; \mathbf{x}_{k-1}, 0) &= \int \frac{\mathrm{d}^D \mathbf{p}_k}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\Big(\mathbf{p}_k \cdot \frac{\Delta \mathbf{x}_k}{\delta t_k} - H_E(\mathbf{x}_k, \mathbf{p}_k)\Big)\delta t_k\right] \\ &= \int \frac{\mathrm{d}^D \mathbf{p}_k}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\Big(\mathbf{p}_k \cdot \frac{\Delta \mathbf{x}_k}{f_l(\mathbf{x}_k) f_r(\mathbf{x}_{k-1})\delta s} - H_E(\mathbf{x}_k, \mathbf{p}_k)\Big) f_l(\mathbf{x}_k) f_r(\mathbf{x}_{k-1})\delta s\right] \\ &= \int \frac{\mathrm{d}^D \mathbf{p}_k}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\Big(\mathbf{p}_k \cdot \frac{\Delta \mathbf{x}_k}{\delta s} - f_l(\mathbf{x}_k) H_E(\mathbf{x}_k, \mathbf{p}_k) f_r(\mathbf{x}_{k-1})\Big)\delta s\right]. \end{aligned} \tag{5.42}$$

Equation (5.41) then becomes

$$\begin{aligned} \mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) &= f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \prod_{k=1}^{N} K_E(\mathbf{x}_k, \delta t_k; \mathbf{x}_{k-1}, 0) \\ &= f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \times \\ &\qquad \prod_{k=1}^{N} \int \frac{\mathrm{d}^D \mathbf{p}_k}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\Big(\mathbf{p}_k \cdot \frac{\Delta \mathbf{x}_k}{\delta s} - f_l(\mathbf{x}_k) H_E(\mathbf{x}_k, \mathbf{p}_k) f_r(\mathbf{x}_{k-1})\Big)\delta s\right] \\ &= f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \int \frac{\mathrm{d}^D \mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D \mathbf{p}_1}{(2\pi\hbar)^D} \times \\ &\qquad \exp\left[\frac{i}{\hbar}\sum_{k=1}^{N}\Big(\mathbf{p}_k \cdot \frac{\Delta \mathbf{x}_k}{\delta s} - f_l(\mathbf{x}_k) H_E(\mathbf{x}_k, \mathbf{p}_k) f_r(\mathbf{x}_{k-1})\Big)\delta s\right], \end{aligned} \tag{5.43}$$

or

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \int \frac{\mathrm{d}^D \mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D \mathbf{p}_1}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}, \mathbf{p}]\right] \tag{5.44}$$

with the **pseudo-time sliced canonical action**

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}, \mathbf{p}] := \sum_{k=1}^{N} \left[\mathbf{p}_k \cdot \frac{\Delta \mathbf{x}_k}{\delta s} - f_l(\mathbf{x}_k)\big[H(\mathbf{x}_k, \mathbf{p}_k) - E\big] f_r(\mathbf{x}_{k-1})\right] \delta s. \tag{5.45}$$

Note that for finite N, we get different $\mathcal{K}_E^{(N)}$ for different choices of the splitting parameter λ. In the continuum limit however, we have seen that $\mathcal{K}_E$ is independent of λ. Thus, in taking the limit $N \to \infty$, we can in particular set $\lambda = 0$ (giving $f_l \equiv f$ and $f_r \equiv 1$). We then obtain

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \lim_{N\to\infty} f(\mathbf{x}_a) \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \int \frac{\mathrm{d}^D\mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D\mathbf{p}_1}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x},\mathbf{p}]\right] \quad (5.46)$$

with the pseudo-time sliced canonical action

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x},\mathbf{p}] = \sum_{k=1}^{N} \left[\mathbf{p}_k \cdot \frac{\Delta\mathbf{x}_k}{\delta s} - f(\mathbf{x}_k)\big[H(\mathbf{x}_k,\mathbf{p}_k) - E\big]\right]\delta s. \quad (5.47)$$

This may formally be written as a phase space path integral

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = f(\mathbf{x}_a) \int_{\mathbf{x}(s_a)=\mathbf{x}_a}^{\mathbf{x}(s_b)=\mathbf{x}_b} \mathcal{D}\big[\mathbf{x}(s)\big] \int \frac{\mathcal{D}\big[\mathbf{p}(s)\big]}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\tilde{\mathcal{S}}_E[\mathbf{x}(s),\mathbf{p}(s);s_a,s_b]\right] \quad (5.48)$$

with the pseudo-action

$$\tilde{\mathcal{S}}_E[\mathbf{x}(s),\mathbf{p}(s);s_a,s_b] = \int_{s_a}^{s_b} \mathrm{d}s \left[\mathbf{p}(s)\cdot\mathbf{x}'(s) - f\big(\mathbf{x}(s)\big)\big[H\big(\mathbf{x}(s),\mathbf{p}(s)\big) - E\big]\right], \quad (5.49)$$

where $\mathbf{x}'(s)$ denotes the derivative of $\mathbf{x}(s)$ with respect to pseudotime s.

5.3 New Path Integral Formula: Configuration Space

The configuration space path integral for the pseudo-propagator is obtained by integrating out the $\mathbf{p}$-variables in the phase space path integral (5.44). Equivalently, we may again use the result (5.41). For large enough N (i.e. small δs), δt_k is small enough so that, using (5.11),

$$\begin{aligned}
K_E(\mathbf{x}_k, \delta t_k; \mathbf{x}_{k-1}, 0) &= \left(\frac{m}{2\pi i\hbar\delta t_k}\right)^{D/2} \exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\left(\frac{\Delta\mathbf{x}_k}{\delta t_k}\right)^2 - V_E(\mathbf{x}_k)\right)\delta t_k\right] = \\
&= \left(\frac{m}{2\pi i\hbar f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})\delta s}\right)^{D/2} \exp\left[\frac{i}{\hbar}\left(\frac{1}{2}m\left(\frac{\Delta\mathbf{x}_k}{f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})\delta s}\right)^2 - V_E(\mathbf{x}_k)\right) f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})\delta s\right] \\
&= \frac{1}{[f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})]^{D/2}}\left(\frac{m}{2\pi i\hbar\delta s}\right)^{D/2} \exp\left[\frac{i}{\hbar}\left(\frac{1}{2f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})}m\left(\frac{\Delta\mathbf{x}_k}{\delta s}\right)^2 - f_l(\mathbf{x}_k)V_E(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})\right)\delta s\right].
\end{aligned} \quad (5.50)$$

Substituting this into (5.41), we obtain

$$\begin{aligned}
\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) &= f_r(\mathbf{x}_b)f_l(\mathbf{x}_a) \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \prod_{k=1}^{N} K_E(\mathbf{x}_k, \delta t_k; \mathbf{x}_{k-1}, 0) = \\
&= f_r(\mathbf{x}_b)f_l(\mathbf{x}_a) \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \left(\prod_{k=1}^{N} \frac{1}{[f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})]^{D/2}}\left(\frac{m}{2\pi i\hbar\delta s}\right)^{D/2} \times \right. \\
&\left. \exp\left[\frac{i}{\hbar}\left(\frac{1}{2f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})}m\left(\frac{\Delta\mathbf{x}_k}{\delta s}\right)^2 - f_l(\mathbf{x}_k)V_E(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})\right)\delta s\right]\right)
\end{aligned} \quad (5.51)$$

or, after expanding the product,

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \left(\frac{m}{2\pi i\hbar\delta s}\right)^{DN/2} \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \left(\prod_{k=1}^{N} \frac{1}{[f_l(\mathbf{x}_k) f_r(\mathbf{x}_{k-1})]^{D/2}}\right) \times$$
$$\exp\left[\frac{i}{\hbar}\sum_{k=1}^{N}\left(\frac{1}{2f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})} m\left(\frac{\Delta\mathbf{x}_k}{\delta s}\right)^2 - f_l(\mathbf{x}_k)V_E(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})\right)\delta s\right]. \quad (5.52)$$

Using $f_r(\mathbf{x})f_l(\mathbf{x}) = f(\mathbf{x})$ we see that the product in f_l, f_r may be written as

$$\prod_{k=1}^{N} \frac{1}{[f_l(\mathbf{x}_k) f_r(\mathbf{x}_{k-1})]^{D/2}} = \frac{1}{[f_l(\mathbf{x}_b) f_r(\mathbf{x}_a)]^{D/2}} \prod_{k=1}^{N-1} \frac{1}{\big(f(\mathbf{x}_k)\big)^{D/2}}, \quad (5.53)$$

giving

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{f_r(\mathbf{x}_b) f_l(\mathbf{x}_a)}{[f_l(\mathbf{x}_b) f_r(\mathbf{x}_a)]^{D/2}} \left(\frac{m}{2\pi i\hbar\delta s}\right)^{DN/2} \int \frac{\mathrm{d}^D\mathbf{x}_{N-1}}{\big(f(\mathbf{x}_{N-1})\big)^{D/2}} \cdots \int \frac{\mathrm{d}^D\mathbf{x}_1}{\big(f(\mathbf{x}_1)\big)^{D/2}} \exp\left[\frac{i}{\hbar}\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}]\right], \quad (5.54)$$

with the **pseudo-time sliced Lagrangian action**

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] := \sum_{k=1}^{N}\left[\frac{1}{2f_l(\mathbf{x}_k)f_r(\mathbf{x}_{k-1})} m\left(\frac{\Delta\mathbf{x}_k}{\delta s}\right)^2 - f_l(\mathbf{x}_k)\big[V(\mathbf{x}_k) - E\big]f_r(\mathbf{x}_{k-1})\right]\delta s. \quad (5.55)$$

As pointed out in the previous section, we get different $\mathcal{K}_E^{(N)}$ for different choices of the splitting parameter λ, but in the continuum limit all choices should converge to the limit $\mathcal{K}_E$, independently of λ. Setting $\lambda = 0$, we obtain

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \lim_{N\to\infty} \frac{f(\mathbf{x}_a)}{[f(\mathbf{x}_b)]^{D/2}} \left(\frac{m}{2\pi i\hbar\delta s}\right)^{DN/2} \int \frac{\mathrm{d}^D\mathbf{x}_{N-1}}{\big(f(\mathbf{x}_{N-1})\big)^{D/2}} \cdots \int \frac{\mathrm{d}^D\mathbf{x}_1}{\big(f(\mathbf{x}_1)\big)^{D/2}} \exp\left[\frac{i}{\hbar}\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}]\right] \quad (5.56)$$

with the pseudo-time sliced Lagrangian action

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] = \sum_{k=1}^{N}\left[\frac{1}{2f(\mathbf{x}_k)} m\left(\frac{\Delta\mathbf{x}_k}{\delta s}\right)^2 - f(\mathbf{x}_k)\big[V(\mathbf{x}_k) - E\big]\right]\delta s. \quad (5.57)$$

This may formally be written as a configuration space path integral

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{f(\mathbf{x}_a)}{[f(\mathbf{x}_b)]^{D/2}} \int_{\mathbf{x}(s_a)=\mathbf{x}_a}^{\mathbf{x}(s_b)=\mathbf{x}_b} \frac{\mathscr{D}\big[\mathbf{x}(s)\big]}{f(\mathbf{x}(s))} \exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}(s); s_a, s_b]\right] \quad (5.58)$$

with the pseudo-action

$$\mathcal{S}[\mathbf{x}(s); s_a, s_b] = \int_{s_a}^{s_b} \mathrm{d}s \left[\frac{1}{2f\big(\mathbf{x}(s)\big)} m\big[\mathbf{x}'(s)\big]^2 - f\big(\mathbf{x}(s)\big)\big[V\big(\mathbf{x}(s)\big) - E\big]\right], \quad (5.59)$$

where $\mathbf{x}'(s)$ denotes the derivative of $\mathbf{x}(s)$ with respect to pseudo-time s.

Summary of Section 5

The fixed-energy amplitude can be obtained from a **pseudo-propagator** $\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a)$ according to

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_0^\infty \mathrm{d}(\Delta s)\, \mathcal{K}_E(\mathbf{x}_b, \Delta s; \mathbf{x}_a, 0). \tag{5.60}$$

By choosing a suitable function $f(\mathbf{x})$ depending on $\mathbf{x}$, and a **splitting parameter** $\lambda \in \mathbb{R}$, we define **regulating functions** $f_l := f^{1-\lambda}$ and $f_r := f^\lambda$. A corresponding pseudo-propagator is then obtained from the **pseudo-time sliced path integral of phase space**,

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = f_r(\mathbf{x}_b) f_l(\mathbf{x}_a) \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \int \frac{\mathrm{d}^D\mathbf{p}_N}{(2\pi\hbar)^D} \cdots \int \frac{\mathrm{d}^D\mathbf{p}_1}{(2\pi\hbar)^D} \exp\left[\frac{i}{\hbar}\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x},\mathbf{p}]\right] \tag{5.61}$$

with the **pseudo-time sliced canonical action**

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x},\mathbf{p}] := \sum_{k=1}^N \left[\mathbf{p}_k \cdot \frac{\Delta\mathbf{x}_k}{\delta s} - f_l(\mathbf{x}_k)\big[H(\mathbf{x}_k, \mathbf{p}_k) - E\big] f_r(\mathbf{x}_{k-1})\right] \delta s, \tag{5.62}$$

or from the **pseudo-time sliced path integral of configuration space**,

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{f_r(\mathbf{x}_b) f_l(\mathbf{x}_a)}{[f_l(\mathbf{x}_b) f_r(\mathbf{x}_a)]^{D/2}} \left(\frac{m}{2\pi i\hbar\delta s}\right)^{DN/2} \int \frac{\mathrm{d}^D\mathbf{x}_{N-1}}{\big(f(\mathbf{x}_{N-1})\big)^{D/2}} \cdots \int \frac{\mathrm{d}^D\mathbf{x}_1}{\big(f(\mathbf{x}_1)\big)^{D/2}} \exp\left[\frac{i}{\hbar}\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}]\right], \tag{5.63}$$

with the **pseudo-time sliced Lagrangian action**

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] := \sum_{k=1}^N \left[\frac{1}{2 f_l(\mathbf{x}_k) f_r(\mathbf{x}_{k-1})} m \left(\frac{\Delta\mathbf{x}_k}{\delta s}\right)^2 - f_l(\mathbf{x}_k)\big[V(\mathbf{x}_k) - E\big] f_r(\mathbf{x}_{k-1})\right] \delta s. \tag{5.64}$$

Taking the limit $N \to \infty$ of (5.61) or (5.63) yields the pseudo-propagator,

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \lim_{N\to\infty} \mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a), \tag{5.65}$$

which is independent of the splitting parameter λ. We then obtain the fixed-energy amplitude from (5.60), the result being independent of the choice of function f. That is, provided that f has been suitably chosen such that the path integral formulas (5.61) and (5.63) are well defined.

Setting $f(\mathbf{x}) = 1$ we recover the original path integrals in Section 4, which diverge for singular potentials such as the Coulomb potential. The presence of suitably chosen regulating functions is therefore essential to solving path integrals for many systems of interest.

6 Exact Solution for the Hydrogen Atom

6.1 The Hydrogenic Path Integral in D Dimensions

Using the formalism developed in section 5, we are now ready to tackle the Coulomb-problem and the hydrogen atom in particular. Consider a D-dimensional electron-proton system with Coulomb interaction, or, in the centre-of-mass system, an electron subjected to the potential

$$V(\mathbf{x}) = -\frac{e^2}{(4\pi\epsilon_0)r}, \tag{6.1}$$

where e is the elementary charge, ϵ_0 the free space permittivity, and $r \equiv |\mathbf{x}|$.

To simplify the formulas, we shall work in **atomic units** in which

$$\hbar = m_e = e = \frac{1}{4\pi\epsilon_0} = 1 \tag{6.2}$$

so that the potential (6.1) takes the simple form

$$V(\mathbf{x}) = -\frac{1}{r}. \tag{6.3}$$

By choosing the function $f(\mathbf{x})$ introduced in section 5 to be

$$f(\mathbf{x}) := r \tag{6.4}$$

and defining regulating functions

$$f_l(\mathbf{x}) := f(\mathbf{x})^{1-\lambda} = r^{1-\lambda} \quad \text{and} \quad f_r(\mathbf{x}) := f(\mathbf{x})^{\lambda} = r^{\lambda}. \tag{6.5}$$

for arbitrary λ, the modified path integral formulas (5.61) and (5.63) become well-defined, as discovered by Duru and Kleinert in 1979 [4]. The pseudo-time sliced configuration space path integral for the pseudo propagator (5.54) then becomes

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{r_b^{\lambda} r_a^{1-\lambda}}{[r_b^{1-\lambda} r_a^{\lambda}]^{D/2}} \left(\frac{1}{2\pi i \delta s}\right)^{DN/2} \int \frac{\mathrm{d}^D \mathbf{x}_{N-1}}{r_{N-1}^{D/2}} \cdots \int \frac{\mathrm{d}^D \mathbf{x}_1}{r_1^{D/2}} \exp\left[i\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}]\right] \tag{6.6}$$

with the pseudo-time sliced action (5.55) given by

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] = \sum_{k=1}^{N} \left[\frac{1}{2 r_k^{1-\lambda} r_{k-1}^{\lambda}} \left(\frac{\Delta \mathbf{x}_k}{\delta s}\right)^2 - r_k^{1-\lambda}\left(-\frac{1}{r_k} - E\right) r_{k-1}^{\lambda}\right] \delta s. \tag{6.7}$$

For our purposes in this Section the freedom in the value of the splitting parameter λ will not be needed. Setting $\lambda = 0$ yields

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{r_a}{r_b^{D/2}} \left(\frac{1}{2\pi i \delta s}\right)^{DN/2} \int \frac{\mathrm{d}^D \mathbf{x}_{N-1}}{r_{N-1}^{D/2}} \cdots \int \frac{\mathrm{d}^D \mathbf{x}_1}{r_1^{D/2}} \exp\left[i\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}]\right] \tag{6.8}$$

with

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] = \sum_{k=1}^{N} \left[\frac{1}{2 r_k} \left(\frac{\Delta \mathbf{x}_k}{\delta s}\right)^2 + E r_k + 1\right] \delta s. \tag{6.9}$$

6.2 Solution for the Two-Dimensional H-atom

Before solving the full three-dimensional problem, we will first consider the simplified case of a two-dimensional Hydrogen atom. In two dimensions ($D = 2$), the pseudo-time sliced path integral (6.8) becomes

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{r_a}{r_b}\left(\frac{1}{2\pi i\delta s}\right)^N \int \frac{\mathrm{d}^2\mathbf{x}_{N-1}}{r_{N-1}} \cdots \int \frac{\mathrm{d}^2\mathbf{x}_1}{r_1} \exp\left[i\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}]\right] \tag{6.10}$$

with the pseudo-time sliced action

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] = \sum_{k=1}^{N}\left[\frac{1}{2r_k}\left(\frac{\Delta\mathbf{x}_k}{\delta s}\right)^2 + Er_k + 1\right]\delta s. \tag{6.11}$$

We shall see that this path integral can be transformed into that of the harmonic oscillator by making a coordinate transformation from $\{x^i\}$ to "square root coordinates" $\{u^i\}$ satisfying $\mathbf{u}^2 = r$. This is accomplished by the **Levi-Civita transformation**

$$\begin{cases} x^1 = (u^1)^2 - (u^2)^2 \\ x^2 = 2u^1u^2 \end{cases} . \tag{6.12}$$

Indeed, with this transformation we have

$$r = \sqrt{(x^1)^2 + (x^2)^2} = \sqrt{\left((u^1)^2 - (u^2)^2\right)^2 + 4(u^1)^2(u^2)^2} = (u^1)^2 + (u^2)^2 \equiv \mathbf{u}^2 \tag{6.13}$$

as desired. Using the relation for x^1 in (6.12) together with (6.13), we find

$$\begin{cases} (u^1)^2 = \frac{1}{2}(r + x^1) \\ (u^2)^2 = \frac{1}{2}(r - x^1) \end{cases} . \tag{6.14}$$

It is important to note that the transformation (6.12) is not a bijection, but two to one. An inverse can be found by restricting it to, say, $u^1 \geq 0$.

The differentials of x^i and u^i are related by

$$[\mathrm{d}\mathbf{x}] = \mathbf{A}(\mathbf{u})\,[\mathrm{d}\mathbf{u}] \tag{6.15}$$

with the Jacobian matrix

$$\mathbf{A}(\mathbf{u}) = \begin{bmatrix} 2u^1 & -2u^2 \\ 2u^2 & 2u^1 \end{bmatrix}. \tag{6.16}$$

The metric g_{ij} in u^i-coordinates then takes the simple form

$$\mathbf{g}(\mathbf{u}) = \mathbf{A}^T\mathbf{A} = \begin{bmatrix} 2u^1 & 2u^2 \\ -2u^2 & 2u^1 \end{bmatrix}\begin{bmatrix} 2u^1 & -2u^2 \\ 2u^2 & 2u^1 \end{bmatrix} = \begin{bmatrix} 4\mathbf{u}^2 & 0 \\ 0 & 4\mathbf{u}^2 \end{bmatrix} = 4\mathbf{u}^2\mathbf{I} \tag{6.17}$$

and in the continuum limit we have, to first order in δs (summation convention implied):

$$(\Delta\mathbf{x})^2 = g_{ij}\Delta u^i\,\Delta u^j = [\Delta\mathbf{u}]^T\mathbf{g}[\Delta\mathbf{u}] = 4\mathbf{u}^2(\Delta\mathbf{u})^2, \tag{6.18}$$

or

$$\frac{1}{r}(\Delta\mathbf{x})^2 = 4(\Delta\mathbf{u})^2. \tag{6.19}$$

Using (6.13) and (6.19), we can now write the pseudo-time sliced action (6.11) in terms of $\mathbf{u}_k$-variables as

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] = \sum_{k=1}^{N} \left[\frac{1}{2} \cdot 4 \left(\frac{\Delta \mathbf{u}_k}{\delta s} \right)^2 + E\mathbf{u}_k^2 + 1 \right] \delta s = \sum_{k=1}^{N} \left[\frac{1}{2} \cdot 4 \left(\frac{\Delta \mathbf{u}_k}{\delta s} \right)^2 - \frac{1}{2} \cdot 4 \left(\frac{-E}{2} \right) \mathbf{u}_k^2 \right] \delta s + \Delta s \quad (6.20)$$

where $\Delta s = s_b - s_a = N\delta s$. Now we see that by letting

$$m := 4m_e = 4 \quad (6.21)$$

and

$$\omega := \sqrt{\frac{-E}{2m_e}} = \sqrt{\frac{-E}{2}} \quad (6.22)$$

the pseudo-time sliced action (6.20) becomes

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] = \sum_{k=1}^{N} \left[\frac{1}{2} m \left(\frac{\Delta \mathbf{u}_k}{\delta s} \right)^2 - \frac{1}{2} m\omega^2 \mathbf{u}_k^2 \right] \delta s + \Delta s = \mathcal{S}_{\text{osc}}^{(N)}[\mathbf{u}] + \Delta s, \quad (6.23)$$

where $\mathcal{S}_{\text{osc}}^{(N)}[\mathbf{u}]$ is the time-sliced action of the harmonic oscillator.

Next, the determinant of $\mathbf{A}$ is

$$|\det \mathbf{A}| = \sqrt{\det \mathbf{g}} = 4\mathbf{u}^2 = 4r, \quad (6.24)$$

so the volume elements $\mathrm{d}^2\mathbf{x}$ and $\mathrm{d}^2\mathbf{u}$ are related by

$$\frac{\mathrm{d}^2\mathbf{x}}{r} = 4\,\mathrm{d}^2\mathbf{u}. \quad (6.25)$$

Using (6.25), we can now transform the integrals over $\mathbf{x}_k$ in (6.10) to integrals over $\mathbf{u}_k$. The factor 4 from each integral combine to an overall factor $4^{N-1} = \frac{1}{4}4^N$, and we can put the factor 4^N inside the prefactor of (6.10), giving the correct prefactor for the harmonic oscillator path integral with $m = 4$. The result is

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{\exp[i\Delta s]}{4} \Big[K_{\text{osc}}^{(N)}(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) + K_{\text{osc}}^{(N)}(-\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) \Big], \quad (6.26)$$

where

$$K_{\text{osc}}^{(N)}(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) = \left(\frac{m}{2\pi i \delta s} \right)^N \int \mathrm{d}^2\mathbf{u}_{N-1} \cdots \int \mathrm{d}^2\mathbf{u}_1 \, \exp\left[i\mathcal{S}_{\text{osc}}^{(N)}[\mathbf{u}] \right] \quad (6.27)$$

is the time-sliced path integral for the two-dimensional harmonic oscillator, and the integrals are over the whole of $\mathbb{R}^2$. The symmetrization in $\mathbf{u}_b$ in (6.26) arises as a consequence of the mapping (6.12) being two to one. For each path going from $\mathbf{x}_a$ to $\mathbf{x}_b$ there are two paths in $\mathbf{u}$-space, one going from $\mathbf{u}_a$ to $\mathbf{u}_b$ and another going from $\mathbf{u}_a$ to $-\mathbf{u}_b$.

By taking the limit $N \to \infty$ of (6.26), we obtain directly

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{\exp[i\Delta s]}{4} \Big[K_{\text{osc}}(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) + K_{\text{osc}}(-\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) \Big] \quad (6.28)$$

with the two-dimensional harmonic oscillator propagator given by (B.45) with $D = 2$, i.e.

$$K_{\text{osc}}(\mathbf{u}_b, s_b; \mathbf{u}_a, s_a) = \frac{m\omega}{2\pi i \sin(\omega\Delta s)} \exp\left[i\frac{m\omega}{2\sin(\omega\Delta s)} \Big((\mathbf{u}_b^2 + \mathbf{u}_a^2)\cos(\omega\Delta s) - 2\mathbf{u}_b \cdot \mathbf{u}_a \Big) \right]. \quad (6.29)$$

The pseudo-propagator (6.28) then becomes

$$
\begin{aligned}
\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) &= \frac{\exp[i\Delta s]}{4} \frac{m\omega}{2\pi i \sin(\omega\Delta s)} \exp\left[i \frac{m\omega}{2\sin(\omega\Delta s)} (\mathbf{u}_b^2 + \mathbf{u}_a^2) \cos(\omega\Delta s) \right] \times \\
&\qquad \left[\exp\left[i \frac{m\omega}{2\sin(\omega\Delta s)} (-2\mathbf{u}_b \cdot \mathbf{u}_a) \right] + \exp\left[i \frac{m\omega}{2\sin(\omega\Delta s)} (+2\mathbf{u}_b \cdot \mathbf{u}_a) \right] \right] \\
&= \frac{m\omega}{4\pi i} \frac{\exp[i\Delta s]}{\sin(\omega\Delta s)} \exp\left[i \frac{m\omega}{2} \frac{\cos(\omega\Delta s)}{\sin(\omega\Delta s)} (\mathbf{u}_b^2 + \mathbf{u}_a^2) \right] \cos\left(\frac{m\omega}{\sin(\omega\Delta s)} \mathbf{u}_b \cdot \mathbf{u}_a \right). \qquad (6.30)
\end{aligned}
$$

After restoring SI units, this reads

$$
\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{m\omega}{4\pi i\hbar} \frac{\exp\left[\frac{i}{\hbar} \frac{e^2}{4\pi\epsilon_0} \Delta s \right]}{\sin(\omega\Delta s)} \exp\left[i \frac{m\omega}{2\hbar} \frac{\cos(\omega\Delta s)}{\sin(\omega\Delta s)} (\mathbf{u}_b^2 + \mathbf{u}_a^2) \right] \cos\left(\frac{m\omega}{\hbar \sin(\omega\Delta s)} \mathbf{u}_b \cdot \mathbf{u}_a \right). \qquad (6.31)
$$

By expressing the trigonometric functions as

$$
\cos(\omega\Delta s) = \frac{1}{2}\Big(\exp[i\omega\Delta s] + \exp[-i\omega\Delta s] \Big) = \frac{1}{2} \exp[i\omega\Delta s] \Big(1 + \exp[-i\, 2\omega\Delta s] \Big) \qquad (6.32)
$$

and

$$
\sin(\omega\Delta s) = \frac{1}{2i}\Big(\exp[i\omega\Delta s] - \exp[-i\omega\Delta s] \Big) = \frac{1}{2i} \exp[i\omega\Delta s] \Big(1 - \exp[-i\, 2\omega\Delta s] \Big), \qquad (6.33)
$$

and introducing the abbreviations

$$
\kappa := \frac{m\omega}{2\hbar} = \sqrt{\frac{-2m_e E}{\hbar^2}} \qquad (6.34)
$$

and

$$
\nu := \frac{e^2/(4\pi\epsilon_0)}{2\omega\hbar} = \sqrt{\frac{m_e e^4/(4\pi\epsilon_0)^2}{-2\hbar^2 E}}, \qquad (6.35)
$$

we can rewrite (6.31) as

$$
\begin{aligned}
\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) &= \frac{\kappa}{\pi} \frac{\exp[-i\, 2\omega\Delta s(-\nu + 1/2)]}{1 - \exp[-i\, 2\omega\Delta s]} \exp\left[-\kappa \frac{1 + \exp[-i\, 2\omega\Delta s]}{1 - \exp[-i\, 2\omega\Delta s]} (\mathbf{u}_b^2 + \mathbf{u}_a^2) \right] \times \\
&\qquad \cos\left(\frac{4i\kappa \exp[-i\omega\Delta s]}{1 - \exp[-i\, 2\omega\Delta s]} \mathbf{u}_b \cdot \mathbf{u}_a \right). \qquad (6.36)
\end{aligned}
$$

Finally, we express the parameters $\mathbf{u}_{a,b}$ in terms of the physical coordinates $\mathbf{x}_{a,b}$. From (6.12) and (6.14) we find

$$
\mathbf{u}_{a,b}^2 = r_{a,b}\,, \quad \mathbf{u}_b \cdot \mathbf{u}_a = \pm\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}, \qquad (6.37)
$$

and the pseudo-propagator (6.36) takes the final form

$$
\begin{aligned}
\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) &= \frac{\kappa}{\pi} \frac{\exp[-i\, 2\omega\Delta s(-\nu + 1/2)]}{1 - \exp[-i\, 2\omega\Delta s]} \exp\left[-\kappa \frac{1 + \exp[-i\, 2\omega\Delta s]}{1 - \exp[-i\, 2\omega\Delta s]} (r_b + r_a) \right] \times \\
&\qquad \cos\left(\frac{4i\kappa \exp[-i\omega\Delta s]}{1 - \exp[-i\, 2\omega\Delta s]} \sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)} \right). \qquad (6.38)
\end{aligned}
$$

Having solved the pseudo-time sliced path integral and obtained the pseudo-propagator, the fixed-energy amplitude (5.29) can now be found from

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_0^\infty \mathrm{d}s\, \mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) \tag{6.39}$$

with

$$\mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) = \frac{\kappa}{\pi} \frac{\exp[-i\,2\omega s(-\nu + 1/2)]}{1 - \exp[-i\,2\omega s]} \exp\left[-\kappa \frac{1 + \exp[-i\,2\omega s]}{1 - \exp[-i\,2\omega s]}(r_b + r_a)\right] \times \\ \cos\left(\frac{4i\kappa \exp[-i\omega s]}{1 - \exp[-i\,2\omega s]} \sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right). \tag{6.40}$$

When evaluating the integral (6.39), we have to pass around the singularities of (6.40) in the complex plane. We can invoke the residue theorem to evaluate (6.39) as an integral in the complex plane according to

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_C \mathrm{d}s\, \mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) \tag{6.41}$$

where the path C may be parametrized as $s(\sigma) = \sigma - i\eta$ with $\sigma \in (0, \infty)$ and η infinitesimal. Since (6.40) is an analytic function in the domain beneath C, the integral is path-independent there, and we may write (6.41) as

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_{C_1} \mathrm{d}s\, \mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) + \int_{C_2} \mathrm{d}s\, \mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) \tag{6.42}$$

where C_1 is the negative imaginary axis, with parametrization $s(\sigma) = -i\sigma$, $\sigma \in (0, R)$, and C_2 the path with parametrization $s(\alpha) = R\exp[i\alpha]$, $-\pi/2 \leq \alpha \leq 0$, and $R \to \infty$. Now, it is readily verified that (6.40) vanishes for $|s(\alpha)| \to \infty$ so that the integral over C_2 vanishes. Thus we are left with

$$\begin{aligned} \tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) &= \int_{C_1} \mathrm{d}s\, \mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) = \int_0^\infty \mathrm{d}\sigma\, \frac{\mathrm{d}s}{\mathrm{d}\sigma}\, \mathcal{K}_E(\mathbf{x}_b, s(\sigma); \mathbf{x}_a, 0) = -i \int_0^\infty \mathrm{d}\sigma\, \mathcal{K}_E(\mathbf{x}_b, -i\sigma; \mathbf{x}_a, 0) \\ &= -i\frac{\kappa}{\pi} \int_0^\infty \mathrm{d}\sigma\, \frac{\exp[-2\omega\sigma(-\nu + 1/2)]}{1 - \exp[-2\omega\sigma]} \exp\left[-\kappa \frac{1 + \exp[-2\omega\sigma]}{1 - \exp[-2\omega\sigma]}(r_b + r_a)\right] \times \\ &\qquad \cos\left(\frac{4i\kappa \exp[-\omega\sigma]}{1 - \exp[-2\omega\sigma]} \sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right). \end{aligned} \tag{6.43}$$

We now change the integration variable to

$$\varrho := \exp[-2\omega\sigma] \tag{6.44}$$

so that

$$\mathrm{d}\varrho = -2\omega \exp[-2\omega\sigma]\, \mathrm{d}\sigma, \quad \mathrm{d}\sigma = -\frac{1}{2\omega} \frac{\mathrm{d}\varrho}{\varrho}, \tag{6.45}$$

and (6.43) becomes

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = -i\frac{\kappa}{2\omega\pi} \int_0^1 \mathrm{d}\varrho\, \frac{\varrho^{-\nu - 1/2}}{1 - \varrho} \exp\left[-\kappa \frac{1 + \varrho}{1 - \varrho}(r_b + r_a)\right] \cosh\left(\frac{4\kappa\sqrt{\varrho}}{1 - \varrho} \sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right). \tag{6.46}$$

From (6.21) and (6.22) we have $\omega = \frac{2\hbar\kappa}{m} = \frac{\hbar\kappa}{2m_e}$ and thus the fixed-energy amplitude of the two-dimensional Hydrogen atom takes the form

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \frac{m_e}{i\pi\hbar} \int_0^1 \mathrm{d}\varrho\, \frac{\varrho^{-\nu - 1/2}}{1 - \varrho} \exp\left[-\kappa \frac{1 + \varrho}{1 - \varrho}(r_b + r_a)\right] \cosh\left(\frac{4\kappa\sqrt{\varrho}}{1 - \varrho} \sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right) \tag{6.47}$$

with κ and ν given by (6.34) and (6.35), respectively.

The integral in (6.47) converges only for $\nu < 1/2$, but we can find another integral representation that converges for all $\nu \neq 1/2, 3/2, \ldots$ by changing the integration variable to

$$\zeta := \frac{1+\varrho}{1-\varrho}. \tag{6.48}$$

with ζ going from 1 to ∞ as ϱ goes from 0 to 1. We then have

$$\varrho = \frac{\zeta-1}{\zeta+1}, \quad \mathrm{d}\varrho = \frac{2}{(\zeta+1)^2}\mathrm{d}\zeta \tag{6.49}$$

so that

$$1-\varrho = \frac{2}{\zeta+1}, \tag{6.50}$$

$$\frac{\sqrt{\varrho}}{1-\varrho} = \frac{\zeta+1}{2}\sqrt{\frac{\zeta-1}{\zeta+1}} = \frac{1}{2}\sqrt{\zeta^2-1}, \tag{6.51}$$

$$\mathrm{d}\varrho\,\frac{\varrho^{-\nu-1/2}}{1-\varrho} = \mathrm{d}\zeta\,\frac{2}{(\zeta+1)^2}\,\frac{\zeta+1}{2}\left(\frac{\zeta-1}{\zeta+1}\right)^{-\nu-1/2} = \mathrm{d}\zeta\,\frac{(\zeta+1)^{\nu-1/2}}{(\zeta-1)^{\nu+1/2}}, \tag{6.52}$$

and the fixed-energy amplitude (6.47) becomes

$$\tilde{K}(\mathbf{x}_b,\mathbf{x}_a;E) = \frac{m_e}{i\pi\hbar}\int_1^\infty \mathrm{d}\zeta\,\frac{(\zeta+1)^{\nu-1/2}}{(\zeta-1)^{\nu+1/2}}\,\exp\left[-\kappa\zeta(r_b+r_a)\right]\cosh\left(2\kappa\sqrt{\zeta^2-1}\sqrt{\frac{1}{2}(r_br_a+\mathbf{x}_b\cdot\mathbf{x}_a)}\right). \tag{6.53}$$

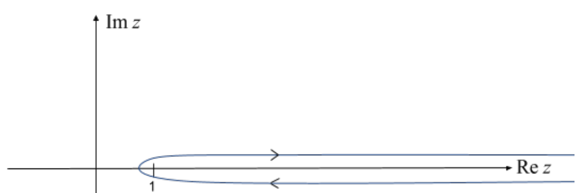

Figure 1. *The integration contour C in the complex plane.*

The integrand of (6.53) has branch cuts in the complex ζ-plane extending from $\zeta = -1$ to $-\infty$ and from $\zeta = 1$ to ∞, the integral running along the latter cut. By invoking the residue theorem, we can evaluate the integral in the complex plane according to [4]

$$\int_1^\infty \frac{\mathrm{d}\zeta}{(\zeta-1)^{\nu+1/2}}\cdots = \frac{\pi\exp\left[i\pi(\nu+1/2)\right]}{\sin[\pi(\nu+1/2)]}\,\frac{1}{2\pi i}\int_C \frac{\mathrm{d}\zeta}{(\zeta-1)^{\nu+1/2}}\cdots = \frac{1}{1+\exp\left[-i\,2\pi\nu\right]}\int_C \frac{\mathrm{d}\zeta}{(\zeta-1)^{\nu+1/2}}\cdots \tag{6.54}$$

along the contour C encircling the right-hand cut clockwise (see fig. 1). The fixed-energy amplitude (6.53) then finally becomes

$$\tilde{K}(\mathbf{x}_b,\mathbf{x}_a;E) = \frac{m_e}{i\pi\hbar}\,\frac{1}{1+\exp\left[-i\,2\pi\nu\right]}\int_C \mathrm{d}\zeta\,\frac{(\zeta+1)^{\nu-1/2}}{(\zeta-1)^{\nu+1/2}}\,\exp\left[-\kappa\zeta(r_b+r_a)\right]\times \cosh\left(2\kappa\sqrt{\zeta^2-1}\sqrt{\frac{1}{2}(r_br_a+\mathbf{x}_b\cdot\mathbf{x}_a)}\right), \tag{6.55}$$

where this integral representation converges for all $\nu \neq 1/2, 3/2, \ldots$.

6.3 Solution for the Three-Dimensional H-atom

The two-dimensional hydrogen atom is of course a toy model, the real world being three-dimensional. In three dimensions ($D = 3$), the pseudo-time sliced path integral (6.8) becomes

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{r_a}{r_b^{3/2}} \left(\frac{1}{2\pi i\delta s}\right)^{3N/2} \int \frac{\mathrm{d}^3\mathbf{x}_{N-1}}{r_{N-1}^{3/2}} \cdots \int \frac{\mathrm{d}^3\mathbf{x}_1}{r_1^{3/2}} \exp\left[i\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}]\right] \tag{6.56}$$

with the pseudo-time sliced action

$$\tilde{\mathcal{S}}_E^{(N)}[\mathbf{x}] = \sum_{k=1}^{N} \left[\frac{1}{2r_k}\left(\frac{\Delta\mathbf{x}_k}{\delta s}\right)^2 + Er_k + 1\right]\delta s. \tag{6.57}$$

As in two dimensions, we shall see that we can transform this path integral into that of the harmonic oscillator by going over to "square root coordinates" u^μ whose sum of squares equals r. This can be done for three dimensions by introducing a mapping from a four-dimensional $\{u^\mu\}$ space to the three-dimensional $\{x^i\}$ space by

$$x^i = \mathbf{z}^\dagger\boldsymbol{\sigma}^i\mathbf{z} \tag{6.58}$$

with

$$\mathbf{z} := \begin{bmatrix} u^1 + iu^2 \\ u^3 + iu^4 \end{bmatrix} \tag{6.59}$$

and the Pauli spin matrices

$$\boldsymbol{\sigma}^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \boldsymbol{\sigma}^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \boldsymbol{\sigma}^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{6.60}$$

With this transformation we indeed have $r = (u^1)^2 + (u^2)^2 + (u^3)^2 + (u^4)^2 \equiv \vec{u}^2$, as shown in Appendix C.

The mapping (6.58) is obviously not invertible, so the inverse relationship will be multivalued. By expressing the x^i in terms of spherical coordinates r, θ, ϕ, we find (see Appendix C)

$$\begin{cases} u^1 = \sqrt{r}\cos\left(\frac{\theta}{2}\right)\cos\left(\frac{\phi+\gamma}{2}\right) \\ u^2 = -\sqrt{r}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\phi+\gamma}{2}\right) \\ u^3 = \sqrt{r}\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\phi-\gamma}{2}\right) \\ u^4 = \sqrt{r}\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{\phi-\gamma}{2}\right) \end{cases} \tag{6.61}$$

with $\gamma \in (0, 4\pi)$. The parameter γ is compliments r, θ, ϕ as coordinates for the four-dimensional $\{u^\mu\}$ space. Accordingly, we introduce a fourth coordinate x^4 and extend the mapping from u^μ to x^i by the differential relation

$$\begin{aligned} \mathrm{d}x^4 &= 2u^2\,\mathrm{d}u^1 - 2u^1\,\mathrm{d}u^2 + 2u^4\,\mathrm{d}u^3 - 2u^3\,\mathrm{d}u^4 \\ &= r\cos\theta\,\mathrm{d}\phi + r\,\mathrm{d}\gamma. \end{aligned} \tag{6.62}$$

The differentials $\mathrm{d}x^\mu$ and $\mathrm{d}u^\nu$ are then related by

$$[\mathrm{d}\vec{x}] = \mathbf{A}(\vec{u})[\mathrm{d}\vec{u}] \tag{6.63}$$

where the Jacobian matrix $\mathbf{A}$, given by (C.23), has the determinant

$$|\det\mathbf{A}(\vec{u})| = 16r^2, \tag{6.64}$$

and the metric $g_{\mu\nu}$ in u^μ coordinates takes the simple form

$$g_{\mu\nu} = 4r\,\delta_{\mu\nu}. \tag{6.65}$$

Equation (6.63) defines a mapping between the four-dimensional $\{x^\mu\}$ and $\{u^\mu\}$ spaces. This mapping becomes bijective once it has been specified at an initial point $u^\mu(\vec{x}_a) = u^\mu_a$.

We now incorporate the fourth dummy dimension x^4 into the path integral (6.56). First note that r is independent of x^4. Writing $\Delta x^4_k \equiv x^4_k - x^4_{k-1}$, we have (with $x^4_0 \equiv x^4_a$ and arbitrary $x^4_N \equiv x^4_b$):

$$\begin{aligned}
&\frac{1}{r_b^{1/2}}\left(\frac{1}{2\pi i\delta s}\right)^{N/2}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x^4_{N-1}}{r_{N-1}^{1/2}}\cdots\int_{-\infty}^{+\infty}\frac{\mathrm{d}x^4_1}{r_1^{1/2}}\int_{-\infty}^{+\infty}\mathrm{d}x^4_0\,\exp\left[i\sum_{k=1}^{N}\frac{1}{2r_k}\Big(\frac{\Delta x^4_k}{\delta s}\Big)^2\delta s\right] = \\
&= \left(\frac{1}{2\pi i\delta s}\right)^{N/2}\int_{-\infty}^{+\infty}\frac{\mathrm{d}(\Delta x^4_N)}{r_N^{1/2}}\exp\left[i\frac{1}{2r_N}\Big(\frac{\Delta x^4_N}{\delta s}\Big)^2\delta s\right]\cdots\int_{-\infty}^{+\infty}\frac{\mathrm{d}(\Delta x^4_1)}{r_1^{1/2}}\exp\left[i\frac{1}{2r_1}\Big(\frac{\Delta x^4_1}{\delta s}\Big)^2\delta s\right] \\
&= \prod_{k=1}^{N}\left(\frac{1}{2\pi i\delta s r_k}\right)^{1/2}\int_{-\infty}^{+\infty}\mathrm{d}(\Delta x^4_k)\,\exp\left[i\frac{1}{2r_k\delta s}(\Delta x^4_k)^2\right] = \prod_{k=1}^{N}\left(\frac{1}{2\pi i\delta s r_k}\right)^{1/2}\left(\frac{i\pi}{1/(2r_k\delta s)}\right)^{1/2} \\
&= 1
\end{aligned} \tag{6.66}$$

where we have used (A.22) for the integrals in the third line. By inserting this identity into the integrand of the pseudo-time sliced path integral (6.56) and changing the order of the integrals, we get

$$\begin{aligned}
\mathcal{K}^{(N)}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) &= \frac{r_a}{r_b^{4/2}}\left(\frac{1}{2\pi i\delta s}\right)^{4N/2}\int_{-\infty}^{+\infty}\mathrm{d}x^4_0\,\times \\
&\qquad \int\frac{\mathrm{d}^3\mathbf{x}_{N-1}}{r_{N-1}^{3/2}}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x^4_{N-1}}{r_{N-1}^{1/2}}\cdots\int\frac{\mathrm{d}^3\mathbf{x}_1}{r_1^{3/2}}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x^4_1}{r_1^{1/2}}\,\exp\left[i\,\tilde{\mathcal{S}}^{(N)}_E[\vec{x}]\right] \\
&= \frac{r_a^2}{r_b^2}\left(\frac{1}{2\pi i\delta s}\right)^{2N}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x^4_a}{r_a}\int\frac{\mathrm{d}^4\vec{x}_{N-1}}{r_{N-1}^2}\cdots\int\frac{\mathrm{d}^4\vec{x}_1}{r_1^2}\,\exp\left[i\,\tilde{\mathcal{S}}^{(N)}_E[\vec{x}]\right]
\end{aligned} \tag{6.67}$$

with the definition

$$\tilde{\mathcal{S}}^{(N)}_E[\vec{x}] := \tilde{\mathcal{S}}^{(N)}_E[\mathbf{x}] + \sum_{k=1}^{N}\frac{1}{2r_k}\left(\frac{\Delta x^4_k}{\delta s}\right)^2\delta s = \sum_{k=1}^{N}\left[\frac{1}{2r_k}\left(\frac{\Delta\vec{x}_k}{\delta s}\right)^2 + Er_k + 1\right]\delta s. \tag{6.68}$$

Here $\vec{x}_k$ denotes the four-vector $(x^1_k, x^2_k, x^3_k, x^4_k)$, not to be confused with the three-vector $\mathbf{x}_k = (x^1_k, x^3_k, x^3_k)$, for which we still denote $|\mathbf{x}_k| \equiv r_k$. With $\Delta\vec{x}_k \equiv \vec{x}_k - \vec{x}_{k-1}$ we can rewrite (6.67) as

$$\begin{aligned}
\mathcal{K}^{(N)}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) &= \frac{r_a^2}{r_b^2}\left(\frac{1}{2\pi i\delta s}\right)^{2N}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x^4_a}{r_a}\int\frac{\mathrm{d}^4(\Delta\vec{x}_N)}{r_{N-1}^2}\cdots\int\frac{\mathrm{d}^4(\Delta\vec{x}_2)}{r_1^2}\,\exp\left[i\,\tilde{\mathcal{S}}^{(N)}_E[\vec{x}]\right] \\
&= \left(\frac{1}{2\pi i\delta s}\right)^{2N}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x^4_a}{r_a}\int\frac{\mathrm{d}^4(\Delta\vec{x}_N)}{r_N^2}\cdots\int\frac{\mathrm{d}^4(\Delta\vec{x}_2)}{r_2^2}\,\frac{r_a^2}{r_1^2}\,\exp\left[i\,\tilde{\mathcal{S}}^{(N)}_E[\vec{x}]\right].
\end{aligned} \tag{6.69}$$

Since, in the continuum limit, the dominant contributions comes from the continuous paths [5], we can approximate $r_a/r_1 = 1$ to first order in δs, giving

$$\mathcal{K}^{(N)}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \left(\frac{1}{2\pi i\delta s}\right)^{2N}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x^4_a}{r_a}\int\frac{\mathrm{d}^4(\Delta\vec{x}_N)}{r_N^2}\cdots\int\frac{\mathrm{d}^4(\Delta\vec{x}_2)}{r_2^2}\,\exp\left[i\,\tilde{\mathcal{S}}^{(N)}_E[\vec{x}]\right]. \tag{6.70}$$

Having incorporated the fourth variable x^4 into the path integral, we can now go over to the u^μ variables. The integral over x^4_a provides a unique mapping between x^ν and u^μ for each value of x^4_a. With $|\det\mathbf{A}(\vec{u}_k)| = 16r_k^2$, the path integral (6.70) transforms as [4]

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \left(\frac{1}{2\pi i\delta s}\right)^{2N} \int_{-\infty}^{+\infty} \frac{\mathrm{d}x_a^4}{r_a} \int \frac{\mathrm{d}^4(\Delta\vec{u}_N)}{r_N^2} |\det \mathbf{A}(\vec{u}_N)| \cdots$$
$$\cdots \int \frac{\mathrm{d}^4(\Delta\vec{u}_2)}{r_2^2} |\det \mathbf{A}(\vec{u}_2)| \exp\left[i\left[\tilde{\mathcal{S}}_E^{(N)}[\vec{x}] + \mathcal{S}_J\right]\right]$$
$$= \frac{1}{16}\left(\frac{4}{2\pi i\delta s}\right)^{2N} \int_{-\infty}^{+\infty} \frac{\mathrm{d}x_a^4}{r_a} \int \mathrm{d}^4\vec{u}_{N-1} \cdots \int \mathrm{d}^4\vec{u}_1 \exp\left[i\left[\tilde{\mathcal{S}}_E^{(N)}[\vec{x}] + \mathcal{S}_J\right]\right]. \quad (6.71)$$

The quantity $\mathcal{S}_J$ appearing here is called the **Jacobian action**. It arises, for a generic variable transformation $\{x^\mu\} \to \{u^\nu\}$, from correction terms due to the finite time-slicing and finite coordinate differences Δu^μ (the technical details of which is beyond the scope of this thesis). For our purposes it suffices to note that it can be expressed as [4]

$$\mathcal{S}_J = \sum_{k=1}^{N} \mathcal{S}_{J,k}(\delta s) \quad (6.72)$$

where (summation convention implied)

$$i\mathcal{S}_{J,k}(\delta s) = \frac{1}{2}\Gamma_\mu{}^\mu{}_\nu\, \Delta u_k^\nu - i\delta s\, \frac{1}{8}\delta^{\alpha\beta}\, \Gamma_\mu{}^\mu{}_\alpha\, \Gamma_\lambda{}^\lambda{}_\beta \quad (6.73)$$

with the **affine connection**

$$\Gamma_{\lambda\kappa}{}^\mu = \frac{\partial u^\mu}{\partial x^i} \frac{\partial^2 x^i}{\partial u^\lambda \partial u^\kappa} \quad (6.74)$$

evaluated at $\vec{u} = \vec{u}_k$. Luckily, in the case of our interest, x^i has no second derivatives with respect to any u^λ, u^κ so the Jacobian action vanishes identically and (6.71) simplifies to

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{1}{16}\left(\frac{4}{2\pi i\delta s}\right)^{2N} \int_{-\infty}^{+\infty} \frac{\mathrm{d}x_a^4}{r_a} \int \mathrm{d}^4\vec{u}_{N-1} \cdots \int \mathrm{d}^4\vec{u}_1 \exp\left[i\,\tilde{\mathcal{S}}_E^{(N)}[\vec{x}]\right]. \quad (6.75)$$

Next we need to write the time-sliced pseudo-action (6.68) in terms of u^μ. To lowest order in δs we have

$$(\Delta\vec{x})^2 = g_{\mu\nu}\Delta u^\mu \Delta u^\nu = [\Delta\vec{u}]^T[g_{\mu\nu}][\Delta\vec{u}] = 4r(\Delta\vec{u})^2.$$

The four-dimensional pseudo-action (6.68) then becomes

$$\tilde{\mathcal{S}}_E^{(N)}[\vec{x}] = \sum_{k=1}^{N}\left[\frac{1}{2r_k}4r_k\left(\frac{\Delta\vec{u}_k}{\delta s}\right)^2 + E\vec{u}_k^2 + 1\right]\delta s = \sum_{k=1}^{N}\left[\frac{1}{2}4\left(\frac{\Delta\vec{u}_k}{\delta s}\right)^2 - \frac{1}{2}4(-E/2)\vec{u}_k^2\right]\delta s + \Delta s \quad (6.76)$$

with $\Delta s \equiv s_b - s_a = N\delta s$. Now we see that by letting

$$m := 4m_e = 4 \quad (6.77)$$

and

$$\omega := \sqrt{-E/2m_e} = \sqrt{-E/2} \quad (6.78)$$

we can write (6.76) as

$$\tilde{\mathcal{S}}_E^{(N)}[\vec{x}] = \sum_{k=1}^{N}\left[\frac{1}{2}m\left(\frac{\Delta\vec{u}_k}{\delta s}\right)^2 - \frac{1}{2}m\omega^2\vec{u}_k^2\right]\delta s + \Delta s = \mathcal{S}_{\mathrm{osc}}^{(N)}[\vec{u}] + \Delta s, \quad (6.79)$$

where $\mathcal{S}_{\mathrm{osc}}^{(N)}[\vec{u}]$ is the time-sliced action for the harmonic oscillator. The path integral (6.75) then becomes

$$\mathcal{K}_E^{(N)}(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{\exp[i\Delta s]}{16} \int_{-\infty}^{+\infty} \frac{\mathrm{d}x_a^4}{r_a} \left(\frac{m}{2\pi i \delta s}\right)^{2N} \int \mathrm{d}^4\vec{u}_{N-1} \cdots \int \mathrm{d}^4\vec{u}_1 \, \exp\left[i\, \mathcal{S}_{\mathrm{osc}}^{(N)}[\vec{u}]\right]$$
$$= \frac{\exp[i\Delta s]}{16} \int_{-\infty}^{+\infty} \frac{\mathrm{d}x_a^4}{r_a} K_{\mathrm{osc}}^{(N)}(\vec{u}_b, s_b; \vec{u}_a, s_a) \tag{6.80}$$

where $K_{\mathrm{osc}}^{(N)}(\vec{u}_b, s_b; \vec{u}_a, s_a)$ is the corresponding time-sliced path integral of the four-dimensional harmonic oscillator. By taking the limit $N \to \infty$ of (6.80) we obtain directly

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{\exp[i\Delta s]}{16} \int_{-\infty}^{+\infty} \frac{\mathrm{d}x_a^4}{r_a} K_{\mathrm{osc}}(\vec{u}_b, s_b; \vec{u}_a, s_a), \tag{6.81}$$

with the four-dimensional harmonic oscillator propagator given by (B.65) with $D = 4$, i.e.

$$K_{\mathrm{osc}}(\vec{u}_b, s_b; \vec{u}_a, s_a) = \left(\frac{m\omega}{2\pi i \sin(\omega\Delta s)}\right)^2 \exp\left[i\frac{m\omega}{2\sin(\omega\Delta s)}\left[(\vec{u}_b^2 + \vec{u}_a^2)\cos(\omega\Delta s) - 2\vec{u}_b\cdot\vec{u}_a\right]\right]. \tag{6.82}$$

The u^μ variables may be expressed directly in terms of r, θ, ϕ, γ using (6.61). Since $\mathbf{x}_a$ is fixed in (6.81), (r_a, θ_a, ϕ_a) are all fixed and (6.62) gives us

$$\mathrm{d}x_a^4 = r_a \, \mathrm{d}\gamma_a. \tag{6.83}$$

Recalling that $\gamma \in (0, 4\pi)$, we can then write (6.81) as

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{\exp[i\Delta s]}{16} \int_0^{4\pi} \mathrm{d}\gamma_a \, K_{\mathrm{osc}}(\vec{u}_b, s_b; \vec{u}_a, s_a)$$
$$= \frac{\exp[i\Delta s]}{16} \int_0^{4\pi} \mathrm{d}\gamma_a \left(\frac{m\omega}{2\pi i \sin(\omega\Delta s)}\right)^2 \exp\left[i\frac{m\omega}{2\sin(\omega\Delta s)}\left[(\vec{u}_b^2 + \vec{u}_a^2)\cos(\omega\Delta s) - 2\vec{u}_b\cdot\vec{u}_a\right]\right] \tag{6.84}$$

or, after restoring SI units, substituting $\vec{u}_{a,b}^2 = r_{a,b}$ and rearranging, as

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = -\frac{1}{16\pi^2}\left(\frac{m\omega}{2\hbar}\right)^2 \frac{\exp\left[\frac{i}{\hbar}\frac{e^2}{4\pi\epsilon_0}\Delta s\right]}{\sin^2(\omega\Delta s)} \exp\left[i\frac{m\omega}{2\hbar}\frac{\cos(\omega\Delta s)}{\sin(\omega\Delta s)}(r_b + r_a)\right] \times$$
$$\int_0^{4\pi} \mathrm{d}\gamma_a \, \exp\left[-i\frac{m\omega}{2\hbar}\frac{2}{\sin(\omega\Delta s)}\vec{u}_b\cdot\vec{u}_a\right]. \tag{6.85}$$

As in the two-dimensional problem, we introduce the abbreviations

$$\kappa := \frac{m\omega}{2\hbar} = \sqrt{\frac{-2m_e E}{\hbar^2}} \tag{6.86}$$

and

$$\nu := \frac{e^2/(4\pi\epsilon_0)}{2\omega\hbar} = \sqrt{\frac{m_e e^4/(4\pi\epsilon_0)^2}{-2\hbar^2 E}}, \tag{6.87}$$

and write (6.85) a little more compactly as

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = -\frac{\kappa^2}{16\pi^2}\frac{\exp[i\,2\omega\nu\Delta s]}{\sin^2(\omega\Delta s)} \exp\left[i\kappa\frac{\cos(\omega\Delta s)}{\sin(\omega\Delta s)}(r_b + r_a)\right] \int_0^{4\pi} \mathrm{d}\gamma_a \, \exp\left[\frac{-i\,2\kappa}{\sin(\omega\Delta s)}\vec{u}_b\cdot\vec{u}_a\right]. \tag{6.88}$$

We proceed to evaluate the integral over γ_a in (6.88). Using (6.61) we find, after some algebra and trigonometric rearrangements,

$$\vec{u}_b \cdot \vec{u}_a = \sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\, \cos\left(\frac{\gamma_a - \gamma_b - \beta}{2}\right), \tag{6.89}$$

where β is an angle independent of γ_a, defined by

$$\tan\left(\frac{\beta}{2}\right) := \frac{\cos\left(\frac{\theta_b+\theta_a}{2}\right)\sin\left(\frac{\phi_b-\phi_a}{2}\right)}{\cos\left(\frac{\theta_b-\theta_a}{2}\right)\cos\left(\frac{\phi_b-\phi_a}{2}\right)}. \tag{6.90}$$

The integral over γ_a in (6.88) then becomes

$$\begin{aligned}\int_0^{4\pi} \mathrm{d}\gamma_a\, \exp\left[\frac{-i\,2\kappa}{\sin(\omega\Delta s)}\vec{u}_b \cdot \vec{u}_a\right] &= \int_0^{4\pi} \mathrm{d}\gamma_a\, \exp\left[\frac{-i\,2\kappa}{\sin(\omega\Delta s)}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\, \cos\left(\frac{\gamma_a - \gamma_b - \beta}{2}\right)\right]\\ &= 2\int_{(-\gamma_b-\beta)/2}^{(-\gamma_b-\beta)/2+2\pi} \mathrm{d}\gamma\, \exp\left[\frac{-i\,2\kappa}{\sin(\omega\Delta s)}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\, \cos\gamma\right].\end{aligned} \tag{6.91}$$

By using the *Jacobi–Anger expansion* [6]

$$\exp[iz\cos\gamma] = \sum_{n=-\infty}^{\infty} i^{-n} J_n(z)\, \exp[in\gamma] \tag{6.92}$$

where the J_n are the Bessel functions of the first kind, we have for arbitrary z and α,

$$\int_\alpha^{\alpha+2\pi} \exp[iz\cos\gamma]\, \mathrm{d}\gamma = \sum_{n=-\infty}^{\infty} i^{-n} J_n(z) \int_\alpha^{\alpha+2\pi} \exp[in\gamma]\, \mathrm{d}\gamma = 2\pi J_0(z), \tag{6.93}$$

due to the integral in the sum being zero for $n \neq 0$. The integral on the right-hand side of (6.91) has precisely the form of (6.93), and thus evaluates to

$$\int_0^{4\pi} \mathrm{d}\gamma_a\, \exp\left[\frac{-i\,2\kappa}{\sin(\omega\Delta s)}\vec{u}_b \cdot \vec{u}_a\right] = 4\pi J_0\left(\frac{-2\kappa}{\sin(\omega\Delta s)}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right). \tag{6.94}$$

Substituting this result into (6.88), the pseudo-propagator now becomes

$$\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = -\frac{\kappa^2}{4\pi}\frac{\exp[i\,2\omega\nu\Delta s]}{\sin^2(\omega\Delta s)}\, \exp\left[i\kappa\frac{\cos(\omega\Delta s)}{\sin(\omega\Delta s)}(r_b + r_a)\right] J_0\left(\frac{-2\kappa}{\sin(\omega\Delta s)}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right). \tag{6.95}$$

As in the two-dimensional problem, we express the trigonometric functions as

$$\cos(\omega\Delta s) = \frac{1}{2}\exp[i\omega\Delta s]\Big(1 + \exp[-i\,2\omega\Delta s]\Big) \tag{6.96}$$

and

$$\sin(\omega\Delta s) = \frac{1}{2i}\exp[i\omega\Delta s]\Big(1 - \exp[-i\,2\omega\Delta s]\Big), \tag{6.97}$$

whereby we can write the pseudo-propagator (6.95) in the final form

$$\begin{aligned}\mathcal{K}_E(\mathbf{x}_b, s_b; \mathbf{x}_a, s_a) = \frac{\kappa^2}{\pi}\frac{\exp[-i\,2\omega\Delta s(1-\nu)]}{(1-\exp[-i\,2\omega\Delta s])^2}\, \exp\left[-\kappa\frac{1+\exp[-i\,2\omega\Delta s]}{1-\exp[-i\,2\omega\Delta s]}(r_b + r_a)\right] \times\\ I_0\left(\frac{4\kappa\exp[-i\omega\Delta s]}{1-\exp[-i\,2\omega\Delta s]}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right)\end{aligned} \tag{6.98}$$

where $I_0(z) = I_0(-z) = J_0(iz)$ is the zeroth order modified Bessel function of the first kind.

Having solved the pseudo-time sliced path integral and obtained the pseudo-propagator, the fixed-energy amplitude (5.29) can now be found from

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_0^\infty \mathrm{d}s\, \mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) \tag{6.99}$$

with

$$\mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) = \frac{\kappa^2}{\pi} \frac{\exp\left[-i\, 2\omega s(1-\nu)\right]}{(1-\exp\left[-i\, 2\omega s\right])^2} \exp\left[-\kappa \frac{1+\exp\left[-i\, 2\omega s\right]}{1-\exp\left[-i\, 2\omega s\right]}(r_b + r_a)\right] \times \\ I_0\left(\frac{4\kappa \exp\left[-i\omega s\right]}{1-\exp\left[-i\, 2\omega s\right]}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right). \tag{6.100}$$

When evaluating the integral (6.99), we have to pass around the singularities of (6.100) in the complex plane. We can invoke the residue theorem to evaluate (6.99) as an integral in the complex plane according to

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_C \mathrm{d}s\, \mathcal{K}_E(\mathbf{x}_b, s; \mathbf{x}_a, 0) \tag{6.101}$$

where the path C may be parametrized as $s(\sigma) = \sigma - i\eta$ with $\sigma \in (0, \infty)$ and η infinitesimal. As for the two-dimensional problem, we convince ourselves that (6.100) vanishes for $|s| \to \infty$ in the fourth quadrant, so that the integral (6.101) may be evaluated along the negative imaginary axis. With the parametrization $s(\sigma) = -i\sigma$, we then have

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \int_0^\infty \mathrm{d}\sigma\, \frac{\mathrm{d}s}{\mathrm{d}\sigma}\, \mathcal{K}_E(\mathbf{x}_b, s(\sigma); \mathbf{x}_a, 0) = -i \int_0^\infty \mathrm{d}\sigma\, \mathcal{K}_E(\mathbf{x}_b, -i\sigma; \mathbf{x}_a, 0) \\ = -i\frac{\kappa^2}{\pi} \int_0^\infty \mathrm{d}\sigma\, \frac{\exp\left[-\, 2\omega\sigma(1-\nu)\right]}{(1-\exp\left[-\, 2\omega\sigma\right])^2} \exp\left[-\kappa \frac{1+\exp\left[-\, 2\omega\sigma\right]}{1-\exp\left[-\, 2\omega\sigma\right]}(r_b + r_a)\right] \times \\ I_0\left(\frac{4\kappa \exp\left[-\omega\sigma\right]}{1-\exp\left[-\, 2\omega\sigma\right]}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right). \tag{6.102}$$

After changing the integration variable to

$$\varrho := \exp\left[-2\omega\sigma\right], \quad \mathrm{d}\sigma = -\frac{1}{2\omega}\frac{\mathrm{d}\varrho}{\varrho}, \tag{6.103}$$

and substituting $\omega = \frac{2\hbar\kappa}{m} = \frac{\hbar\kappa}{2m_e}$, the fixed-energy amplitude (6.102) takes the form

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \frac{m_e\kappa}{i\pi\hbar} \int_0^1 \mathrm{d}\varrho\, \frac{\varrho^{-\nu}}{(1-\varrho)^2} \exp\left[-\kappa\frac{1+\varrho}{1-\varrho}(r_b + r_a)\right] I_0\left(\frac{4\kappa\sqrt{\varrho}}{1-\varrho}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b \cdot \mathbf{x}_a)}\right). \tag{6.104}$$

The integral in (6.104) converges only for $\nu < 1$, but we can find another integral representation that converges for all $\nu \neq 1, 2, \ldots$ by changing the integration variable to

$$\zeta := \frac{1+\varrho}{1-\varrho}. \tag{6.105}$$

as in the two-dimensional case. We then have

$$\varrho = \frac{\zeta - 1}{\zeta + 1}, \quad \mathrm{d}\varrho = \frac{2}{(\zeta+1)^2}\mathrm{d}\zeta, \tag{6.106}$$

so that

$$1-\varrho = \frac{2}{\zeta+1}, \tag{6.107}$$

$$\frac{\sqrt{\varrho}}{1-\varrho} = \frac{1}{2}\sqrt{\zeta^2-1}, \tag{6.108}$$

$$\mathrm{d}\varrho\, \frac{\varrho^{-\nu}}{(1-\varrho)^2} = \mathrm{d}\zeta\, \frac{2}{(\zeta+1)^2}\frac{(\zeta+1)^2}{4}\left(\frac{\zeta-1}{\zeta+1}\right)^{-\nu} = \mathrm{d}\zeta\, \frac{1}{2}\left(\frac{\zeta+1}{\zeta-1}\right)^{\nu}, \tag{6.109}$$

and the fixed-energy amplitude (6.104) becomes

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \frac{m_e\kappa}{2\pi i\hbar}\int_1^\infty \mathrm{d}\zeta\, \left(\frac{\zeta+1}{\zeta-1}\right)^{\nu} \exp\left[-\kappa\zeta(r_b+r_a)\right] I_0\left(2\kappa\sqrt{\zeta^2-1}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b\cdot\mathbf{x}_a)}\right). \tag{6.110}$$

As in the two-dimensional case, the integrand has branch cuts extending from -1 to $-\infty$ and from 1 to ∞, with the integral running along the second cut. We again transform this integral into an integral over a contour C encircling the right-hand branch cut in the clockwise sense, as in figure 1, Section 6.2. The replacement rule is now [4]

$$\int_1^\infty \frac{\mathrm{d}\zeta}{(\zeta-1)^\nu}\cdots = \frac{\pi\exp\left[i\pi\nu\right]}{\sin\pi\nu}\frac{1}{2\pi i}\int_C \frac{\mathrm{d}\zeta}{(\zeta-1)^\nu}\cdots = \frac{1}{1-\exp\left[-i\,2\pi\nu\right]}\int_C \frac{\mathrm{d}\zeta}{(\zeta-1)^\nu}\cdots, \tag{6.111}$$

and the fixed-energy amplitude (6.110) finally becomes

$$\tilde{K}(\mathbf{x}_b, \mathbf{x}_a; E) = \frac{m_e\kappa}{2\pi i\hbar}\frac{1}{1-\exp\left[-i\,2\pi\nu\right]}\int_C \mathrm{d}\zeta\, \left(\frac{\zeta+1}{\zeta-1}\right)^{\nu} \exp\left[-\kappa\zeta(r_b+r_a)\right]\times$$
$$I_0\left(2\kappa\sqrt{\zeta^2-1}\sqrt{\frac{1}{2}(r_b r_a + \mathbf{x}_b\cdot\mathbf{x}_a)}\right), \tag{6.112}$$

where this integral representation converges for all $\nu \neq 1, 2, \ldots$.

7 Conclusion

We have given analytical solutions of path integrals for the two– and three-dimensional Hydrogen atom, thereby obtaining integral representations for the corresponding fixed-energy amplitudes. To do so, we had to construct a new path integral formula for an auxiliary quantity called the pseudo-propagator, from which the fixed-energy amplitude is obtained. The new path integral formula incorporates a functional degree of freedom that can be exploited when dealing with singular potentials to bring the path integral to a form that is easier to deal with. For the two- and three-dimensional Hydrogen atoms, the resulting path integrals could then, by means of a coordinate transformation, be transformed into the Gaussian form of a harmonic oscillator, whereby the solution was readily obtained.

We now summarize the main results. For the two-dimensional Hydrogen atom, we found integral representations for the fixed-energy amplitude given by (6.47) and (6.55), namely,

$$\tilde{K}(\mathbf{x}_b,\mathbf{x}_a;E)=\frac{m_e}{i\pi\hbar}\int_0^1 \mathrm{d}\varrho\,\frac{\varrho^{-\nu-1/2}}{1-\varrho}\,\exp\left[-\kappa\frac{1+\varrho}{1-\varrho}(r_b+r_a)\right]\cosh\left(\frac{4\kappa\sqrt{\varrho}}{1-\varrho}\sqrt{\frac{1}{2}(r_br_a+\mathbf{x}_b\cdot\mathbf{x}_a)}\right),$$

which converges for $\nu<1/2$, and

$$\tilde{K}(\mathbf{x}_b,\mathbf{x}_a;E)=\frac{m_e}{i\pi\hbar}\frac{1}{1+\exp\left[-i\,2\pi\nu\right]}\int_C \mathrm{d}\zeta\,\frac{(\zeta+1)^{\nu-1/2}}{(\zeta-1)^{\nu+1/2}}\,\exp\left[-\kappa\zeta(r_b+r_a)\right]\times$$
$$\cosh\left(2\kappa\sqrt{\zeta^2-1}\sqrt{\frac{1}{2}(r_br_a+\mathbf{x}_b\cdot\mathbf{x}_a)}\right),$$

which converges for all $\nu\neq 1/2,3/2,\ldots$. The integration contour C encircles the branch cut of the integrand from 1 to ∞ in the clockwise sense (see fig. 1, Section 6.2), and the quantities ν and κ are defined by

$$\nu:=\sqrt{\frac{m_ee^4/(4\pi\epsilon_0)^2}{-2\hbar^2E}}\quad\text{and}\quad\kappa:=\sqrt{\frac{-2m_eE}{\hbar^2}}.$$

For the three-dimensional Hydrogen atom, we found integral representations for the fixed-energy amplitude given by (6.104) and (6.112), namely,

$$\tilde{K}(\mathbf{x}_b,\mathbf{x}_a;E)=\frac{m_e\kappa}{i\pi\hbar}\int_0^1 \mathrm{d}\varrho\,\frac{\varrho^{-\nu}}{(1-\varrho)^2}\,\exp\left[-\kappa\frac{1+\varrho}{1-\varrho}(r_b+r_a)\right]I_0\left(\frac{4\kappa\sqrt{\varrho}}{1-\varrho}\sqrt{\frac{1}{2}(r_br_a+\mathbf{x}_b\cdot\mathbf{x}_a)}\right),$$

which converges for $\nu<1$, and

$$\tilde{K}(\mathbf{x}_b,\mathbf{x}_a;E)=\frac{m_e\kappa}{2\pi i\hbar}\frac{1}{1-\exp\left[-i\,2\pi\nu\right]}\int_C \mathrm{d}\zeta\,\left(\frac{\zeta+1}{\zeta-1}\right)^{\nu}\exp\left[-\kappa\zeta(r_b+r_a)\right]\times$$
$$I_0\left(2\kappa\sqrt{\zeta^2-1}\sqrt{\frac{1}{2}(r_br_a+\mathbf{x}_b\cdot\mathbf{x}_a)}\right),$$

which converges for all $\nu\neq 1,2,\ldots$, and where $I_0(z)$ is the zeroth order modified Bessel function of the first kind. The contour C is the same as for the two-dimensional case, as well as the quantities ν and κ.

The success in calculating the path integrals demonstrates the power of the new path integral formulas, developed in Section 5, involving the regulating functions f_l and f_r. In fact, this method has made it possible to solve a large class of previously unsolvable Feynman path integrals [4].

Having obtained the fixed-energy amplitude of the Hydrogen atom, the next step is to extract from it the various physical quantities. The integral representations are enough to obtain the well known energy eigenvalues and eigenfunctions. This procedure is done in the Duru–Kleinert article [2] as well as in the book [4] by Kleinert. To take the study of the Hydrogen atom one step further, we may take into account relativistic effects. The corresponding relativistic path integral is solved in Kleinert's 1996 article [7].

A Gaussian Integrals

When solving some standard path integrals, we often encounter D-dimensional integrals of the form

$$\int \mathrm{d}^D\mathbf{q}\,\exp\left[\frac{i}{\hbar}(\alpha\mathbf{q}^2+\mathbf{q}'\cdot\mathbf{q})\right]$$

where $\alpha \neq 0$ is a real parameter not depending on $\mathbf{q}$, and the integral is over the whole $\mathbf{q}$-space. To solve this integral, we begin by completing the square in the exponential as

$$\alpha\mathbf{q}^2+\mathbf{q}'\cdot\mathbf{q}=\alpha\left(\mathbf{q}^2+2\frac{\mathbf{q}'}{2\alpha}\cdot\mathbf{q}\right)=\alpha\left(\mathbf{q}+\frac{\mathbf{q}'}{2\alpha}\right)^2-\alpha\left(\frac{\mathbf{q}'}{2\alpha}\right)^2. \tag{A.1}$$

We then have

$$\begin{aligned}\int \mathrm{d}^D\mathbf{q}\,\exp\left[\frac{i}{\hbar}(\alpha\mathbf{q}^2+\mathbf{q}'\cdot\mathbf{q})\right]&=\exp\left[-\frac{i}{\hbar}\alpha\left(\frac{\mathbf{q}'}{2\alpha}\right)^2\right]\int \mathrm{d}^D\mathbf{q}\,\exp\left[\frac{i}{\hbar}\alpha\left(\mathbf{q}+\frac{\mathbf{q}'}{2\alpha}\right)^2\right]\\&=\exp\left[-\frac{i}{\hbar}\alpha\left(\frac{\mathbf{q}'}{2\alpha}\right)^2\right]\int \mathrm{d}^D\mathbf{q}\,\exp\left[\frac{i}{\hbar}\alpha\mathbf{q}^2\right]\\&=\exp\left[-\frac{i}{\hbar}\alpha\left(\frac{\mathbf{q}'}{2\alpha}\right)^2\right]\left[\int_{-\infty}^{+\infty}\mathrm{d}q\,\exp\left[\frac{i}{\hbar}\alpha q^2\right]\right]^D.\end{aligned} \tag{A.2}$$

We first treat the case $\alpha < 0$. Then the integral on the right-hand side of (A.2) can be written as

$$\int_{-\infty}^{+\infty}\mathrm{d}q\,\exp\left[\frac{i}{\hbar}\alpha q^2\right]=2\int_0^{\infty}\mathrm{d}q\,\exp\left[-\frac{i}{\hbar}|\alpha|q^2\right]=2\left(\frac{\hbar}{|\alpha|}\right)^{1/2}\int_0^{\infty}\mathrm{d}\xi\,\exp\left[-i\xi^2\right]. \tag{A.3}$$

We can write the integral over ξ in (A.3) as an integral in the complex plane,

$$\int_0^{\infty}\mathrm{d}\xi\,\exp\left[-i\xi^2\right]=\int_C \mathrm{d}z\,\exp\left[-iz^2\right], \tag{A.4}$$

over the contour $C : z(\xi) = \xi$, $0 \leq \xi < \infty$. By invoking the residue theorem, we can integrate along a different contour according to

$$\int_0^{\infty}\mathrm{d}\xi\,\exp\left[-i\xi^2\right]=\lim_{R\to\infty}\left[\int_{C_1(R)}\mathrm{d}z\,\exp\left[-iz^2\right]+\int_{C_2(R)}\mathrm{d}z\,\exp\left[-iz^2\right]\right], \tag{A.5}$$

where C_1 and C_2 are given by

$$C_1:\ z(\xi)=\exp\left[-i\pi/4\right]\xi,\quad 0\leq\xi<R \tag{A.6}$$

and

$$C_2:\ z(\theta)=R\exp\left[i\theta\right],\quad -\pi/4\leq\theta\leq 0, \tag{A.7}$$

respectively. The integral along C_2 becomes

$$\int_{C_2(R)}\mathrm{d}z\,\exp\left[-iz^2\right]=\int_{-\pi/4}^{0}\mathrm{d}\theta\,\frac{\mathrm{d}z}{\mathrm{d}\theta}\exp\left[-iz(\theta)^2\right]. \tag{A.8}$$

The derivative $\frac{\mathrm{d}z}{\mathrm{d}\theta}$ is linear in R, whereas

$$\exp\left[-iz(\theta)^2\right]=\exp\left[-iR^2(\cos 2\theta+i\sin 2\theta)\right]=\exp\left[R^2\sin 2\theta\right]\exp\left[-iR^2\cos 2\theta\right]. \tag{A.9}$$

For $\theta \in (-\pi/4, 0)$ we have $\sin 2\theta < 0$. Therefore the product $\frac{\mathrm{d}z}{\mathrm{d}\theta} \exp\left[-iz(\theta)^2\right] \to 0$ as $R \to \infty$ so that the integral (A.8) vanishes, and (A.5) reduces to

$$\begin{aligned}\int_0^\infty \mathrm{d}\xi \, \exp\left[-i\xi^2\right] &= \lim_{R\to\infty} \int_{C_1(R)} \mathrm{d}z \, \exp\left[-iz^2\right] = \lim_{R\to\infty} \int_0^R \mathrm{d}\xi \, \frac{\mathrm{d}z}{\mathrm{d}\xi} \exp\left[-iz(\xi)^2\right] \\ &= \int_0^\infty \mathrm{d}\xi \, \exp\left[-i\pi/4\right] \exp\left[-i(-i\xi^2)\right] = \exp\left[-i\pi/4\right] \int_0^\infty \mathrm{d}\xi \, \exp\left[-\xi^2\right] \\ &= \frac{1}{2} \exp\left[-i\pi/4\right] \int_{-\infty}^{+\infty} \mathrm{d}\xi \, \exp\left[-\xi^2\right]. \end{aligned} \tag{A.10}$$

We now use the well known result for the Gaussian integral,

$$\int_{-\infty}^{\infty} \mathrm{d}\xi \, \exp\left[-\xi^2\right] = \sqrt{\pi}, \tag{A.11}$$

giving

$$\int_0^\infty \mathrm{d}\xi \, \exp\left[-i\xi^2\right] = \frac{1}{2} \exp\left[-i\pi/4\right] \sqrt{\pi} = \frac{1}{2} \left(\frac{\pi}{i}\right)^{1/2}, \tag{A.12}$$

where we use the branch $\sqrt{i} \equiv \exp\left[i\pi/4\right]$. Using this result, (A.3) becomes

$$\int_{-\infty}^{+\infty} \mathrm{d}q \, \exp\left[\frac{i}{\hbar}\alpha q^2\right] = 2\left(\frac{\hbar}{|\alpha|}\right)^{1/2} \frac{1}{2}\left(\frac{\pi}{i}\right)^{1/2} = \left(\frac{\pi\hbar}{i|\alpha|}\right)^{1/2} = \left(\frac{i\pi\hbar}{\alpha}\right)^{1/2}, \tag{A.13}$$

and (A.2) becomes

$$\int \mathrm{d}^D \mathbf{q} \, \exp\left[\frac{i}{\hbar}(\alpha \mathbf{q}^2 + \mathbf{q}' \cdot \mathbf{q})\right] = \left(\frac{i\pi\hbar}{\alpha}\right)^{D/2} \exp\left[-\frac{i}{\hbar}\alpha\left(\frac{\mathbf{q}'}{2\alpha}\right)^2\right], \tag{A.14}$$

valid for $\alpha < 0$.

Next, we treat the case $\alpha > 0$. Then the integral on the right-hand side of (A.2) can be written as

$$\int_{-\infty}^{+\infty} \mathrm{d}q \, \exp\left[\frac{i}{\hbar}\alpha q^2\right] = 2\left(\frac{\hbar}{\alpha}\right)^{1/2} \int_0^\infty \mathrm{d}\xi \, \exp\left[i\xi^2\right]. \tag{A.15}$$

We can again invoke the residue theorem and integrate according to

$$\int_0^\infty \mathrm{d}\xi \, \exp\left[i\xi^2\right] = \lim_{R\to\infty} \left[\int_{C_1(R)} \mathrm{d}z \, \exp\left[iz^2\right] + \int_{C_2(R)} \mathrm{d}z \, \exp\left[iz^2\right]\right], \tag{A.16}$$

where this time we take C_1 and C_2 to be

$$C_1: \; z(\xi) = \exp\left[i\pi/4\right]\xi, \quad 0 \le \xi < R \tag{A.17}$$

and

$$C_2: \; z(\theta) = R\exp\left[i\theta\right], \quad \pi/4 \ge \theta \ge 0, \tag{A.18}$$

respectively. The integral along C_2 becomes

$$\int_{C_2(R)} \mathrm{d}z \, \exp\left[iz^2\right] = \int_{\pi/4}^0 \mathrm{d}\theta \, \frac{\mathrm{d}z}{\mathrm{d}\theta} \exp\left[iz(\theta)^2\right]. \tag{A.19}$$

The derivative $\frac{\mathrm{d}z}{\mathrm{d}\theta}$ is linear in R, whereas

$$\exp\left[iz(\theta)^2\right] = \exp\left[iR^2(\cos 2\theta + i\sin 2\theta)\right] = \exp\left[-R^2\sin 2\theta\right]\exp\left[iR^2\cos 2\theta\right]. \tag{A.20}$$

For $\theta \in (0, \pi/4)$ we have $\sin 2\theta > 0$. Therefore the product $\frac{\mathrm{d}z}{\mathrm{d}\theta}\exp\left[iz(\theta)^2\right] \to 0$ as $R \to \infty$ so that the integral (A.19) vanishes, and (A.16) reduces to

$$\begin{aligned}\int_0^\infty \mathrm{d}\xi\, \exp\left[i\xi^2\right] &= \lim_{R\to\infty}\int_{C_1(R)} \mathrm{d}z\, \exp\left[iz^2\right] = \lim_{R\to\infty}\int_0^R \mathrm{d}\xi\, \frac{\mathrm{d}z}{\mathrm{d}\xi}\exp\left[iz(\xi)^2\right] \\ &= \int_0^\infty \mathrm{d}\xi\, \exp\left[i\pi/4\right]\exp\left[i(i\xi^2)\right] = \exp\left[i\pi/4\right]\int_0^\infty \mathrm{d}\xi\, \exp\left[-\xi^2\right] \\ &= \frac{1}{2}\exp\left[i\pi/4\right]\int_{-\infty}^{+\infty} \mathrm{d}\xi\, \exp\left[-\xi^2\right] = \frac{1}{2}\exp\left[i\pi/4\right]\sqrt{\pi} = \frac{1}{2}\left(i\pi\right)^{1/2}, \end{aligned} \tag{A.21}$$

again using the branch $\sqrt{i} \equiv \exp\left[i\pi/4\right]$. Using this result, (A.15) becomes

$$\int_{-\infty}^{+\infty} \mathrm{d}q\, \exp\left[\frac{i}{\hbar}\alpha q^2\right] = 2\left(\frac{\hbar}{\alpha}\right)^{1/2}\frac{1}{2}\left(i\pi\right)^{1/2} = \left(\frac{i\pi\hbar}{\alpha}\right)^{1/2}, \tag{A.22}$$

and (A.2) becomes

$$\int \mathrm{d}^D\mathbf{q}\, \exp\left[\frac{i}{\hbar}(\alpha\mathbf{q}^2 + \mathbf{q}'\cdot\mathbf{q})\right] = \left(\frac{i\pi\hbar}{\alpha}\right)^{D/2}\exp\left[-\frac{i}{\hbar}\alpha\left(\frac{\mathbf{q}'}{2\alpha}\right)^2\right], \tag{A.23}$$

valid for $\alpha > 0$. This is the same as the formula (A.14) and is therefore valid for both $\alpha < 0$ and $\alpha > 0$.

B Exact Solutions for some Simple Path Integrals

B.1 The Free Particle

We will now derive the propagator for a free particle in D dimensions by solving the configuration space path integral

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b} \mathscr{D}\big[\mathbf{x}(t)\big] \; \exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}(t); t_a, t_b]\right] \tag{B.1}$$

with the action integral

$$\mathcal{S}[\mathbf{x}(t); t_a, t_b] = \int_{t_a}^{t_b} \mathrm{d}t \, \frac{1}{2} m \dot{\mathbf{x}}^2. \tag{B.2}$$

The time-sliced form of (B.1) reads

$$K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \Big(\frac{m}{2\pi i \hbar \delta t}\Big)^{DN/2} \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \; \exp\left[\frac{i}{\hbar}\mathcal{S}^{(N)}[\mathbf{x}]\right] \tag{B.3}$$

with the time-sliced action

$$\mathcal{S}^{(N)}[\mathbf{x}] = \sum_{k=1}^{N} \frac{1}{2} m \left(\frac{\Delta \mathbf{x}_k}{\delta t}\right)^2 \delta t = a \sum_{k=1}^{N} (\mathbf{x}_k - \mathbf{x}_{k-1})^2 \tag{B.4}$$

where

$$a := \frac{m}{2\delta t}. \tag{B.5}$$

Letting

$$\mathcal{N} := \Big(\frac{m}{2\pi i \hbar \delta t}\Big)^{D/2} = \Big(\frac{a}{i\pi\hbar}\Big)^{D/2} \tag{B.6}$$

we can write (B.3) as

$$\begin{aligned} K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) &= \mathcal{N}^N \int \mathrm{d}^D\mathbf{x}_{N-1} \cdots \int \mathrm{d}^D\mathbf{x}_1 \; \exp\left[\frac{i}{\hbar} a \sum_{k=1}^{N} (\mathbf{x}_k - \mathbf{x}_{k-1})^2\right] \\ &= \int \mathrm{d}^D\mathbf{x}_{N-1} \mathcal{N} \; \exp\left[\frac{i}{\hbar} a (\mathbf{x}_N - \mathbf{x}_{N-1})^2\right] \cdots \\ &\qquad \cdots \int \mathrm{d}^D\mathbf{x}_1 \mathcal{N} \; \exp\left[\frac{i}{\hbar} a (\mathbf{x}_2 - \mathbf{x}_1)^2\right] \mathcal{N} \; \exp\left[\frac{i}{\hbar} a (\mathbf{x}_1 - \mathbf{x}_0)^2\right]. \end{aligned} \tag{B.7}$$

The integral over $\mathbf{x}_1$ in (B.7) is a special case of the following integral in which we have replaced a in the last exponential with an arbitrary constant b, and $\mathbf{x}_2$ with $\mathbf{x}'$. We solve this case instead, for later convenience:

$$\begin{aligned} &\int \mathrm{d}^D\mathbf{x} \mathcal{N} \exp\left[\frac{i}{\hbar} a (\mathbf{x}' - \mathbf{x})^2\right] \mathcal{N} \; \exp\left[\frac{i}{\hbar} b (\mathbf{x} - \mathbf{x}_0)^2\right] = \\ &= \mathcal{N}^2 \int \mathrm{d}^D\mathbf{x} \; \exp\left[\frac{i}{\hbar}\Big(a(\mathbf{x}'^2 + \mathbf{x}^2 - 2\mathbf{x}' \cdot \mathbf{x}) + b(\mathbf{x}^2 + \mathbf{x}_0^2 - 2\mathbf{x} \cdot \mathbf{x}_0)\Big)\right] \\ &= \mathcal{N}^2 \; \exp\left[\frac{i}{\hbar}\Big(a\mathbf{x}'^2 + b\mathbf{x}_0^2\Big)\right] \int \mathrm{d}^D\mathbf{x} \; \exp\left[\frac{i}{\hbar}\Big((a+b)\mathbf{x}^2 - 2(a\mathbf{x}' + b\mathbf{x}_0) \cdot \mathbf{x}\Big)\right]. \end{aligned} \tag{B.8}$$

Using (A.23), the integral on the right-hand side evaluates to

$$\int \mathrm{d}^D\mathbf{x}\,\exp\left[\frac{i}{\hbar}\Big((a+b)\mathbf{x}^2-2(a\mathbf{x}'+b\mathbf{x}_0)\cdot\mathbf{x}\Big)\right]=\left(\frac{i\pi\hbar}{a+b}\right)^{D/2}\exp\left[-\frac{i}{\hbar}(a+b)\left(\frac{-2(a\mathbf{x}'+b\mathbf{x}_0)}{2(a+b)}\right)^2\right]$$
$$=\left(\frac{i\pi\hbar}{a+b}\right)^{D/2}\exp\left[-\frac{i}{\hbar}\frac{(a\mathbf{x}'+b\mathbf{x}_0)^2}{a+b}\right] \tag{B.9}$$

so that (B.8) becomes

$$\int \mathrm{d}^D\mathbf{x}\,\mathcal{N}\exp\left[\frac{i}{\hbar}a(\mathbf{x}'-\mathbf{x})^2\right]\mathcal{N}\,\exp\left[\frac{i}{\hbar}b(\mathbf{x}-\mathbf{x}_0)^2\right]=$$
$$=\mathcal{N}^2\,\exp\left[\frac{i}{\hbar}\Big(a\mathbf{x}'^2+b\mathbf{x}_0^2\Big)\right]\left(\frac{i\pi\hbar}{a+b}\right)^{D/2}\exp\left[-\frac{i}{\hbar}\frac{(a\mathbf{x}'+b\mathbf{x}_0)^2}{a+b}\right]$$
$$=\mathcal{N}^2\left(\frac{i\pi\hbar}{a+b}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{1}{a+b}\Big((a+b)(a\mathbf{x}'^2+b\mathbf{x}_0^2)-(a\mathbf{x}'+b\mathbf{x}_0)^2\Big)\right]$$
$$=\mathcal{N}\left(\frac{a}{i\pi\hbar}\right)^{D/2}\left(\frac{i\pi\hbar}{a+b}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{1}{a+b}\Big((a^2+ab)\mathbf{x}'^2+(ab+b^2)\mathbf{x}_0^2-(a^2\mathbf{x}'^2+b^2\mathbf{x}_0^2+2ab\mathbf{x}'\cdot\mathbf{x}_0)\Big)\right]$$
$$=\mathcal{N}\left(\frac{a}{a+b}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{1}{a+b}\Big(ab\mathbf{x}'^2+ab\mathbf{x}_0^2-2ab\mathbf{x}'\cdot\mathbf{x}_0\Big)\right]$$
$$=\left(\frac{a}{a+b}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{ab}{a+b}(\mathbf{x}'-\mathbf{x}_0)^2\right]. \tag{B.10}$$

Using this result with $b=a$ and $\mathbf{x}'=\mathbf{x}_2$, the integral over $\mathbf{x}_1$ in (B.7) becomes

$$\int \mathrm{d}^D\mathbf{x}_1\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_2-\mathbf{x}_1)^2\right]\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_1-\mathbf{x}_0)^2\right]=\left(\frac{1}{2}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{a}{2}(\mathbf{x}_2-\mathbf{x}_0)^2\right] \tag{B.11}$$

and using this result, the integral over $\mathbf{x}_2$ in (B.7) becomes

$$\int \mathrm{d}^D\mathbf{x}_2\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_3-\mathbf{x}_2)^2\right]\int \mathrm{d}^D\mathbf{x}_1\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_2-\mathbf{x}_1)^2\right]\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_1-\mathbf{x}_0)^2\right]$$
$$=\left(\frac{1}{2}\right)^{D/2}\int \mathrm{d}^D\mathbf{x}_2\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_3-\mathbf{x}_2)^2\right]\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{a}{2}(\mathbf{x}_2-\mathbf{x}_0)^2\right]$$
$$=\left(\frac{1}{2}\right)^{D/2}\left(\frac{a}{a+a/2}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{aa/2}{a+a/2}(\mathbf{x}_3-\mathbf{x}_0)^2\right]$$
$$=\left(\frac{1}{3}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{a}{3}(\mathbf{x}_3-\mathbf{x}_0)^2\right] \tag{B.12}$$

where we have again used (B.10). Thus for $n-1=1,2$ we have

$$\int \mathrm{d}^D\mathbf{x}_{n-1}\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_n-\mathbf{x}_{n-1})^2\right]\cdots\int \mathrm{d}^D\mathbf{x}_1\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_2-\mathbf{x}_1)^2\right]\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_1-\mathbf{x}_0)^2\right]=$$
$$=\left(\frac{1}{n}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{a}{n}(\mathbf{x}_n-\mathbf{x}_0)^2\right]. \tag{B.13}$$

Suppose (B.13) holds for $n-1=1,2,\ldots,k-1$ for some k. Then by integrating k times we get

$$\int \mathrm{d}^D\mathbf{x}_k \,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_{k+1}-\mathbf{x}_k)^2\right]\int \mathrm{d}^D\mathbf{x}_{k-1}\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_k-\mathbf{x}_{k-1})^2\right]\cdots \tag{B.14}$$

$$\cdots\int \mathrm{d}^D\mathbf{x}_1\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_2-\mathbf{x}_1)^2\right]\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_1-\mathbf{x}_0)^2\right]=$$

$$=\int \mathrm{d}^D\mathbf{x}_k\,\mathcal{N}\,\exp\left[\frac{i}{\hbar}a(\mathbf{x}_{k+1}-\mathbf{x}_k)^2\right]\left(\frac{1}{k}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{a}{k}(\mathbf{x}_k-\mathbf{x}_0)^2\right]$$

$$=\left(\frac{1}{k}\right)^{D/2}\left(\frac{a}{a+a/k}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{aa/k}{a+a/k}(\mathbf{x}_{k+1}-\mathbf{x}_0)^2\right]$$

$$=\left(\frac{1}{k+1}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{a}{k+1}(\mathbf{x}_{k+1}-\mathbf{x}_0)^2\right] \tag{B.15}$$

where we have used (B.10) once again. Thus (B.13) holds for $n-1=k$ as well, and by induction must hold for all $n-1=1,2,\ldots$. After $N-1$ integrations we therefore get

$$K^{(N)}(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a)=\left(\frac{1}{N}\right)^{D/2}\mathcal{N}\,\exp\left[\frac{i}{\hbar}\frac{a}{N}(\mathbf{x}_N-\mathbf{x}_0)^2\right]$$

$$=\left(\frac{1}{N}\right)^{D/2}\left(\frac{m}{2\pi i\hbar\delta t}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{m/2\delta t}{N}(\mathbf{x}_N-\mathbf{x}_0)^2\right]$$

$$=\left(\frac{m}{2\pi i\hbar N\delta t}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(\mathbf{x}_N-\mathbf{x}_0)^2}{N\delta t}\right]$$

$$=\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(\mathbf{x}_b-\mathbf{x}_a)^2}{\Delta t}\right] \tag{B.16}$$

with $\Delta t\equiv t_b-t_a=N\delta t$. Note that this result is independent of the number of time slices. Thus the D-dimensional free-particle propagator is given by

$$K(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a)=\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{m}{2}\frac{(\mathbf{x}_b-\mathbf{x}_a)^2}{\Delta t}\right]. \tag{B.17}$$

B.2 The Harmonic Oscillator

We will now derive the propagator for a particle in D dimensions subjected to a harmonic oscillator potential

$$V(\mathbf{x})=\frac{1}{2}m\omega^2\mathbf{x}^2 \tag{B.18}$$

by solving the configuration space path integral

$$K(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a)=\int_{\mathbf{x}(t_a)=\mathbf{x}_a}^{\mathbf{x}(t_b)=\mathbf{x}_b}\mathscr{D}\big[\mathbf{x}(t)\big]\,\exp\left[\frac{i}{\hbar}\mathcal{S}[\mathbf{x}(t);t_a,t_b]\right] \tag{B.19}$$

with the action integral

$$\mathcal{S}[\mathbf{x}(t);t_a,t_b]=\int_{t_a}^{t_b}\mathrm{d}t\,\left[\frac{1}{2}m\dot{\mathbf{x}}^2-\frac{1}{2}m\omega^2\mathbf{x}^2\right]. \tag{B.20}$$

The time-sliced form of (B.19) reads

$$K^{(N)}(\mathbf{x}_b,t_b;\mathbf{x}_a,t_a)=\left(\frac{m}{2\pi i\hbar\delta t}\right)^{DN/2}\int \mathrm{d}^D\mathbf{x}_{N-1}\cdots\int \mathrm{d}^D\mathbf{x}_1\,\exp\left[\frac{i}{\hbar}\mathcal{S}^{(N)}[\mathbf{x}]\right]. \tag{B.21}$$

Instead of using the expression (4.35) for the time-sliced action, we write it as

$$\mathcal{S}^{(N)}[\mathbf{x}] = \sum_{k=1}^{N} \left[\frac{1}{2} m \left(\frac{\Delta \mathbf{x}_k}{\delta t} \right)^2 - \frac{1}{2} m \omega^2 \left(\frac{\mathbf{x}_k^2 + \mathbf{x}_{k-1}^2}{2} \right) \right] \delta t, \tag{B.22}$$

which differs from (4.35) in that we have replaced $V(\mathbf{x}(t_k))$ with the average $\frac{1}{2}\big[V(\mathbf{x}(t_k)) + V(\mathbf{x}(t_{k-1}))\big]$, the large N limit still being (B.20). We can then rewrite it as

$$\begin{aligned} \mathcal{S}^{(N)}[\mathbf{x}] &= \sum_{k=1}^{N} \frac{m}{2\delta t^2} \left[(\mathbf{x}_k - \mathbf{x}_{k-1})^2 - \omega^2 \delta t^2 \left(\frac{\mathbf{x}_k^2 + \mathbf{x}_{k-1}^2}{2} \right) \right] \delta t \\ &= \sum_{k=1}^{N} \frac{m}{2\delta t} \left[\left(1 - \frac{1}{2} \omega^2 \delta t^2 \right) (\mathbf{x}_k^2 + \mathbf{x}_{k-1}^2) - 2 \mathbf{x}_k \cdot \mathbf{x}_{k-1} \right] \\ &= \sum_{k=1}^{N} \left[a_1 (\mathbf{x}_k^2 + \mathbf{x}_{k-1}^2) - 2 b_1 \mathbf{x}_k \cdot \mathbf{x}_{k-1} \right] \end{aligned} \tag{B.23}$$

with

$$a_1 := \frac{m}{2\delta t} \left(1 - \frac{1}{2} \omega^2 \delta t^2 \right) \quad \text{and} \quad b_1 := \frac{m}{2\delta t}. \tag{B.24}$$

Also letting

$$\mathcal{N}_1 := \left(\frac{m}{2\pi i \hbar \delta t} \right)^{D/2} \tag{B.25}$$

the time-sliced path integral (B.21) becomes

$$\begin{aligned} K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) &= \mathcal{N}_1^N \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \, \exp \left[\frac{i}{\hbar} \sum_{k=1}^{N} \Big(a_1 (\mathbf{x}_k^2 + \mathbf{x}_{k-1}^2) - 2 b_1 \mathbf{x}_k \cdot \mathbf{x}_{k-1} \Big) \right] \\ &= \int \mathrm{d}^D \mathbf{x}_{N-1} \cdots \int \mathrm{d}^D \mathbf{x}_1 \prod_{k=1}^{N} \mathcal{N}_1 \, \exp \left[\frac{i}{\hbar} \Big(a_1 (\mathbf{x}_k^2 + \mathbf{x}_{k-1}^2) - 2 b_1 \mathbf{x}_k \cdot \mathbf{x}_{k-1} \Big) \right] \\ &= \int \mathrm{d}^D \mathbf{x}_{N-1} \, \mathcal{N}_1 \, \exp \left[\frac{i}{\hbar} \Big(a_1 (\mathbf{x}_N^2 + \mathbf{x}_{N-1}^2) - 2 b_1 \mathbf{x}_N \cdot \mathbf{x}_{N-1} \Big) \right] \cdots \\ &\quad \cdots \int \mathrm{d}^D \mathbf{x}_1 \, \mathcal{N}_1 \, \exp \left[\frac{i}{\hbar} \Big(a_1 (\mathbf{x}_2^2 + \mathbf{x}_1^2) - 2 b_1 \mathbf{x}_2 \cdot \mathbf{x}_1 \Big) \right] \times \\ &\qquad \mathcal{N}_1 \, \exp \left[\frac{i}{\hbar} \Big(a_1 (\mathbf{x}_1^2 + \mathbf{x}_0^2) - 2 b_1 \mathbf{x}_1 \cdot \mathbf{x}_0 \Big) \right]. \end{aligned} \tag{B.26}$$

The integral over $\mathbf{x}_1$ in (B.26) is a special case of the following integral in which we have replaced a_1, b_1 in the last exponential with arbitrary nonzero constants a, b, and $\mathbf{x}_2$ with $\mathbf{x}'$. We solve this case instead, for later convenience:

$$\begin{aligned} &\int \mathrm{d}^D \mathbf{x} \, \exp \left[\frac{i}{\hbar} \Big(a_1 (\mathbf{x}'^2 + \mathbf{x}^2) - 2 b_1 \mathbf{x}' \cdot \mathbf{x} \Big) \right] \exp \left[\frac{i}{\hbar} \Big(a (\mathbf{x}^2 + \mathbf{x}_0^2) - 2 b \mathbf{x} \cdot \mathbf{x}_0 \Big) \right] = \\ &\quad = \exp \left[\frac{i}{\hbar} \Big(a_1 \mathbf{x}'^2 + a \mathbf{x}_0^2 \Big) \right] \int \mathrm{d}^D \mathbf{x} \, \exp \left[\frac{i}{\hbar} \Big((a_1 + a) \mathbf{x}^2 - 2 (b_1 \mathbf{x}' + b \mathbf{x}_0) \cdot \mathbf{x} \Big) \right]. \end{aligned} \tag{B.27}$$

Using (A.23), the integral on the right-hand side evaluates to

$$\begin{aligned} \int \mathrm{d}^D \mathbf{x} \, \exp \left[\frac{i}{\hbar} \Big((a_1 + a) \mathbf{x}^2 - 2 (b_1 \mathbf{x}' + b \mathbf{x}_0) \cdot \mathbf{x} \Big) \right] &= \left(\frac{i \pi \hbar}{a_1 + a} \right)^{D/2} \exp \left[-\frac{i}{\hbar} (a_1 + a) \left(\frac{-2 (b_1 \mathbf{x}' + b \mathbf{x}_0)}{2 (a_1 + a)} \right)^2 \right] \\ &= \left(\frac{i \pi \hbar}{a_1 + a} \right)^{D/2} \exp \left[-\frac{i}{\hbar} \frac{(b_1 \mathbf{x}' + b \mathbf{x}_0)^2}{a_1 + a} \right] \end{aligned} \tag{B.28}$$

so that (B.27) becomes

$$\int \mathrm{d}^D\mathbf{x}\,\exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}'^2+\mathbf{x}^2)-2b_1\mathbf{x}'\cdot\mathbf{x}\Big)\right]\exp\left[\frac{i}{\hbar}\Big(a(\mathbf{x}^2+\mathbf{x}_0^2)-2b\mathbf{x}\cdot\mathbf{x}_0\Big)\right]=$$
$$=\exp\left[\frac{i}{\hbar}\Big(a_1\mathbf{x}'^2+a\mathbf{x}_0^2\Big)\right]\left(\frac{i\pi\hbar}{a_1+a}\right)^{D/2}\exp\left[-\frac{i}{\hbar}\frac{(b_1\mathbf{x}'+b\mathbf{x}_0)^2}{a_1+a}\right]$$
$$=\left(\frac{i\pi\hbar}{a_1+a}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{1}{a_1+a}\Big((a_1+a)(a_1\mathbf{x}'^2+a\mathbf{x}_0^2)-(b_1\mathbf{x}'+b\mathbf{x}_0)^2\Big)\right]$$
$$=\left(\frac{i\pi\hbar}{a_1+a}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{1}{a_1+a}\Big((a_1+a)(a_1\mathbf{x}'^2+a\mathbf{x}_0^2)-b_1^2\mathbf{x}'^2-b^2\mathbf{x}_0^2-2b_1b\mathbf{x}'\cdot\mathbf{x}_0\Big)\right]$$
$$=\left(\frac{i\pi\hbar}{a_1+a}\right)^{D/2}\exp\left[\frac{i}{\hbar}\frac{1}{a_1+a}\Big(\big[(a_1+a)a_1-b_1^2\big]\mathbf{x}'^2+\big[(a_1+a)a-b^2\big]\mathbf{x}_0^2-2b_1b\mathbf{x}'\cdot\mathbf{x}_0\Big)\right]$$
$$=\left(\frac{i\pi\hbar}{a_1+a}\right)^{D/2}\exp\left[\frac{i}{\hbar}\Big(\frac{a_1^2-b_1^2+a_1a}{a_1+a}\mathbf{x}'^2+\frac{a^2-b^2+a_1a}{a_1+a}\mathbf{x}_0^2-2\frac{b_1b}{a_1+a}\mathbf{x}'\cdot\mathbf{x}_0\Big)\right]. \tag{B.29}$$

Using this result (with $a=a_1$, $b=b_1$, $\mathbf{x}'=\mathbf{x}_2$) the integral over $\mathbf{x}_1$ in (B.26) becomes

$$\int \mathrm{d}^D\mathbf{x}_1\,\mathcal{N}_1\exp\left[\frac{i}{\hbar}\Big(a_1({\mathbf{x}_2}^2+\mathbf{x}_1^2)-2b_1\mathbf{x}_2\cdot\mathbf{x}_1\Big)\right]\mathcal{N}_1\exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_1^2+\mathbf{x}_0^2)-2b_1\mathbf{x}_1\cdot\mathbf{x}_0\Big)\right]=$$
$$=\mathcal{N}_1^2\left(\frac{i\pi\hbar}{2a_1}\right)^{D/2}\exp\left[\frac{i}{\hbar}\Big(\frac{2a_1^2-b_1^2}{2a_1}{\mathbf{x}_2}^2+\frac{2a_1^2-b_1^2}{2a_1}\mathbf{x}_0^2-2\frac{b_1^2}{2a_1}\mathbf{x}_2\cdot\mathbf{x}_0\Big)\right]$$
$$=\mathcal{N}_2\,\exp\left[\frac{i}{\hbar}\Big(a_2({\mathbf{x}_2}^2+\mathbf{x}_0^2)-2b_2\mathbf{x}_2\cdot\mathbf{x}_0\Big)\right] \tag{B.30}$$

with

$$a_2:=\frac{2a_1^2-b_1^2}{2a_1},\qquad b_2:=\frac{b_1^2}{2a_1}\qquad\text{and}\qquad \mathcal{N}_2:=\mathcal{N}_1^2\left(\frac{i\pi\hbar}{2a_1}\right)^{D/2}. \tag{B.31}$$

Using (B.30) the integral over $\mathbf{x}_2$ in (B.26) then becomes

$$\int \mathrm{d}^D\mathbf{x}_2\;\mathcal{N}_1\;\exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_3^2+\mathbf{x}_2^2)-2b_1\mathbf{x}_3\cdot\mathbf{x}_2\Big)\right]\times$$
$$\int \mathrm{d}^D\mathbf{x}_1\;\mathcal{N}_1\;\exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_2^2+\mathbf{x}_1^2)-2b_1\mathbf{x}_2\cdot\mathbf{x}_1\Big)\right]\mathcal{N}_1\;\exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_1^2+\mathbf{x}_0^2)-2b_1\mathbf{x}_1\cdot\mathbf{x}_0\Big)\right]=$$
$$=\int \mathrm{d}^D\mathbf{x}_2\;\mathcal{N}_1\;\exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_3^2+\mathbf{x}_2^2)-2b_1\mathbf{x}_3\cdot\mathbf{x}_2\Big)\right]\mathcal{N}_2\;\exp\left[\frac{i}{\hbar}\Big(a_2({\mathbf{x}_2}^2+\mathbf{x}_0^2)-2b_2\mathbf{x}_2\cdot\mathbf{x}_0\Big)\right]$$
$$=\mathcal{N}_2\mathcal{N}_1\left(\frac{i\pi\hbar}{a_1+a_2}\right)^{D/2}\exp\left[\frac{i}{\hbar}\Big(\frac{a_1^2-b_1^2+a_1a_2}{a_1+a_2}{\mathbf{x}_3}^2+\frac{a_2^2-b_2^2+a_1a_2}{a_1+a_2}\mathbf{x}_0^2-2\frac{b_1b_2}{a_1+a_2}\mathbf{x}_3\cdot\mathbf{x}_0\Big)\right]. \tag{B.32}$$

where in the last step we have used the result (B.29) with $\mathbf{x}'=\mathbf{x}_3$, $\mathbf{x}=\mathbf{x}_2$, $a=a_2$ and $b=b_2$. From (B.31) we see that $a_2=a_1-b_2$ and

$$a_2^2-b_2^2=(a_1-b_2)^2-b_2^2=a_1^2-2a_1b_2=a_1^2-b_1^2 \tag{B.33}$$

so that (B.32) becomes

$$\int \mathrm{d}^D\mathbf{x}_2\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_3^2+\mathbf{x}_2^2)-2b_1\mathbf{x}_3\cdot\mathbf{x}_2\Big)\right]\times$$
$$\int \mathrm{d}^D\mathbf{x}_1\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_2^2+\mathbf{x}_1^2)-2b_1\mathbf{x}_2\cdot\mathbf{x}_1\Big)\right]\mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_1^2+\mathbf{x}_0^2)-2b_1\mathbf{x}_1\cdot\mathbf{x}_0\Big)\right]=$$
$$=\mathcal{N}_3\ \exp\left[\frac{i}{\hbar}\Big(a_3({\mathbf{x}_3}^2+\mathbf{x}_0^2)-2b_3\mathbf{x}_3\cdot\mathbf{x}_0\Big)\right] \tag{B.34}$$

with

$$a_3:=\frac{a_1^2-b_1^2+a_1a_2}{a_1+a_2},\qquad b_3:=\frac{b_1b_2}{a_1+a_2}\qquad\text{and}\qquad \mathcal{N}_3:=\mathcal{N}_2\mathcal{N}_1\left(\frac{i\pi\hbar}{a_1+a_2}\right)^{D/2}. \tag{B.35}$$

Thus for $n-1=1,2$ we have

$$\int \mathrm{d}^D\mathbf{x}_{n-1}\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_n^2+\mathbf{x}_{n-1}^2)-2b_1\mathbf{x}_n\cdot\mathbf{x}_{n-1}\Big)\right]\cdots$$
$$\cdots\int \mathrm{d}^D\mathbf{x}_1\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_2^2+\mathbf{x}_1^2)-2b_1\mathbf{x}_2\cdot\mathbf{x}_1\Big)\right]\mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_1^2+\mathbf{x}_0^2)-2b_1\mathbf{x}_1\cdot\mathbf{x}_0\Big)\right]=$$
$$=\mathcal{N}_n\ \exp\left[\frac{i}{\hbar}\Big(a_n({\mathbf{x}_n}^2+\mathbf{x}_0^2)-2b_n\mathbf{x}_n\cdot\mathbf{x}_0\Big)\right] \tag{B.36}$$

with

$$a_n=\frac{a_1^2-b_1^2+a_1a_{n-1}}{a_1+a_{n-1}}=\frac{a_{n-1}^2-b_{n-1}^2+a_1a_{n-1}}{a_1+a_{n-1}}, \tag{B.37}$$
$$b_n=\frac{b_1b_{n-1}}{a_1+a_{n-1}}, \tag{B.38}$$
$$\mathcal{N}_n=\mathcal{N}_{n-1}\mathcal{N}_1\left(\frac{i\pi\hbar}{a_1+a_{n-1}}\right)^{D/2}. \tag{B.39}$$

Suppose (B.36) holds for $n-1=1,2,\ldots,k-1$ for some k. Then by integrating k times we get

$$\int \mathrm{d}^D\mathbf{x}_k\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_{k+1}^2+\mathbf{x}_k^2)-2b_1\mathbf{x}_{k+1}\cdot\mathbf{x}_k\Big)\right]\cdots$$
$$\cdots\int \mathrm{d}^D\mathbf{x}_1\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_2^2+\mathbf{x}_1^2)-2b_1\mathbf{x}_2\cdot\mathbf{x}_1\Big)\right]\mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_1^2+\mathbf{x}_0^2)-2b_1\mathbf{x}_1\cdot\mathbf{x}_0\Big)\right]=$$
$$=\int \mathrm{d}^D\mathbf{x}_k\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_{k+1}^2+\mathbf{x}_k^2)-2b_1\mathbf{x}_{k+1}\cdot\mathbf{x}_k\Big)\right]\mathcal{N}_k\ \exp\left[\frac{i}{\hbar}\Big(a_k({\mathbf{x}_k}^2+\mathbf{x}_0^2)-2b_k\mathbf{x}_k\cdot\mathbf{x}_0\Big)\right]$$
$$=\mathcal{N}_k\mathcal{N}_1\left(\frac{i\pi\hbar}{a_1+a_k}\right)^{D/2}\exp\left[\frac{i}{\hbar}\Big(\frac{a_1^2-b_1^2+a_1a_k}{a_1+a_k}\mathbf{x}_{k+1}^2+\frac{a_k^2-b_k^2+a_1a_k}{a_1+a_k}\mathbf{x}_0^2-2\frac{b_1b_k}{a_1+a_k}\mathbf{x}_{k+1}\cdot\mathbf{x}_0\Big)\right] \tag{B.40}$$

where in the last step we have again used (B.29). Now, since a_k, b_k by assumption satisfy (B.37)–(B.38), we have

$$a_k^2-b_k^2=\frac{(a_1^2-b_1^2+a_1a_{k-1})^2-(b_1b_{k-1})^2}{(a_1+a_{k-1})^2}$$
$$=\frac{a_1^4+b_1^4-2a_1^2b_1^2+a_1^2a_{k-1}^2+2a_1^3a_{k-1}-2a_1a_{k-1}b_1^2+b_1^2(a_1^2-b_1^2-a_{k-1}^2)}{(a_1+a_{k-1})^2} \tag{B.41}$$

where in the second line we have substituted $-b_{k-1}^2 = a_1^2 - b_1^2 - a_{k-1}^2$ from (B.37). After some algebra, this reduces to

$$a_k^2 - b_k^2 = a_1^2 - b_1^2 \tag{B.42}$$

and (B.40) becomes

$$\begin{aligned}
&\int \mathrm{d}^D\mathbf{x}_k\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_{k+1}^2 + \mathbf{x}_k^2) - 2b_1\mathbf{x}_{k+1}\cdot\mathbf{x}_k\Big)\right]\cdots \\
&\cdots\int \mathrm{d}^D\mathbf{x}_1\ \mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_2^2 + \mathbf{x}_1^2) - 2b_1\mathbf{x}_2\cdot\mathbf{x}_1\Big)\right]\mathcal{N}_1\ \exp\left[\frac{i}{\hbar}\Big(a_1(\mathbf{x}_1^2 + \mathbf{x}_0^2) - 2b_1\mathbf{x}_1\cdot\mathbf{x}_0\Big)\right] = \\
&\quad = \mathcal{N}_k\mathcal{N}_1\left(\frac{i\pi\hbar}{a_1 + a_k}\right)^{D/2}\exp\left[\frac{i}{\hbar}\Big(\frac{a_1^2 - b_1^2 + a_1a_k}{a_1 + a_k}(\mathbf{x}_{k+1}^2 + \mathbf{x}_0^2) - 2\frac{b_1b_k}{a_1 + a_k}\mathbf{x}_{k+1}\cdot\mathbf{x}_0\Big)\right] \\
&\quad = \mathcal{N}_{k+1}\ \exp\left[\frac{i}{\hbar}\Big(a_{k+1}(\mathbf{x}_{k+1}^2 + \mathbf{x}_0^2) - 2b_{k+1}\mathbf{x}_{k+1}\cdot\mathbf{x}_0\Big)\right]
\end{aligned} \tag{B.43}$$

with

$$a_{k+1} = \frac{a_1^2 - b_1^2 + a_1a_k}{a_1 + a_k} = \frac{a_k^2 - b_k^2 + a_1a_k}{a_1 + a_k}, \quad b_{k+1} = \frac{b_1b_k}{a_1 + a_k}, \quad \mathcal{N}_{k+1} = \mathcal{N}_k\mathcal{N}_1\left(\frac{i\pi\hbar}{a_1 + a_k}\right)^{D/2}, \tag{B.44}$$

so that (B.36) holds for $n - 1 = k$ as well. By induction, then, (B.36) must hold for all $n - 1 = 1, 2, \ldots$. After $N - 1$ integrations, we therefore have

$$K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \mathcal{N}_N\ \exp\left[\frac{i}{\hbar}\Big(a_N(\mathbf{x}_N^2 + \mathbf{x}_0^2) - 2b_N\mathbf{x}_N\cdot\mathbf{x}_0\Big)\right] \tag{B.45}$$

where we need to find $a_N, b_N, \mathcal{N}_N$ recursively from (B.37)–(B.39).

From (B.37) we have, for arbitrary n,

$$a_n = \sqrt{b_n^2 - (b_1^2 - a_1^2)} \tag{B.46}$$

and the recursion formula for b_n may then be written

$$b_n = \frac{b_1b_{n-1}}{a_1 + a_{n-1}} = \frac{b_1b_{n-1}}{a_1 + \sqrt{b_{n-1}^2 - (b_1^2 - a_1^2)}} = \frac{b_1}{\frac{a_1}{b_{n-1}} + \sqrt{1 - \frac{b_1^2 - a_1^2}{b_{n-1}^2}}} \tag{B.47}$$

or

$$\frac{1}{b_n} = \frac{1}{b_1}\left(\frac{a_1}{b_{n-1}} + \sqrt{1 - \frac{b_1^2 - a_1^2}{b_{n-1}^2}}\right). \tag{B.48}$$

By introducing an auxiliary frequency $\tilde{\omega}$ defined such that

$$\sin\frac{\tilde{\omega}\delta t}{2} := \frac{\omega\delta t}{2}, \tag{B.49}$$

we can express a_1 as

$$a_1 = \frac{m}{2\delta t}\left(1 - \frac{(\omega\delta t)^2}{2}\right) = \frac{m}{2\delta t}\left(1 - 2\sin^2\frac{\tilde{\omega}\delta t}{2}\right) = \frac{m}{2\delta t}\cos(\tilde{\omega}\delta t). \tag{B.50}$$

The relation (B.48) then becomes

$$\frac{1}{b_n} = \frac{1}{\frac{m}{2\delta t}} \left(\frac{\frac{m}{2\delta t}\cos(\tilde{\omega}\delta t)}{b_{n-1}} + \sqrt{1 - \frac{\frac{m^2}{4\delta t^2} - \frac{m^2}{4\delta t^2}\cos^2(\tilde{\omega}\delta t)}{b_{n-1}^2}} \right)$$
$$= \frac{\cos(\tilde{\omega}\delta t)}{b_{n-1}} + \frac{2\delta t}{m}\sqrt{1 - \frac{m^2}{4\delta t^2}\frac{\sin^2(\tilde{\omega}\delta t)}{b_{n-1}^2}}. \tag{B.51}$$

For notational convenience, we now introduce reduced quantities

$$\beta_n := \frac{b_n}{b_1} = \frac{2\delta t}{m} b_n. \tag{B.52}$$

Then the recursion formula for β_n reads

$$\frac{1}{\beta_n} = \frac{\cos(\tilde{\omega}\delta t)}{\beta_{n-1}} + \sqrt{1 - \frac{\sin^2(\tilde{\omega}\delta t)}{\beta_{n-1}^2}} \tag{B.53}$$

with $\beta_1 = 1$. For $n = 2, 3$ we get

$$\frac{1}{\beta_2} = \cos(\tilde{\omega}\delta t) + \sqrt{1 - \sin^2(\tilde{\omega}\delta t)} = \frac{\sin(2\tilde{\omega}\delta t)}{\sin(\tilde{\omega}\delta t)} \tag{B.54}$$

and

$$\frac{1}{\beta_3} = \cos(\tilde{\omega}\delta t)\frac{\sin(2\tilde{\omega}\delta t)}{\sin(\tilde{\omega}\delta t)} + \sqrt{1 - \sin^2(\tilde{\omega}\delta t)\frac{\sin^2(2\tilde{\omega}\delta t)}{\sin^2(\tilde{\omega}\delta t)}} = \frac{\sin(3\tilde{\omega}\delta t)}{\sin(\tilde{\omega}\delta t)}, \tag{B.55}$$

so in general we expect that

$$\frac{1}{\beta_n} = \frac{\sin(n\tilde{\omega}\delta t)}{\sin(\tilde{\omega}\delta t)}. \tag{B.56}$$

Suppose (B.56) holds for all $n = 1, 2, \ldots, k$ for some k. Then

$$\frac{1}{\beta_{k+1}} = \cos(\tilde{\omega}\delta t)\frac{\sin(k\tilde{\omega}\delta t)}{\sin(\tilde{\omega}\delta t)} + \sqrt{1 - \sin^2(\tilde{\omega}\delta t)\frac{\sin^2(k\tilde{\omega}\delta t)}{\sin^2(\tilde{\omega}\delta t)}} = \frac{\sin((k+1)\tilde{\omega}\delta t)}{\sin(\tilde{\omega}\delta t)} \tag{B.57}$$

so that (B.56) holds for $k+1$ as well. By induction it must hold for all $n = 1, 2, \ldots$ and hence solves the recursion relation (B.53). Thus we have

$$b_n = \frac{m}{2\delta t}\beta_n = \frac{m}{2\delta t}\frac{\sin(\tilde{\omega}\delta t)}{\sin(n\tilde{\omega}\delta t)}. \tag{B.58}$$

From (B.46) and (B.50) we then get

$$a_n = \sqrt{b_n^2 - (b_1^2 - a_1^2)} = \sqrt{\left(\frac{m}{2\delta t}\right)^2 \frac{\sin^2(\tilde{\omega}\delta t)}{\sin^2(n\tilde{\omega}\delta t)} - \left[\left(\frac{m}{2\delta t}\right)^2 - \left(\frac{m}{2\delta t}\right)^2\cos^2(\tilde{\omega}\delta t)\right]}$$
$$= \frac{m}{2\delta t}\sqrt{\frac{\sin^2(\tilde{\omega}\delta t)}{\sin^2(n\tilde{\omega}\delta t)} - \sin^2(\tilde{\omega}\delta t)} = \frac{m}{2\delta t}\sin(\tilde{\omega}\delta t)\frac{\cos(n\tilde{\omega}\delta t)}{\sin(n\tilde{\omega}\delta t)}. \tag{B.59}$$

We have now determined the a_n and the b_n. Finally, we need to determine the normalisation constant (B.39). For $n = 2, 3$ we get

$$\mathcal{N}_2 = \mathcal{N}_1 \mathcal{N}_1 \left(\frac{i\pi\hbar}{a_1 + a_1} \right)^{D/2} = \mathcal{N}_1^2 \left(\frac{i\pi\hbar}{2 \frac{m}{2\delta t} \cos(\tilde{\omega}\delta t)} \right)^{D/2} = \mathcal{N}_1 \left(\frac{\sin(\tilde{\omega}\delta t)}{\sin(2\tilde{\omega}\delta t)} \right)^{D/2} \tag{B.60}$$

and

$$\begin{aligned}\mathcal{N}_3 &= \mathcal{N}_2 \mathcal{N}_1 \left(\frac{i\pi\hbar}{a_1 + a_2} \right)^{D/2} = \mathcal{N}_1^2 \left(\frac{\sin(\tilde{\omega}\delta t)}{\sin(2\tilde{\omega}\delta t)} \right)^{D/2} \left(\frac{i\pi\hbar}{\frac{m}{2\delta t} \left(\cos(\tilde{\omega}\delta t) + \sin(\tilde{\omega}\delta t) \frac{\cos(2\tilde{\omega}\delta t)}{\sin(2\tilde{\omega}\delta t)} \right)} \right)^{D/2} \\ &= \mathcal{N}_1 \left(\frac{\sin(\tilde{\omega}\delta t)}{\sin(3\tilde{\omega}\delta t)} \right)^{D/2}\end{aligned} \tag{B.61}$$

so we expect the general result

$$\mathcal{N}_n = \mathcal{N}_1 \left(\frac{\sin(\tilde{\omega}\delta t)}{\sin(n\tilde{\omega}\delta t)} \right)^{D/2} . \tag{B.62}$$

Suppose (B.62) holds for all $n = 1, 2, \ldots, k$ for some k. Then

$$\begin{aligned}\mathcal{N}_{k+1} &= \mathcal{N}_k \mathcal{N}_1 \left(\frac{i\pi\hbar}{a_1 + a_k} \right)^{D/2} = \mathcal{N}_1^2 \left(\frac{\sin(\tilde{\omega}\delta t)}{\sin(k\tilde{\omega}\delta t)} \right)^{D/2} \left(\frac{i\pi\hbar}{\frac{m}{2\delta t} \left(\cos(\tilde{\omega}\delta t) + \sin(\tilde{\omega}\delta t) \frac{\cos(k\tilde{\omega}\delta t)}{\sin(k\tilde{\omega}\delta t)} \right)} \right)^{D/2} \\ &= \mathcal{N}_1 \left(\frac{\sin(\tilde{\omega}\delta t)}{\sin((k+1)\tilde{\omega}\delta t)} \right)^{D/2} ,\end{aligned} \tag{B.63}$$

so that (B.62) holds for $k + 1$ as well. By induction it must hold for all $n = 1, 2, \ldots$ and hence solves the recursion relation (B.39). Having obtained the constants (B.59), (B.58) and (B.62), we now plug them into (B.45) and get

$$\begin{aligned}
&K^{(N)}(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \\
&= \mathcal{N}_N \exp \left[\frac{i}{\hbar} \Big(a_N (\mathbf{x}_N^2 + \mathbf{x}_0^2) - 2 b_N \mathbf{x}_N \cdot \mathbf{x}_0 \Big) \right] \\
&= \mathcal{N}_1 \left(\frac{\sin(\tilde{\omega}\delta t)}{\sin(N\tilde{\omega}\delta t)} \right)^{D/2} \exp \left[\frac{i}{\hbar} \Big(\frac{m}{2\delta t} \sin(\tilde{\omega}\delta t) \frac{\cos(N\tilde{\omega}\delta t)}{\sin(N\tilde{\omega}\delta t)} (\mathbf{x}_N^2 + \mathbf{x}_0^2) - 2 \frac{m}{2\delta t} \frac{\sin(\tilde{\omega}\delta t)}{\sin(N\tilde{\omega}\delta t)} \mathbf{x}_N \cdot \mathbf{x}_0 \Big) \right] \\
&= \left(\frac{m}{2\pi i\hbar\delta t} \right)^{D/2} \left(\frac{\sin(\tilde{\omega}\delta t)}{\sin(N\tilde{\omega}\delta t)} \right)^{D/2} \exp \left[\frac{i}{\hbar} \frac{m}{2\delta t} \frac{\sin(\tilde{\omega}\delta t)}{\sin(N\tilde{\omega}\delta t)} \Big((\mathbf{x}_N^2 + \mathbf{x}_0^2) \cos(N\tilde{\omega}\delta t) - 2\mathbf{x}_N \cdot \mathbf{x}_0 \Big) \right] \\
&= \left(\frac{m}{2\pi i\hbar} \frac{\tilde{\omega}}{\sin(N\tilde{\omega}\delta t)} \frac{\sin(\tilde{\omega}\delta t)}{\tilde{\omega}\delta t} \right)^{D/2} \exp \left[\frac{i}{\hbar} \frac{m\tilde{\omega}}{2\sin(N\tilde{\omega}\delta t)} \frac{\sin(\tilde{\omega}\delta t)}{\tilde{\omega}\delta t} \Big((\mathbf{x}_N^2 + \mathbf{x}_0^2) \cos(N\tilde{\omega}\delta t) - 2\mathbf{x}_N \cdot \mathbf{x}_0 \Big) \right] \\
&= \left(\frac{m}{2\pi i\hbar} \frac{\tilde{\omega}}{\sin(\tilde{\omega}\Delta t)} \frac{\sin(\tilde{\omega}\delta t)}{\tilde{\omega}\delta t} \right)^{D/2} \exp \left[\frac{i}{\hbar} \frac{m\tilde{\omega}}{2\sin(\tilde{\omega}\Delta t)} \frac{\sin(\tilde{\omega}\delta t)}{\tilde{\omega}\delta t} \Big((\mathbf{x}_b^2 + \mathbf{x}_a^2) \cos(\tilde{\omega}\Delta t) - 2\mathbf{x}_b \cdot \mathbf{x}_a \Big) \right]
\end{aligned} \tag{B.64}$$

with $\Delta t \equiv t_b - t_a = N\delta t$. In taking the limit $N \to \infty, \delta t \to 0$, we have $\frac{\sin(\tilde{\omega}\delta t)}{\tilde{\omega}\delta t} \to 1$ and the auxiliary frequency $\tilde{\omega}$ defined by (B.49) simply becomes the oscillator frequency ω. We then finally obtain the following expression for the propagator of the D-dimensional harmonic oscillator:

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \left(\frac{m\omega}{2\pi i\hbar \sin(\omega\Delta t)} \right)^{D/2} \exp \left[\frac{i}{\hbar} \frac{m\omega}{2\sin(\omega\Delta t)} \Big((\mathbf{x}_b^2 + \mathbf{x}_a^2) \cos(\omega\Delta t) - 2\mathbf{x}_b \cdot \mathbf{x}_a \Big) \right] . \tag{B.65}$$

C Square-root Coordinates for the 3-D H-atom

For the solution of the path integral for the three-dimensional Hydrogen atom, we introduced a mapping from a four-dimensional $\{u^\mu\}$ space to the three-dimensional $\{x^i\}$ space by

$$x^i = \mathbf{z}^\dagger \boldsymbol{\sigma}^i \mathbf{z} \tag{C.1}$$

with

$$\mathbf{z} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} := \begin{bmatrix} u^1 + iu^2 \\ u^3 + iu^4 \end{bmatrix} \tag{C.2}$$

and the Pauli spin matrices

$$\boldsymbol{\sigma}^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \boldsymbol{\sigma}^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \boldsymbol{\sigma}^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{C.3}$$

Explicitly, the transformation (C.1) reads

$$\begin{bmatrix} x^1 \\ x^2 \\ x^3 \end{bmatrix} = \begin{bmatrix} \mathbf{z}^\dagger \boldsymbol{\sigma}^1 \mathbf{z} \\ \mathbf{z}^\dagger \boldsymbol{\sigma}^2 \mathbf{z} \\ \mathbf{z}^\dagger \boldsymbol{\sigma}^3 \mathbf{z} \end{bmatrix} = \begin{bmatrix} z_1^* z_2 + z_2^* z_1 \\ -iz_1^* z_2 + iz_2^* z_1 \\ z_1^* z_1 - z_2^* z_2 \end{bmatrix} = \begin{bmatrix} 2\,\mathrm{Re}(z_1^* z_2) \\ 2\,\mathrm{Im}(z_1^* z_2) \\ |z_1|^2 - |z_2|^2 \end{bmatrix} = \begin{bmatrix} 2u^1u^3 + 2u^2u^4 \\ 2u^1u^4 - 2u^2u^3 \\ (u^1)^2 + (u^2)^2 - (u^3)^2 - (u^4)^2 \end{bmatrix} \tag{C.4}$$

and the relations between the differentials are

$$\begin{bmatrix} \mathrm{d}x^1 \\ \mathrm{d}x^2 \\ \mathrm{d}x^3 \end{bmatrix} = \begin{bmatrix} 2u^3 & 2u^4 & 2u^1 & 2u^2 \\ 2u^4 & -2u^3 & -2u^2 & 2u^1 \\ 2u^1 & 2u^2 & -2u^3 & -2u^4 \end{bmatrix} \begin{bmatrix} \mathrm{d}u^1 \\ \mathrm{d}u^2 \\ \mathrm{d}u^3 \\ \mathrm{d}u^4 \end{bmatrix}. \tag{C.5}$$

The transformation (C.1) has been chosen so that $r = \vec{u}^2$. Indeed, we have

$$r^2 = \sum_i (x^i)^2 = (z_1^* z_2 + z_2^* z_1)^2 + (-iz_1^* z_2 + iz_2^* z_1)^2 + (z_1^* z_1 - z_2^* z_2)^2 = (|z_1|^2 + |z_2|^2)^2 \tag{C.6}$$

so that

$$r = |z_1|^2 + |z_2|^2 = (u^1)^2 + (u^2)^2 + (u^3)^2 + (u^4)^2 \equiv \vec{u}^2. \tag{C.7}$$

The mapping (C.4) is obviously not invertible, so the inverse relationship will be multivalued. To find an inverse relationship, we first express the x^i in terms of spherical coordinates

$$\begin{cases} x^1 = r\sin\theta\cos\phi \\ x^2 = r\sin\theta\sin\phi \\ x^3 = r\cos\theta \end{cases}. \tag{C.8}$$

Next, by writing

$$z_1 = |z_1| \exp[i\theta_1], \quad z_2 = |z_2| \exp[i\theta_2] \tag{C.9}$$

we have, from (C.4) and (C.7),

$$\begin{cases} |z_1|^2 + |z_2|^2 = r \\ |z_1|^2 - |z_2|^2 = r\cos\theta \end{cases} \quad \text{or} \quad \begin{cases} |z_1|^2 = \frac{1}{2}r(1+\cos\theta) = r\cos^2(\theta/2) \\ |z_2|^2 = \frac{1}{2}r(1-\cos\theta) = r\sin^2(\theta/2) \end{cases} \tag{C.10}$$

giving

$$\begin{cases} z_1 = \sqrt{r}\cos(\theta/2)\ \exp[i\theta_1] \\ z_2 = \sqrt{r}\sin(\theta/2)\ \exp[i\theta_2] \end{cases} . \tag{C.11}$$

To find the phase angles, we calculate

$$z_1^* z_2 = r\cos(\theta/2)\sin(\theta/2)\ \exp[i(\theta_2-\theta_1)] = \frac{1}{2} r\sin\theta\ \exp[i(\theta_2-\theta_1)] \tag{C.12}$$

and use, from (C.4),

$$r\sin\theta\cos\phi = x^1 = 2\,\mathrm{Re}(z_1^* z_2) = r\sin\theta\cos(\theta_2-\theta_1) \tag{C.13}$$

and

$$r\sin\theta\sin\phi = x^2 = 2\,\mathrm{Im}(z_1^* z_2) = r\sin\theta\sin(\theta_2-\theta_1), \tag{C.14}$$

to find that

$$\theta_2 - \theta_1 = \phi + 2\pi n. \tag{C.15}$$

Letting

$$\theta_1 = -\frac{\phi+\gamma}{2}, \quad \text{with } \gamma\in\mathbb{R}, \tag{C.16}$$

then gives us

$$\theta_2 = -\frac{\phi+\gamma}{2} + \phi + 2\pi n = \frac{\phi-\gamma}{2} + 2\pi n. \tag{C.17}$$

Thus

$$\begin{cases} z_1 = \sqrt{r}\cos(\theta/2)\ \exp[-i(\phi+\gamma)/2] \\ z_2 = \sqrt{r}\sin(\theta/2)\ \exp[i(\phi-\gamma)/2] \end{cases} \tag{C.18}$$

or

$$\begin{cases} u^1 = \ \ \sqrt{r}\cos\left(\frac{\theta}{2}\right)\cos\left(\frac{\phi+\gamma}{2}\right) \\ u^2 = -\sqrt{r}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\phi+\gamma}{2}\right) \\ u^3 = \ \ \sqrt{r}\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\phi-\gamma}{2}\right) \\ u^4 = \ \ \sqrt{r}\sin\left(\frac{\theta}{2}\right)\sin\left(\frac{\phi-\gamma}{2}\right) \end{cases} . \tag{C.19}$$

For fixed (r,θ,ϕ), this describes a curve in $\{u^\mu\}$ space parametrized by γ. Each point on this curve maps to the same point (r,θ,ϕ) in $\{x^i\}$ space. Note that the curve is closed, since $u^\mu(\gamma+4\pi) = u^\mu(\gamma)$. Thus we can restrict γ to the interval $[0, 4\pi)$.

We can then interpret γ as an additional angle that compliments r,θ,ϕ as coordinates for the four-dimensional $\{u^\mu\}$ space. Accordingly, we introduce a fourth coordinate x^4 and extend the mapping from u^μ to x^i by the differential relation

$$\mathrm{d}x^4 = 2u^2\,\mathrm{d}u^1 - 2u^1\,\mathrm{d}u^2 + 2u^4\,\mathrm{d}u^3 - 2u^3\,\mathrm{d}u^4 \tag{C.20}$$

so that

$$\begin{bmatrix}\mathrm{d}x^1\\ \mathrm{d}x^2\\ \mathrm{d}x^3\\ \mathrm{d}x^4\end{bmatrix} = \begin{bmatrix} 2u^3 & 2u^4 & 2u^1 & 2u^2 \\ 2u^4 & -2u^3 & -2u^2 & 2u^1 \\ 2u^1 & 2u^2 & -2u^3 & -2u^4 \\ 2u^2 & -2u^1 & 2u^4 & -2u^3 \end{bmatrix} \begin{bmatrix}\mathrm{d}u^1\\ \mathrm{d}u^2\\ \mathrm{d}u^3\\ \mathrm{d}u^4\end{bmatrix} \tag{C.21}$$

or

$$[\mathrm{d}\vec{x}] = \mathbf{A}(\vec{u})[\mathrm{d}\vec{u}] \tag{C.22}$$

with the Jacobian matrix

$$\mathbf{A}(\vec{u}) = \begin{bmatrix} 2u^3 & 2u^4 & 2u^1 & 2u^2 \\ 2u^4 & -2u^3 & -2u^2 & 2u^1 \\ 2u^1 & 2u^2 & -2u^3 & -2u^4 \\ 2u^2 & -2u^1 & 2u^4 & -2u^3 \end{bmatrix}. \tag{C.23}$$

The relation (C.20) has been chosen such that the metric in u^μ coordinates,

$$g_{\mu\nu} = \frac{\partial x^\alpha}{\partial u^\mu}\frac{\partial x^\beta}{\partial u^\nu}\delta_{\alpha\beta} \quad \text{(summation convention implied)}, \tag{C.24}$$

takes the simple form

$$\begin{aligned} \mathbf{g}(\vec{u}) = \mathbf{A}^T\mathbf{A} &= 4\begin{bmatrix} u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & u^2 & -u^1 \\ u^1 & -u^2 & -u^3 & u^4 \\ u^2 & u^1 & -u^4 & -u^3 \end{bmatrix}\begin{bmatrix} u^3 & u^4 & u^1 & u^2 \\ u^4 & -u^3 & -u^2 & u^1 \\ u^1 & u^2 & -u^3 & -u^4 \\ u^2 & -u^1 & u^4 & -u^3 \end{bmatrix} = 4\begin{bmatrix} \vec{u}^2 & 0 & 0 & 0 \\ 0 & \vec{u}^2 & 0 & 0 \\ 0 & 0 & \vec{u}^2 & 0 \\ 0 & 0 & 0 & \vec{u}^2 \end{bmatrix} \\ &= 4r\mathbf{I} \end{aligned} \tag{C.25}$$

so that the determinant of $\mathbf{A}$ is

$$|\det\mathbf{A}| = \sqrt{\det\mathbf{g}} = \sqrt{(4r)^4} = 16r^2. \tag{C.26}$$

Note that the relation (C.20) is not integrable since the mixed partial derivatives don't commute, e.g.:

$$\frac{\partial^2 x^4}{\partial u^2\partial u^1} = -\frac{\partial^2 x^4}{\partial u^1\partial u^2}. \tag{C.27}$$

Nevertheless, the relation between $\{x^\mu\}$ and $\{u^\mu\}$ becomes bijective once it has been specified at an initial point $u^\mu(\vec{x}_a) = u^\mu_a$.

Using the relations in (C.19) we can express the differentials $\mathrm{d}u^\mu$ in terms of $(\mathrm{d}r, \mathrm{d}\theta, \mathrm{d}\phi, \mathrm{d}\gamma)$ and substitute these into (C.20) to find

$$\mathrm{d}x^4 = r\cos\theta\,\mathrm{d}\phi + r\,\mathrm{d}\gamma. \tag{C.28}$$

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