PATH INTEGRATION IN NON-RELATIVISTIC QUANTUM MECHANICS

Cécile DeWITT-MORETTE

Department of Astronomy and Center for Relativity, University of Texas, Austin, TX 78712, USA

Amar MAHESHWARI

Department of Physics, Regional College of Education, Mysore 570006, India

and

Bruce NELSON

Department of Physics and Center for Relativity, University of Texas, Austin, TX 78712, USA

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Contents

Abstract

A new method for computing path integrals explicitly is developed and applied to problems in non-relativistic quantum mechanics, such as wave functions, propagators on configuration spaces and on phase space, caustic problems, bound states Path integrals for paths on curved spaces and for paths on multiply-connected spaces are computed

Introduction

"In 1932 Dirac [125, p 312] laid the foundation stone of what was destined to become in the hands of Feynman a new formulation of quantum mechanics Feynman raised the subject to the rank of a new discipline"

"A physicist needs that his equations should be mathematically sound" Dirac [42]

A path integral is often a beautiful answer to a physical problem [e.g. 35] – provided one knows how to compute it! Admittedly one can extract some information from a path integral without computing it, but unless one has developed a versatile path integration technology one is severely restricted in the use of this powerful method.

Path integrals and partial differential equations serve different purposes. Path integrals are more than solutions of differential equations satisfying given boundary conditions. Their formulation incorporate global properties of the system and they can give answers which cannot be given by partial differential equations (see section 3.1).

When functional integration was introduced in physics independently by the work of Wiener on brownian motion* in 1922 and by Feynman's formalism of quantum physics [53, 56] in 1942, partial differential equations were such an omnipotent formulation of physical laws that it was difficult to appreciate path integrals. Nevertheless they have wormed themselves in, and appear nowadays in nearly all branches of physics. But because a workable theory of integration on function spaces cannot be constructed as a formal generalization of integration on $\mathbf{R}^n$ (see appendix A), path integration has on the whole remained a rudimentary tool. Note however that even in its rudimentary form, it has produced an illustrious offspring, the Feynman diagram technique. But the general user who cannot progress as well as Feynman with crude instruments needs a reliable formulation.

A great example of functional integration is the Wiener integral. Unfortunately despite their similarities with Wiener integrals, Feynman (path) integrals cannot *readily* be defined in the same manner because they cannot be built from bounded measures. Analytic continuation of Wiener integrals has served well in some problems, in particular in constructive field theory. Albeverio and Høegh-Krøhn [3] have developed a general theory of oscillatory integrals on real Hilbert spaces and applied it to the mathematical foundation of Feynman path integrals. Truman [135–137] has carefully investigated the polygonal definition of Feynman path integrals and its applications. In this monograph we shall present another approach to Feynman integration – one which does not treat Feynman integrals as the limit of an integral over $\mathbf{R}^p$ when $p = \infty$.

The possibility of defining path integrals without the "lattice approximation" dawned on one of us while reading the marvelous chapter of Bourbaki [13]** on integration on topological vector spaces: one could define an object, later called a "prodistribution", and with it build and compute some Feynman integrals. The potential of this formulation appealed to the second author who immediately

*There are many books and articles on the subject [e g 117]

**To those who do not receive instant gratification from such readings, it should be said that it was read under duress, but that is another story

used it to obtain, on the back of an envelope, the partition function of an electron in a random potential in closed form [93]. The third author, who likes topology, geometry and physics, found in the theory of prodistributions a rewarding field of investigations. Together, and several papers later, we hope to present this formulation of path integration not as a recipe, but as a tool which everyone can fashion to one's own needs.*

This tool meshes gears with product integrals (section 2) and a small turn of the crank gives the path integral representation of the wave function known as the Feynman–Kac formula and the Møller wave operators (sections 2.3, 2.4). The Feynman–Kac formula is used, in particular, in sections 3.3 and 3.4 to compute wave functions and propagators on curved spaces.

The Gaussian prodistributions built with the Jacobi fields of the system (appendix B) and linear transformations on the domain of integration (sections 1.4, 1.5) are simple to manipulate and well suited to solving many problems of quantum physics. In a nutshell, the elementary kernels of the Jacobi operators make excellent covariances for the gaussian prodistribution of lagrangian and hamiltonian systems. A natural application is the semiclassical expansion to all orders in $\hbar$ (section 3.4). The method does not break down on the caustics and gives the phase losses at conjugate points (section 3.5). It can also be combined with the diagram technique whose primary usefulness is for computing power series in a coupling constant, so that the coupled perturbation is indeed small (section 3.6).

A useful by-product: The Fredholm determinants of the linear transformations discussed in this monograph (Volterra equations) can now be computed explicitly via path integrals; i.e. the Cameron–Martin formula can be turned around and used to compute Fredholm determinants (section 1.5).

Another aspect of the method is the possibility in some cases of associating in a well defined sense a prodistribution on $X \subset Y$ to a given prodistribution on Y. For instance given a gaussian on the space of paths with only one end fixed, one can associate, in the Leray sense, a gaussian on the space of paths with both ends fixed (sections 1.6 and 3.4).

It has been said that the method presented here is difficult. Different, yes; difficult, "no" say the users, and depending on one's background one could even add "obvious". Moreover, it is always possible to project an infinite dimensional space into a finite one (but not vice versa) and to compare the new results with the familiar lattice approximation.

Originally this monograph was to include several other topics which had to be shelved for inclusion in another monograph. Most prominent among the questions in holding pattern is the problem of paths "going backward in proper time" and related subjects such as: pair production in classical relativistic mechanics, causality lost with the existence of paths going backward in time and restored by quantum mechanics, and the Schwinger effective lagrangian formalism in field theory. When lack of space forced us to eliminate these questions it became natural to focus on nonrelativistic quantum mechanics and to give the lion's share to the gaussian method.

This monograph takes up where the book by Feynman and Hibbs [56] and the article by Keller and McLaughlin [80]** leave off. We hope it can be a user's manual and we have let reliability dictate the level of mathematical rigor. All expressions are explicitly given, *not* modulo an unknown (infinite!) factor. The definition of mathematical terms is included only when needed for computational purposes. To define terms needed to state a theorem correctly but of no concern to the practicing physicist would have cluttered this monograph to no benefit.† For instance we do not define "Hausdorff" but we

*A promeasure is a particular case of prodistribution, and all results derived here apply obviously to Wiener integrals

**On the whole, we do not repeat the discussions found in references [56] and [80]

†If desired these definitions can be found in standard mathematical texts We have used basic notation and terminology, as for instance ref [23], which gathers in a single volume different areas of contemporary mathematics, references are made to this book in order to use only one reference for different areas of mathematics

define "derivative mapping". When it can be done without loss of generality, we often give the proof of a proposition in the context of an application. On the other hand, it would have been cumbersome in many cases to introduce a theorem by presenting an example. When such is the case, the example follows right on the heels of the general statement and can be read before the theorem if one is so inclined. For instance if the following paragraphs seem too abstract, go right on to example 1.

Mathematical introduction

1. Prodistributions

1.1. Promeasures

It is easier, even for a user's manual, to start from the theory of promeasures* (also called **cylindrical measures**), and we give a brief introduction** to the subject. The theory of promeasures generalizes the theory of integration on $\mathbf{R}^n$ to spaces which are not locally compact.† It is restricted to topological vector spaces that are Hausdorff and locally convex. Let $X, Y, \ldots$ be such spaces.†† A promeasure on X is a family of bounded measures on finite dimensional spaces appropriately related to X, satisfying some coherence conditions. The family of finite dimensional spaces form a so-called "projective system of X" defined as follows.

Let $\mathcal{F}(X)$ be the set of closed subspaces V, W of X of finite codimension,§ partially ordered by the inclusion relation $\subset$. Let p_v be the canonical mapping from X into the quotient space X/V. Let $W \subset V$ and let p_{vw} be defined by $p_v = p_{vw} \circ p_w$. The quotient spaces X/V, $X/W, \ldots$ together with the canonical mappings $p_{vw} : X/W \to X/V \ldots$ form the **projective system of finite dimensional quotient spaces of X indexed by $\mathcal{F}(X)$** – in brief, the projective system of X.

Example 1. Let X be the space of continuous functions f, f', $g, \ldots$ defined on $T \subset \mathbf{R}$. Let the functions f, f' which take the same values at a certain partition $\theta_v = \{t_1 \ldots t_v\}$ of T be called equivalent, i.e.

$$f \sim f' \quad \Leftrightarrow \quad f' = f + g \quad \text{with } g(t_i) = 0 \text{ for every } t_i \in \theta_v.$$

The set of functions g which vanish on the set θ_v forms a closed subspace $V \subset X$ of finite codimension v. X/V is the space of equivalence classes $[f] \overset{\text{def}}{=} \{f'; f' \sim f\}$.

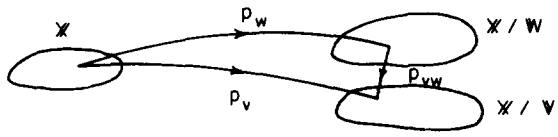


Fig 1

*Introduced by Segal [127] under the name **weak canonical distribution.**

**For further details see for instance refs [13, 23]

†See appendix A

††$X, Y,$ can be either finite or infinite dimensional, here they usually are infinite dimensional but not necessarily so

§Also called **cofinite space**

The canonical mapping $p_v : X \to X/V$ is given by $f, f', \ldots \mapsto [f]$. The space X/V has dimension v, since we need only the v quantities $\{f(t_i)\}$ to define $[f]$. Similarly another partition θ_w defines another closed subspace $W \subset X$. If $\theta_v \subset \theta_w$, then $W \subset V$ and $X/V \subset X/W$.

Definition. A **promeasure** μ on X is a family of bounded measures $\{\mu_V\}$ on X/V with $V \in \mathcal{F}(X)$ which satisfies the following coherence conditions:

$\mu_V(X/V)$ is independent of V and is noted $\mu(X)$.
When $W \subset V$, μ_V is the image* under p_{vw} of μ_w.

The projective system $\{X/V, p_{vw};\ V \in \mathcal{F}(X)\}$ of X on which the promeasure is built is determined by the topological dual X' of X, i.e. by the set of linear containuous functions** on X: Let $x \in X$ and $x' \in X'$ then $\langle x', x\rangle_X = x'(x) \in \mathbf{R}$. The space V belongs to $\mathcal{F}(X)$ if and only if it consists of $x \in X$ such that $\langle x'_j, x\rangle = 0$ for a finite number of $x'_j \in X'$. The set $V_0 = \{x'_j\}$ is said to be **orthogonal** to V.

In example 1, X' is the space of bounded measures on X and V is defined by the finite set $\{\langle \delta_{t_j}, g\rangle = g(t_j) = 0;\ t_j \in \theta_v\}$.

The topological dual X' of X is the corner stone of our formulation and we shall make extensive use of linear mappings and their transposes. Let $P : X \to Y$ be a linear continuous mapping. Its transpose $\tilde{P}$ maps $Y' \to X'$ and is defined by the relationship

$$\langle \tilde{P}y', x\rangle_X = \langle y', Px\rangle_Y.$$

Example 2. With the notation of example 1, let $p_v : X \to \mathbf{R}^v$ by $f \mapsto \{f(t_1) \ldots f(t_v)\} \in \mathbf{R}^v$; the transpose $\tilde{p}_v : \mathbf{R}^v \to X'$ by $\xi = \{\xi_1, \ldots \xi_v\} \in \mathbf{R}^v \mapsto \sum_{j=1}^{v} \xi_j \delta_{t_j}$. Indeed

$$\langle \tilde{p}_v \xi, f\rangle_X = \langle \{\xi_1, \ldots \xi_v\}, \{f(t_1) \ldots f(t_v)\}\rangle_{\mathbf{R}^v} = \sum_j \xi_j f(t_j). \qquad \blacksquare$$

Because we can identify X/V and $\mathbf{R}^v$, this example shows that if $p_v : X \to X/V$, $\tilde{p}_v : (X/V)' \to V_0 \subset X'$ where V_0 is orthogonal to V. It is easy to show that $\tilde{p}_v$ is an isomorphism of $(X/V)'$ into V_0. The mapping p_v of the examples 1 and 2 will be used whenever we want to compare our results with results obtained with the original definition in which a path is replaced by v of its values. Many other linear continuous mappings will be used (see for instance sections 1.2, 1.4, 1.5, 2.3, 3.2, 3.3, 4.4, 4.5). The transpose of an arbitrary linear continuous mapping from X into $\mathbf{R}^v$ is given in the following example.

Example 3. Let X be the space of continuous functions defined on $\mathsf{T} \subset \mathbf{R}$ X' is the space of bounded measures on T. Let $P : X \to \mathbf{R}^v$ by $x \mapsto u$ where u is the v-tuple $\{u^i = \langle x'_i, x\rangle\}$. The dual of $\mathbf{R}^v$ is the set of v-tuples $\xi = \{\xi_i\}$ and $\langle \xi, u\rangle_{\mathbf{R}^v} = \sum_{i=1}^{v} \xi_i u^i$. The transpose $\tilde{P} : \xi \mapsto \Sigma \xi_i x'_i$.

Proof:

$$\langle \tilde{P}\xi, x\rangle_X = \langle \xi, Px\rangle_{\mathbf{R}^v} = \sum_i \xi_i \langle x'_i, x\rangle = \sum_i \langle \xi_i x'_i, x\rangle. \qquad \blacksquare$$

*Let $A \subset X/W$ and $B \subset X/V$ such that $A = p_{vw}^{-1}(B)$ then μ_V is the image under p_{vw} of μ_W if $\mu_V(B) = \mu_W(A)$ One writes $\mu_V = p_{vw}(\mu_W)$ or $\mu_V = p_{vw}\mu_W$

**Also called functionals, or forms We use the word function for any mapping with values in R or C, whether its domain is a finite or infinite dimensional space

Fourier transforms. We recall first some properties of Fourier transforms of tempered distributions $\mathcal{S}'$ based on $\mathbf{R}^n$. Let $\mathcal{S}$ be the space of rapidly decreasing functions ϕ on $\mathbf{R}^n$. The Fourier transform $\mathcal{F}T$ of $T \in \mathcal{S}'$ is defined by

$$\langle \mathcal{F}T, \phi \rangle = \langle T, \mathcal{F}\phi \rangle$$

where

$$\mathcal{F}\phi(x') = \int_{R^n} \exp(-i\langle x', x\rangle)\phi(x)\, dx.$$

In particular if T is a vector valued* measure μ on $\mathbf{R}^n$, then

$$\langle \mu, \phi \rangle = \int_{\mathbf{R}^n} d\mu_\alpha(x)\phi^\alpha(x) \qquad \alpha = 1, \ldots n,$$

and

$$\langle \mathcal{F}\mu, \phi \rangle = \int_{\mathbf{R}^n} dx' \int_{\mathbf{R}^n} \exp(-i\langle x, x'\rangle)\, d\mu_\alpha(x)\phi^\alpha(x').$$

Note that a measure is not defined pointwise but setwise, $\mu(U) = \int_U d\mu(x)$. Its Fourier transform, on the other hand, is defined pointwise

$$\mathcal{F}\mu(x') = \int_{\mathbf{R}^n} \exp(-i\langle x', x\rangle)\, d\mu(x).$$

In other words, a measure is a **distribution of order zero**, i.e. a distribution defined** on the space of continuous (not necessarily smooth) functions with compact support. But the Fourier transform of a measure μ on X is a distribution equivalent to the function $\mathcal{F}\mu$ on the dual X' of X. If $X = \mathbf{R}^n$ is the space of n-dimensional contravariant vectors, $X' = \mathbf{R}^n$ is the space of n-dimensional covariant vectors.

Image of a Fourier transform under a linear mapping P. Let $P: X \to Y$ and $\tilde{P}: Y' \to X'$. Let μ be a measure on X and ν its image under P. Then

$$\mathcal{F}\nu = \mathcal{F}\mu \circ \tilde{P}. \tag{1.1}$$

The **Fourier transform of a promeasure** μ is defined by the family of Fourier transforms $\{\mathcal{F}\mu_V;\ V \in \mathcal{F}(X)\}$.

Let x' be in the space V_0, orthogonal to V, and let u be in $\mathbf{R}^v$ and u' in the dual of $\mathbf{R}^v$. Then

$$\mathcal{F}\mu(x') = \mathcal{F}\mu_V(u') = \int_{X/V} \exp(-i\langle u', u\rangle)\, d\mu_V(u), \qquad x' \in V_0.$$

Since

$$X' = \bigcup_{V \in \mathcal{F}(X)} V_0$$

*Coordinate expressions will be written explicitly only when desirable

**We say that a distribution is *defined* on a space of test functions of domain $\mathbf{R}^n$, or that a distribution is *based* on $\mathbf{R}^n$. The theory of distributions on general spaces has been studied by Kree [82]. It is not simply a formal generalization of distributions on $\mathbf{R}^n$

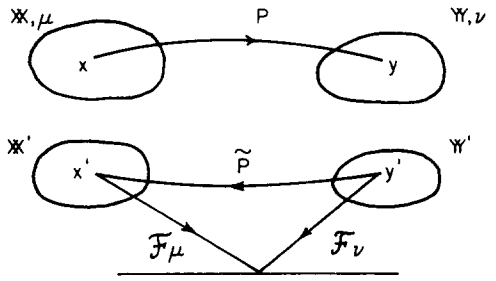


Fig 2 $\mathcal{F}_\mu$ is a function on X' If $\nu = P(\mu)$, then $\mathcal{F}\nu(y') = (\mathcal{F}_\mu \circ \tilde{P})(y')$

this equation defines $\mathcal{F}_\mu$ on X'. It is straightforward to show that eq. (1.1) is valid for promeasures. Equation (1.1) is one of the basic tools in computing path integrals.

1.2. Prodistributions

A promeasure is a family of bounded measures. For instance, the Wiener promeasure* is a family of gaussian measures. To show why promeasures, and in particular the Wiener measure cannot readily be used in the case of Feynman integrals we shall contrast real and imaginary gaussian measures on $\mathbf{R}^v$. Let

$$d\gamma_\lambda(x) = (2\pi\lambda)^{-v/2}(\det A^{-1})^{1/2} \exp(-(A^{-1})_{ij}x^i x^j/2\lambda)\, dx^1 \ldots dx^v$$

where $\lambda = 1$ for real gaussians and $\lambda = i$ for imaginary gaussians. $\sqrt{i} = \exp(i\pi/4)$. The real gaussian γ_1 is a bounded measure**: $\int_{\mathbf{R}^v} |d\gamma_1(x)| < \infty$. The imaginary gaussian γ_i is not bounded, and we cannot use it to define an integral in the usual sense. One can define $\int_{\mathbf{R}} d\gamma_i(x)$ as the limit when $a = \infty$ of $\int_{-a}^{a} d\gamma_i(x)$, but for $v > 1$ one cannot define $\int_{\mathbf{R}^v} d\gamma_i(x)$ as the limit of an integral over a finite domain. For example

$$\int_{\mathbf{R}^2} (2\pi i)^{-1} \exp(i(x^2+y^2)/2)\, dx\, dy = \begin{cases} 1 & \text{if computed in Cartesian coordinates as the limit of} \\ & \int_{-a}^{a} dx \int_{-b}^{b} dy. \\ 1 - (\lim \exp i a^2/2) & \text{if computed in polar coordinates as the limit of} \\ & \int_0^a r\, dr \int_0^{2\pi} d\theta. \end{cases}$$

One can hardly build a theory of integration where change of variables of integration is not allowed, let alone a theory of integration over infinite dimensional spaces.

Although γ_i is a measure unsuitable for integration in the sense of set theory, it is an excellent measure in the sense of distribution theory.

*It can be shown that the Wiener promeasure is equivalent to a measure [e g 13, p 87], it is thus perfectly correct to speak of the Wiener measure

**When A^{-1} is a positive definite form on $\mathbf{R}^v$

(a) It is a tempered distribution,* $\gamma_\lambda \in \mathcal{S}'$. Its Fourier transform is the normalized complex gaussian function of **covariance** A^{ij}, **variance** $A^{ij}x'_i x'_j$,

$$\mathcal{F}\gamma_\lambda(x') = \exp\left(-\frac{i}{2} A^{ij}x'_i x'_j\right).$$

(b) It is in the space of operators on $\mathcal{S}'$: both multiplication $\gamma_\lambda T$ and convolution $\gamma_\lambda * T$ are defined for every $T \in \mathcal{S}'$.

Since there is a one-to-one correspondence between the set of promeasures on X and their Fourier transforms on X', one can define a promeasure by its Fourier transform and state the coherence conditions as conditions satisfied by the Fourier transforms. *At this point we shall remove the restriction to bounded measures* since $\mathcal{F}\gamma_\lambda$ is defined equally well for $\lambda = 1$ and for $\lambda = i$, and we shall call** "**prodistributions**" the generalization of promeasures thus obtained

Definition. **The Fourier transform** $\mathcal{F}\mu$ **on** X' **of a prodistribution** μ **on** X **is a family** $\{\mathcal{F}\mu_V;\ V \in \mathcal{F}(X)\}$ **such that**

$$\begin{cases} \mathcal{F}\mu_V(0) \text{ is independent of } V. \\ \text{When } W \subset V,\ \mathcal{F}\mu_V = \mathcal{F}_{\mu W} \circ \tilde{p}_{vw}. \end{cases}$$

$\mathcal{F}\mu$ is coherently defined: If $x' \in V^0 \cap W^0$, then $\mathcal{F}\mu_V(x') = \mathcal{F}\mu_W(x')$. It is easy to check that a promeasure is a prodistribution.

Gaussian prodistributions. A prodistribution w on X is said to be **gaussian** if

$$\mathcal{F}w(x') = w(X)\exp\left(-\frac{\lambda}{2} W(x', x')\right), \qquad \lambda = 1 \text{ or } i$$

where W is a bilinear function on X' (positive definite if $\lambda = 1$). $W(x', x')$ is called the **variance**. The normalization $w(X)$ is not necessarily equal to one. We are using the letter w for gaussian prodistributions because its famous prototype, the Wiener measure, is usually called w.

Example 4. Let X_- be the space of continuous paths x on $T = [t_a, t_b]$ with values in $\mathbf{R}^n$ vanishing at t_a. The bilinear function W on X' is of the form

$$W(\mu, \nu) = \int_T d\mu_\alpha(t) \int_T d\nu_\beta(s)\, G^{\alpha\beta}(t, s).$$

$G^{\alpha\beta}(t, s)$ is called the **covariance** of w.

Definition. The **Wiener measure** on the space X of paths with values in $\mathbf{R}$ is the gaussian prodistribution characterized by $\lambda = 1$, $w(X) = 1$, and

$$G(t, s) = \theta(t - s)(s - t_a) + \theta(s - t)(t - t_a) = \inf(s - t_a, t - t_a)$$

*The space of tempered distributions, labeled $\mathcal{S}'$, is the space of distributions defined on the space $\mathcal{S}$ of test functions ϕ such that ϕ has a Fourier transform It follows that $\mathcal{S}'$ is the space of distributions which have Fourier transforms

**Originally called pseudomeasures The word "prodistribution" has been suggested by Dieudonné, to describe a projective family of distributions

where θ is the step function equal to one for positive arguments and zero otherwise. For simplicity we shall often use the term "**Wiener measure**" for both the complex and real normalized gaussians of covariance infinum and label it w^W See p 266 for the relationship between the Wiener measure and the Brownian motion.

Example 5. The space introduced in example 4 is used extensively in the diffusion problem. A particle is known to be somewhere at time t_a; how will it diffuse? A different, but similar space is used in quantum physics, namely the space of paths $x \cdot T \to \mathbf{R}^n$ vanishing at t_b. One knows the wave function at time t_a, one wants the wave function at t_b, hence one sums over all the paths taking the same value at t_b.

Let X_- be the space introduced in example 4 and X_+ be the space of paths vanishing at t_b Let $P : X_- \to X_+$ by $x \mapsto y$ such that $y(t) = x(t) - x(t_b)$. P is a linear mapping. Its transpose $\tilde{P}$ is such that

$$\tilde{P}\mu = \mu - \mu(T)\delta_{t_b} \quad \text{with } \mu(T) = \int_T \mathrm{d}\mu(t).$$

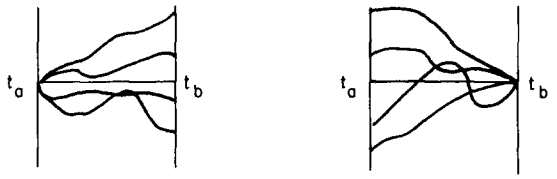
Let w_-, W_- and G_- be respectively the Wiener measure on X_-, its variance and covariance, and let w_+, W_+, G_+ be the corresponding quantities on X_+. Then

$$W_+(\mu, \mu) = W_-(\tilde{P}\mu, \tilde{P}\mu) = \int_T \mathrm{d}\mu(r) \int_T \mathrm{d}\mu(s)[\theta(r-s)(t_b - r) + \theta(s-r)(t_b - s)].$$

The covariance G_+ of the Wiener measure on X_+ is

$$G_+(t, s) = \theta(t-s)(t_b - t) + \theta(s-t)(t_b - s) = \inf(t_b - t, t_b - s)$$

The skill in computing a path integral consists in choosing the covariance and the normalization best suited for the problem at hand. We shall give in sections 3 and 4, a method for computing covariances naturally suited to given lagrangian and hamiltonian systems. The versatility of the path integration technology based on prodistribution comes in part from the great choice of covariances at our disposal. It comes also from the fact that we work with the variance $W(\mu, \mu)$ rather than the covariance $G^{\alpha\beta}(t, s)$. For instance the image under a linear mapping P of a gaussian of variance W is the gaussian of variance $W \circ \tilde{P}$. No such simple relation exists between covariances. Moreover the variance is a coordinate free expression, and the problems connected with change of coordinate system on the configuration space do not exist.



Example 4 Example 5

Fig 3

Gaussian and gaussian induced* prodistributions are the only ones we have been able to use in a practical way so far. It is not too severe a restriction for quantum physics since the covariance constructed from the Jacobi fields of the system contains the essence of all quantum effects. Nevertheless it would be valuable to be able to integrate with respect to other prodistributions.

1.3. Integration

The computation of integrals with respect to a prodistribution w (known by its Fourier transform $\mathcal{F}w$) will proceed entirely in terms of $\mathcal{F}w$. But we shall also use the usual notation to write down a path integral

$$\int_X F(x)\,\mathrm{d}w(x) \in \mathbf{R}.$$

We shall use the following properties of integration:

a) linearity:

$$\int_X \alpha(F(x)+G(x))\,\mathrm{d}w(x) = \alpha \int_X F(x)\,\mathrm{d}w(x) + \alpha \int_X G(x)\,\mathrm{d}w(x);$$

b) change of variable of integration:** Let $F = f \circ P$ where $P : X \to Y$ by $x \mapsto y$. Let Pw be the image of w under P. Then

$$\int_X F(x)\,\mathrm{d}w(x) = \int_Y f(u)\,\mathrm{d}Pw(u) \tag{1.2}$$

where

$$\mathcal{F}(Pw) = \mathcal{F}w \circ \tilde{P}. \tag{1.3}$$

If P is a linear continuous mapping of X into a finite dimensional space, F is called a **cylindrical** or a **tame** function. A cylindrical integral is equal to an integral over a finite dimensional space.

Let w be a normalized gaussian prodistribution of variance W, $\mathcal{F}w = \exp(-\mathrm{i}W/2)$, then

$$\int_X F(x)\,\mathrm{d}w(x) = \int_{R^v} f(u)\,\mathrm{d}Pw(u);$$

Pw is a normalized complex gaussian measure of variance

$$W_P = W \circ \tilde{P}. \tag{1.4}$$

The most general† linear continuous mapping $P : X \to \mathbf{R}^v$ is defined by $x \mapsto u = \{u^1, \ldots u^v\}$ where $u^j = \langle x'_j, x\rangle$ for some $x'_j \in X'$. Let $\xi = \{\xi_1, \ldots \xi_v\}$ be in the dual of $\mathbf{R}^v$; then (see example 3) $\tilde{P}(\xi) =$

*See p 268

**Other notations such as $E[F]$ often used in probability theory are not as convenient when performing change of variables of integration

†v is not necessarily finite See for instance section 3 5

$\Sigma_{i=1}^{v} \xi_i x_i'$ and

$$W \circ \tilde{P}(\xi, \xi) = W\left(\sum \xi_i x_i', \sum \xi_j x_j'\right) = \sum_{i,j} \xi_i \xi_j W(x_i', x_j').$$

Set $W(x_i', x_j') = \mathcal{W}^{ij}$. Pw is a normalized complex gaussian measure on $\mathbf{R}^v$ of covariance $\mathcal{W}^{ij}$;

$$\mathrm{d}Pw(u) = (2\pi\mathrm{i})^{-v/2} |\det(\mathcal{W}^{-1})_{ij}|^{1/2} \exp\left(\frac{\mathrm{i}}{2}(\mathcal{W}^{-1})_{ij} u^i u^j\right) \mathrm{d}u^1 \ldots \mathrm{d}u^v. \tag{1.5}$$

Example 6. Wiener measure and Brownian motion. The Brownian motion is a random motion such that, if $t > s$, $x(t) - x(s)$ is a random variable with gaussian distribution of mean $x(s)$ and mean square deviation $t - s$. We can readily use eq. (1.5) to compute

$$I = \int_{X_-} f(x(t_1), x(t_2) - x(t_1), \ldots, x(t_{n+1}) - x(t_n)) \, \mathrm{d}w_-^{\mathrm{W}}(x),$$

where w_-^{W} is the real Wiener measure on X_-. Indeed, let

$$P : x \mapsto u = \{u^k = \delta_{t_{k+1}} - \delta_{t_k}, x; k = 0, \ldots, n\},$$

then

$$\mathcal{W}^{ij} = W_-(\delta_{t_{i+1}} - \delta_{t_i}, \delta_{t_{j+1}} - \delta_{t_j}) = \delta_{ij}(t_{i+1} - t_i)$$

$$I = \int_{\mathbf{R}^{n+1}} f(u^1, \ldots, u^{n+1}) \, \mathrm{d}\gamma_1(u^1), \ldots, \mathrm{d}\gamma_{n+1}(u^{n+1}),$$

where

$$\mathrm{d}\gamma_k(u^k) = (2\pi(t_{k+1} - t_k))^{-1/2} \exp(-(u^k)^2/2(t_{k+1} - t_k)).$$

The random process* $\{x(t); t \geqslant 0\}$ defined by the Wiener measure is the Brownian motion.

Example 7. Let $P : X \to \mathbf{R}^v$ by $x \mapsto u = \{u^1, u^{2\alpha}\}$ where $u^1 = \int_T g_\alpha(t) x^\alpha(t) \, \mathrm{d}t$, $u^{2\alpha} = x^\alpha(t)$. Introducing the Lebesgue measure λ defined by

$$\langle \lambda, \phi \rangle = \int_T \phi(t) \, \mathrm{d}t$$

and the vector valued Dirac measure δ_t^α of components $\delta_\beta^\alpha \delta_t$, we can write

$$u^1 = \langle \lambda g, x \rangle, \qquad u^{2\alpha} = \langle \delta_t^\alpha, x \rangle.$$

Let $\xi = \{\xi_1, \xi_{2\alpha}\}$, then

$$\begin{aligned} \tilde{P}\xi = \mu_\alpha &= \xi_1 \lambda g_\alpha + \xi_{2\beta} \delta_{\alpha t}^{\beta} \\ &= \xi_1 \lambda g_\alpha + \xi_{2\alpha} \delta_t, \end{aligned}$$

*A random process, in probability theory, is a family of random variables indexed by time See appendix D

$$W(\mu,\mu)=\int_T \mathrm{d}\mu_\alpha(t)\int_T \mathrm{d}\mu_\beta(s)\,G^{\alpha\beta}(t,s),$$

and

$$W(\tilde{P}\xi,\tilde{P}\xi)=\xi_i\xi_j\mathcal{W}^{ij}$$
$$=(\xi_1,\xi_{2\alpha})\begin{pmatrix}\mathcal{W}^{11} & \mathcal{W}^{12\beta}\\ \mathcal{W}^{2\alpha 1} & \mathcal{W}^{2\alpha 2\beta}\end{pmatrix}\begin{pmatrix}\xi_1\\ \xi_{2\beta}\end{pmatrix}$$

with $\mathcal{W}^{11}=\int_T \mathrm{d}t\int_T \mathrm{d}s\,g_\alpha(t)g_\beta(s)G^{\alpha\beta}(t,s)$, $\mathcal{W}^{12\beta}=\int_T \mathrm{d}s\,g_\alpha(s)G^{\alpha\beta}(s,t)$,

$\mathcal{W}^{2\alpha 1}=\int_T \mathrm{d}s\,g_\beta(s)G^{\alpha\beta}(t,s)$, and $\mathcal{W}^{2\alpha 2\beta}=G^{\beta\alpha}(t,t)$.

To complete the calculation of $\int_{R^v} f(u)\,\mathrm{d}Pw(u)$ it remains to invert the covariance $\mathcal{W}^{ij}$ and to compute its determinant. For v small, as is often the case, this not particularly difficult. Large v's come usually when $u^j=\langle\delta_{t_j},x\rangle=x(t_j)$; then $W(\delta_{t_i},\delta_{t_j})=G(t_i,t_j)$. The inverse and the determinant of $\mathcal{W}^{ij}=G(t_i,t_j)$ have been computed [40] in the cases of greatest interest in quantum physics and statistical mechanics, namely when the covariances are elementary kernels of the Jacobi equation of the system. (See appendix B.)

Application: The moment integrals and the Feynman diagram technique. Let w be a normalized gaussian on X of variance W, covariance G; then

$$I_2\overset{\text{def}}{=}\int_X \langle\delta_r,x\rangle\langle\delta_s,x\rangle\,\mathrm{d}w(x)=\lambda G(r,s), \tag{1.6}$$

where $\lambda=1$ for real gaussian and $\lambda=\mathrm{i}$ for complex gaussians. More generally, if n is even, the moment integral

$$I_n=\int_X \langle\mu_1,x\rangle\langle\mu_2,x\rangle\cdots\langle\mu_n,x\rangle\,\mathrm{d}w(x)=(\lambda)^{n/2}\sum_{\text{part}} W(\mu_{i_1},\mu_{i_2})W(\mu_{i_3},\mu_{i_4})\ldots W(\mu_{i_{n-1}},\mu_{i_n}), \tag{1.7}$$

where the sum is taken over all partitions of $\{1,\ldots n\}$. If n is odd the moment integral vanishes.

Proof. The moment integral is a cylindrical integral which can be computed by the method outlined above. It simplifies the calculation to write first $2\langle\delta_r,x\rangle\langle\delta_s,x\rangle=\langle\delta_r+\delta_s,x\rangle^2-\langle\delta_r,x\rangle^2-\langle\delta_s,x\rangle^2$ and similar expressions* for I_n. By eq. (1.5)

$$\int_X \langle\delta_r+\delta_s,x\rangle^2\,\mathrm{d}w(x)=(2\pi\lambda\mathcal{W})^{-1/2}\int_R u^2\exp(-u^2/2\lambda\mathcal{W})\,\mathrm{d}u=\lambda\mathcal{W}/2$$

where $\mathcal{W}=W(\delta_r+\delta_s,\delta_r+\delta_s)=W(\delta_r,\delta_r)+2W(\delta_r,\delta_s)+W(\delta_s,\delta_s)$. ■

*See details in ref. [38] Mizrahi has proved this result using generalized Hermite polynomials [106]

The moment integral I_n is the key integral of the Feynman diagram technique. For instance

$$K \overset{\text{def}}{=} \int_X P_{\alpha_1 \quad \alpha_p}(t_1, \dots t_p)\langle \delta_{t_1}^{\alpha_1}, x\rangle \cdots \langle \delta_{t_p}^{\alpha_p}, x\rangle \, dw(x)$$

$$= \sum_{\text{part}} P_{\alpha_1 \quad \alpha_p}(t_1, \dots t_p) G^{\alpha_{i_1}\alpha_{i_2}}(t_{i_1}, t_{i_2}) \dots G^{\alpha_{i_{p-1}}\alpha_{i_p}}(t_{i_{p-1}}, t_{i_p}).$$

When $P_{\alpha_1 \quad \alpha_p}(t_1, \dots t_p) = P_{\alpha_1}(t_1) \dots P_{\alpha_p}(t_p)$ one speaks of vertex functions $P_\alpha(t)$ and propagator lines $G^{\alpha\beta}(r, s)$. The propagator lines are hooked up to the vertices in all possible ways, and the Σ_{part} is represented by $1, 3 \dots (p-1)$ different diagrams.

We do not develop further the diagram technique which has been extensively studied. Equation (1.7) shows how the diagram technique can be obtained from path integration.

Although all the examples given here have been worked out with gaussian prodistributions, the basic equations (1.2) and (1.3) apply to any prodistributions and can be used to integrate any cylindrical function. Mizrahi [108] often uses gaussian induced prodistributions. For instance, let w be a gaussian prodistribution and let F be a cylindrical function of the form $F(\int_T x(t)f(t)\,dt)$. One can define a gaussian induced prodistribution $\bar{w}$ by the equation $\int_X d\bar{w}(x) = \int_X F(\int_T x(t)f(t)\,dt)\,dw(x)$.

If F is not a cylindrical function but can be approximated by a sequence of cylindrical functions F^n, one defines the **sequential path integral**

$$\int_X F(x)\,dw(x) = \lim \int_X F^n(x)\,dw(x).$$

The convergence of a sequential path integral is a difficult subject which is not attempted here.

Albeverio and Høegh-Krøhn [3] consider path integrals $\int_X F(x)\,dw(x)$ where F is the Fourier transform of a bounded complex measure on X':

$$F(x) = \int_{X'} \exp(-i\langle x', x\rangle)\,dv(x').$$

Thus

$$\int_X F(x)\,dw(x) = \int_{X'} dv(x') \int_X dw(x) \exp(-i\langle x', x\rangle) = \int_{X'} dv(x') \exp\left(-\frac{i}{2} W(x', x')\right).$$

This method does not require the inversion of W, but it does require finding v. It is well defined but only for integrands which are the Fourier transforms of bounded complex measures on X', and this is restrictive. Albeverio and Høegh-Krøhn have proved that their definition is equivalent to the one proposed by Itô [71].

1.4. Some properties of the Wiener measure

The following mappings establish important and useful properties of the Wiener measure.

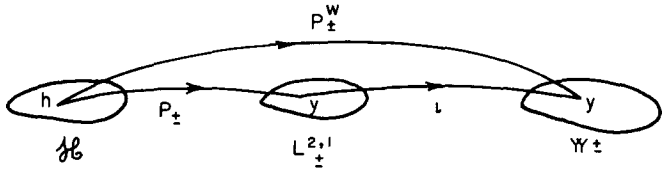


Fig 4

Let $\mathscr{H}$ be the space of real square-integrable functions h on T:

$$\|h\|^2 = \int_T g_{\alpha\beta} h^\alpha(t) h^\beta(t)\, dt$$

Let $L^{2,1}$ be the Sobolev space of square-integrable functions on T whose first weak* derivatives are square-integrable. Let $L_-^{2,1} \subset L^{2,1}$ and $L_+^{2,1} \subset L^{2,1}$ be the subspaces of $L^{2,1}$ of functions vanishing at t_a and of functions vanishing at t_b respectively.

$$\|y\|^2_{L_\pm^{2,1}} = \int_T g_{\alpha\beta} y^\alpha(t) y^\beta(t)\, dt, \qquad \dot{y}(t) = dy/dt.$$

The action $S(f) = \int_T L(f(t), \dot{f}(t))\, dt$ of the physical systems considered here are mappings $S: L^{2,1} \to \mathbf{R}$. Path integrals, on the other hand, are not defined over $L^{2,1}$ but over the spaces of continuous functions, for instance over space Y_- [the space Y_+] of continuous functions vanishing at t_a [at t_b]. Fortunately $L_-^{2,1}$ is dense in Y_-, i.e. any path in Y_- is the limit in the $L_-^{2,1}$ topology of a sequence of paths in $L_-^{2,1}$. Similarly $L_+^{2,1}$ is dense in Y_+.

Holder continuous paths. So far when talking about the paths in $Y_\pm$ we have used the word "continuous" loosely. The precise statement is as follows [e.g. 121, p. 279]. A path f is said to be **Holder continuous** of order α if $|f(t) - f(s)| \leq M|t - s|^\alpha$.

Theorem. Let Ω_α be the set of Holder continuous paths of order α. Let w^W be the Wiener gaussian on Ω_α. If $0 < \alpha < 1/2$ then $w^W(\Omega_\alpha) = 1$. If $1/2 \leq \alpha \leq 1$, then $w^W(\Omega_\alpha) = 0$.

Theorem. $L_\pm^{2,1}$ is contained in Ω_α if $\alpha \leq 1/2$ but not if $\alpha > 1/2$.

Proof.

$$f \in L_\pm^{2,1} \quad \Rightarrow \quad f(t) - f(s) = \int_s^t f'(u)\, du$$

$$\Rightarrow \quad |f(t) - f(s)|^2 = \left| \int_s^t f'(u)\, du \right|^2 \leq \int_s^t |f'(u)|^2\, du \int_s^t 1^2\, du \leq \|f\|^2_{L^{2,1}} (t - s). \qquad \blacksquare$$

*Derivatives in the sense of distribution theory Sobolev's spaces $L^{p\,m}$ are also labelled W_p^m, the spaces $L^{2\,m}$ are also labelled H^m

Intuitively this theorem says that $|y(t)-y(s)|^n$ is of order $|t-s|^{\alpha n}$, a fact worth remembering when expanding in powers of $|t-s|$.

The **primitive mapping maps** $\mathscr{H}$ **onto** $L^{2,1}_{\pm}$ and $\mathscr{H}$ ***into*** $Y_{\pm}$ by

$$h(t) \mapsto y(t) = \int_T \mp\theta_{\pm}(s-t)h(s)\,\mathrm{d}s$$

where θ_+ is the usual step up function θ equal to one for positive arguments and to zero otherwise, and θ_- is the step down function equal to one for negative arguments and zero otherwise. Let $P_{\pm}: \mathscr{H} \to L^{2,1}_{\pm}$ and $P^{\mathrm{W}}_{\pm}: \mathscr{H} \to Y_{\pm}$; the mappings $P_{\pm}$ and $P^{\mathrm{W}}_{\pm}$ do the same thing but their difference will show up strikingly below (compare theorems 1 and 2). The inclusion mapping i maps $L^{2,1}_{\pm}$ into Y by $y \mapsto y$. Innocuous it appears, but powerful it will be ... (see theorem 3).

The **canonical gaussian on a Hilbert space** is the normalized gaussian prodistribution whose variance is equal to the square of the norm. Thus the variance of the canonical gaussian on $\mathscr{H}$ and on $L^{2,1}$ are

$$I_{\mathscr{H}}(h,h) = \|h\|^2_{\mathscr{H}} = \int_T g^{\alpha\beta}h_\alpha(t)h_\beta(t)\,\mathrm{d}t$$

$$I_{L^{2,1}}(y,y) = \|y\|^2_{(L^{2,1})'} = \int_T g^{\alpha\beta}\dot{y}_\alpha(t)y_\beta(t)\,\mathrm{d}t.$$

Theorem 1. *The Wiener measure on* $Y_{\pm}$ *is the image, under the primitive mapping* $P^{\mathrm{W}}_{\pm}$ *of the canonical gaussian on* $\mathscr{H}$.

Proof: The transpose map $\tilde{P}$ is defined by

$$\langle \tilde{P}_-\mu, h\rangle_{\mathscr{H}} = \langle \mu, P_-h\rangle_{Y_-} = \int_T \mathrm{d}\mu(t) \int_T \theta(t-s)h(s)\,\mathrm{d}s;$$

thus

$$\tilde{P}_-\mu(s) = \int_T \theta(t-s)\,\mathrm{d}\mu(t),$$

and the variance is

$$I \circ \tilde{P}_-(\mu,\mu) = \int_T \mathrm{d}s \int_T \theta(t-s)\,\mathrm{d}\mu(t) \int_T \theta(t'-s)\,\mathrm{d}\mu(t') = \int_T \mathrm{d}\mu(t) \int_T \mathrm{d}\mu(t')\inf(t-t_a, t'-t_a)$$

$$I \circ \tilde{P}_- = W_-. \qquad \blacksquare$$

A similar calculation gives

$$I \circ \tilde{P}_+(\mu,\mu) = \int_T \mathrm{d}\mu(t) \int_T \mathrm{d}\mu(t')\inf(t_b-t, t_b-t').$$

Theorem 2. The canonical gaussian on $L^{2,1}_{\pm}$ is the image, under the primitive mapping $P_{\pm}$, of the canonical gaussian on $\mathscr{H}$,

$$I_{L^{2,1}} = I_{\mathscr{H}} \circ \tilde{P}_{\pm}.$$

The proof proceeds as in the previous theorem.

Theorem 3. The Wiener measure on Y is the image, under the inclusion mapping, of the canonical gaussian on $L^{2,1}$.

Proof:

$$P^{W}_{\pm} = i \circ P_{\pm}$$

$$W_{\pm} = I_{\mathscr{H}} \circ \tilde{P}^{W}_{\pm} = I_{\mathscr{H}} \circ \tilde{P}_{\pm} \circ \tilde{i} = I_{L^{2,1}_{\pm}} \circ \tilde{i}.$$

To display how the inclusion mapping works we compute $I_{L^{2,1}_{\pm}} \circ \tilde{i}$:

$$\langle \tilde{i}\mu, y\rangle_{L^{2,1}_{-}} = \langle \mu, iy\rangle_{Y_{-}} = \int_T \frac{d}{dt}(\tilde{i}\mu(t))\dot{y}(t)\,dt = \int_T y(t)\,d\mu(t).$$

It follows that

$$\frac{d}{dr}(\tilde{i}\mu(r)) = \int_T \theta(t-r)\,d\mu(t)$$

$$I_{L^{2,1}_{-}} \circ \tilde{i}(\mu,\mu) = \int_T \frac{d}{dr}(\tilde{i}\mu(r))\frac{d}{dr}(\tilde{i}\mu(r))\,dr$$

$$= \int_T d\mu(t) \int_T d\mu(t') \inf(t-t_a, t-t_a).$$

Therefore $I_{L^{2,1}_{-}} \circ \tilde{i} = W_{-}$.
If $y \in L^{2,1}_{+}$, then $d(\tilde{i}\mu(r))/dr = \int_T \theta(r-t)\,d\mu(t)$. It follows that $I_{L^{2,1}_{-}} \circ \tilde{i} = W_{+}$. ■

Theorem 3 gives the Wiener measure in terms of the space $L^{2,1}$ which is of physical interest, theorem 2 shows that the same result is obtained by using the mapping $P^{W}_{\pm}: \mathscr{H} \to Y_{\pm}$ which is usually simpler to handle. In section 1.5 we shall work with $P^{W}_{\pm}$ to compute some Fredholm determinants.

1.5. The Cameron–Martin transformation. Fredholm determinants. Affine transformations

It is easy to compute the image of a gaussian under a linear mapping. It is more difficult but often necessary to solve the inverse problem: Given two gaussians, w_A on Y and w_B on X (with variances A, B, and covariances G_A, G_B), what is the linear mapping $M: Y \to X$ which transforms one into the other? For example, in section 3.2 we have to compute the integral

$$I = \int_{Y_{+}} dw_A(y) \exp\left(\frac{-i}{2}\int_T V_{\alpha\beta}(t)y^{\alpha}(t)y^{\beta}(t)\,dt + \frac{i}{2}S_{\alpha\beta}y^{\alpha}(t_a)y^{\beta}(t_a)\right) \tag{1.8}$$

where w_A is the Wiener measure on Y_+. Obviously we need to find the linear mapping which maps w_A into a new gaussian w_B "incorporating" the integrand. A similar problem occurs in sections 3.2, 3.3, 3.4, 4.6 where, given a lagrangian system or a hamiltonian system, we seek the variable of integration best adapted to the computation of path integrals. Such problems can be solved by a generalized Cameron-Martin formula.*

The Cameron–Martin formula. Consider a normalized gaussian w_A of variance A defined on Y. Its image under the linear continuous mapping $M: Y \to X$ is the normalized gaussian w_B of variance $B = A \circ \tilde{M}$. Although $dw_A(y)$ and $dw_B(x)$ cannot be defined for arbitrary prodistributions, their ratio is defined** and given by the Cameron–Martin formula when M has a unique inverse M^{-1}.

$$dw_B(x)/dw_A(x) = \operatorname{Det} M^{-1} \exp\left(\frac{i}{2}(A^{-1}(M^{-1}x, M^{-1}x) - A^{-1}(x, x))\right) \tag{1.9}$$

Proof of the Cameron–Martin formula. Let X' and Y' be the duals of X and of Y, let $\xi \in X'$ In the finite dimensional case, $A(\xi, \xi) = A^{ij}\xi_i\xi_j$, i.e. the covariance G_A is the dyadic A^{ij},

$$dw_A(y) = \frac{dy^1}{\sqrt{2\pi i}} \cdots \frac{dy^b}{\sqrt{2\pi i}} (\det A^{-1}_{ij})^{1/2} \exp\left(\frac{i}{2} A^{-1}_{ij} y^i y^j\right)$$

$$dw_B(x) = dw_A(x)\left(\frac{\det B^{-1}_{ij}}{\det A^{-1}_{ij}}\right)^{1/2} \exp \frac{1}{2}(B^{-1} - A^{-1})_{ij} x^i x^j$$

The mapping M is defined by the matrix M^i_j,

$$B^{ij} = M^i_k M^j_l A^{kl}; \qquad B^{-1}_{ij} = A^{-1}_{kl}(M^{-1})^k_i (M^{-1})^l_j$$

$$\det B^{ij} / \det A^{kl} = (\det M^m_n)^2 \tag{1.10}$$

The infinite dimensional case is obtained by rewriting the finite dimensional case in terms of linear and bilinear continuous mappings rather than matrices and dyadics. Inverse bilinear forms are defined below. ■

We prove later on (p. 279) that Det M is the Fredholm determinant of the linear mapping M. Stated in a terminology valid both for the finite and infinite dimensional case, eq. (1.10) says

Lemma. The determinant of M, squared, is the ratio of the determinants of the covariances of w_B and w_A.

This ratio can be evaluated in closed form by the method given in appendix B, p. 358.

Inverse bilinear forms. We have to define the "inverse" of a bilinear form† on X'. The inverse, in the sense defined below, of a bilinear form on X' is a bilinear form on X''. Since†† X'' is not

*Early in the development of the theory of prodistributions, Mizrahi used the Cameron–Martin mapping to absorb part of the integrand and create new gaussians See ref [107] for his techniques and their applications

**See the proof that the ratio is defined in appendix B, p 358

†A fruitful discussion with J Dollard is gratefully acknowledged

††In general $X'' \supset X$

necessarily equal to X, it is better to work backwards: define a bilinear form on X, compute its inverse on X', i.e. assume we know A^{-1} on X and compute a bilinear form A on X' which can legitimately be called its inverse.

Let $x, y, \ldots \in X$ and $x', y' \ldots \in X'$. A bilinear form $A^{-1}(x, y)$ defines a linear map $A_y^{-1}: X \to R$ for every $y \in X$ by

$$A_y^{-1}(x) = A^{-1}(x, y).$$

Hence $A_y^{-1} \in X'$. Since A_y^{-1} is linear in y it defines a linear map $\hat{A}^{-1}: X \to X'$ by

$$\hat{A}^{-1} y = A_y^{-1}.$$

If $\hat{A}^{-1}$ is a bijection (one-one, onto) then it has an inverse $\hat{A}: X' \to X$ such that

$$A^{-1}(\hat{A}x', \hat{A}y') = \langle A^{-1}_{\hat{A}x'}, \hat{A}y' \rangle = (\hat{A}^{-1}\hat{A}x')(\hat{A}y') = \langle x', \hat{A}y' \rangle.$$

Definition. The bilinear form A on X' is said to be the **inverse of the bilinear** form A^{-1} on X if

$$A(x', y') = A^{-1}(\hat{A}x', \hat{A}y'). \tag{1.11}$$

Equation (1.11) provides a method for computing $\hat{A}$, hence a method for computing A.

Example 1. Let X be the space of $L_{\pm}^{2,1}$ paths $x, y \ldots$ (defined p. 269). The most general symmetric bilinear form on X is $\int_T (\alpha(t)x(t)\dot{y}(t) + \beta(t)(\dot{x}(t)y(t) + x(t)\dot{y}(t)) + \gamma(t)x(t)y(t))\,dt$. Assume that

$$A^{-1}(x, y) = \int_T (\dot{x}(y) \mid \dot{y}(t))\,dt = \int_T g_{\alpha\beta}\dot{x}^{\alpha}(t)\dot{y}^{\beta}(t)\,dt$$

and compute $A(x', y')$. Equation (1.11) gives

$$A^{-1}(\hat{A}x', \hat{A}y') = \int_T dt\ (\nabla_t \hat{A}x'(t) \mid \nabla_t \hat{A}y'(t)) = \langle x', \hat{A}y' \rangle_{L_{\pm}^{2,1}}.$$

The duality in $L_{\pm}^{2,1}$ is $\langle x', y \rangle = \int_T \dot{x}'_{\alpha}(t)\dot{y}^{\alpha}(t)\,dt$. Hence $\hat{A}$ is the canonical isomorphism $X' \to X$ defined by the metric on X. And

$$A(x', y') = A^{-1}(\hat{A}x', \hat{A}y') = \int_T dt\ g^{\gamma\delta}\dot{x}'_{\gamma}(t)\dot{y}'_{\delta}(t).$$

This example is possibly too trivial because the space of $L_{\pm}^{2,1}$ paths can be identified with its dual.

Example 2. Let X_+ be the space of continuous paths $x, y, \ldots$ vanishing at t_b. Let i be the inclusion mapping from the space of $L_{\pm}^{2,1}$ paths vanishing at t_b into X_+, $i: y \mapsto y$. Let A^{-1} be the bilinear form on X_+ induced by i from the bilinear form A^{-1} on X defined in example 1. The duality in X_+ is

$$\langle x', y \rangle = \int_T y^{\alpha}(t)\,dx'_{\alpha}(t)$$

and an arbitrary mapping $\hat{A}: X' \to X$ is of the form

$$(\hat{A}y')^{\alpha}(t) = \int_T G_+^{\alpha\beta}(t, s)\, \mathrm{d}y'_{\beta}(s) \qquad \text{with } G_+(t_b, s) = 0.$$

Equation (1.11) gives

$$A^{-1}(\hat{A}x', \hat{A}y') = \int_T \mathrm{d}t\, g_{\alpha\beta} \nabla_t \Big(\int_T G_+^{\alpha\gamma}(t, s)\, \mathrm{d}x'_{\gamma}(s) \Big) \nabla_t \Big(\int_T G_+^{\beta\delta}(t, r)\, \mathrm{d}y'_{\delta}(r) \Big)$$

$$= \int_T \mathrm{d}x'_{\alpha}(t) \int_T G_+^{\alpha\beta}(t, s)\, \mathrm{d}y'_{\beta}(s).$$

It is satisfied if $G_+(t, s)$ is the elementary kernel of $-\nabla_t \nabla_t$ such that $\mathrm{d}G_+(t_a, s)/\mathrm{d}t_a = 0$. Together with the previous condition $G_+(t_b, s) = 0$ and the fact that $G_+(t, s) = G_+(s, t)$ this determines G_+ uniquely.

In conclusion, the inverse of $A^{-1}(x, y) = \int_T (x(t) \mid y(t))\, \mathrm{d}t$ in the space of $L^{2,1}$ paths is $A(x', y') = \int_T (\dot{x}'(t) \mid y'(t))\, \mathrm{d}t$; its inverse in the spaces $X_{\pm}$ of continuous paths vanishing at t_b [vanishing at t_a] is the Wiener variance $A_{\pm}(x', y') = \int_T \mathrm{d}x'_{\alpha}(t) \int_T \mathrm{d}y'_{\beta}(s)\, G_{\pm}^{\alpha\beta}(t, s)$.

We have computed the inverse of A^{-1}, not the inverse of A. We may occasionally speak colloquially of A^{-1} as the inverse of A; we may also say that the elementary kernel G_A of an operator D_A that satisfies the boundary conditions C_A is the inverse of (D_A, C_A), and vice versa.

We have noted previously that it is simpler to work with the variance A than the covariance G_A; similarly it is easier to work with the "inverse" variance A^{-1} than with the "inverse" covariance (D_A, C_A) Covariances and inverse covariances are introduced in the last stages of the calculation.

Remark. $G_{\pm}$ are the reproducing kernels in the spaces of $L^{2,1}_{\pm}$ paths vanishing at t_b [vanishing at t_a], $(G_{\pm}(s, \cdot) \mid x(\cdot))_{L^{2,1}} = x(s)$.

How to use the Cameron–Martin formula for computing or simplifying path integrals. Consider the integral

$$I = \int_Y \mathrm{d}w_A(y) \exp\Big(\frac{-\mathrm{i}}{2} \int_T V_{\alpha\beta}(t) y^{\alpha}(t) y^{\beta}(t)\, \mathrm{d}t \Big) F(y).$$

We give first three different methods for simplifying this integral and then proceed to compute an example.

Method 1. Change of variable $M: Y \to X$

$$I = \int_X \mathrm{d}w_B(x) \exp\Big(\frac{-\mathrm{i}}{2} \int_T V_{\alpha\beta}(t) (M^{-1}x)^{\alpha}(t) (M^{-1}x)^{\beta}(t)\, \mathrm{d}t \Big) F(M^{-1}x)$$

By the Cameron–Martin formula

$$\mathrm{d}w_B(x) = \mathrm{d}w_A(x)\, \mathrm{Det}\, M^{-1} \exp\Big(\frac{1}{2} (A^{-1}(M^{-1}x, M^{-1}x) - A^{-1}(x, x)) \Big).$$

Choose M^{-1} such that

$$A^{-1}(M^{-1}x, M^{-1}x) - A^{-1}(x, x) - \int_T V_{\alpha\beta}(t)(M^{-1}x)^{\alpha}(t)(M^{-1}x)^{\beta}(t)\,dt = 0$$

i.e. choose M such that

$$A^{-1}(My, My) - A^{-1}(y, y) + \int_T V_{\alpha\beta}(t)y^{\alpha}(t)y^{\beta}(t)\,dt = 0. \tag{1.12}$$

Then

$$I = \operatorname{Det} M^{-1} \int_X dw_A(x)\, F(M^{-1}x).$$

Method 2. Change of prodistribution. Since the exponent is quadratic in y, there is a mapping $M^{-1}: X \to Y$ such that the image of w_A on X is w_B on Y satisfying

$$dw_A(y) \exp\left(\frac{-i}{2} \int_T V_{\alpha\beta}(t)y^{\alpha}(t)y^{\beta}(t)\,dt\right) = \operatorname{Det} M^{-1}\, dw_B(y).$$

Find w_B such that $B^{-1}(y, y) = A^{-1}(y, y) - \int_T V_{\alpha\beta}(t)y^{\alpha}(t)y^{\beta}(t)\,dt$, then

$$I = \operatorname{Det} M^{-1} \int_Y dw_B(y)\, F(y).$$

The second method (change of gaussian) is in general simpler than the first one (change of variable) because F is usually simpler than $F \circ M^{-1}$. The gaussian w_B incorporates more information about the system than w_A but it is still a gaussian and as easy to handle as w_A.

The second method is used in the application p. 276 and in sections 3.2, 3.3 and 3.4. Obviously both methods give the same answer:

$$\operatorname{Det} M^{-1} \int_X dw_A(x)\, F(M^{-1}x) = \operatorname{Det} M^{-1} \int_Y dw_B(y)\, F(y).$$

It is pleasing, nevertheless, to check it on an example. For instance if $F(y) = f(y(t_a))$ then

$$I = \operatorname{Det} M^{-1} \int_R du(2\pi i)^{-1/2}(\det G_B(t_a, t_a))^{-1/2} \exp\left(\frac{i}{2} u^2 / G_B(t_a, t_a)\right) f(u).$$

Using the first method and assuming M^{-1} to be of the form

$$M^{-1}: x \mapsto y \qquad \text{by } y(t) = x(t) + \int_T k(t, s)x(s)\,ds$$

then

$$F \circ M^{-1}(x) = f\Big(x(t_a) + \int_T k(t_a, s)x(s)\,\mathrm{d}s\Big).$$

Set $u = \langle \delta_{t_a} + \nu, x\rangle = x(t_a) + \int_T k(t_a, s)x(s)\,\mathrm{d}s,$

then

$$I = \operatorname{Det} M^{-1} \int_R \mathrm{d}u(2\pi\mathrm{i})^{-1/2}(\det W_A(\delta_{t_a} + \nu, \delta_{t_a} + \nu))^{-1/2} \exp\Big(\frac{\mathrm{i}}{2}u^2 \Big/ W_A(\delta_{t_a} + \nu, \delta_{t_a} + \nu)\Big) f(u)$$

$$W_A(\delta_{t_a} + \nu, \delta_{t_a} + \nu) = G_A(t_a, t_a) + 2\int_T k(t_a, s)G_A(s, t_a)\,\mathrm{d}s$$

$$+ \int_T \mathrm{d}s \int_T \mathrm{d}r\, k(t_a, s)k(t_a, r)G_A(s, r) = G_B(t_a, t_a)$$

Method 3. Any term in F which is an exponential of a linear or quadratic form in the variable of integration can be incorporated with w_A and give a new gaussian w_B. The following example will show the general procedure for incorporating quadratic forms. See the paragraph (p. 281) on affine transformation for incorporating linear forms.

Application. Compute the path integral given by eq. (1.8). We shall use the second method. The problem consists in finding $M^{-1}: X_+ \to Y_+$ such that

$$A^{-1}(My, My) - A^{-1}(y, y) = -\int_T V_{\alpha\beta}(t)y^\alpha(t)y^\beta(t)\,\mathrm{d}t + S_{\alpha\beta}y^\alpha(t_a)y^\beta(t_a)$$

for the case where A is the Wiener variance

$$A(\mu, \nu) = \int_T \mathrm{d}\mu_\alpha(r) \int_T \mathrm{d}\nu_\beta(s)G_A^{\alpha\beta}(r, s), \tag{1.13}$$

with

$$G_A^{\alpha\beta}(t, s) = g^{\alpha\beta}(\theta(t - s)(t_b - t) + \theta(s - t)(t_b - s)),$$

$g_{\alpha\beta}$ being the euclidean metric on $\mathbf{R}^n$. $G_A(t, s)$ is the elementary kernel of $D_A = -g_{\alpha\beta}\,\mathrm{d}^2/\mathrm{d}s^2$ with boundary conditions $C_A \cdot G_A(t, t_b) = 0$, $\mathrm{d}G_A(t, t_a)/\mathrm{d}t_a = 0$.

A^{-1} is a bilinear form on Y_+ which is determined by G_A, and vice versa. For instance if A is the Wiener variance, then

$$A^{-1}(y, y) = \int_T \|y(t)\|^2\,\mathrm{d}t \qquad y \in Y_+ \tag{1.14}$$

$$= -\int_T (y(t) \mid y(t))\,\mathrm{d}t - (y(t_a) \mid y(t_a)). \tag{1.15}$$

We seek G_B such that

$$B^{-1}(y, y) = A^{-1}(My, My)$$

$$= -\int_T (g_{\alpha\beta}y^\alpha(t) + V_{\alpha\beta}(t)y^\alpha(t))y^\beta(t)\,dt - (g_{\alpha\beta}\dot{y}^\alpha(t_a) - S_{\alpha\beta}y^\alpha(t_a))y^\beta(t_a) \tag{1.16}$$

It follows that $G_B(t, s)$ is the elementary kernel of $D_B = -g_{\alpha\beta}\,d^2/dt^2 - V_{\alpha\beta}(t)$.

In appendix B (p. 357) we give the elementary kernel G of an operator D in terms of its solutions $K(r, t_a)$, $J(r, t_b)$ and their inverses. Covariances G_+ of gaussians on Y_+ are given by

$$G_+(r, s) = \theta(s - r)K(r, t_a)N(t_a, t_b)J(t_b, s) - \theta(r - s)J(r, t_b)\tilde{N}(t_b, t_a)\tilde{K}(t_a, s).$$

Let $K_A(t, t_a)$ and $K_B(t, t_a)$ be the solutions of D_A and D_B respectively satisfying the boundary conditions

$$K_A^{\alpha\beta}(t_a, t_a) = g^{\alpha\beta}, \qquad dK_A^{\alpha\beta}(t, t_a)/dt_a\Big|_{t=t_a} = 0$$

$$K_B^{\alpha\beta}(t_a, t_a) = g^{\alpha\beta}, \qquad dK_B^{\alpha\beta}(t, t_a)/dt_a\Big|_{t=t_a} = S_{\alpha\beta}(t_a).$$

Let $J_A(t, t_a)$ and $J_B(t, t_a)$ be the solutions of D_A and D_B respectively satisfying the same boundary conditions: $J^{\alpha\beta}(t_a, t_a) = 0$, $dJ^{\alpha\beta}(t, t_a)/dt_a|_{t=t_a} = g^{\alpha\beta}$. Let C_B be the corresponding boundary conditions for G_B. Note that the boundary conditions for G_B are more complicated than the boundary conditions for G_A because we chose an application in which $S_{\alpha\beta}(t_a) \neq 0$ for greater generality.

Having determined the covariances G_A, G_B as the elementary kernels of (D_A, C_A) and (D_B, C_B), we obtain immediately the ratio of their determinants from equation (B.18). Thus the integral I given by eq. (1.8) can be written

$$I = \operatorname{Det} M^{-1} \int_{X_+} dw_B(x) = \operatorname{Det} M^{-1} = (\operatorname{Det} G_B^{\alpha\beta}(t, s)/\operatorname{Det} G_A^{\alpha\beta}(t, s))^{1/2}$$

$$= (\det K_B^{\alpha\beta}(t_b, t_a)/\det K_A^{\alpha\beta}(t_b, t_a))^{-1/2}. \tag{1.17}$$

The problem is solved without computing M, without even computing w_B. We only know G_B as being the elementary kernel of (D_B, C_B). The path integral I given by eq. (1.8) appears in section 3.2 as the solution of a partial differential equation satisfying some Cauchy data; it is computed here in terms of the determinant of two finite dimensional matrices, themselves obtained by solving ordinary, second order, linear homogeneous differential equations.

Fredholm determinants. In the previous application we have unobtrusively computed the determinant of a linear mapping $M^{-1}: X_+ \to Y_+$. But of which mapping M^{-1} we do not know yet. We know that M^{-1} is such that the image of the gaussian w_A on X_+ is w_B on Y_+; we do not know explicitly w_A and w_B, we only know that their covariances are the elementary kernels of D_A and D_B satisfying some boundary conditions C_A and C_B respectively. We shall proceed to determine M^{-1} explicitly on this basis. Since all our computations can be made only with the second method, we work with M^{-1}, not with M.

Problem: Let w_A be the Wiener measure on X_+, let the covariance G_B of its image under M^{-1} be the elementary kernel of (D_B, C_B). Find M^{-1}.

Answer: Since the Wiener measure w_A on X_+ is the image of the canonical gaussian on $\mathscr{H}$ under the primitive mapping P^{W} introduced on p. 270,

$$P_+^{\mathrm{W}}: \mathscr{H} \to X_+ \qquad \text{by } x(t) = -\int_t^{t_b} h(s)\,\mathrm{d}s, \tag{1.18}$$

we expect the gaussian w_B on Y_+ to be the image of the canonical gaussian on $\mathscr{H}$ under the generalized primitive mapping [94]

$$P_+: \mathscr{H} \to Y_+ \qquad \text{by } y(t) = -\int_t^{t_b} F(t,s)h(s)\,\mathrm{d}s \tag{1.19}$$

where the kernel F is such that $F(\cdot, s)h(s) \in \mathscr{H}$. The covariance of w_B is then

$$G_B^{\alpha\beta}(r,s) = \theta(r-s)\int_r^{t_b} F_\gamma^\alpha(r,t)F_\delta^\beta(s,t)g^{\gamma\delta}\,\mathrm{d}t + \theta(s-r)\int_s^{t_b} F_\gamma^\alpha(r,t)F_\delta^\beta(s,t)g^{\gamma\delta}\,\mathrm{d}t. \tag{1.20}$$

F is uniquely determined by the conditions imposed on G_B and found to be equal to*

$$F_\gamma^\alpha(r,t) = K_B^{\alpha\beta}(r,t_a)N_{\beta\gamma}^B(t_a,t) \tag{1.21}$$

where $K_B(r,t_a)$ as a function of r is the solution of

$$D_B K_B(r,t_a) = 0, \qquad K_B^{\alpha\beta}(t_a,t_a) = g^{\alpha\beta}, \qquad \mathrm{d}K_B^{\alpha\beta}(r,t_a)/\mathrm{d}r|_{r=t_a} = S^{\alpha\beta}(t_a), \tag{1.22}$$

$N(t_a,r)$ is the "inverse" of $K(r,t_a)$ in the sense that:

$$K_B^{\alpha\beta}(r,t_a)N_{\beta\gamma}^B(t_a,r) = \delta_\gamma^\alpha \tag{1.23}$$

Knowing P_+ and P_+^{W}, we can easily determine M since

$$P_+ = M^{-1} \circ P_+^{\mathrm{W}}.$$

A straightforward calculation gives $M^{-1}: X_+ \to Y_+$ by

$$y(t) = x(t) + \int_t^{t_1} \frac{\partial F(t,s)}{\partial s} x(s)\,\mathrm{d}s \;=\; x(t) + K_B(t,t_a)\int_t^{t_b} \frac{\mathrm{d}N^B(t_a,s)}{\mathrm{d}s} x(s)\,\mathrm{d}s \tag{1.24}$$

and the problem is solved. ■

Remark. The spaces Y_- and X_- are as important in practice as the spaces Y_+ and X_+, and to have on record the corresponding expressions for them we summarize the procedure for finding $M_\pm^{-1}: X_\pm \to Y_\pm$ and their determinants for both cases together.

$$\text{Let } P_\pm: \mathscr{H} \to Y_\pm \quad \text{by} \quad y(t) = \mp\int_T \theta_\pm(s-t)F_\pm(t,s)h(s)\,\mathrm{d}s$$

*No summation over B intended, the labels B are placed in upper or lower position solely for typographical convenience

where θ_+ is the usual step up function θ equal to one for positive arguments and zero otherwise, and θ_- is the step down function $\theta_-(t-s)=\theta_+(s-t)$. The image under $P_\pm$ of the canonical gaussian on $\mathscr{H}$ is the gaussian of covariance

$$G_B^\pm(r,s)=\theta_\pm(r-s)\int_T \theta_\pm(t-r)F_\pm(s,t)F_\pm(r,t)g^{-1}\,dt+\theta_\pm(s-r)\int_T \theta_\pm(t-s)F_\pm(r,t)F_\pm(s,t)g^{-1}\,dt.$$

$G_B^\pm$ is the elementary kernel of $(D_B, C_B^\pm)$ if and only if

$$F_+(t,s)=K_B(t,t_a)N^B(t_a,s),\qquad F_-(t,s)=K_B(t,t_b)N^B(t_b,s)$$

where, $S_{\alpha\beta}$ being the matrix in eq. (1.8),

$$D_BK_B(t,t_a)=0,\qquad K_B(t_a,t_a)=g^{-1},\qquad \left.\frac{dK_B(t,t_a)}{dt}\right|_{t=t_a}=S.$$

Since $P_\pm=M_\pm^{-1}\circ P_\pm^W$, $\quad M_\pm^{-1}: x\mapsto y$ by

$$y(t)=x(t)\pm\int\theta_\pm(s-t)\frac{\partial F_\pm(t,s)}{\partial s}x(s)\,ds.$$

Set

$$k_+(r)=\frac{dK_B(r,t_a)}{dr}N_B(t_a,r),\qquad k_-(r)=\frac{dK_B(r,t_b)}{dr}N_B(t_b,r).$$

Then $M: y\mapsto x$ by

$$x(t)=y(t)\pm\int_T\theta_\pm(s-t)k_\pm(s)y(s)\,ds.$$

$$\text{Det } M_+^{-1}=(\det K_B(t_b,t_a)/\det K_A(t_b,t_a))^{-1/2},\qquad \text{Det } M_-^{-1}=(\det K_B(t_a,t_b)/\det K_A(t_a,t_b))^{-1/2}.$$

Now that M^{-1} has been determined, we can check on this example that Det M^{-1} given by

$$(\text{Det } M^{-1})^2=\text{Det } G_B(r,s)/\text{Det } G_A(r,s)$$

is the Fredholm determinant of the linear mapping M^{-1}. One expects this to be so from the analysis of the finite dimensional case, but saying that the infinite dimensional case is the limit of the finite dimensional case when the number of dimension goes to infinity is a treacherous procedure, best to be avoided. We shall thus compute Det M^{-1} by a procedure which exhibits the Fredholm determinant in its usual form – or rather we shall compute Det M which is simpler.

$M: Y_+\to X_+$ is given by

$$x(t)=y(t)+\int_t^{t_b}\frac{dK_B}{dr}(r,t_a)N^B(t_a,r)y(r)\,dr. \tag{1.25}$$

Indeed eq. (1.24) gives

$$N^B(t_a,t)(y(t)-x(t))=\int_t^{t_b}\frac{dN^B}{ds}(t_a,s)x(s)\,ds.$$

Differentiation and simple algebraic manipulation gives (1.25). This derivation shows that M is unique ■

Knowing M, the computation of Det M goes as follows: Set

$$k^{\alpha}_{\beta}(t, r) = \theta(r-t)k^{\alpha}_{\beta}(r) = \theta(r-t)\frac{dK^{\alpha\gamma}_{B}(r, t_a)}{dr}N^{B}_{\gamma\beta}(t_a, r)$$

and assume that the undefined quantity $k(r, r)$ equals

$$\tfrac{1}{2}k(r^{+}, r) + \tfrac{1}{2}k(r^{-}, r) = \tfrac{1}{2}k(r).$$

This assumption, standard in theory of Fredholm determinants of Volterra equations, can be justified here by the fact that both calculations of Det M (eqs. (1.16) and (1.26)) give the same result:

$$\text{Det } M = \exp(tr \log(1 + k(t, r))) = \sum_{n=0}^{\infty}\frac{1}{n!}\int_{T} dr_1 \ldots \int_{T} dr_n \det_{(i,j)}[\theta(r_j - r_i)k^{\alpha_i}_{\alpha_j}(r_j)]$$

$$= \exp\int_{T}\tfrac{1}{2}tr\, k(t)\, dt = \exp\int_{T} -\tfrac{1}{2}tr\, K_B(t, t_a)\frac{dN_B}{dt}(t_a, t)\, dt$$

$$= (\det K_B(t_b, t_a)/\det K_B(t_a, t_a))^{1/2}. \tag{1.26}$$

Since $\det K^{\alpha\beta}_{A}(t_b, t_a) = g^{\alpha\beta}$ and $\det K_B(t_a, t_a) = g^{\alpha\beta}$, the result is proved. ■

The various games we have played in this section have given us two methods for computing the Fredholm determinants of linear mappings from $L^{2,1}_{\pm}(T)$ into $L^{2,1}_{\pm}(T)$ of the type defined by eq. (1.24).

1. Take a simple gaussian w_A on Y_+, map Y_+ into X_+ by M, and compute the image of w_A under M. Determine the "inverses" (D_A, C_A) and (D_B, C_B) of the covariances G_A, G_B of w_A and w_B,

$$(\text{Det } M)^2 = \det K_B(t_b, t_a)/\det K_A(t_b, t_a)$$

where

$$D_A K_A(t, t_a) = 0, \qquad K^{\alpha\beta}_{A}(t_a, t_a) = g^{\alpha\beta}, \qquad \left.\frac{dK^{\alpha\beta}_{A}(t, t_a)}{dt}\right|_{t=t_a} = 0$$

and where K_B is given by a similar equation. The Fredholm determinant of linear mappings from Y_- into X_- is obtained similarly.

2. It often happens that there are two mappings $P_A : H \to X_+$ and $P_B : H \to Y_+$, simpler than M, such that $P_B = M^{-1} \circ P_A$. Take a simple gaussian on H. Let w_A and w_B be its images under P_A and P_B respectively and then proceed as above.

In this section the key elements have been the coordinate free symmetric bilinear forms A^{-1} on X_+ and B^{-1} on Y_+ (eqs. (1.14) and (1.16)), induced by the variances A and B on the duals of X_+ and Y_+ respectively. Y_+ and X_+ are $L^{2,1}(T)$ spaces, i.e. spaces of $L^{2,1}$ functions* on T. So is the action $S(f) = \int_T L(f(t), \dot{f}(t))\, dt$ Moreover the second variation of S is, like A^{-1} and B^{-1}, a symmetric bilinear form on $L^{2,1}(T)$ and the methods developed here have wide application in physics [e.g. 37, 40].

*A function is $L^{2,1}$ if it is square integrable as well as its first order weak derivatives (derivatives in the sense of distributions)

Affine transformations. The linear Cameron–Martin transformations were introduced to simplify the computation of integrals of type (1.8) with quadratic terms. In this section we study the image of a gaussian under an affine mapping and develop a method for computing or simplifying integrals with linear terms in the exponent.

Recall the finite dimensional case with $x, y, l \in \mathbb{R}^n$. Under the affine transformation $x = y + l$, the gaussian w on $\mathbb{R}^n$ of variance $\mathcal{W}$ becomes a shifted gaussian w_l whose Fourier transform is

$$\mathcal{F}w_l(x') = \exp(-\mathrm{i}x'_i l^i) \exp(-\tfrac{1}{2}\mathrm{i}\mathcal{W}^{ij}x'_i x'_j).$$

Let $M: Y_+ \to Y_+$ by $M(y) = y + l$. Let w be the gaussian of variance W on Y_+, let w_l be its image under the affine mapping M. Then

$$\mathcal{F}w_l(\mu) = \exp(-\mathrm{i}\langle \mu, l\rangle) \exp(-\tfrac{1}{2}\mathrm{i}W(\mu, \mu)).$$

Again $\mathrm{d}w$ and $\mathrm{d}w_l$ are not defined but their ratio is defined:

$$\mathrm{d}w_l(x) = \mathrm{d}w(x) \exp\left\{\frac{\mathrm{i}}{2}\int_T \|l(t)\|^2\,\mathrm{d}t - \mathrm{i}\int_T (l(t) \mid \mathrm{d}x(t))\right\}.$$

The affine mapping, like the linear mapping (see p. 274) can be used in two different ways depending on whether one prefers to integrate the original integrant with respect to w_l or to integrate the shifted integrand with respect to w. Consider the integral

$$I = \int_{Y_+} \mathrm{d}w(y) \exp\left\{\mathrm{i}\int_T (a(t) \mid \mathrm{d}y(t))\right\} F(y).$$

Under the affine change of variable $M: Y_+ \to X_+$ the integral becomes

$$I = \int_{X_+} \mathrm{d}w_l(x) \exp\left(\mathrm{i}\int_T (a(t) \mid \mathrm{d}(M^{-1}x)(t))\right) F(M^{-1}x).$$

Choose M^{-1} such that

$$\mathrm{i}\int_T \|l(t)\|^2\,\mathrm{d}t - \mathrm{i}\int_T (\dot{l}(t) \mid \mathrm{d}x(t)) + \mathrm{i}\int_T (a(t) \mid \mathrm{d}(M^{-1}x)(t)) = 0$$

i.e. choose M such that $M^{-1}x = x - l$ with $a(t) = \dot{l}(t)$, $l(t) = -\int_t^{t_b} a(s)\,\mathrm{d}s$. Then

$$I = \exp\left(-\frac{1}{2}\int_T \|\dot{l}(t)\|^2\,\mathrm{d}t\right) \int_{X_+} \mathrm{d}w(x)\, F(x - l). \tag{1.27}$$

Note that under the mapping $M^{-1}: X_+ \to Y_+$ the image of w on X_+ *is* $w_{(-l)}$ on Y_+ satisfying

$$\mathrm{d}w_{(-l)}(y) = \mathrm{d}w(y) \exp\left(\frac{\mathrm{i}}{2}\int \|l(t)\|^2\,\mathrm{d}t + \mathrm{i}\int (l(t) \mid \mathrm{d}y(t))\right).$$

Then, if $l(t) = -\int_t^{t_b} a(s)\,ds$,

$$I = \exp\left(-\tfrac{1}{2}\int_T \|\dot{l}(t)\|^2\,dt\right)\int_{Y_+} dw_{(-l)}(y)\,F(y) \tag{1.28}$$

and we have obtained another expression for computing I.

If $l(t_b) \neq 0$, then $M: Y_+ \to Y_+^l$ where Y_+^l is not a vector space unless one defines addition by the prescription given p. 291. The formulae given in this section are still valid. Note that the dual of Y_+^l is slightly different from the dual of Y_+.

1.6. *Space of paths with both ends fixed*

A path integral is often over a space of paths with both ends fixed. A space of paths x such that $x(t_a) = a$, $x(t_b) = b$ is a vector space only if $a = b = 0$. Indeed $x, y \in X$ implies $x + y \in X$ only if $(x + y)(t_a) = x(t_a) = y(t_a)$ which in turn implies $a = b = 0$. Let X be the space of continuous paths x on T such that $x(t_a) = x(t_b) = 0$. X can be treated equally well as a subspace of X_+ or X_-. Say $X \subset X_-$. Given a prodistribution w_- on X_-, one can define a prodistribution w on X associated to w_- as follows.

Recall first the finite dimensional case: Given a measure on $\mathbf{R}^n$, the measure of an $n-1$ dimensional surface $S \subset \mathbf{R}^n$ is zero. Nevertheless there is a natural and convenient way to introduce a measure on S associated to the measure on $\mathbf{R}^n$, namely the **Leray form**: Let S be a subset of $\mathbf{R}^n$ of codimension one* defined by the irreducible equation $S(u) = C$, $u \in \mathbf{R}^n$. The **Leray form ω on S associated to the measure γ on $\mathbf{R}^n$** is defined by the equation

$$dS \wedge d\omega = d\gamma. \tag{1.29}$$

For example the Leray form on the plane $u_2 = C$ associated to the gaussian γ on $\mathbf{R}^2$

$$d\gamma(u_1, u_2) = (2\pi a)^{-1/2}(2\pi b)^{-1/2}\exp(-u_1^2/2a - u_2^2/2b)\,du_1\,du_2$$

is

$$d\omega(u) = (2\pi a)^{-1/2}(2\pi b)^{-1/2}\exp(-u^2/2a - C^2/2b)\,du.$$

Note that ω is not the normalized gaussian on $\mathbf{R}$.

The Leray form ω on S associated to the Lebesgue measure on $\mathbf{R}^n$ defines the Dirac measure δ_S on S by

$$\langle \delta_S, \psi\rangle = \int_S \psi\,d\omega. \tag{1.30}$$

The space X of paths with both ends fixed is a subset of X_- of codimension one and we can generalize the notion of Leray forms to define a prodistribution w on X associated in the Leray sense to a given prodistribution w_- on X_-. A prodistribution is by definition a family of distributions on a projective system of finite dimensional spaces. To each finite dimensional space X_-/V_- of the

* I.e. the dimension of S is $n-1$. The more general terminology is introduced here to prepare the infinite dimensional case.

projective system of X_- corresponds a finite dimensional space X/V of the projective system of X such that V is defined by one more equation than V_-, namely $\langle \delta_{t_b}, x\rangle = 0$.

Definition. Let $V \in X_-$, and let V be defined by $\langle \delta_{t_b}, x\rangle = 0$ and by the equations defining V_-. A **prodistribution** w **on** X is said to be **associated in the Leray sense to the prodistribution** w_- **on** X_- if the distribution on X/V is Leray related to the distribution on X_-/V_-.

Leray associated gaussians. Let χ be the characteristic function* of $X \subset X_-$. Let w_- be a gaussian on X_- with variance W_- and covariance G_-. It follows from the definition that the prodistribution w on X, Leray related to w_- on X_-, is the gaussian normalized to

$$w(X) = \int_{X_-} \chi(x)\, \mathrm{d}w_-(x) \tag{1.31}$$

of covariance (see eq. (1.6))

$$\mathrm{i}G(r, s) = \int_{X_-} \chi(x)\langle \delta_r, x\rangle\langle \delta_s, x\rangle\, \mathrm{d}w_-(x)/w(X). \tag{1.32}$$

These cylindrical integrals are readily computed. Let

$$P : X_- \to \mathbf{R}^n \text{ by } x \to \{u^\alpha = \langle \delta^\alpha_{t_b}, x\rangle = x^\alpha(t_b)\}, \text{ then} \tag{1.33}$$

$$w(X) = \int \mathrm{d}u^1 \ldots \mathrm{d}u^n\, \delta(u^1)\ldots\delta(u^n)(2\pi\mathrm{i})^{-n/2}|\det G_-^{\alpha\beta}(t_b, t_b)|^{-1/2} \exp\left(\frac{1}{2}u^\alpha u^\beta (G_-(t_b, t_b))^{-1}_{\alpha\beta}\right)$$
$$= (2\pi 1)^{-n/2}|\det G_-^{\alpha\beta}(t_b, t_b)|^{-1/2}. \tag{1.34}$$

The covariance $G(r, s)$ can be computed by the same method.

*Prodistributions on $L^{2,1}$ spaces.*** The covariances $G_\pm$ on spaces of $L^{2,1}$ paths vanishing either at t_b or t_a are elementary kernels of a second order linear differential operator D. It follows from the definition† that the covariance G of the prodistribution w on X Leray associated to either w_- or w_+ is the elementary kernel of the same operator D such that

$$G(r, s) = 0 \qquad \text{for } r \text{ or } s \text{ equal to } t_a \text{ or } t_b.$$

The covariance G is the Green's function of the operator D in the strict sense of the term, namely G is the elementary kernel of a positive second order linear differential operator that vanishes on the boundary and that is C^∞ except on the diagonal. When D is the Jacobi operator (alias the operator for small disturbances) G is known as the **Feynman–Green function**.

Example. The gaussian w^{W} on X associated in the Leray sense to the Wiener gaussian w^{W}_- on X_- is the gaussian normalized to

$$w^{\mathrm{W}}(X) = (2\pi\mathrm{i}(t_b - t_a))^{-n/2}(\det g_{\alpha\beta})^{1/2},$$

*$\chi(x) = 1$ for every $x \in X$ and zero otherwise

**See footnote, p 280

†Use the definition together with the expression given p 272 for $\mathrm{d}w_A(y)$ on finite dimensional spaces and note that A^{-1} is the same for $w_\pm$ and w

its covariance is

$$G^{W\alpha\beta}(t,s) = -g^{\alpha\beta}(\theta(s-t)(t-t_a)(t_a-t_b)^{-1}(t_b-s) + \theta(t-s)(t-t_b)(t_b-t_a)^{-1}(t_a-s)). \tag{1.35}$$

Lemma.

$$\int_{X_+} F(x)\,\mathrm{d}w_+(x)\delta(x(t_a)) = \int_{X_-} F(x)\,\mathrm{d}w_-(x)\delta x(t_b) = \int_X F(x)\,\mathrm{d}w(x). \tag{1.36}$$

Proof. It is sufficient to prove that this equation is true for cylindrical functions, $F(x) = f \circ P(x)$. Without loss of generality we shall prove it with $P: x \mapsto u^1 = \langle \mu, x \rangle$.

$$I = \int_{X_+} f \circ P(x)\,\mathrm{d}w_+(x)\delta(x(t_a)) = (2\pi\mathrm{i})^{-1}(\det \mathcal{W}_{+ij})^{-1/2} \int_{R^2} f(u^1)\delta(u^2)\,\mathrm{d}u^1\,\mathrm{d}u^2 \exp\tfrac{\mathrm{i}}{2}u^i u^j (\mathcal{W}_+^{-1})_{ij}$$

where

$$\mathcal{W}_{+ij} = \begin{pmatrix} W_+(\mu,\mu) & W_+(\mu,\delta_{t_a}) \\ W_+(\delta_{t_a},\mu) & W_+(\delta_{t_a},\delta_{t_a}) \end{pmatrix}.$$

On the other hand

$$J = \int_X f \circ P(x)\,\mathrm{d}w(x) = (2\pi\mathrm{i})^{-1/2}(G_+(t_a,t_a))^{-1/2}(2\pi\mathrm{i})^{-1/2}\mathcal{W}^{-1/2} \int_R f(u)\,\mathrm{d}u \exp\tfrac{1}{2}u^2\mathcal{W}^{-1}$$

where $\mathcal{W} = W(\mu,\mu)$. The integrals I and J are equal if $(\mathcal{W}_+^{-1})_{11} = \mathcal{W}^{-1}$, i.e.

$$\mathcal{W}G_+(t_a,t_a) = \det \mathcal{W}_{+ij}. \tag{1.37}$$

If $\mu = \delta_{t_k}$ for an arbitrary t_k then eq. (1.37) follows from eq. (B17). The proof for arbitrary μ can be checked on specific examples. ∎

2. Product integrals

Introduced by Volterra [140] in 1896, product integrals are a simple and rigorous vehicle for Feynman's operator calculus [55]: They yield results quickly and provide explicit error estimates. Product integration has been developed recently by Dollard and Friedman [44] who have used it, in particular, to obtain the asymptotic behavior of positive energy solutions of the Schrödinger equation. As an immediate application of their theorems they prove the non-existence of positive energy bound states for some classes of potentials and the possible existence of such states for others. For example they show that $E = 1$ is the only positive energy for which the Wigner–Von Neumann potential [141, 130] can have a positive-energy bound state.

Interesting applications of product integrals to Brownian motions on a Lie group have been developed by McKean [99, p. 115 and references quoted therein].

After a brief introduction to product integrals, we shall use them to obtain a path integral solution of the Schrodinger equation, known as the Feynman–Kac formula, or the Trotter–Kato–Nelson [117] product formula.

2.1. Definition and properties of product integrals

There is a strong formal analogy between the theory of product integration and the usual theory of Riemann integration; product integration is to products what Riemann integration is to sums. The additive neutral element 0 becomes the multiplicative neutral element 1 (the identity matrix), the additive inverse $-A$ becomes the multiplicative inverse A^{-1}, etc.

A Riemann integral $f(t) = \int_{t_a}^{t} g(s)\,\mathrm{d}s$ can be introduced as the solution of the differential equation $\mathrm{d}f(t)/\mathrm{d}t = g(t)$ such that $f(t_a) = 0$. Similarly a product integral

$$U(t) = \prod_{t_a}^{t} \exp(A(s)\,\mathrm{d}s)U(t_a)$$

can be introduced as the solution of the differential equation

$$\frac{\mathrm{d}U}{\mathrm{d}t} = A(t)U(t), \qquad \text{equal to } U(t_a) \text{ at } t = t_a. \tag{2.1}$$

Let $\mathbb{C}_n$ be the set of $n \times 1$ matrices with complex entries, and $\mathbb{C}_{n\times n}$ be the set of $n \times n$ matrices with complex entries. The norms are defined as follows. Let α^i be the entries of $\alpha \in \mathbb{C}_n$, and let $\beta \in \mathbb{C}_{n\times n}$,

$$\|\alpha\| = \left(\sum_{i=1}^{n} |\alpha^i|^2\right)^{1/2}, \qquad \|\beta\| = \sup\|\beta\alpha\|$$

where the supremum is over all α in $\mathbb{C}_n$ such that $\|\alpha\| = 1$. Throughout this section A, B are continuous functions from $[t_a, t_b]$ into $\mathbb{C}_{n\times n}$ and V is a differentiable function from $[t_a, t_b]$ into $\mathbb{C}_n$.

An approximate solution of eq. (2.1) can be obtained by making a partition* $\theta_{v+1} = \{t_a, s_1, \ldots, s_{v+1} = t\}$ of $[t_a, t]$ with $\Delta s_i = s_i - s_{i-1}$. Let $\mu(\theta_{v+1})$ denote the mesh of θ_{v+1}, i.e. the length of its longest subinterval. Then**

$$U(t) \approx \left\{\prod_{i=1}^{v+1} \exp(A(s_i)\Delta s_i)\right\}U(t_a). \tag{2.2}$$

Volterra has shown [140] the existence of the limit of this product when $\mu(\theta_{v+1})$ goes to zero; it is thus possible to define a product integral as follows.

Definition. Let $A:[t_a, t_b] \to \mathbb{C}_{n\times n}$. The **product integral** of A over $[t_a, t_b]$ is defined by

$$\prod_{T} \exp(A(t)\,\mathrm{d}t) = \lim_{\mu(\theta_{v+1})=0} \prod_{i=1}^{v+1} \exp(A(t_i)\Delta t_i).$$

Some of the properties of product integrals are well known by physicists who have done similar manipulations. The notation of product integrals allows a swift presentation of these properties and of others. It makes possible concise statements of rigorous results which otherwise would be cumbersome. We shall begin by a property which simplifies many other statements.

Property 0. Let $A:[t_a, t_b] \to \mathbb{C}_{n\times n}$, then $\Pi_s^t \exp(A(r))\,\mathrm{d}r$ is non-singular, in the sense that the mapping $\Pi_s^t \exp(A(r)\,\mathrm{d}r)$: $\mathbb{C}_n \to \mathbb{C}_n$ has a non-vanishing determinant.

*The partitions of a time interval $[t_a, t_b]$ are chosen throughout so that $t_a = t_0$, $t_b = t_{v+1}$ for later convenience in going from $X_\pm$ to X

**$\exp(B) = \Sigma_{n=0}^{\infty} B^n/n!$

Proof. Use the definition and the determinant trace relationship,

$$\det \prod_s^t \exp(A(r)\,dr) = \exp \int_s^t tr\,A(r)\,dr \neq 0.$$

Property 0 allows the following definitions, analogous to that in the ordinary theory of integration:

$$\prod_t^t \exp(A(r)\,dr) = \mathbf{1},$$

$$\prod_t^s \exp(A(r)\,dr) = \left\{\prod_s^t \exp(A(r)\,dr)\right\}^{-1}.$$

This definition removes in many statements the necessity of ordering the limits of integration. In the following properties, several proofs are obvious for $s < t$ and generalized to arbitrary s and t by this definition.

Property 1

$$\frac{d}{dt}\prod_s^t \exp(A(r)\,dr) = A(t)\prod_s^t \exp(A(r)\,dr), \qquad \frac{d}{ds}\prod_s^t \exp(A(r)\,dr) = -\prod_s^t \exp(A(r)\,dr)A(s).$$

Property 2

$$\prod_s^t \exp(A(u)\,du) = \prod_r^t \exp(A(u)\,du)\prod_s^r \exp(A(u)\,du).$$

Property 3. Let $\{A(r); r \in [t_a, t_b]\}$ *be a commutative family, then*

$$\prod_s^t \exp(A(r)\,dr) = \exp \int_s^t A(r)\,dr.$$

Property 4 (The sum rule). *Let* $P(t, s) = \prod_s^t \exp(A(r)\,dr)$, *then one can write either*

$$\prod_s^t \exp(A(r)\,dr + B(r)\,dr) = P(t, s)\prod_s^t \exp(P(s, r)B(r)P(r, s)\,dr)$$

or

$$\prod_s^t \exp(A(r)\,dr + B(r)\,dr) = \prod_s^t \exp\{P(t, r)B(r)P(r, t)\,dr\}P(t, s).$$

Proof. If $F(t, s)$ denotes either side of these equations, compute $\partial F(t, s)/\partial s$ to prove the second.

Property 5 (The similarity rule). *Suppose that* $T : [t_a, t_b] \to \mathbf{C}_{n\times n}$ *has a continuous derivative* T' *and suppose that* $T(t)$ *is non-singular for all* $t \in [t_a, t_b]$, *then*

$$T^{-1}(t)\prod_s^t \exp\{A(r)\,dr\}T(s) = \prod_s^t \exp\{T^{-1}(r)A(r)T(r)\,dr - T^{-1}(r)T'(r)\,dr\}.$$

The proof is similar to the previous one after multiplying both sides on the left by $T(t)$.

The following properties give error estimates and make possible the definition of improper product integrals when one of the limits of integration goes to infinity.

Property 6. Let $s \leqslant t$, then

$$\left\| \prod_s^t \exp(A(r)\,dr) \right\| \leqslant \exp \int_s^t \|A(r)\|\,dr.$$

Property 7. Let $s \leqslant t$, then

$$\left\| \prod_s^t \exp(A(v)\,dv) - 1 \right\| \leqslant \exp\left(\int_s^t \|A(r)\|\,dr \right) - 1.$$

Proof. Because of property 1

$$\prod_s^t \exp(A(r)\,dr) = 1 + \int_s^t dr\, A(r) \prod_s^r \exp(A(u)\,du).$$

Using Property 6

$$\left\| \prod_s^t \exp(A(r)\,dr) - 1 \right\| \leqslant \int_s^t dr \|A(r)\| \exp\left\{ \int_s^r \|A(u)\|\,du \right\} = \exp\left\{ \int_s^t \|A(u)\|\,du \right\} - 1.$$

Improper product integrals. Provided the indicated limit exists, we define the improper product integral

$$\prod_{t_a}^{\infty} \exp(A(t)\,dt) = \lim_{t_b=\infty} \prod_{t_a}^{t_b} \exp(A(t)\,dt).$$

An improper integral can be singular. For instance, let $A(t) = -1$ for all t then

$$\lim_{t_b=\infty} \prod_{t_a}^{t_b} \exp(-1\,ds) = \lim_{t_b=\infty} \exp(-1(t_b - t_a)) = 0.$$

Since we are interested in product integrals as solutions of eq. (2.1) we need to determine the conditions under which the improper integral of A over $[t_a, \infty)$ exists and is nonsingular. When it is singular det $U(t)$ has a zero limit for $t = \infty$, for nonzero $U(t_a)$.

The following properties have been used to determine the possible existence of positive-energy bound states, and to study cases of "anomalous" behavior of the wave-function [43]. They give existence theorems for the Feynman-Kac formula (see section 2.3).

Property 8. Let $A : [t_a, \infty) \to C_{n\times n}$ be in $L^1(t_a, \infty)$, i.e.

$$\int_{t_a}^{\infty} \|A(t)\|\,dt < \infty, \quad \textit{then} \prod_{t_a}^{\infty} \exp(A(t)\,dt) \textit{ exists and is nonsingular.}$$

Corollary. Let A and $B:[t_a,\infty)\to C_{n\times n}$; suppose that $\prod_{t_a}^{\infty}\exp(A(t)\,dt)$ exists and is non-singular and suppose that B is in $L^1(t_a,\infty)$ (A is not necessarily in $L^1(t_a,\infty)$), then

$$\prod_{t_a}^{\infty}\exp\{A(r)\,dr+B(r)\,dr\}\ \text{exists and is non-singular}$$

Property 9. Suppose that the improper integral $H(t_a)=\operatorname{imp}\int_{t_a}^{\infty}A(s)\,ds=\lim_{t_b=\infty}\int_{t_a}^{t_b}A(s)\,ds$ exists. Suppose also that $HA\in L^1(t_a,\infty)$ (A is not necessarily in $L^1(t_a,\infty)$), then $\prod_{t_a}^{\infty}\exp(A(t))\,dt$ exists and is non-singular

2.2. Asymptotic solutions of the Schrodinger equation for large positive energies

For simplicity consider the one dimensional dimensionless Schrodinger equation

$$-d^2\psi/dx^2+V(x)\psi=E\psi.$$

Set

$$U(x)=\begin{pmatrix}\psi(x)\\ \psi'(x)\end{pmatrix},\qquad A_1(x)=\begin{pmatrix}0 & 1\\ V(x)-E & 0\end{pmatrix},\qquad E>V(x).$$

Its solution expressed as a product integral is

$$\begin{pmatrix}\psi(x)\\ \psi'(x)\end{pmatrix}=\prod_{x_0}^{x}\exp(A_1(y)\,dy)\begin{pmatrix}\psi(x_0)\\ \psi'(x_0)\end{pmatrix}.$$

Set

$$k(x)=+\sqrt{E-V(x)}.$$

The matrix $A_1(x)$ can be diagonalized:

$$A_1(x)=M(x)\Lambda(x)M^{-1}(x),\qquad \Lambda(x)=\begin{pmatrix}ik(x) & 0\\ 0 & -ik(x)\end{pmatrix},\qquad M(x)=\begin{pmatrix}1 & 1\\ ik(x) & -ik(x)\end{pmatrix}$$

The similarity rule (property 5) now yields

$$\prod_{x_0}^{x}\exp M(y)\Lambda(y)M^{-1}(y)\,dy=M(x)\prod_{x_0}^{x}\exp\{\Lambda(y)\,dy-M^{-1}(y)M'(y)\,dy\}M^{-1}(x_0).$$

Property 4 gives

$$\prod_{x_0}^{x}\exp(\Lambda(y)\,dy-M^{-1}(y)M'(y)\,dy)=\begin{pmatrix}e^{iK(x)} & 0\\ 0 & e^{-iK(x)}\end{pmatrix}\prod_{x_0}^{x}\exp A_2(y)\,dy,$$

$$K(x)=\int_{x_0}^{x}k(y)\,dy,\qquad A_2(y)=\frac{V'(y)}{4(V(y)-E)}\begin{pmatrix}-1 & e^{-2iK(y)}\\ e^{2iK(y)} & -1\end{pmatrix}.$$

Combining these results we get

$$\begin{pmatrix}\psi(x)\\ \psi'(x)\end{pmatrix}=\begin{pmatrix}1 & 1\\ ik(x) & -ik(x)\end{pmatrix}\begin{pmatrix}e^{iK(x)} & 0\\ 0 & e^{-iK(x)}\end{pmatrix}\prod_{x_0}^{x}\exp A_2(y)\,dy\begin{pmatrix}\frac{1}{2} & \frac{1}{2ik(x_0)}\\ \frac{1}{2} & -\frac{1}{2ik(x_0)}\end{pmatrix}\begin{pmatrix}\psi(x_0)\\ \psi'(x_0)\end{pmatrix}.$$

Using the inequality on the norm of product integrals (property 7), it is easily estimated that

$$\prod_{x_0}^{x}\exp A_2(y)\,dy = 1 + R(x, x_0, E) \text{ where}$$

$$\|R(x, x_0, E)\| \leq \exp\left\{\frac{1}{2}\int_{x_0}^{x}\frac{|V'(y)|\,dy}{E - V(y)}\right\} - 1.$$

By matrix multiplication we find

$$\psi(x, E) = \psi(x_0)\cos\left(\int_{x_0}^{x}(E - V(y))^{1/2}\,dy\right) + \frac{\psi'(x_0)}{(E - V(x_0))^{1/2}}\sin\left(\int_{x_0}^{x}(E - V(y))^{1/2}\,dy\right) + r(x, x_0E).$$

2.3. Feynman operator calculus and the Feynman–Kac formulae

The Feynman operator calculus, colloquially called the **disentangling of non-commutating operators**, starts with the remark that the order of two operators, say A and B, need not be given by their position, say AB, but by an ordering label $A(s_2)\,B(s_1)$. Once the ordering labels have been attached to the operators, they can be manipulated nearly as if they commuted and their order restored only when needed.

Example 2. Let $\hat{H}_0 = \hat{p}^2/2m = -\hbar^2\,\Delta_x/2m$. The solution of the Schrodinger equation

$$\partial\psi/\partial t = -(i/\hbar)\hat{H}_0\psi$$

with Cauchy data $\psi(t_a, x) = \phi(x)$ can be written

$$\psi(t_b, x) = \exp\left(-\frac{i}{\hbar}\hat{H}_0(t_b - t_a)\right)\phi(x) = \exp\left(-\frac{1}{\hbar}\int_T H_0(t)\,dt\right)\phi(x) = \prod_T \exp\left(-\frac{i}{\hbar}H_0(t)\,dt\right)\phi(x).$$

Although it seems hardly interesting to have attached an ordering label to $\hat{H}_0$, we shall see that it leads to a path integral representation of $\psi(t_b, x)$ which is convenient for deriving the Feynman–Kac formula. Indeed: Let $\mathcal{H}$ be the space of square integrable functions h on T, and let w_c be the canonical gaussian on $\mathcal{H}$ of variance I:

$$I(h, h) = \int_T g^{\alpha\beta}h_\alpha(t)h_\beta(t)\,dt.$$

We shall prove that

$$U_0(t_b, t_a) = \exp\left(-\frac{\mathrm{i}}{\hbar}\int_T H_0(t)\,\mathrm{d}t\right) = \exp\left(-\mathrm{i}\frac{1}{2m\hbar}\int_T g^{\alpha\beta}p_\alpha(t)p_\beta(t)\,\mathrm{d}t\right)$$

$$= \int_{\mathscr{H}} \mathrm{d}w_c(h)\exp\left(-\mathrm{i}\sqrt{\frac{m}{\hbar}}\frac{1}{m}\int_T h^\alpha(t)p_\alpha(t)\,\mathrm{d}t\right) \tag{2.3}$$

$$= \int_{\mathscr{H}} \mathrm{d}w_c(h)\exp\left(-\frac{1}{\mu m}\hat{p}_\alpha\int_T h^\alpha(t)\,\mathrm{d}t\right), \qquad \text{with } \mu = \sqrt{\hbar/m}. \tag{2.4}$$

To prove eq. (2.3) compute the path integral by the method given p. 265. Let $P:\mathscr{H}\to\mathbb{R}$ by $h\mapsto u = (1/\mu m)\int_T p_\alpha(t)h^\alpha(t)\,\mathrm{d}t = \langle p/\mu m, h\rangle_{\mathscr{H}}$. The image of w_c under P is the gaussian Pw_c on $\mathbb{R}$ of variance

$$\xi^2 I(p/\mu m, p/\mu m) = \xi^2(\mu m)^{-2}\int_T g^{\alpha\beta}p_\alpha(t)p_\alpha(t)\,\mathrm{d}t,$$

hence

$$\mathrm{d}Pw_c(u) = \mathrm{d}u\{2\pi\mathrm{i}I(p/\mu m, p/\mu m)\}^{-1/2}\exp\{\mathrm{i}u^2/2I(p/\mu m, p/\mu m)\}$$

and

$$\int_{\mathscr{H}} \mathrm{d}w_c(h)\exp\left\{-\frac{\mathrm{i}}{\mu m}\int_T h^\alpha(t)p_\alpha(t)\,\mathrm{d}t\right\} = \int_R \exp(-\mathrm{i}u)\,\mathrm{d}Pw_c(u) = \exp\{-\mathrm{i}I(p/\mu m, p/\mu m)/2\}. \quad \blacksquare$$

Equation (2.4) reexpresses eq. (2.3) in terms of the operator $\hat{p}$. The operator $\hat{p}$ enters the path integral representation of $U_0(t_b, t_a)$ *linearly*.

The Feynman–Kac formula. The solution of the Schrodinger equation

$$\partial\psi/\partial t = -\frac{1}{\hbar}(\hat{H}_0 + \hat{V}(x))\psi(t, x)$$

with Cauchy data $\psi(t_a, x) = \phi(x)$ can be written*

$$\psi(t_b, x) = \prod_T \exp\left(-\frac{\mathrm{i}}{\hbar}(H_0(t) + V(x(t))\,\mathrm{d}t\right)\phi(x)$$

$$= \int_{\mathscr{H}} \mathrm{d}w_c(h)\prod_T \exp\left(\left(-\frac{1}{\mu m}p_\alpha(t)h^\alpha(t) - \frac{1}{\hbar}V(x(t))\right)\mathrm{d}t\right)\phi(x).$$

On using property 4 (the sum rule) of the product integrals we get

*The equation $\psi(t_b, x) = \exp\{-(\mathrm{i}/\hbar)\int_T (H_0(t) + V(t))\,\mathrm{d}t\}\phi(x)$ is not correct without additional prescription because the family $\{H_0(t) + V(t)\}$ is not a commuting family

$$\psi(t_b, x) = \int_{\mathscr{H}} \mathrm{d}w_c(h) \prod_T \exp\left\{-\frac{\mathrm{i}}{\hbar}\left[\exp\left\{-\frac{\mathrm{i}}{\mu m}\hat{p}_\alpha \int_t^{t_b} h^\alpha(s)\,\mathrm{d}s\right\} V(x(t))\right.\right.$$
$$\left.\left. \times \exp\left\{+\frac{1}{\mu m}\hat{p}_\alpha \int_t^{t_b} h^\alpha(s)\,\mathrm{d}s\right\}\right]\mathrm{d}t\right\} \exp\left\{-\frac{\mathrm{i}}{\mu m}\hat{p}_\alpha \int_{t_a}^{t_b} h^\alpha(s)\,\mathrm{d}s\right\} \phi(x).$$

Use $\exp(\mathrm{i}\alpha\hat{p})V(x) = V(x + \hbar\alpha)$ to get

$$\psi(t_b, x) = \int_{\mathscr{H}} \mathrm{d}w_c(h) \exp\left(-\frac{\mathrm{i}}{\hbar}\int_T V\left(x(t) - \mu\int_t^{t_b} h(s)\,\mathrm{d}s\right)\mathrm{d}t\right) \cdot \phi\left(x - \mu\int_T h(s)\,\mathrm{d}s\right).$$

This path integral representation of $\psi(t_b, x)$ is readily simplified by the primitive mapping $P_+ : \mathscr{H} \to Y_+$ defined by

$$P_+h(t) = y(t) = -\int_t^{t_b} h(s)\,\mathrm{d}s.$$

The image of w_c under P_+ is the Wiener measure w_+^{W} (see p. 271),

$$\psi(t_b, x) = \int_{Y_+} \mathrm{d}w_+^{\mathrm{W}}(y) \exp\left(-\frac{\mathrm{i}}{\hbar}\int_T V(x + \mu y(t))\,\mathrm{d}t\right) \phi(x + \mu y(t_a)). \tag{2.5}$$

The Kac formula is often written by probabilists as an integral over Y_-. The probabilists' formula can be obtained from the physicists' formula by the mapping $y \mapsto z$ such that $z(t) = y(t_a + t_b - t)$, i.e. y and z are the same path traversed in opposite directions. This mapping gives

$$\psi(t_b, x) = \int_{Y_-} \mathrm{d}w_-^{\mathrm{W}}(z) \exp\left(-\frac{1}{\hbar}\int_T V(x + \mu z(t))\,\mathrm{d}t\right) \phi(x + \mu z(t_b)). \tag{2.6}$$

Note that in the Kac formula all the paths are at x at time t_a, whereas in the Feynman formula all the paths are at x at time t_b. Thus the Kac formula runs the movie backwards, it gives the final wave function at the origin of the paths in terms of the initial wave function evaluated at the end points of the paths.*

The domains of integration $Y_\pm$ are vector spaces, as it should be since prodistributions are defined on vector spaces. The space of paths f such that $f(t_b) = x$ is not a vector space unless $x = 0$. Indeed f_1 and f_2 being in a vector space such that $f_1(t_b) = f_2(t_b)$ implies $(f_1 + f_2)(t_b) = f_1(t_b) = f_2(t_b)$ which in turn implies $f_1(t_b) = 0$.

Usually no sum of paths is needed: The "sum over all paths" is *not* a sum of paths but a sum of *functions* of paths, for example $\exp \mathrm{i}\int_T V(f(t))\,\mathrm{d}t$. If however one needs to "add" f_1 and f_2 so that $(f_1 \text{ "+" } f_2)(t_b) = f_1(t_b) = f_2(t_b) = c$, one can define the "sum" to be

$$f_1 \text{ "+" } f_2 = (f_1 - c) + (f_2 - c) + c.$$

*See note I added in proof

Remark. The fact that in the integrand y appears multiplied by $\mu = \sqrt{\hbar/m}$ is not a novelty [e.g. 80, p. 459]. Here, however, it has not been put in "by hand" but follows naturally from the derivation of the Feynman–Kac formula. In the next chapter we shall expand the integrand in powers of μ – not in powers of $\hbar$ – and obtain the semiclassical expansion (eq 3.20)

Remark. There is another form of the Feynman–Kac formula [117, 121 p. 279, 3] based on the Trotter product formula valid for potentials $V \in L^2(R^n) + L^\infty(R^n)$. We shall give later (Remark p. 315) a class of potentials for which our results are valid.

2.4. *The Møller wave operators*

Let $\hat{H} = \hat{H}_0 + V$ be the Hamiltonian operator of a system S, with $\hat{H}_0 = \hat{p}^2/2m$. The Møller wave operators $W_\pm$ defined formally by

$$W_\pm = \lim_{t=\mp\infty} W_\pm^t, \qquad W_\pm^t = \exp(+\mathrm{i}t\hat{H}/\hbar)\exp(-\mathrm{i}t\hat{H}_0/\hbar)$$

play an important role in scattering theory.* Albeverio and Høegh-Krøhn [3, p. 32–41] have obtained a path integral representation of the Møller wave operators using their theory of oscillatory integrals. Their formula is readily obtained from the Feynman–Kac formula by linear mappings on the spaces Y_- and Y_+ of paths with one end fixed. Let the initial wave function be

$$\phi(x) = \int_R \exp(\mathrm{i}px/\hbar)a(p)\,\mathrm{d}p, \text{ then}$$

$$\exp(-\mathrm{i}t\hat{H}_0/\hbar)\phi(x) = \int_R \exp(-\mathrm{i}p^2t/2m\hbar)\exp(\mathrm{i}px/\hbar)a(p)\,\mathrm{d}p.$$

Let Y_+ be the space of paths y defined on $[t, 0]$ such that $y(0) = 0$. The path integral representation of $W_+^t\phi$ is, according to the Feynman–Kac formula,

$$(W_+^t\phi)(x) = \int_{Y_+} \mathrm{d}w_+^{\mathrm{W}}(y)\exp\left\{-\frac{1}{\hbar}\int_t^0 V(x+\mu y(s))\,\mathrm{d}s\right\}\int_R \exp(-\mathrm{i}p^2t/2m\hbar) \times \exp\{\mathrm{i}p(x+\mu y(t))/\hbar\}a(p)\,\mathrm{d}p.$$

Let $P : Y_+ \to Y_+$ by $y \mapsto z$ such that

$$z(s) = y(s) - \mu ps/\hbar.$$

It follows from the Cameron–Martin formula that

$$(W_+^t\phi)(x) = \int_R \mathrm{d}p\,a(p)\int_{Y_+}\mathrm{d}w_+^{\mathrm{W}}(y)\exp\left\{\mathrm{i}\int_t^0\left(\frac{\mu^2p^2}{2\hbar^2}+\frac{\mu pz(s)}{\hbar}\right)\mathrm{d}s\right\} \times \exp\left\{-\frac{1}{\hbar}\int_t^0 V\left(x+\mu z(s)+\frac{\mu^2ps}{\hbar}\right)\mathrm{d}s\right\}\exp\left(-\frac{\mathrm{i}p^2t}{2m\hbar}\right)\exp\left\{\frac{\mathrm{i}}{\hbar}p\left(x+\mu z(t)-\frac{\mu^2pt}{\hbar}\right)\right\}.$$

*There is an abundant literature on scattering theory For the operator formalism of scattering theory [e g 36], for the mathematical scattering theory [e g 77, 89] Also [149, pp 210–212] and [151]

The oscillatory terms cancel. The limit of $W_+^t\phi$ when $t = -\infty$ is

$$(W_+\phi)(x) = \int_R \mathrm{d}p\ W_+(x,p)\exp(\mathrm{i}px/\hbar)a(p),$$

where

$$W_+(x,p) = \int_{Y_+} \mathrm{d}w_+^{\mathrm{W}}(z)\exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{0} V(x+\mu z(s)+ps/m)\,\mathrm{d}s\right\}. \tag{2.7}$$

A similar calculation gives $W_-\phi(x) = \int_R \mathrm{d}p\ W_-(x,p)\exp(\mathrm{i}px/\hbar)a(p)$ where

$$W_-(x,p) = \int_{Y_-} \mathrm{d}w_-^{\mathrm{W}^*}(z)\exp\left\{\frac{1}{\hbar}\int_{0}^{\infty} V(x+\mu z(s)+ps/m)\,\mathrm{d}s\right\}. \tag{2.8}$$

The path integral representations of W_+ and W_-^* are over the space of paths defined on $(-\infty, 0]$ and $[0, +\infty)$, respectively, vanishing at 0.

The scattering operator S is defined by $S = W_-^* W_+$. Its matrix elements are (see note II added in proof)

$$\langle p_f|S|p_i\rangle = \int_R W_-^*(x,p_f)\exp(-\mathrm{i}(p_f-p_i)x/\hbar)W_+(x,p_i)\,\mathrm{d}x.$$

Non Relativistic Quantum Mechanics

Consider a dynamical system whose state at time t is represented by a point $f(t)$ of its configuration space M. As t varies from t_a to t_b, $f(t)$ defines a path $f: T \to M$. The Feynman formalism of quantum physics begins with the identification of the space of all the possible, non-equivalent, paths f satisfying some appropriate boundary conditions. Thus a path integral "probes" the whole configuration space and reflects its global features (see for instance section 3.1). In this respect, a path integral is not just a solution of a differential equation satisfying some chosen boundary conditions: A differential equation is an excellent way of presenting a whole class of functions. It states a local law satisfied by a class of physical systems. The boundary conditions are then chosen to answer specific questions. These two parts, on the one hand finding the differential equation (equation of motion), and on the other hand choosing the boundary conditions and global characteristic which determine the solution may not be independent [67]. A path integral is a statement which incorporates these two parts organically, and insures that they are compatible.

The configuration space of a system, even the most trivial one, is rarely $\mathbf{R}^n$: A pendulum, a system of indistinguishable particles, a rigid body with one fixed point, etc. have configuration spaces which are Riemannian multiply-connected manifolds.

We begin with systems whose configuration spaces are multiply-connected in order to show how to use path integrals to obtain global features of a system without actually computing the path integrals. Computing path integrals is the purpose of the other sections in this chapter. The following cases are

treated: In section 3 the paths x, y, h, X, Y, .. map a finite time interval $T = [t_a, t_b]$ into the configuration space M of the system; in section 4 they map T into its phase space T^*M. Path integrals of quantum mechanics can further be classified by the boundary conditions imposed on the paths:

1. The path integral representation of the wave function, known as the Feynman–Kac formula, is an integral over the space X_+ of paths which vanish at t_b and which are arbitrary at t_a In section 3.2 the Feynman–Kac path integral is computed to the WKB approximation. This calculation serves three purposes:

a. It displays the use of prodistribution on a simple example.

b. It gives a precise meaning to the statement "quantum mechanics goes to classical mechanics when h goes to zero because of destructive interference of the amplitudes attached to neighboring paths."

c. It sets up the stage for calculating the wave functions of systems whose configuration space is a riemannian manifold.

2. The path integral representation of the probability amplitude $K(b, t_b; a, t_a)$ that a system known to be in the state $a \in M$ at t_a be found in the state $b \in M$ at t_b is a path integral over the space X of paths vanishing at t_a and t_b (sections 3.4, 3.5, 3.6)

At this point, physicists may immediately object to the nature of the space of paths X considered· Feynman expressed $K(b, t_b; a, t_a)$ as the "sum" over all possible paths f, such that $f(t_a) = a$ and $f(t_b) = b$, of $\exp \mathrm{i}S(f)/\hbar$ with $S(f) = \int_T L(f(t), \dot{f}(t))\,\mathrm{d}t$ – not as the sum over all possible paths vanishing at t_a and t_b. The reason one works with integrals over X is that functional integration has been defined only on vector spaces. Paths f_1, f_2 satisfying Feynman boundary conditions form a vector space only if $a = b = 0$ (see p. 291). In practice one first makes the transformations necessary for the Feynman path integral to be an integral over a vector space: For instance an affine transformation (see p. 281), or a semiclassical expansion as in section 3 Mizrahi has developed techniques for integration in function spaces which are not necessarily vector spaces and has given practical expressions [108] for such integrals.

In section 3.4 the theory of prodistribution is used to give a workable method for computing the semiclassical expansion of $K(b, t_b; a, t_a)$ in principle to any desired order in $\hbar$. This method does not break down "on the caustics" and the caustic problem is treated in section 3.5. The semiclassical expansion is combined with perturbative methods in section 3.6.

The game in both sections 3 and 4 is to find the prodistribution best suited to the problem at hand, i.e. the prodistribution which makes it possible to express the given integrals as cylindrical integrals or as series of cylindrical integrals.

3. Path integration on configuration space

3.1. Multiply connected configuration spaces

Let $a, a', b \ldots \in M$ and let $A = (a, t_a)$, $A' = (a', t_a)$, $B = (b, t_b)$ characterize the initial and final states of a system. Starting from an analysis of quantum effects, Feynman showed that the probability amplitude $K(B, A)$ of a transition $A \to B$ is the sum of the probability amplitudes associated with all possible paths from A to B. If all the paths are not homotopically equivalent, the Feynman theory says only that $K(B; A)$ is a linear combination of the partial probability amplitudes $\{K^{\hat{\alpha}}(B; A)\}$ where $K^{\hat{\alpha}}(B; A)$ is obtained by summing over all paths from A to B in the homotopy class $\hat{\alpha}$:

$$K(B;A)=\sum_{\{\alpha\}}\chi(\alpha)K^{\hat{\alpha}}(B;A). \tag{3.1}$$

The coefficients $\chi(a)$ are so far undetermined. We expect them to be related to the fundamental group π of the configuration space M: The elements $\{\alpha_i\}$ of π are the homotopy classes of closed loops at a point $c \in M$, together with the multiplication law $\alpha_i\alpha_j = \alpha_{ij}$, where α_{ij} is the homotopy class of closed loops obtained by linking a path in α_j with a path in α_i. It can be shown [e g. 131] that there is an isomorphism between the fundamental groups based at two different points c and c' but there is no canonical (i.e. no preferred) isomorphism between them. By connecting c and c', a closed loop at c' becomes a closed loop at c, but there is no unique way of connecting c and c'.

By the same token, there is no unique way of labeling the homotopy classes $\hat{\alpha}$ of paths from a to b by the elements of the fundamental group. The coefficients $\{\chi(\alpha);\ \alpha \in \pi\}$ cannot be paired with the partial amplitudes $K^{\hat{\alpha}}$ in a unique fashion and eq. (3.1) is meaningless

There are two equivalent ways of giving meaning to eq. (3.1). We give here the one [84] which does not require auxiliary concepts; the other one [45] proceeds via the universal covering of M.

1. Choose an "homotopy mesh", i.e. choose an arbitrary point $c \in M$, and arbitrary paths $C(a)$ and $C(b)$ from c to a and c to b respectively. This homotopy mesh associates a unique closed loop $cabc$ to any given path ab.
2. Require that the quantity of physical interest $K(B;A)$ be independent of the chosen homotopy mesh. No other condition is necessary to determine the set $\{\chi(\alpha)\}$.

Let us for simplicity speak of a loop α, or a path $\hat{\alpha}$, from a to b, instead of a loop [a path] in the homotopy class α [class $\hat{\alpha}$].

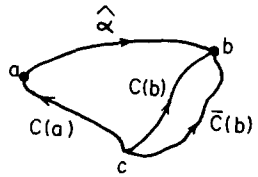


Fig 5

Let us choose two different paths $C(b)$ and $\bar{C}(b)$ from c to b. In the C mesh the path $\hat{\alpha}$ is part of the loop $\alpha = c^{-1}(b)\hat{\alpha}c(a)$. In the $\bar{C}$ mesh it is part of

$$\bar{\alpha} = \bar{C}^{-1}(b)\hat{\alpha}C(a) = \bar{C}^{-1}(b)C(b)C^{-1}(b)\hat{\alpha}C(a) = \beta\alpha, \quad \text{with } \beta = \bar{C}^{-1}(b)C(b).$$

In the C mesh

$$K = \sum_{\alpha\in\pi}\chi(\alpha)K^{\hat{\alpha}}.$$

In the $\bar{C}$ mesh

$$\bar{K} = \sum_{\bar{\alpha}\in\pi}\chi(\bar{\alpha})K^{\hat{\alpha}} = \sum_{\alpha\in\pi}\chi(\beta\alpha)K^{\hat{\alpha}}$$

Physical results are independent of the mesh if and only if

$$|K| = |\bar{K}| \Leftrightarrow \left|\sum_{\alpha\in\pi}\chi(\alpha)K^{\hat{\alpha}}\right| = \left|\sum_{\alpha\in\pi}\chi(\beta\alpha)K^{\hat{\alpha}}\right|$$
$$\Leftrightarrow \{\chi(\alpha);\ \alpha \in \pi\} \text{ is a unitary representation of } \pi.$$

Proof. If $\{\chi(\alpha); \alpha \in \pi\}$ is a unitary representation of the fundamental group, $\chi(\beta\alpha) = \chi(\beta)\chi(\alpha)$ and $\chi(\beta)\chi^+(\beta) = 1$. It follows that $|K| = |\bar{K}|$ Conversely, it can be shown [338] that $\{K^\alpha; \alpha \in \pi\}$ is a linearly independent set. Hence $|K| = |\bar{K}|$ implies that

$$\chi(\beta\alpha) = \exp(i\xi(\beta))\chi(\alpha).$$

If $\alpha = e$ is the unit element of π, then $\chi(\beta) = \exp(i\xi(\beta))\chi(e)$ and

$$\chi(\beta\alpha) = \chi(\beta)\chi(\alpha)[\chi(e)]^{-1}, \qquad \chi(\beta)\chi^+(\beta) = |\chi(e)|^2.$$

Without loss of generality one can set $\chi(e) = 1$. ■

In conclusion.

Theorem. The probability amplitude $K(B; A)$ is a linear combination of the probability amplitudes $K^{\hat{\alpha}}(B; A)$ whose coefficients $\{\chi(\alpha)\}$ form a one dimensional unitary representation of the fundamental group.

There are as many answers for $K(B; A)$ as there are one dimensional unitary representations of π. These different answers correspond to different systems, and because of the orthogonality theorem of representations, there is no transition between these different systems.

Example. Systems of indistinguishable particles [84]. The configuration space of a system of p indistinguishable particles in R^n for $n \geq 3$ is multiply-connected. Its fundamental group is the permutation group S_p which has two and only two one-dimensional unitary representations. The two possible expressions for the probability amplitude correspond to systems of bosons and systems of fermions:

$$K^B = \sum_{\alpha \in S_p} \chi^B(\alpha) K^{\hat{\alpha}} \qquad \text{with } \chi^B(\alpha) = 1 \text{ for every } \alpha,$$

$$K^F = \sum_{\alpha \in S_p} \chi^F(\alpha) K^{\hat{\alpha}} \qquad \text{with } \chi^F(\alpha) = \pm 1.$$

K^F is determined modulo a minus sign.

This example shows how the dynamical symmetries of a system can be obtained, via path integration, from the symmetries of its configuration space, i.e. from the symmetries of its states: If a system is invariant under a group of transformation R, all the points in the configuration space M which are R-related must be identified in order that M be in a one-to-one correspondence with the states of the system. As a general rule, M will then be multiply-connected. Its fundamental group is determined by R. The fundamental group in turn determines the propagator K, hence its invariance group, say T. The example treated here shows that a system of n indistinguishable particles (invariance group R) can be propagated only by totally symmetric and totally antisymmetric propagators (invariance group T).

R may or may not be identical with T. The phenomena observed when R is not identical with T have been given different names such as symmetry rearrangements, broken symmetries, etc.*

Other multiply-connected spaces occuring in physics include SO(3) (e.g. a spherical top [123]), the 2 torus (e.g. electrons in a lattice [124]). SO(3) is doubly connected, its fundamental group is Z^2 The

*For an analysis of these phenomena in terms of R and T see refs [97] and [139]

two possible expressions for the probability amplitudes which can be constructed [123] for the spherical top correspond to half integer spins if one uses the trivial representation $\chi(\alpha) = 1$ for every α, and to integer spins if one uses the representation $\chi(\alpha) = \pm 1$

Path integrals have been used to extract information about a physical system, without computing the integral, in situations other than multiply-connected configuration spaces. For example, the existence of ghost particles in gauge fields [52], and the black hole radiance [66], to name a few of current interest.

The computation of path integrals remains nevertheless a primary task and will be treated in the remaining part of this section 3.

3.2. *WKB approximation of the wave function in flat space*

Consider a system S whose action is

$$S(f) = \int_T L(f(t), \dot{f}(t))\,\mathrm{d}t = \int_T \left\{\frac{m}{2}\|\dot{f}(t)\|^2 - V(f(t))\right\}\mathrm{d}t,$$

$$T = [t_a, t_b], \qquad f: T \to R^n, \qquad \|\dot{f}(t)\|^2 = (\dot{f}(t) \mid \dot{f}(t)) = g_{\alpha\beta}\dot{f}^{\alpha}(t)\dot{f}^{\beta}(t).$$

Let ψ be the wave function of the system S whose initial wave function ϕ at time t_a is known. Following Truman's method [136]* we shall compute the WKB approximation of ψ starting from its path integral representation, known as the Feynman–Kac formula (p. 290). Set $(\hbar/m)^{1/2} = \mu$, and $c = 1$. Let w_+^{W} be the Wiener gaussian on the space Y_+ of paths vanishing at t_b. Then the Feynman–Kac formula states that

$$\psi(t_b, b, \mu) = \int_{Y_+} \mathrm{d}w_+^{\mathrm{W}}(y) \exp\left\{\frac{-\mathrm{i}}{\mu^2 m}\int_T V(b + \mu y(t))\,\mathrm{d}t\right\}\phi(b + \mu y(t_a)). \tag{3.2}$$

The dependence of the wave function on μ is explicitly stated since all quantities will be expanded in powers of μ.

We could assume that the initial wave function is a plane wave of momentum p_a, or a wave packet which in the limit $\hbar = 0$ describes a particle of momentum p_a at t_a. In order to generalize easily the calculation in flat space to the case where the configuration space is a riemannian space we shall assume the same initial wave function as Truman [136], namely

$$\phi(a) = \exp(\mathrm{i}S_0(a)/\hbar)T(a).$$

T is an arbitrary well behaved function on $\mathbf{R}^n$ whose support determines the localization of the system. S_0 is the initial value of the solution of the Hamilton–Jacobi equation for the system S. Thus the initial probability density $\rho = \phi^*\phi$ is $\rho(a) = |T_0(a)|^2$, and the limit when $\hbar = 0$ of the initial current density

$$j = \hbar(\phi^*\nabla\phi - (\nabla\phi)^*\phi)/2\mathrm{i}m$$

is

$$\lim_{\hbar=0} j(a) = \rho(a)\nabla S_0(a)/m.$$

*See p 312 for precise comparison with Truman's method A formal derivation can be found in ref [80, p 460]

We could choose $\nabla S_0(a) = p^0$ at every point $a \in \mathbb{R}^n$, i.e. $S_0(a) = p^0_\alpha a^\alpha$, it is sufficient however to choose S_0 such that

$$\nabla S_0(q(t_a)) = p^0 \tag{3.3}$$

where q is the classical path, solution of

$$m g_{\alpha\beta}\dot{q}^\beta(t) + \nabla_\alpha V(q(t)) = 0, \qquad mq(t_a) = p^0, \qquad q(t_b) = b$$

I.e. the surface $S_0(a) = 0$ need not be a plane, it is only required that it be orthogonal to p_a at $q(t_a)$. Since $\lim_{\hbar=0} -i\hbar\nabla\phi(a) = \nabla S_0(a)\phi(a)$, we sometimes say, loosely, that, in the limit $\hbar = 0$, ϕ is an eigenstate of the momentum operator $\hat{p} = -i\hbar\nabla$ with eigenvalue $p^0(a) = \nabla S_0(a)$.

The semiclassical expansion of ψ is conveniently obtained by expanding about the classical path q the integrand of the Feynman–Kac formula (3.1). Make the change of variable of integration $y \mapsto x$ such that

$$b + \mu y(t) = q(t) + \mu x(t).$$

The new variable of integration* x is the deviation of an arbitrary path from the classical path. Under this change of variable, the Cameron–Martin formula (p. 274) gives**

$$\psi(t_b, b, \mu) = \int_{Y_+} dw_+^{W}(x) \exp\left\{\frac{1}{2}\int_T \left(\frac{1}{2\mu^2}\|q(t)\|^2 - \frac{1}{\mu^2 m} V(q(t) + \mu x(t))\, dt\right) + i\int_T \frac{1}{\mu}(\dot{q}(t) \mid dx(t))\right\}$$

$$\times \phi(q(t_a) + \mu x(t_a)). \tag{3.4}$$

Integrate by parts the stochastic integral**.

$$\int_T (q(t) \mid dx(t)) = -(q(t_a) \mid x(t_a)) - \int_T (q(t) \mid x(t))\, dt;$$

expand $V(q(t) + \mu x(t))$, $S_0(q(t_a) + \mu x(t_a))$ and $T(q(t_a) + \mu x(t_a))$ in powers of μ; and use the classical equation of motion to obtain $\psi = \psi_{WKB}(1 + O(\hbar))$ where ψ_{WKB} is the WKB approximation:

$$\psi_{WKB}(t_b, b, \mu) = \exp\left\{\frac{1}{\hbar}\bar{S}(t_b, b)\right\} \int_{Y_+} dw_+^{W}(x) \exp\left\{\frac{-i}{2m}\int_T x^\alpha(t)x^\beta(t)\nabla_\alpha\nabla_\beta V(q(t))\, dt\right.$$

$$\left. + \frac{1}{2m} x^\alpha(t_a)x^\beta(t_a)\nabla_\alpha\nabla_\beta S_0(q(t_a))\right\} T(q(t_a)) \tag{3.5}$$

where $\bar{S}(t_b, b)$ is the general solution [e.g. 23, p. 260] of the Hamilton–Jacobi equation of the system with Cauchy data S_0 at t_a.

$$\bar{S}(t_b, b) = S_0(q(t_a)) + \int_T \left\{\frac{m}{2}\|q(t)\|^2 - V(q(t))\right\} dt.$$

*For simplicity we give the same label to the vector field x along q and to the path $x\ T \to \mathbb{R}^n$ such that $x(t)$ is equal to $x(t)$ at $q(t)$, we also identify under the label Y_+ the space of vector fields x along q vanishing at $q(t_b)$ with the space of paths $x\ T \to \mathbb{R}^n$ vanishing at t_b.

**See appendix D

Here $q(t_a)$ is a function of $q(t_b)$, i.e. a function of (t_b, b).

The path integral (3.5) has already been computed (eq. 1.17):

$$\psi_{\mathrm{WKB}}(t_b, b, \mu) = (\det \bar{K}(t_a, t_a)/\det \bar{K}(t_b, t_a))^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar}\bar{S}(t_b, b)\right\} T(q(t_a))$$

where $\bar{K}(t, t_a)$ is the solution of the differential equation

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\bar{K}^{\alpha}_{\beta}(t, t_a) + \nabla^{\alpha}\nabla_{\delta}V(q(t))\bar{K}^{\delta}_{\beta}(t, t_a) = 0$$

such that

$$\bar{K}^{\alpha}_{\beta}(t_a, t_a) = \delta^{\alpha}_{\beta} \qquad \text{and} \qquad (\mathrm{d}\bar{K}^{\alpha}_{\beta}/\mathrm{d}t)(t = t_a, t_a) = \nabla^{\alpha}\nabla_{\beta}S_0(q(t_a)).$$

Since the classical path has been defined by its initial momentum and its final position, $q(t_a)$ is understood as a function of the initial momentum and the equation of motion can be written

$$mg_{\alpha\beta}q^{\beta}(t, \nabla S_0(q(t_a)), b) + \nabla_{\alpha}V\{q(t, \nabla S_0(q(t_a)), b)\} = 0.$$

Differentiating with respect to $q(t_a)$ and interchanging the order of differentiation shows that

$$\bar{K}^{\alpha}_{\beta}(t, t_a) = \partial q^{\alpha}(t)/\partial q^{\beta}(t_a)$$

satisfies the required conditions. In conclusion

$$\psi_{\mathrm{WKB}}(t_b, b, \mu) = (\det|\partial q^{\alpha}(t_a)/\partial q^{\beta}(t_b)|)^{1/2} \exp\{\mathrm{i}\bar{S}(t_b, b)/\hbar\} T(q(t_a)). \tag{3.6}$$

We give in appendix B practical methods for computing the WKB approximation.

Physical interpretation of the WKB *approximation.* The localization of the system at time t_a on its configuration space M is the support* of its wave function, here Supp T. Consider a flow of classical paths surrounding the classical path q defined above by $q(t_b) = b$ and $mq(t_a) = p^0$. More specifically consider the flow $\{\bar{q}(t, a, p_a); a \in N\}$ where N is a neighborhood of $a_0 = q(t_a)$ and where the initial momenta $p_a = \nabla S_0(a)$. Note $\bar{q}(t, a_0, p^0) = q(t)$. This flow generates a group of transformations $\{\mathscr{C}_t; t \in T\}$, each transformation

$$\mathscr{C}_t : M \to M \qquad \text{by } a \to \bar{q}(t, a, p_a).$$

Let $\mathrm{d}\omega_0$ be the volume element at a_0. Under the transformation $\mathscr{C}_t$, the volume element $\mathrm{d}\omega$ becomes $\mathrm{d}\omega_t = \det|\partial q^{\alpha}(t)/\partial q^{\beta}(t_a)|\,\mathrm{d}\omega_0$. We shall say that the determinant of $\partial q^{\alpha}(t)/\partial q^{\beta}(t_a)$ gives the rate at which the flow $\{\bar{q}(t, a, p_a); a \in N\}$ diverges or converges around q. Equation (3.6) says that in the limit $\hbar = 0$,

$$\int_{\Omega} |\psi(t, b, \mu)|^2\,\mathrm{d}\omega_t = \int_{\mathscr{C}_t^{-1}\Omega} |\phi(a)|^2\,\mathrm{d}\omega_0.$$

In the classical limit, the probability of finding in Ω at time t a system known to be in $\mathscr{C}_t^{-1}\Omega$ at time t_a is unity. The case when $\det|\partial q^{\alpha}(t)/\partial q^{\beta}(t_a)| = 0$ is studied in section 3.5.

*The support of $T: M \to \mathbf{R}$ is the set of points $a \in M$ such that $T(a) \neq 0$ together with their limits. The limit points are included so that, for instance if $T(a)$ vanishes at isolated points, these points belong nevertheless to Supp T.

3.3. WKB *approximation of the wave function in curved spaces*

What is the Schrodinger equation for a system whose configuration space is a riemannian manifold? How does one compute a path integral over the space of paths $X: T \to M$ where M is an n-dimensional riemannian manifold? These questions have been discussed since Pauli remarked [118] in 1952 that the Feynman propagator for a short time interval does not quite obey the Schrodinger equation. It "misses" it by a term proportional to $\hbar^2$ which vanishes in simple cases but does not generally vanish on curved spaces. Alternatively one can ask what is the short time interval propagator which obeys the Schrodinger equation $i\hbar\partial_t\psi(t,x) = -\hbar^2\Delta\psi(t,x)/2m + V(x)\psi(t,x)$ on curved spaces? Or what is the path integral representation of a wave function which satisfies this Schrodinger equation?

Recently the works of Elworthy on Wiener integrals on curved spaces and the work of Truman on the classical limit of the solutions of the Schrödinger equation have provided a method for computing the semiclassical approximation of the wave function on curved spaces. The key element for extending the results of section 3.2 to curved spaces is the development mapping as used by Eells and Elworthy [46–49]

The development mapping was first introduced in differential geometry for describing the rolling of a riemannian manifold on a plane. It has been used by Yosida [145] in describing brownian motion on a 2 sphere and has appeared more or less explicitly in later papers* on brownian motion on manifolds. It is defined as follows.

Let T_bM be the tangent space to the configuration space M at b. **The development mapping** is a bijection between the space of $L^{2,1}$ paths** on T_bM which vanish at t_b and the space of $L^{2,1}$ paths on M which are at b at t_b. It is defined as follows:

Consider† a path z on T_bM. A path Dev z on M is said to be the development of z if its derivative at t,

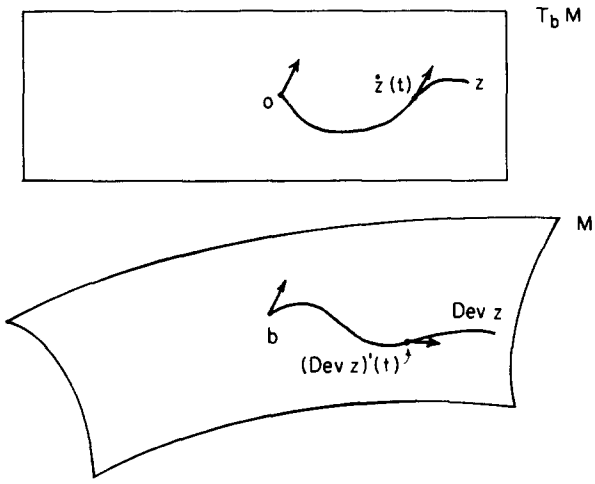


Fig 6 $z(t)$ is equal to (Dev z)'(t) parallel transported along Dev z to b The development mapping is a mapping from the space of $L^{2,1}_{+}$ paths on T_bM into the space of $L^{2,1}_{+}$ paths on M It is not a mapping from T_bM into M

*See references quoted in refs [46] and [49]

**Defined p 280

†As usual one identifies T_bM and $\mathbf{R}^n$ The metric on T_bM and $\mathbf{R}^n$ is $g(b)$

parallel transported to b, is equal to $z(t)$, when it exists. When $z(t^+) \neq z(t^-)$, then $(\mathrm{Dev}\, z)'(t^+)$ and $(\mathrm{Dev}\, z)'(t^-)$ parallel transported to b are equal respectively to $z(t^+)$ and $z(t^-)$

It follows immediately from the definition that

1 The development mapping maps a straight line on T_bM into a geodesic on M such that $(\mathrm{Dev}\, z)'(t_b) = z(t_b)$.

2. The development mapping preserves angles

3. Closed loops on T_bM are not developed into closed loops on M: a mapping from the space of paths on T_bM into the space of paths on M cannot both map closed loops into closed loops and conserve angles. A closed loop is a particular case of paths with both ends fixed. Hence a family of paths with both ends fixed is not developed into a family with both ends fixed.*

The space of $L^{2,1}$ paths on T_bM vanishing at the origin is dense in the space Y_+ of continuous paths on T_bM vanishing at the origin; the space of $L^{2,1}$ paths on M going through b at t_b is dense in the space $\mathscr{C}_b(M)$ of continuous paths on M going through b at t_b. The development mapping determines [49] a measurable map between the space of continuous paths on T_bM which vanish at t_b and the space of continuous paths on M which are at b and t_b. To simplify the notation we may sometimes use the same label for the development mapping and the mapping it determines on the space of continuous paths, and write

$$\mathrm{Dev}\colon Y_+ \to \mathscr{C}_b(M) \qquad \text{by} \quad z \mapsto \mathrm{Dev}\, z$$

but it should remembered that by so doing we create a treacherous legerdemain.**

Since paths are variables of integration, we shall consider a path X on M as a mapping from $T \times Y_+$ into M:

$$X(t, z) = (\mathrm{Dev}\, z)(t).$$

The theory of prodistributions makes it possible to extend to the Schrodinger equation the results obtained by Elworthy† for the heat equation; the solution of the Schrodinger equation

$$i\hbar\partial_t\psi(t, x) = -\hbar^2\Delta\psi(t, x)/2m + V(x)\psi(t, x), \qquad \psi(t_a, x) = \phi(x)$$

is then

$$\psi(t_b, b, \mu) = \int_{Y_+} \mathrm{d}w_+^{\mathrm{W}}(y) \exp\left\{\frac{-1}{\mu^2 m}\int_T V(X(t, b + \mu y))\,\mathrm{d}t\right\}\phi(X(t_a, b + \mu y)). \tag{3.7}$$

This is also the equation one would have written if asked to generalize formally eq. (3.1) to curved spaces As before assume

$$\phi(a) = \exp(iS_0(a)/\hbar)T(a).$$

In the previous section V and ϕ have been expanded about the classical path defined by a given initial velocity and a given final point. Here consider the classical path $X(\cdot, q)$ such that $q(t_a) = v_a$ and $X(t_b, q) = b$. In practice it may be difficult to find q such that its development is a classical path but q is not needed in the final expression. It is sufficient that it exist and be unique.

*See section 3 4

**Having, in a first draft, excused this notation with the conventional "By a convenient abuse of language" our mentor (K D E) wrote back. "That 'convenient abuse of language' phrase is almost as strong an abuse of the word 'convenient' as the Mafia could ever have made! since it knocks out one of the major mathematical difficulties!" See p 313, the effect of the inclusion mapping $i\colon L^{2,1} \to Y^+$

†Reference [49] and private communication

Set $X(\cdot, q) = Z(\cdot)$ and call $v(t)v_a$ the parallel transport of v_a from $Z(t_b)$ to $Z(t)$ along Z. Then

$$mg_{\alpha\beta}Z^{\beta}(t) + \nabla_{\alpha}V(Z(t)) = 0, \qquad Z(t_a) = v(t_a)v_a, \qquad Z(t_b) = b.$$

$Z(t_a)$ is a complicated function of v_a. In this section the time interval $[t_a, t_b]$ is assumed sufficiently short so that there is a unique classical path between $Z(t_a)$ and $Z(t_b)$. This restriction is removed in section 3.5.

Returning to the initial wave function, assume that

$$\nabla_{\alpha}S_0(Z(t_a)) = mg_{\alpha\beta}(Z(t_a))\dot{Z}^{\beta}(t_a).$$

Here as in the previous section, the surface $S_0(a) = 0$ is assumed to be perpendicular to the classical path at $Z(t_a)$.

The development mapping is not linear, it is not even given explicitly but via an integro-differential equation and computing the wave function given by eq. (3.7) seems a formidable task. It is however possible to compute its semiclassical expansion. As before make the change of variable of integration defined by

$$q + \mu x = b + \mu y$$

where q is now the path such that Dev $q = Z$. Set

$$Y(t, x, \mu) = X(t, q + \mu x) = \mathrm{Dev}(q + \mu x)(t).$$

In the following μ is a variable $\mu \in U = [0, (\hbar/m)^{1/2}]$ which defines a one-parameter* family of paths $\{Y(\cdot, x, \mu);\ \mu \in U\}$. $Y(t, x, \mu)$ defines a surface on M parametrized by t and μ. Let ∇_{μ} be the covariant derivative along the curve Y (t = constant, x, μ). The expansion of $V(Y(t, x, \mu))$ about $Z(t)$ reads

$$\begin{aligned} V(Y(t, x, \mu)) = {} & V(Z(t)) + \mu\nabla_{\alpha}V(Z(t))\delta Y^{\alpha}(t, x) + \tfrac{1}{2}\mu^2\nabla_{\alpha}\nabla_{\beta}V(Z(t))\delta Y^{\alpha}(t, x)\delta Y^{\beta}(t, x) \\ & + \tfrac{1}{2}\mu^2\nabla_{\alpha}V(Z(t))\delta^2 Y^{\alpha}(t, x) + \cdots \end{aligned} \tag{3.8}$$

where

$$\delta Y(t, x) = \partial_{\mu}Y(t, x, \mu)\Big|_{\mu=0} \quad \text{and} \quad \delta^2 Y(t, x) = \nabla_{\mu}\partial_{\mu}Y(t, x, \mu)\Big|_{\mu=0}$$

$\delta Y(\cdot, x)$ is a vector field** along Z generated by varying μ in $\mathrm{Dev}(q + \mu x)$. Let $T_Z M$ be the space of vector fields† along Z The following lemma shows that the mapping from Y_+ into $T_Z M$ by $x \mapsto \delta Y(\cdot, x)$ is linear; it will then be easy to reexpress the integral (3.7) as an integral over the space of vector fields along Z via the linear mappings $y \mapsto x \mapsto \delta Y(\cdot, x)$.

Formal Lemma. The mapping $\delta Y(\cdot, \cdot): x \mapsto \delta Y(\cdot, x)$ is the derivative†† of the development mapping at the path q.

Proof.

$$\mathrm{Dev}: Y_+ \to \mathscr{C}_b M.$$

*Look up appendix B for the use of one parameter variations and the use of covariant derivatives in Taylor expansions

**This notation gives the erroneous feeling that $\delta Y(t, x)$ is a small increment, it is used nevertheless for its obvious convenience

†Strictly speaking it should be called $T_Z(\mathscr{C}_b(M))$

††The derivative mapping $f'(x)$ of a mapping $f\ \mathbf{R}^n \to \mathbf{R}^n$ by $x \mapsto y$ is the linear mapping $f'(x)\ T_x R^n \to T_y R^n$ by $f'(x)v = w$ such that $(\partial f^{\alpha}(x)/\partial x^{\beta})v^{\beta} = w^{\alpha}$ In general the derivative mapping of $f\ X \to Y$ is a linear mapping $f'(x)\ T_x X \to T_y Y$ such that $f(x) = f(x_0) + f'(x_0)(x - x_0) + O(\|x - x_0\|)$

In particular

$$\mathrm{Dev}(q+\mu x) = Y(\cdot, x, \mu).$$

By definition

$\mathrm{Dev}'(q): T_q Y_+ \to T_Z(\mathscr{C}_b(M))$, also called $T_Z M$, by

$$\partial_\mu \mathrm{Dev}(q+\mu x)\Big|_{\mu=0} = \mathrm{Dev}'(q)x = \partial_\mu Y(\cdot, x, \mu)\Big|_{\mu=0} = \delta Y(\cdot, x). \qquad \blacksquare$$

The lemma and its proof are only formal because the development mapping is only measurable so does not really have a derivative. Elworthy* has derived essentially the same result via the Girsanov–Cameron–Martin formula.

Note that $\mathrm{Dev}'(q)$ is a linear mapping $x \mapsto \delta Y(\cdot, x)$ but that there is no linear mapping $x(t) \mapsto \delta Y(t, x)$.

Lemma. Let $V = 0$. Let h be a Jacobi field along q defined by $h(t_b)$ and $\dot{h}(t_b)$. Then $\delta Y(\cdot, h)$ is a Jacobi field along Z defined by $\delta Y(t_b, h) = h(t_b)$, $\nabla_t \delta Y(t = t_b, h) = \dot{h}(t_b)$.

Proof. When $V = 0$, $q(t) =$ constant, the development of q is the geodesic Z on M such that $\dot{Z}(t_b) = q(t)$. We shall compute $\nabla_t \nabla_t \delta Y(t, x)$ for an arbitrary vector field x along q and show that, if x is a Jacobi field vanishing at t_b, $\delta Y(\cdot, x)$ is a Jacobi field along Z,

$$\nabla_t \delta Y(t, x) = \nabla_\mu \partial_t Y(t, x, \mu)\Big|_{\mu=0}.$$

By definition of the development map, $\partial_t Y(t, x, \mu)$ is equal to $\dot{q}(t) + \mu \dot{x}(t)$ parallel propagated along $Y(t, x, \mu)$. Parallel propagation can be expressed in terms of orthogonal frames. A frame $v(t, x, \mu)$ at $Y(t, x, \mu)$ is a mapping from R^n into $T_{Y(t,x,\mu)}M$. Indeed, an n-tuple and a frame determine a unique vector whose components in the given frame is the given n-tuple. Then

$$\partial_t Y(t, x, \mu) = v(t, x, \mu)(\dot{q}(t) + \mu x(t)) \tag{3.9}$$

and

$$\nabla_t \delta Y(t, x) = \nabla_\mu \partial_t Y(t, x, \mu)\Big|_{\mu=0} = v(t)x(t) + \nabla_\mu v(t, x, \mu) q(t)\Big|_{\mu=0}$$

where $v(t) = v(t, x, 0)$ is the parallel transport along Z from $Z(t_b)$ to $Z(t)$. Since $\nabla_t v(t, x, \mu) = 0$ and $\dot{q}(t) = 0$,

$$\nabla_t \nabla_t \delta Y(t, x) = v(t)\ddot{x}(t) + R(\dot{Z}(t), \delta Y(t, x))\dot{Z}(t).$$

If x is a Jacobi field along q, $x(t) = 0$ and $\delta Y(\cdot, x)$ satisfies the equation of geodetic deviation. $\blacksquare$

$\delta Y(\cdot, x)$ is not the only vector field along Z which enters the calculation; so does the vector field vx obtained by parallel transporting $x(t)$ along Z from b to $Z(t)$. Note that

$$\delta Y(t, x) \neq v(t)x(t).$$

*Private communication

In other words developing a family of paths $\{q + \mu x\}$ and then making a one-parameter variation is not equivalent to making a one-parameter variation of $\{q + \mu x\}$ and then parallel propagating x along Dev q. Set

$$\bar{\delta}Y(t, x) = \delta Y(t, x) - v(t)x(t).$$

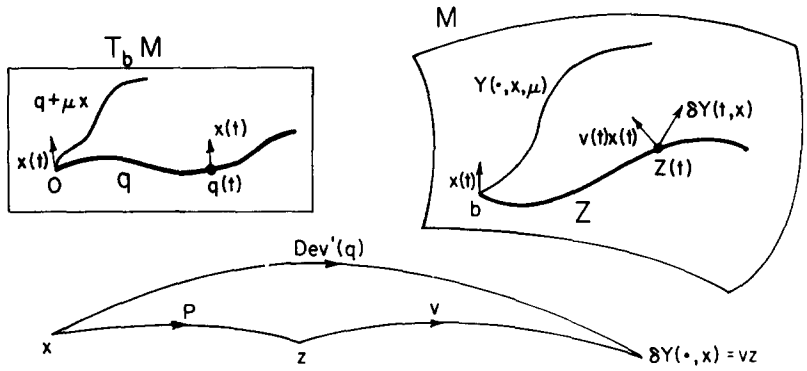


Fig 7

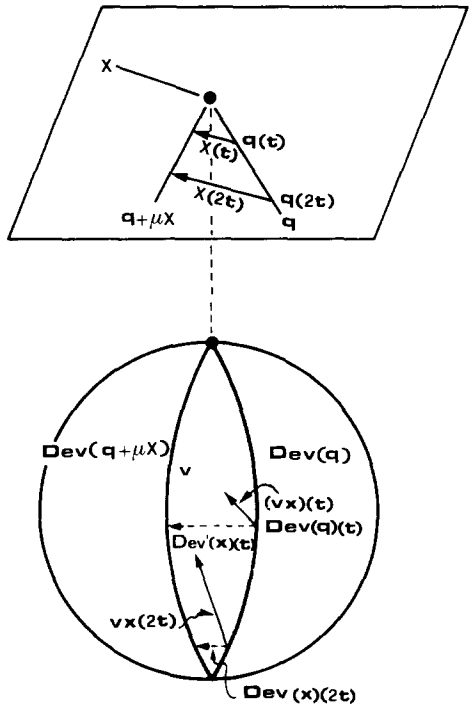


Fig 8 Consider a sphere and its tangent space at the north pole The two lines q and $q + \mu x$ develop into two geodesics The vector field vx along Dev(Q) is such that $vx(t)$ is obtained by parallel propagating $x(t)$ from the north pole to Dev$(q)(t)$ The vector field Dev'$(q)x$ along Dev(q) is obtained by making a one-parameter variation of the family of paths $\{\text{Dev}(q + \mu x),\ 0 \leq \mu \leq (\hbar/m)^{1/2}\}$ Its value at Dev$(q)(t)$ is Dev'$(q)(x)(t)$ abbreviated on the picture as Dev'$(x)(t)$

The marvelous thing is that $\bar{\delta}Y(\cdot, x)$ is differentiable [49],* of class C^2, although $\delta Y(\cdot, x)$ and vx are not differentiable. Indeed, the differentiability of $\bar{\delta}Y(\cdot, x)$ follows from

$$(\bar{\delta}Y(t,x) \mid Z(t)) = \int_t^{t_b} \frac{1}{m} \nabla V(Z(s)) \bar{\delta}Y(s,x)\, \mathrm{d}s. \tag{3.10}$$

Proof of eq. (3.10). Compute $\partial_\mu \| \dot{Y}(t,x,\mu)\|^2$ at $\mu = 0$ in two different ways. On the one hand

$$\partial_\mu (\dot{Y}(t,x,\mu) \mid \dot{Y}(t,x,\mu))\Big|_{\mu=0} = 2\partial_t (\partial Y(t,x) \mid \dot{Z}(t)) + \frac{2}{m} \nabla V(Z(t)) \delta Y(t,x).$$

On the other hand, since the frames are orthogonal, eq. (3.9) gives

$$\partial_\mu \| \dot{Y}(t,x,\mu)\|^2 \Big|_{\mu=0} = 2(v(t)\dot{x}(t) \mid \dot{Z}(t)) = 2\partial_t (v(t)x(t) \mid Z(t)) + \frac{2}{m} (\nabla V(Z(t)) \mid v(t)x(t)). \qquad \blacksquare$$

After this long but necessary and fruitful digression on δY, return to the calculation of eq. (3.7). The change of variable $y \mapsto x$ defined by $b + \mu y = q + \mu x$ proceeds as before. The Cameron–Martin formula gives, after the usual integration by parts,

$$\mathrm{d}w(x) = \mathrm{d}w^{\mathrm{W}}(x) \exp \mathrm{i}\left\{ \int_T \mathrm{d}t \left(\frac{1}{2\mu^2} \|Z(t)\|^2 - \frac{1}{\mu} (Z(t) \mid v(t)x(t)) \right) - \frac{1}{\mu} (\dot{Z}(t_a) \mid v(t_a)x(t_a)) \right\}.$$

Replace V, S_0 and T by their expansion (3.8) about Z. The terms proportional to $\hbar^{-1}$ are independent of x and combine to give as before the general solution $\bar{S}(t_b, b)$ of the Hamilton–Jacobi equation with Cauchy data S_0 at t_a. The terms proportional to $\hbar^{-1/2}$ cancel, not readily as before, but by virtue of eq. (3.10), giving

$$\psi_{\mathrm{WKB}}(t_b, b, \mu) = \exp\left\{ \frac{\mathrm{i}}{\hbar} \bar{S}(t_b, b) \right\} \int_{Y_+} \mathrm{d}w^{\mathrm{W}}(x) \exp\left\{ -\frac{\mathrm{i}}{2m} \int_T \mathrm{d}t \left[\nabla_\alpha \nabla_\beta V(Z(t)) \delta Y^\alpha(t,x) \delta Y^\beta(t,x) + \nabla_\alpha V(Z(t)) \delta^2 Y^\alpha(t,x) \right] + \frac{1}{2m} \left[\nabla_\alpha \nabla_\beta S_0(Z(t_a)) \delta Y^\alpha(t_a, x) \delta Y^\beta(t_a, x) + \nabla_\alpha S_0(Z(t_a)) \delta^2 Y^\alpha(t_a, x) \right] \right\} T(Z(t_a)). \tag{3.11}$$

Following Elworthy we show that

$$(\delta^2 Y(t,x) \mid Z(t)) - \int_t^{t_b} \langle \delta^2 Y(r,x), \frac{1}{m} \nabla V(Z(r)) \rangle \, \mathrm{d}r = \int_t^{t_b} (R(\delta Y, \dot{Z}(r)) \delta Y \mid Z(r))\, \mathrm{d}r + \int_t^{t_b} \mathrm{d}r (\|\nabla_r \delta Y(r,x)\|^2 - \|x(r)\|^2). \tag{3.12}$$

For $t = t_a$, the left hand side of eq. (3.12) is precisely the combination which enters eq. (3.11). The quadratic term in δY combines with the other quadratic terms in eq. (3.11) and enters the calculation

*Earlier calculations of path integrals had introduced apparently miraculous cancellation between factors of the undefined quantity $\delta(0)$, [B S DeWitt, private communication] The $\delta(0)$ terms are introduced by the time derivatives of $\delta Y(\,, x)$ and vx, they cancel because the integrand is not a function of $\delta Y(\,, x)$ and vx but of their difference

of the wave function on curved spaces (3.11) in a straightforward generalization of the calculation in flat space. The remaining terms are eliminated by the change of variable $x \to \delta Y(\cdot, x)$.

Proof of equation (3.12). Compute $\nabla_\mu \partial_\mu \|\partial_t Y(t, x, \mu)\|^2$ at $\mu = 0$ in two different ways. On the one hand

$$\nabla_\mu \partial_\mu \|\partial_t Y(t, x, \mu)\|^2 = 2(\nabla_\mu \nabla_t \partial_\mu Y(t, x, \mu) \mid \partial_t Y(t, x, \mu)) + 2(\nabla_t \partial_\mu Y(t, x, \mu) \mid \nabla_t \partial_\mu Y(t, x, \mu))$$

$$\nabla_\mu \partial_\mu \|\partial_t Y(t, x, \mu)\|^2 \Big|_{\mu=0} = 2(\nabla_t \delta^2 Y(t, x) \mid Z(t)) + 2(R(\delta Y, \dot{Z}(t))\delta Y \mid \dot{Z}(t)) + 2\|\nabla_t \delta Y\|^2$$

where the argument of δY is (t, x). On the other hand, since the frames are orthogonal, (3 9) gives

$$\nabla_\mu \partial_\mu \|\partial_t Y(t, x, \mu)\|^2 \Big|_{\mu=0} = 2\|x(t)\|^2$$

Equation (3.12) follows. ■

Insert (3.12) into the wave equation (3.11) and map $x \mapsto \delta Y(\ , x)$ by the derivative of the development mapping at q. Let w be the image under $\mathrm{Dev}'(q)$ of the Wiener gaussian w^{W} on Y_+. Then according to the Cameron–Martin formula

$$dw(\delta Y) = dw^{\mathrm{W}}(\delta Y)(\mathrm{Det}\,\mathrm{Dev}'(q))^{-1} \exp\left\{\frac{1}{2}\int_T (\|x(t)\|^2 - \|\nabla_t \delta Y(t)\|^2)\, dt\right\}$$

where we have simplified the notation and written $\mathrm{Dev}'(q)x = \delta Y$. In the δY-variable, the wave function (3.11) reads

$$\psi_{\mathrm{WKB}}(t_b, b, \mu) = \exp\left(\frac{i}{\hbar}\bar{S}(t_b, b)\right)(\mathrm{Det}\,\mathrm{Dev}'(q))^{-1} T(Z(t_a))I \tag{3.13}$$

where

$$I = \int_{T_Z M} dw^{\mathrm{W}}(\delta Y) \exp\left\{\frac{-1}{2}\int_T \left[\frac{1}{m}\nabla_\alpha \nabla_\beta V(Z(t))\delta Y^\alpha(t)\delta Y^\beta(t) - (R(Z(t), \delta Y(t)\, \dot{Z}(t))\mid \delta Y(t))\right] dt \right.$$
$$\left. + \frac{i}{2m}\nabla_\alpha \nabla_\beta S_0(Z(t_a))\delta Y^\alpha(t_a)\delta Y^\beta(t_a)\right\}.$$

The computation of the path integral I is straightforward and proceeds as in the flat case.

$$I = (\det \bar{K}(t_a, t_a)/\det \bar{K}(t_b, t_a))^{1/2}$$

where $\bar{K}(t, t_a)$ is the solution of the Jacobi equation such that

$$\bar{K}^{\alpha\beta}(t_a, t_a) = g^{\alpha\beta}(Z(t_a)) \text{ and } m\nabla_t \bar{K}^{\alpha\beta}\ (t = t_a, t_a) = \nabla^\alpha \nabla^\beta S_0(Z(t_a))$$

Let $V_a \in T_{Z(t_a)}M$, and $\bar{H}(t) = \bar{K}(t, t_a)V_a \in T_{Z(t)}M$, then

$$m\nabla_t \nabla_t H^\alpha(t) + \nabla^\alpha \nabla_\gamma V(Z(t))H^\gamma(t) + R_{\gamma\delta\epsilon}{}^\alpha H^\gamma(t)Z^\delta(t)\dot{Z}^\epsilon(t) = 0.$$

We prove that

$$\bar{K}^\alpha_\beta(t_b, t_a) = \partial Z^\alpha(t_b)/\partial Z^\beta(t_a).$$

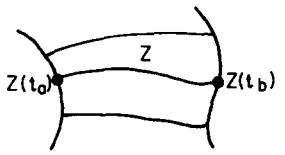


Fig 9

Indeed consider an n parameter flow of classical paths $\{A(t, u_1 \dots u_n) = A(t, u)\}$ originating in a neighborhood of $a = Z(t_a)$ such that $A(t, 0) = Z(t)$ and $m\dot{A}^\alpha(t_a, u) = \nabla^\alpha S_0(A(t_a, u))$.
Consider the group of transformations $\mathscr{C}$ generated by this flow:

$$\mathscr{C} : T \times M \to M$$

in such a way that $(t_b, A(t_a, u)) \mapsto A(t_b, u)$. Its derivative $\mathscr{C}'(t, Z(t_a))$ maps a vector $V_a \in T_{Z(t_a)}M$ into a vector in $V(t) \in T_{Z(t)}M$ such that

$$V^\alpha(t) = (\partial Z^\alpha(t)/\partial Z^\beta(t_a)) V_a^\beta.$$

$V(t)$ is a Jacobi field which can be obtained by a variation through the family $\{A(t, u)\}$ such that

$$\partial_u A(t_a, u)\Big|_{u=0} = V_a.$$

Its covariant derivative along $Z(t)$ is $\dot{V}^\alpha(t) = (D\dot{Z}^\alpha(t)/\partial Z^\beta(t_a)) V_a^\beta$ and at the origin $\dot{V}^\alpha(t_a) = \nabla_\beta \nabla^\alpha S_0(Z(t_a))/m$. Hence

$$V(t) = \bar{H}(t) = \bar{K}(t, t_a) V_a. \qquad \blacksquare$$

Thus the integral I in eq. (3.11) is given by

$$I^2 = \det(\partial Z^\alpha(t_a)/\partial Z^\beta(t_b)).$$

It gives the rate at which a flow of classical paths originating in a neighborhood $N(a)$ of $S_0(Z(t_a))$ diverges or converges. It reflects both the choice of the initial wave function and the dynamical properties of the system.

If we choose $\nabla_\beta \nabla^\alpha S_0(Z(t_a)) = 0$, i.e. if $N(a)$ has first order contact with its tangent space at $Z(t_a)$, the matrix $\bar{K}_\beta^\alpha(t_a, t_b)$ is equal to $K_\beta^\alpha(t_a, t_b)$ defined in appendix B. The matrix $K_\beta^\alpha(t_a, t_b)$ is not the apparently similar matrix (called D^{-1}) constructed by B.S. DeWitt [37, p. 150] from the geodetic interval (alias the world function), nor the matrix (called A) used by Hawking and Ellis [67, p. 96] to define the vorticity, shear and expansion of a family of geodesics. Their matrix satisfies also the equation of geodetic deviation but with the boundary conditions defining the matrix called here $J_\beta^\alpha(t_a, t_b)$. The determinant of $J_\beta^\alpha(t_a, t_b)$ gives the rate at which *geodesics emanating from a fixed point diverge faster or slower than straight lines emanating from a fixed point.*

The determinant of K gives the rate at which a flow of geodesics originating in a neighborhood of $b \subset M$ diverges or converges. More precisely, let $V_b \in T_b M$ and $H(t) = K(t, t_b) V_b$, then H is a Jacobi field along Z such that $H(t_b) = V_b$, $\dot{H}(t_b) = 0$. This Jacobi field can be generated by a variation through geodesics originating in a neighborhood $N(b)$ of b such that $N(b) \subset M$ and

$$\begin{cases} N(b) \text{ has first order contact with its tangent space at } b; \\ \text{the flow of geodesics is orthogonal to } N(b). \end{cases}$$

In flat space for $V = 0$, $K^{\alpha}_{\beta}(t_a, t_b) = K^{W\alpha}_{\beta}(t_a, t_b) = \delta^{\alpha}_{\beta}$. In curved space, $\det K^{\alpha}_{\beta}(t_a, t_b)$ gives the rate at which *geodesics diverge faster or slower than parallel lines orthogonal to the tangent space to $N(b)$ at b.*

In conclusion, the WKB approximation of the wave function in curved space is

$$\psi_{\mathrm{WKB}}(t_b, b, \mu) = \exp\left\{\frac{\mathrm{i}}{\hbar}\bar{S}(t_b, b)\right\}(\det \partial Z^{\alpha}(t_a)/\partial Z^{\beta}(t_b))^{1/2}(\mathrm{Det}\,\mathrm{Dev}'(q))^{-1}T(Z(t_a)). \tag{3.14}$$

It remains to compute $\mathrm{Det}\,\mathrm{Dev}'(q)$. First some general properties of $\mathrm{Dev}'(q)$.

1. The mapping $\mathrm{Dev}'(q): Y_+ \to T_Z M$ by $x \mapsto \delta Y(\cdot, x)$ can be decomposed into two mappings: $\mathrm{Dev}'(q) = v \circ P$ where $P: Y_+ \to Y_+$ by $x \mapsto z = v^{-1}\delta Y(\cdot, x)$. P is the essence of the development mapping. It maps a vector $x(t) \in T_b M$ which parallel transported from b to $Z(t)$ is equal to $\delta Y(t, x)$:

$$v(t)z(t) = \delta Y(t, x) = \mathrm{Dev}'(q)x(t).$$

The mapping P induces a mapping P_v

$$P_v: T_Z M \to T_Z M \qquad \text{by} \quad vx \mapsto \delta Y(\cdot, x).$$

Since parallel transport is norm preserving,

$$\mathrm{Det}\,\mathrm{Dev}'(q) = \mathrm{Det}\,P = \mathrm{Det}\,P_v. \tag{3.15}$$

2. We have previously measured the difference $\delta Y(\cdot, x) - vx$ by $\bar{\delta} Y(\cdot, x)$:

$$P_v = 1 \;\Leftrightarrow\; \bar{\delta} Y(\cdot, x) = 0$$

$$\mathrm{Det}\,P_v \neq 1 \;\Leftrightarrow\; \mathrm{Det}\,\mathrm{Dev}'(q) \neq 1$$

$$\mathrm{Det}\,\mathrm{Dev}'(q) \neq 1 \;\Rightarrow\; \delta \bar{Y}(\cdot, x) \neq 0 \quad \text{but not vice versa.}$$

It follows that a family of paths with both ends fixed in $T_b M$ does not develop into a family of paths in M with both ends fixed. Indeed, the vector fields generated by a family of paths with both ends fixed vanishes at t_a and t_b. If $x(t_a) = 0$, then $v(t_a)x(t_a) = 0$. But $v(t_a)x(t_a) = 0$ does not imply $\delta Y(t_a, x) = 0$; it implies $\delta Y(t_a, x) = \bar{\delta} Y(t_a, x)$. See p. 313 under which conditions a family of paths on $T_b M$ develops into a family on M with both ends fixed.

Lemma. When q develops into a classical path, $\mathrm{Det}\,\mathrm{Dev}'(q) = 1$. (3.16)

Proof. We shall prove the result first when $V = 0$, i.e. when q is a straight line.

$\mathrm{Det}\,\mathrm{Dev}'(q) = \mathrm{Det}\,P$ (eq. 3.15) where $P: x \mapsto z$ with

$$z(t) - x(t) = v^{-1}(t)\bar{\delta} Y(t, x), \qquad \nabla_t \nabla_t \bar{\delta} Y(t, x) = R(\dot{Z}(t), \delta \bar{Y}(t, x))\dot{Z}(t).$$

Hence, since $x(t_b) = z(t_b) = 0$ and $\dot{x}(t_b) = y(t_b)$,

$$x(t) = z(t) - \int_T \theta(s - t)(s - t)R(\dot{Z}(s), z(s))\dot{Z}(t)\,\mathrm{d}s,$$

where the integral is assumed to be written in Fermi coordinates so that the Rieman tensor can be

contracted with vectors at different points.* This linear mapping is of the form

$$x(t) = z(t) - \int_t^{t_b} k(t, s) z(s)\, \mathrm{d}s.$$

Since $k(t, s)$ vanishes on the diagonal, it is continuous on $T \times T$ and its determinant is simply

$$\mathrm{Det}\, P^{-1} = \exp\left(\frac{-1}{2} \int_t^{t_b} \mathrm{tr}(k(s, s))\, \mathrm{d}s\right) = 1.$$

When $V \neq 0$, the following relationship** can be used to prove the result by an argument similar to the previous one:

$$\nabla_\mu (v(t, x, \mu) q(t))\Big|_{\mu=0} = -\int_t^{t_b} R(Z(r), \delta Y(r)) \dot{Z}(t)\, \mathrm{d}r \tag{3.17}$$

where $v(t, x, \mu)q(t)$ is the parallel transport of $q(t)$ along $q(t) + \mu x(t)$ and where the right hand side is assumed to be written in Fermi coordinates.* ■

The WKB approximation of the wave function for a particle in curved space is

$$\psi_{\mathrm{WKB}}(t_b, b) = (\det \partial Z^\alpha(t_a)/\partial Z^\beta(t_b))^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar} \bar{S}(t_b, b)\right\} T(Z(t_a)). \tag{3.18}$$

The method developed here can be used to go beyond the WKB approximation. Terms such as $\delta^{(n)} Y$ enter the calculation and have to be expressed by recurrence formulae in terms of δY (see eq. 3.12). The so-called "two-loop" approximation is being investigated.

3.4. The semiclassical expansion of the propagator $\mathscr{K}(B; A)$

The probability amplitude $\mathscr{K}(B; A)$ that the system which is known to be in the state $a \in M$ at t_a be found in the state $b \in M$ at t_b can be obtained from the Feynman–Kac formula (3.1), by choosing the initial wave function $\phi(b + \mu y(t_a)) = \delta(b + \mu y(t_a) - a)$. This choice makes the computation of the Feynman–Kac formula simple in principle to any order in μ and we shall show that

$$\mathscr{K}(B; A) = \int_{Y_+} \mathrm{d}w_+^{\mathrm{W}}(y) \exp\left\{\frac{-\mathrm{i}}{\mu^2 m} \int_T V(b + \mu y(t))\, \mathrm{d}t\right\} \delta(b + \mu y(t_a) - a) \tag{3.19}$$

$$= \mathscr{K}_{\mathrm{WKB}}(B; A)\left(1 + \sum_{n=1}^{\infty} (\mathrm{i}h)^n \mathscr{A}_n\right), \tag{3.20}$$

where $\mathscr{A}_n$ are finite dimensional integrals. The right hand side of eq. (3.20) is known as the **semiclassical expansion** of $\mathscr{K}(B; A)$.

*If one wishes not to use Fermi coordinates one can parallel transport vectors along Z back and forth to $Z(t_b)$, and the equation reads $x(t) = Z(t) - \oint_t^{t_b} (s - t) R(Z(s), z(s)) v(s) v^{-1}(t) Z(t)\, \mathrm{d}s$ where $\oint_t^{t_b}$ means $v(t) \int_t^{t_b} v^{-1}(s)\ \ \mathrm{d}s$

**Reference [49] and Elworthy private communication

To compute (3.20), proceed as in section 3.2:

1. Change of variable $b + \mu y = q + \mu x$ such that q is the classical path

$$m\dot{q}(t) + \nabla V(q(t)) = 0, \qquad q(t_a) = a, \qquad q(t_b) = b. \tag{3.21}$$

In this section the end points of the classical path $q(t_a) = a$ and $q(t_b) = b$ are within focal distance of each other. This restriction is removed in the following section.

2. Integrate $\int_T (\dot{q}(t) \mid x(t))\, dt$ by parts and use the equation of motion.
3. Expand $V(q(t) + \mu x(t))$ in powers of μ:

$$V(q(t) + \mu x(t)) = V(q(t)) + \mu x^\alpha(t)\nabla_\alpha V(q(t)) + \tfrac{1}{2}\mu^2 x^\alpha(t)x^\beta(t)\nabla_\alpha\nabla_\beta V(q(t)) + \mu^2\Omega(q(t), \mu x(t)) \tag{3.22}$$

$$\mu^2\Omega(q(t), \mu x(t)) = \sum_{|n|=3}^{\infty} \mu^{|n|}\nabla_n V(q(t))(x(t))^n/n!$$

where n is a multi index.* Then

$$\mathcal{K}(B; A) = \exp(i\bar{S}(B; A)/\hbar) \int_{Y_+} dw_+^{W}(x) \exp\left\{-\frac{1}{m}\int_T dt(\tfrac{1}{2}\nabla_\alpha\nabla_\beta V(q(t))x^\alpha(t)x^\beta(t) + \Omega(q(t), \mu x(t))\right\}\delta(\mu x(t_a)) \tag{3.23}$$

where $\bar{S}(B; A) = S(q)$.

We can again use the Cameron–Martin formula to find a new gaussian w_+ which "incorporates" the exponent:

Let $G_+(t, s)$ be the elementary kernel of the Jacobi equation

$$-\frac{d^2}{dt^2}G_+^{\alpha\beta}(t, s) - \frac{1}{m}\nabla^\alpha\nabla_\gamma V(q(t))G_+^{\gamma\beta}(t, s) = \delta_s, \qquad G_+(t_b, s) = 0, \qquad \partial G_+(t_a, s)/\partial t_a = 0. \tag{3.24}$$

It has been shown in section 1.5 that the gaussian w_+ of covariance G_+ satisfies the equation

$$dw_+(x)/dw_+^{W}(x) = (\det K(t_b, t_a)/\det K(t_a, t_a))^{+1/2} \exp\left\{\frac{-1}{2m}\int_T \nabla_\alpha\nabla_\beta V(q(t))x^\alpha(t)x^\beta(t)\, dt\right\} \tag{3.25}$$

where $K(t, t_a)$ is the solution of the homogeneous Jacobi equation corresponding to eq. (3.24), such that $K^{\alpha\beta}(t_a, t_a) = g^{\alpha\beta}$ and such that its derivative vanishes at $t = t_a$. Hence

$$\mathcal{K}(B; A) = \exp\{i\bar{S}(B; A)/\hbar\}(\det K(t_b, t_a)/\det K(t_a, t_a))^{-1/2} I \tag{3.26}$$

where

$$I = \int_{X_+} dw_+(w)\delta(\mu x(t_a)) \exp\left(\frac{-i}{m}\int_T dt\, \Omega(q(t), \mu x(t))\right)$$

I can be reexpressed as an integral over the space X of paths vanishing both at t_a and t_b. Let w be

*n is a multi index $n = \{n_1, \ldots, n_j\}$, $|n| = n_1 + \cdots + n_j$, $n! = n_1! \cdots n_j!$, $\nabla_n = D^{|n|}/(\partial q^{\alpha_1}(t))^{n_1} \cdots (\partial q^{\alpha_j}(t))^{n_j}$, $(x(t))^n = (x^{\alpha_1}(t))^{n_1} \cdots (x^{\alpha_j}(t))^{n_j}$

the gaussian on X, Leray related to w_+ on X_+. The gaussian w is normalized to (see p. 283):

$$w(X) = \int_{X_+} \mathrm{d}w_+(x)\delta(x(t_a)) = (2\pi\mathrm{i})^{-n/2}|\det G_+^{\alpha\beta}(t_a, t_a)|^{-1/2}. \tag{3.27}$$

Its covariance G is the elementary kernel of the Jacobi equation (3.24) vanishing on the boundary and is known as the Feynman–Green function. Since $\delta(\mu x(t_a)) = \mu^{-n}\delta(x(t_a))$,

$$I = \mu^{-n} \int_X \mathrm{d}w(x) \exp\left\{\frac{-\mathrm{i}}{m}\int_T \mathrm{d}t\, \Omega(q(t), \mu x(t))\right\}.$$

The WKB approximation consists in setting $\Omega \equiv 0$. Using eq. (3.27) and the expression for G_+ given in appendix B together with the fact that $(J(t_b, t_a))^{-1}$ is the Van Vleck matrix (off diagonal block of the hessian of the action function, eq. B9) we obtain*

$$\mathscr{K}_{\mathrm{WKB}}(B; A) = \exp\{\mathrm{i}\bar{S}(B; A)/\hbar\}(2\pi\mathrm{i}\hbar)^{-n/2}|\det \partial^2\bar{S}(B; A)/\partial b^\alpha \partial a^\beta|^{1/2}, \tag{3.28}$$

$$\mathscr{K}(B; A) = \mathscr{K}_{\mathrm{WKB}}(B; A) \int_X \mathrm{d}w(x) \exp\left\{\frac{-\mathrm{i}}{m}\int_T \mathrm{d}t\, \Omega(q(t), \mu x(t))\right\} \Big/ w(X).$$

To compute this path integral, expand the exponential and regroup the terms in powers of $\mu = (\hbar/m)^{1/2}$. A typical term is of the following form

$$\int_X \mathrm{d}w(x) \int_T \mathrm{d}t\, \nabla_n V(q(t))(x(t))^n \ \ldots \int_T \mathrm{d}s\, \nabla_k V(q(s))(x(s))^k. \tag{3.29}$$

If we can interchange the order of integration then the problem is reduced to computing cylindrical integrals

$$\int_X \mathrm{d}w(x)\, F_{\alpha \quad \beta}(t, \ldots s)x^\alpha(t)\ldots x^\beta(s)$$

i.e. finite dimensional integrals. The integral of an odd polynomial in x vanishes and the expansion of (3.28) is an expansion in powers of μ^2, i.e. an expansion in powers of $\hbar$. Its terms have been computed in section 1.3 (eq. 1.7). The integration of the Feynman–Kac formula (3.19) gives the semiclassical expansion (3.20). Equation (3.20) is known to be a solution of the Schrodinger equation [56, also 108].

The lattice approximation of $\mathscr{K}(B; A)$. We shall relate eq. (3.28) to the path integral definition proposed by Feynman. Equation (3.28) has been obtained from the Feynman–Kac formula for the system whose action is

$$S(f) = \int_T \left[\frac{m}{2}\|f(t)\|^2 - V(f(t))\right]\mathrm{d}t, \qquad f: T \to R^n \text{ with } f(t_a) = a, \quad f(t_b) = b.$$

*Since eq (3 28) has been computed from first principles, the normalization comes in automatically and we are spared the complicated arguments used in its previous derivations

Let q be the classical path, $f = q + \mu x$,

$$S(f) = S(q) + \tfrac{1}{2}S''(q)xx - \mu^2 \int_T \Omega(q(t), x(t))\,dt$$

Let $t_a = t_0 < t_1 \cdot \cdot < t_k < \cdots t_{p+1} = t_b$. Without loss of generality we assume $t_{k+1} - t_k = (t_b - t_a)/(p+1) = \epsilon$ and to avoid unwieldy notations we assume the system to be one dimensional, $f\ T \to \mathbb{R}$. Replace $\int_T \Omega(q(t), x(t))\,dt$ by its lattice approximation

$$\int_T \Omega(q(t), x(t))\,dt \approx \epsilon \sum_{k=0}^{p} \Omega(q^k, x^k), \quad \text{where } q^k = q(t_k),\ x^k = x(t_k).$$

Equation (3.28) becomes a cylindrical integral which can immediately (eq. 1.5) be expressed as an integral over $\mathbb{R}^{p+1}$ under the mapping $P: x \to \{x^0, \ldots x^p\}$, namely

$$\mathcal{K}(B; A) = \mathcal{K}_{\mathrm{WKB}}(B; A) \int_{\mathbb{R}^{p+1}} \delta(\mu x^0)(2\pi\mathrm{i})^{-(p+1)/2} |\det \mathcal{W}_{ij}^{-1}|^{1/2} \exp\left\{\frac{\mathrm{i}}{2}\mathcal{W}_{ij}^{-1}x^i x^j\right\} dx^0 \ldots dx^p$$
$$\times \exp\left\{\frac{-\mathrm{i}\epsilon}{m}\sum_{k=0}^{p}\Omega(q^k, x^k)\right\}$$

where $\mathcal{W}^{ij} = W(\delta_{t_i}, \delta_{t_j}) = G(t_i, t_j)$. The inverse and the determinant of $\mathcal{W}$ has been computed in a previous paper [40, p. 391–392].* Set $f^k = q^k + \mu x^k$. It has been shown [40] that

$$\bar{S}(a, \ldots f^k \ldots b) = \bar{S}(B, A) + \tfrac{1}{2}\sum \mathcal{W}_{ij}^{-1}x^i x^j - \epsilon\mu^2 \sum_{k=0}^{p}\Omega(q^k, x^k).$$

In the limit $\epsilon = 0$ the determinant of $\mathcal{W}_{ij}^{-1}$ takes a simple form (eqs B17, B18)

$$\det \mathcal{W}_{ij}^{-1} = \epsilon^{-(p+1)}/\det M(t_b, t_a)$$

Since $dx^k = df^k/\mu$

$$\tilde{\mathcal{K}}(B; A) = \int_{\mathbb{R}^{p+1}} \exp\left\{\frac{1}{\hbar}\bar{S}(a, \ldots f^k, \ldots b)\right\}\delta(q^0 - a)\prod_{k=0}^{p}(df^k(m/2\pi\mathrm{i}h\epsilon)^{1/2}).$$

Feynman's original path integral representation is

$$\mathcal{K}(B; A) = \lim_{p=\infty} \tilde{\mathcal{K}}(B; A).$$

Semiclassical expansion, quasiclassical representation, asymptotic expansion. The first steps in the calculation of $\mathcal{K}(B; A)$ follow the method introduced by Truman [135, 136] in his derivation of the solution of the diffusion equation, with initial value given by eq. (3.2), which he called the quasi-classical representation. Adjusting for the different initial value of the wave function, eq. (3.23) is the quasiclassical representation of the Schrödinger equation. The calculation leading from eq. (3.23) to the final result (eq. 3.28) shows how the semiclassical expansion can be obtained from the quasiclassical

*See eq (B20) for $\det \mathcal{W}_{ij}^{-1}$

representation. Truman has given the conditions under which the quasiclassical representation is valid as well as the WKB approximation of the solution of the Schrodinger equation and we refer to his papers for a precise discussion of these matters.

Gervais and Sakita [63]* have developed an improved WKB method where the potential is not assumed to vary slowly in all directions of the configuration space.

The WKB approximation of the propagator on curved spaces. With the notation of section 3.3, p. 301, the propagator $\mathscr{K}$ can be written on curved spaces as

$$\mathscr{K}(B;A)=\int_{Y_+} \mathrm{d}w^{\mathrm{W}}(y)\exp\left\{\frac{-\mathrm{i}}{\mu^2 m}\int_T V(X(t,b+\mu y))\,\mathrm{d}t\right\}\delta(X(t_a,b+\mu y)-a).$$

It can be computed as before; the interesting point is that the expansion in powers of μ leads to

$$\delta(Y(t_a,x,\mu)-a)=\delta(\mu\delta Y(t_a,x)+\tfrac{1}{2}\mu^2\delta^2 Y(t_a,x)+\ \cdots),$$

and the term

$$\exp\left\{\frac{-1}{\mu}(\dot{Z}(t_a)\mid v(t_a)x(t_a))\right\}\delta(\mu\delta Y(t_a,x)+\tfrac{1}{2}\mu^2\delta^2 Y(t_a,x)+\cdots)$$

combines precisely with the terms arising from the change of variables $y\mapsto x\mapsto \delta Y$ to give, after a calculation similar to the one leading from equation (3.19) to (3.28),

$$\mathscr{K}_{\mathrm{WKB}}(B;A)=\exp\{\mathrm{i}\bar{S}(B;A)/\hbar\}(2\pi\mathrm{i}\hbar)^{-n/2}|\det\partial^2\bar{S}(B;A)/\partial b^\alpha\partial a^\beta|^{1/2} \tag{3.30}$$

where now $\bar{S}(B;A)=S(Z)$ where Z is the classical path on M such that $Z(t_a)=a$, $Z(t_b)=b$.

Equation (3.30) shows that the WKB approximation of $\mathscr{K}(B;A)$ is equal to the limit of $\mathscr{K}(B;A)$ when t_b-t_a goes to zero [114].

Remark. It has already been noted that the development of a closed loop is not a closed loop, or that the development of a family of paths with both ends fixed is not a family of paths with both ends fixed. We can now complete the statement made on p. 301.

1. Given a family of paths on T_bM with both ends fixed, it develops into a family of paths on M such that $\delta Y(t_a,x)=\bar{\delta}Y(t_a,x)$.

2. Given a family of paths on M with both ends fixed, it is obtained from a family $\{q+\mu x\}$ of paths on T_bM such that

$$\mathrm{Dev}'(q)x(t_a)=-\tfrac{1}{2}\mu\delta^2 Y(t_a,x)+\mathrm{O}(\mu^2). \tag{3.31}$$

3.5. On and beyond the caustics

The results derived in sections 3.2–3.4 are valid only when t_b-t_a is sufficiently small for the end points a and b of the classical path to be within focal distance of each other. We examine now situations in which $q(t_a)$ and $q(t_b)$ are conjugate** along q, or in which there are conjugate points $q(t_0)$ for $t_a<t_0<t_b$.

*This method has been applied to barrier penetration problems and to instantons [34]

**See appendix B for the definition and properties of caustics and conjugate points

On the caustic. Consider first the case in which $q(t_a)$ and $q(t_b)$ are conjugate but there is no other conjugate point along q between $q(t_a)$ and $q(t_b)$. Notice that if $q(t_b)$ is on the caustic of $q(t_a)$ formed by the family of classical paths with common origin, then* $\det J(t_b, t_a) = 0$, its inverse $\det M(t_a, t_b)$ is infinite and the WKB approximation of $\mathcal{K}(B; A)$ is not defined. Similarly if $q(t_b)$ is on the caustic of $q(t_a)$ formed by the family of classical paths with equal initial velocities,** then $\det K(t_b, t_a) = 0$ and the WKB approximation of the wave function $\psi(t_b, b)$ is not defined. These results could have been anticipated: geometrical optics is not a good approximation of wave optics in the neighborhood of a caustic [e.g. 86, p. 146; 16, p. 60].

To compute† $\mathcal{K}(B; A)$ when a and b are conjugate along q we need to go beyond the WKB approximation. Following an idea of Schulman [5, p. 152] we shall make a change of variable of integration which diagonalizes the variance. This procedure is often useful [56] and we present it in a more general context.

Diagonalization of the variance. Let X be the space of continuous paths $x: T \to \mathbf{R}^n$ vanishing on the boundary $x(t_a) = x(t_b) = 0$. Consider an integral over X with respect to a gaussian w whose covariance G is the elementary kernel of a differential operator D, that vanishes on the boundary:

$$D_t G(t, s) = \delta(t - s), \qquad G(t, s) = 0 \quad \text{for } t \text{ or } s \text{ equal to } t_a \text{ or } t_b.$$

Let $\{\psi_k\}$ be a complete orthogonal set of eigenfunctions of D:

$$D\psi_k^\alpha(t) = \alpha_k \psi_k^\alpha(t), \qquad \psi_k(t_a) = \psi_k(t_b) = 0, \qquad \int_T (\psi_k(t) \mid \psi_j(t))\, \mathrm{d}t = \delta_{kj}. \tag{3.32}$$

Expand x and G in the basis $\{\psi_k; k = 1, \ldots \infty\}$:

$$x^\alpha(t) = \sum u^k \psi_k^\alpha(t), \qquad u^k = \int_T (x(t) \mid \psi^k(t))\, \mathrm{d}t \tag{3.33}$$

$$G^{\alpha\beta}(t, s) = \sum u^{kj} \psi_k^\alpha(t) \psi_j^\beta(s) \tag{3.34}$$

$$u^{kj} = \int_T \mathrm{d}t \int_T \mathrm{d}s\, \psi_\alpha^k(t) \psi_\beta^j(s) G^{\alpha\beta}(t, s). \tag{3.35}$$

The change of variable $x \mapsto \{u^k; k = 1, \ldots \infty\}$ is a linear change of variable which can be treated by the methods developed in section 1.3. Let $P: X \to \mathbf{R}^\infty$ by $x \mapsto u = \{u^k\}$, and let $\xi = \{\xi_k\}$ be in the dual of $\mathbf{R}^\infty$.

Lemma. The image w_P of w under P is a gaussian of covariance $\delta^{kj}\alpha_k^{-1}$. Its normalization is the same as that of w.

Proof. The image of w under P is a gaussian of variance

$$U(\xi, \xi) = \sum \xi_k \xi_j \int_T \mathrm{d}t \int_T \mathrm{d}s\, \psi_\alpha^k(t)\, \psi_\beta^j(s) G^{\alpha\beta}(t, s) \tag{3.36}$$

$$= \sum \xi_j \xi_j u^{kj} \tag{3.37}$$

*See appendix B for the definition and properties of caustics and conjugate points

**See p 353 for the meaning to be given to this condition on a curved space

†We can also compute the wave function when b is on the caustics formed by the family of classical paths with equal initial velocities

The inverse of U, in the sense defined in section 1.5, is a bilinear form on $\mathbb{R}^\infty$

$$U^{-1}(u, u) = \sum u^k u^l u^{-1}_{kj} \qquad \text{with} \quad \sum u^{kj} u^{-1}_{jl} = \delta^l_l.$$

It can be obtained from the inverse of the variance of w. Indeed

$$W^{-1}(x, x) = \int_T (Dx(t) \mid x(t))\, dt = \sum u^k u^l \alpha_k \delta_{jk} = U^{-1}(u, u).$$

Hence $u^{-1}_{kj} = \alpha_k \delta_{jk}$, and the first part of the lemma is proved. A linear mapping always preserves the normalization. Indeed

$$\mathcal{F}w^P(0) = \mathcal{F}w \circ \tilde{P}(0) = \mathcal{F}w(0).$$

We mention explicitly the normalization of w^P because w, in contrast to $w_\pm$, is not normalized to unity.* ■

It follows from eq. (3.34) that

$$G^{\alpha\beta}(t, s) = \sum \alpha_k^{-1} \psi^\alpha_k(t) \psi^\beta_k(s). \tag{3.38}$$

Similar results can be derived for $G_\pm$ by choosing appropriately the boundary conditions of the basis $\{\psi_k\}$.

Remark. The diagonalization of the variance shows that the gaussian method is defined for space of paths X and potentials V such that $\mathcal{J}(\bar{q})$ is a Sturm–Liouville operator on X.

Returning to the study of $\mathcal{K}(B; A)$ near the caustics, we compute $\mathcal{K}(B'; A')$ where $B' = (b', t_b)$ and $A' = (a', t_a)$, but expand all quantities around the classical path q such that $q(t_a) = a$, $q(t_b) = b$. According to the Feynman–Kac formula

$$\mathcal{K}(B'; A') = \int_{Y_+} dw^w_+(y) \exp\left\{\frac{-i}{\mu^2 m} \int_T V(b' + \mu y(t))\, dt\right\} \delta(b' + \mu y(t_a) - a').$$

Since in the basis $\{\psi_k\}$ we can expand only functions which vanish at t_a and t_b, we have to choose a' and b' such that $a' - a = b' - b$. Set

$$a' - a = b' - b = \mu\Delta$$

and make the change of variable $y \mapsto x$ such that

$$b' + \mu y(t) = q(t) + \mu(x(t) + \Delta).$$

Then

$$\mathcal{K}(B'; A') = \exp\left\{\frac{i}{\hbar} S(B; A) - \frac{i}{\mu m} \Delta^\alpha \int_T \nabla_\alpha V(q(t))\, dt + O(\Delta^2)\right\} \mu^{-n}(I + O(\Delta^2, \mu^2)) \tag{3.39}$$

*See Leray associated gaussians, p 283

with*

$$I = \int_{Y_+} \mathrm{d}w_+^{\mathrm{W}}(x) \exp\left\{-\frac{1}{2m}\int_T \left[\nabla_\alpha\nabla_\beta V(q(t))(x^\alpha(t)x^\beta(t) + 2x^\alpha(t)\Delta^\beta) + \frac{\mu}{3}\nabla_\alpha\nabla_\beta\nabla_\gamma V x^\alpha x^\beta x^\gamma\right]\mathrm{d}t\right\}\delta(x(t_a)).$$

To compute I we have the choice of two routes:

(a) Proceed as in section 3.4. Use the Cameron–Martin formula to introduce a new gaussian w_+ which incorporates the terms quadratic in x. Then rewrite I as an integral over the space Y of paths which vanish at both ends, using the gaussian w associated in the Leray sense to w_+. Or, vice versa.

(b) Rewrite I as an integral over Y, using the gaussian w^{W} Leray related to w_+^{W}, then introduce a new gaussian $\bar{w}$ which incorporates the terms quadratic in x. The results can be shown to be identical although $w(Y) \neq \bar{w}(Y)$.

We shall follow the second route which is simpler in this case. The essential steps are:

$$\int_{Y_+} \mathrm{d}w_+^{\mathrm{W}}(x)\delta(x(t_a))F(x) = \int_Y \mathrm{d}w^{\mathrm{W}}(x)F(x)$$

where the Wiener gaussian w^{W} on Y (p. 283) is normalized to

$$w^{\mathrm{W}}(Y) = (2\pi\mathrm{i})^{-n/2}(\det G_+^{\mathrm{W}}(t_a, t_a))^{-1/2} = (2\pi\mathrm{i})^{-n/2}(\det M^{\mathrm{W}}(t_b, t_a))^{1/2}$$
$$= (2\pi\mathrm{i}(t_b - t_a))^{-n/2}\det g_{\alpha\beta}.$$

Use the Cameron–Martin formula, together with the ratio of the covariances G and G^{W} eq. (B.18), to incorporate the quadratic terms

$$\mathrm{d}\bar{w}(x) = \mathrm{d}w^{\mathrm{W}}(x)\exp\left\{-\frac{1}{2m}\int_T \nabla_\alpha\nabla_\beta V(q(t))x^\alpha(t)x^\beta(t)\,\mathrm{d}t\right\}$$
$$\times(\det M^{\mathrm{W}}(t_b, t_a)/\det M(t_b, t_a))^{1/2}.$$

Make the change of variable $x \mapsto u$ which diagonalizes the variance. With Δ defined p. 315, set

$$\Delta^\beta\int_T \nabla_\beta\nabla_\alpha V(q(t))\psi_k^\alpha(t)\,\mathrm{d}t = \Delta^\alpha V_{\alpha k}$$

$$\int_T \nabla_\alpha\nabla_\beta\nabla_\gamma V(q(t))\psi_k^\alpha(t)\psi_j^\beta(t)\psi_l^\gamma(t)\,\mathrm{d}t = V_{kjl}.$$

Then

$$I = (\det M(t_b, t_a)/\det M^{\mathrm{W}}(t_b, t_a))^{1/2}\int_{R^\infty} \mathrm{d}w_P(u)\exp\left\{\frac{-\mathrm{i}}{m}\Delta^\alpha V_{\alpha k}u^k - \frac{1\mu}{6m}V_{kjl}u^k u^j u^l\right\}$$

where

$$\mathrm{d}w_P(u) = (2\pi\mathrm{i})^{-n/2}(\det M^{\mathrm{W}}(t_b, t_a))^{1/2}\exp\left\{\frac{\mathrm{i}}{2}\sum \alpha_k u^k u^k\right\}\prod_1^\infty (\alpha_k/2\pi 1)^{1/2}\,\mathrm{d}u^k. \tag{3.40}$$

*Some arguments not written explicitly are obvious

The integration over u^k when all $\alpha_k \neq 0$ is straightforward; in the limit $\Delta = 0$ and $\mu = 0$, $I = (2\pi i)^{-n/2}(\det M(t_b, t_a))^{1/2}$.

Consider now the case where one and only one eigenvalue, say α_1, is zero; then $\psi_1^\alpha(t)$ is a non zero Jacobi field vanishing on the boundary, $q(t_a)$ and $q(t_b)$ are conjugate, $\det J(t_b, t_a) = 0$ and we have to compute the apparently undefined quantity $\alpha_1 \det M(t_b, t_a) = \alpha_1/\det J(t_b, t_a)$. Each column of $J_\beta^\alpha(t, t_a)$ consists of the components of a Jacobi field $h_{(\beta)}^\alpha(t) = J_\beta^\alpha(t, t_a)$ such that $h_{(\beta)}^\alpha(t_a) = 0$ and $h_{(\beta)}^\alpha(t_a) = \delta_\beta^\alpha$. After a similarity transformation which does not change the determinant we can assume that $\det J(t_b, t_a) = 0$ implies $J_1^\alpha(t_b, t_a) = 0$. Since we have assumed only one vanishing eigenvalue, there is only one non zero Jacobi field vanishing on the boundary. This one field is also a column of $J_\beta^\alpha(t, t_b)$ again possibly after a similarity transformation. The three fields $\psi_1(t)$, $J_1(t, t_a)$ and $J_1(t, t_b)$ satisfy the same equation and the same boundary conditions:

$$\psi_1(t) = J_1(t, t_a) = J_1(t, t_b).$$

Choose the system of coordinates such that $J_1^\alpha \propto \delta_1^\delta$, i.e. the 1-axis is perpendicular to the caustics. Near the caustics $J_1^1(t_b, t_a) = \epsilon$, then $M_{11}(t_b, t_a) = \epsilon^{-1}$, $M_{1\alpha}(t_b, t_a) = 0$ and

$$\lim_{\epsilon=0} G^{\alpha\beta}(t, s) = \theta(s-t)J^{\alpha 1}(t, t_a)M_{11}(t_a, t_b)J^{1\beta}(t_b, s) - \theta(t-s)J^{\alpha 1}(t, t_b)M_{11}(t_b, t_a)J^{1\beta}(t_a, s).$$

On the other hand when α_1 tends to zero, eq. (3.38) gives

$$\lim_{\alpha_1=0} G^{\alpha\beta}(t, s) = \alpha_1^{-1}\psi_1^\alpha(t)\psi_1^\beta(s).$$

Hence $M_{11} = \alpha_1^{-1}$ and $\alpha_1 \det M(t_b, t_a) = \text{cofactor } M_{11}$. The integral over u_1 is an Airy function. Set $u^1 = u/\mu$;

$$\nu = -V_{111}/2\hbar, \qquad c = -2(b'-b)^\alpha V_{\alpha 1}/V_{111}, \qquad \text{and} \qquad I(\nu, c) = \int_R du \exp i\nu(\tfrac{1}{3}u^3 - cu).$$

Then

$$\underset{\lim \hbar = \Delta = 0}{\mathcal{K}(B'; A')} = \exp\left\{\frac{i}{\hbar}\bar{S}(B; A)\right\}(m/2\pi i\hbar)^{(n+1)/2}\text{cofactor } M_{11}I(\nu, c) \tag{3.41}$$

in the system of coordinates where the 1-axis is perpendicular to the caustic. A similar analysis gives the value of $\mathcal{K}(B'; A')$ when there is more than one zero eigenvalue. Since there can be at most n nonzero Jacobi fields vanishing on the boundary, the zero eigenvalue is at most n-degenerate. When there are k nonzero Jacobi fields vanishing on the boundary, b is said to be a conjugate point of multiplicity k. The behavior of $\mathcal{K}$ near the caustics had been obtained by Schulman [5, p. 152], largely from qualitative arguments. Equation (3.41) confirms his results and gives all the factors explicitly.

The Airy regime of the propagator near the caustics has an immediate physical interpretation. When $\hbar$ tends to zero, the leading contribution to $I(\nu, c)$ is found by making the argument of the exponential stationary, i.e. by solving

$$u^2 - c = 0.$$

The sign of c, i.e. the sign $(b'-b)^\alpha V_{\alpha 1}$, has a dramatic effect or as we shall see a catastrophic effect in

the technical sense of the term: Asymptotically

$$I(\nu, c) \sim \begin{cases} (\pi/\nu c^{1/2})^{1/2} \exp(\frac{2}{3}\nu c^{1/2}) + (-\pi/\nu c^{1/2})^{1/2} \exp(-\frac{2}{3}\nu c^{3/2}) & \text{for } c > 0 \\ (\pi/\nu|c|^{1/2})^{1/2} \exp(-\frac{1}{3}\nu|c|^{3/2}) & \text{for } c < 0. \end{cases} \tag{3.42}$$

For $c < 0$ we are in the "shadow" region of exponential decay, while for $c > 0$ we are in the illuminated region.

Classically, it has been shown* that the caustics are the projections of the catastrophe sets on the control space of system: here a state of the system is a particular solution of the Hamilton–Jacobi equation $\bar{S}(B; A)$, the control space is the space of points $B \in M \times T$. Given B there may be $0, 1, \ldots n$ stationary paths from A to B. If there is one and only one, A and B are within focal distance of each other If there is none, B is in the shadow region of A; if there is more than one B is in the illuminated region. The boundaries between regions with different illuminations are the caustics. If there are k stationary paths from A to B, the caustics relative to A is an $n - k$ dimensional surface.

Set $\bar{S}_k(B; A)$ the value of the action function computed along the stationary path q_k. Let Σ be the set of points $\{B, \bar{S}_k(B; A)\}$ for all $B \in M \times T$. The catastrophe set of the system is the set of points $\sigma \in \Sigma$ where the projection $\Pi: \Sigma \to M \times T$ is singular, i.e. the set of points where $\Pi'(\sigma)$: $T_\sigma \Sigma \to T_{\Pi(\sigma)}(M \times T)$ is not one-one. This means that $\{\sigma\}$ is also the set of points where $T_\sigma \Sigma$ is "vertical", hence the set of points where an "upper" and a "lower" sheet of Σ coalesce. This occurs precisely at the points B where two stationary paths coalesce. The caustics are indeed the projections of the sets $\{\sigma\}$. We see that quantum mechanics softens the boundaries between regions of different illuminations

Beyond the caustics. In 1890 Gouy** observed and explained the phase gained by a wave as it goes through a focus. Similar phase shifts occur in the wave function of quantum systems; they have been derived by Keller [79] from the single valuedness of the wave function and by Gutzwiller [64] who established their relationship with the Morse index of the corresponding classical trajectory. A recent careful analysis [26] of the path integral solutions of the harmonic oscillator display the inner workings of these phase shifts.

The Morse† index. Once again we begin at the second variation $S''(q)xx$ from which all blessings flow. Here q is a stationary path defined by its end points $q(t_a) = a$, $q(t_b) = b$ and X is the space of vector fields x along q vanishing at the end points $x(t_a) = x(t_b) = 0$,

$$S''(q)xx = \int_T (\mathscr{J}(q(t))x(t) \mid x(t))\, dt$$

where $\mathscr{J}(q(t))h(t) = Dh(t) = 0$ is the Jacobi equation.††

$S''(q)xx > 0$ for every $x \in X \Leftrightarrow$ a and b within focal distance of each other.

$S''(q)hh = 0$ for some $h \in X \Leftrightarrow$ a and b are conjugate along q.

*DeWitt-Morette in ref [133], see also appendix B

**"Les ondes en traversant le foyer prennent une avance d'une demi ondulation" See also ref [16] p 60

†Maslov [96] has obtained the Morse index by an entirely different approach For the precise relationship between the Maslov index and the Morse index see refs [4] and [95]

††See appendix B

The **Morse index** λ of the hessian $S''(q)$ is defined to be the maximum dimension of a subspace of X on which $S''(q)$ is negative definite.

Morse theorem. The index λ of $S''(q)$ is equal to the number of points $q(t)$, with $t_a < t < t_b$, such that $q(t)$ is conjugate to $q(t_a)$ along q; each conjugate point being counted with its multiplicity. This index λ is always finite.

*Proof.** Let $\{\psi_j\}$ be a complete orthogonal set of eigenfunctions of D vanishing on the boundary and let $\{\alpha_j\}$ be the corresponding eigenvalues. Set $x^\alpha(t) = \Sigma\, u^j \psi_j^\alpha(t)$, then

$$S''(q)xx = \sum \alpha_j (u^j)^2. \tag{3.43}$$

a and b within focal distance of each other $\Leftrightarrow \alpha_j > 0$ for every j

a and b conjugate along q with multiplicity k $\Leftrightarrow \alpha_j = 0$ for k values of j, say, $j = 1, \ldots k$.

We shall prove that

weighted number of conjugate points between a and b equal to $\lambda \Leftrightarrow \alpha_j < 0$ for λ values of j.

Assume that there is one conjugate point between a and b with multiplicity k, then $\lambda = k$. Let ν be a unit vector perpendicular to the caustic at b and set $J_k^\perp(t_b, t_a) = \nu_\alpha J_k^\alpha(t_b, t_a)$. It has been shown that near the caustic

$$J_k^\perp(t_b, t_a) = \alpha_k. \tag{3.44}$$

It suffices to prove that $\nabla_{t_b} J_k^\perp(t_b, t_a) \neq 0$. Indeed, if $\nabla_{t_b} J_k^\perp(t_b, t_a) = 0$, the Jacobi field $J_k^\perp(t, t_a)$ vanishes at t_b as well as its first derivative, hence is identically zero (cf. for instance eq. B20) which contradicts eq. (3.44). ■

We shall show that the propagator $\mathcal{K}(B; A)$ loses a phase equal to $ik\pi/2$ when B goes through a conjugate point of multiplicity k. Indeed, according to eqs. (3.39) and (3.40)

$$\mathcal{K}(B; A) \propto \int \cdots \int \cdots \exp\left\{\tfrac{1}{2}\mathrm{i} \sum \alpha_k (u^k)^2\right\} \prod_1^\infty ((|\alpha_k|/2\pi) \exp(\mathrm{i}\pi/4))^{1/2}\, \mathrm{d}u^k, \qquad \alpha_k > 0. \tag{3.45}$$

Set $B^\pm = (q(t_b^\pm), t_b^\pm)$ where $q(t_b)$ is conjugate to a with multiplicity k. Then

$$\mathcal{K}(B^+; A) = \mathcal{K}(B^-; A) \exp(-\mathrm{i}k\pi/2),$$

since $\int_R \exp(\pm\mathrm{i}|\alpha|u^2/2)\, \mathrm{d}u = \exp(\pm\mathrm{i}\pi/4)(2\pi/|\alpha|)^{1/2}$.

In conclusion if B is not on the caustic of A

$$\mathcal{K}_{\mathrm{WKB}}(B; A) = \sum_j \exp\left\{\frac{\mathrm{i}}{\hbar} \bar{S}_j(B: A)\right\} (\det|M_j(t_b, t_a)|)^{1/2} (2\pi\hbar)^{-n/2} \exp(-\mathrm{i}n\pi/4 - \mathrm{i}\lambda_j\pi/2) \tag{3.46}$$

the sum being performed over all stationary paths q_j such that $q_j(t_b) = b$ and $q_j(t_a) = a$.

The case "B on a caustic with conjugate points between $q(t_b)$ and $q(t_a)$" is obtained by combining in a straightforward fashion the two previous cases.

*By diagonalizing $S''(q)xx$ the proof given by Milnor [105, p 83] is shortened

Levit and Smilansky [90] have constructed a semiclassical uniform approximation for path integrals which approaches both the WKB approximation at and away from conjugate points. It is based on the results given by Connor [28] for the uniform asymptotic evaluation of finite dimensional integrals.

3.6. *Perturbation and gaussian methods combined*

The two techniques which have been developed so far for computing path integrals are the Feynman diagram technique (p. 267) and the gaussian method. They can easily and fruitfully be combined. The gaussian method is based on the assumption that one can solve the Euler–Lagrange equation of the system $S'(q) = 0$. If this is not possible one can decompose the action

$$S = S_0 + S_1$$

so that the equation $S_0'(q_0) = 0$ is soluble and treat S_1 as a perturbation of the S_0-system. We shall show on a simple example but without loss of generality how to proceed when the action has been decomposed into an unperturbed plus a perturbed action.

The forced harmonic oscillator

$$S(f) = \int_T \left[\frac{m}{2}\|\dot{f}(t)\|^2\,\mathrm{d}t - \tfrac{1}{2}\omega^2\|f(t)\|^2 + g_\alpha(t)f^\alpha(t)\right]\mathrm{d}t.$$

This case can obviously be computed without decomposing the action, since, for a quadratic action, the propagator is equal to its WKB approximation:

$$\mathscr{K}(B;A) = (2\pi\mathrm{i}\hbar)^{-n/2}\exp\{\mathrm{i}\bar{S}(B;A)/\hbar\}|\det\partial^2\bar{S}(B;A)/\partial b^\alpha\partial a^\beta|^{1/2} \tag{3.47}$$

where $\bar{S}(B;A) = S(q)$ with

$$-q(t) - \omega^2 q(t) + g(t) = 0, \qquad q(t_a) = a, \qquad q(t_b) = b. \tag{3.48}$$

We shall now compute $\mathscr{K}(B;A)$ by decomposing $S = S_0 + S_1$ where

$$S_1(f) = \int_T V_1(f(t))\,\mathrm{d}t = \int_T g_\alpha(t)f^\alpha(t)\,\mathrm{d}t. \tag{3.49}$$

Proceed as in section 3.4 but make the change of variable $b + \mu y = q_0 + \mu x$ where q_0 is the classical path

$$-\ddot{q}_0(t) - \omega^2 q_0(t) = 0, \qquad q_0(t_a) = a, \qquad q_0(t_b) = b. \tag{3.50}$$

Let $K_0(t, t_a)$ be the solution of $D_0 = -\mathrm{d}^2/\mathrm{d}t^2 - \omega^2$ such that $K_0^{\alpha\beta}(t_a, t_a) = g^{\alpha\beta}$, $\nabla_t K_0(t = t_a, t_a) = 0$. Let G_{0+} and G_0 be the elementary kernels of D_0 such that

$$G_{0+}(t_b, s) = 0, \qquad \partial G_{0+}(t_a, s)/\partial t_a = 0, \qquad G_{0+}(t, s) = G_{0+}(s, t) \tag{3.51}$$

$$G_0(t, s) = 0 \qquad \text{for } t \text{ or } s \text{ equal to } t_a \text{ or } t_b.$$

Let w_0 be the gaussian of covariance* G_0 normalized to

$$w_0(X) = (2\pi\mathrm{i})^{-n/2}|\det G_{0+}(t_a, t_a)|^{1/2},$$

*See appendix B

then

$$\mathcal{K}(B;A)=\exp\left\{\frac{\mathrm{i}}{\hbar}\bar{S}_0(B;A)-\frac{1}{\hbar}\int_T V_1(q_0(t))\,\mathrm{d}t\right\}(\det K^{\mathrm{W}}(t_b,t_a)/\det K_0(t_b,t_a))^{1/2}\mu^{-n}I \tag{3.52}$$

where

$$I=\int_X \mathrm{d}w_0(x)\exp\left\{-\frac{\mathrm{i}}{\mu m}\int_T \nabla_\alpha V_1(q_0(t))x^\alpha(t)\,\mathrm{d}t\right\}.$$

I is a cylindrical integral which can be computed by mapping $x\mapsto u=-(1/\mu m)\int_T \nabla_\alpha V_1(q_0(t))x^\alpha(t)\,\mathrm{d}t$. The image of w_0 under this mapping is a gaussian with the same normalization as w_0. Its covariance is

$$\mathcal{W}=\hbar^{-1}\int_T \mathrm{d}t\int_T \mathrm{d}s\,\nabla_\alpha V_1(q_0(t))\nabla_\beta V_1(q_0(s))G_0^{\alpha\beta}(t,s)$$

$$I[w_0(X)=(2\pi\mathrm{i}\mathcal{W})^{-1/2}\int_R \mathrm{d}u\exp(\mathrm{i}u)\exp\left(\frac{1}{2}u^2\mathcal{W}^{-1}\right)=\exp(-\mathrm{i}\mathcal{W}/2)$$

and

$$\mathcal{K}(B;A)=(2\pi\mathrm{i}\hbar)^{-n/2}\exp\left\{\frac{\mathrm{i}}{\hbar}\bar{S}_0(B;A)-\frac{\mathrm{i}}{\hbar}\int_T V_1(q_0(t))\,\mathrm{d}t-\frac{1}{2}\mathcal{W}\right\}|\det\partial^2\bar{S}_0(B;A)/\partial b^\alpha\partial a^\beta|^{1/2}. \tag{3.53}$$

One recognizes the propagator [56, eq. 3.66, p. 64] which has played a key role in the Feynman formulation of Quantum Electrodynamics. In general this expression would not be the propagator but its WKB approximation. The subsequent terms would be integrals with respect to the gaussian w_0.

Although one knows that both calculations (eqs. (3.47) and (3.53)) must give the same result for $\mathcal{K}(B;A)$, it is gratifying to check it for the chosen example.

Here $q_0(t)=q(t)+\int_T g(s)G_0(t,s)\,\mathrm{d}s$ and a simple calculation gives

$$S(q)=S(q_0)-\int_T (g(t)\,|\,q_0(t))\,\mathrm{d}t-\tfrac{1}{2}\int_T \mathrm{d}t\int_T \mathrm{d}s\,g_\alpha(t)g_\beta(s)G_0^{\alpha\beta}(t,s).$$

The hessian of $\bar{S}$ is equal to the hessian of $\bar{S}_0$ and the equivalence of both methods is proved. Obviously the first one is the simplest; the more information is put in the gaussian the simpler is the integral. In the case of the forced harmonic oscillator the covariance of the gaussian which enters the first calculation is an elementary kernel of $-\mathrm{d}^2/\mathrm{d}t^2-\omega^2+g(t)$ whereas the covariance of the gaussian which enters the second calculation is an elementary kernel of $-\mathrm{d}^2/\mathrm{d}t^2-\omega^2$.

Remark: In some cases the gaussian method can give results where a perturbation method is meaningless. For instance consider the anharmonic oscillator $S(f)=\int_T[\frac{1}{2}f^2(t)-\frac{1}{2}\omega^2f^2(t)+\lambda f^4(t)]\,\mathrm{d}t$; one is tempted, and many have succumbed to the temptation of decomposing the action $S=S_0+S_1$ and treating $S_1(f)=\lambda\int_T f^4(t)\,\mathrm{d}t$ as a perturbation. It is a disaster because the propagator is not

analytic in λ. The semi-classical expansion on the contrary gives a meaningful expansion [108] in powers of $\hbar$.

4. Path integration in phase space

4.1. Introduction

Path integrals on the configuration space of a system are not the only path integrals of interest in quantum physics. The arena of nonrelativistic quantum mechanics is phase space; indeed the uncertainty principle is a relation between measurements of position and momentum. The statement "sum over all paths q such that $q(t_a) = a$ and $q(t_b) = b$" which implies infinite precision of position measurements at t_a and t_b should imply total uncertainty on the measurement of the momentum at t_a and t_b. How does it? Moreover infinite precision of position measurement is not always the best assumption and we need a formulation of quantum physics with greater flexibility. Since the early days of the Feynman path integral formalism of quantum physics, the potential and the challenges of phase space path integration have come up many times. To mention only a few landmarks in the subject we recall the following remarks.

1. Feynman has noted [54, p. 376] that the normalization of the short time interval propagator is the square root of "the density in coordinate space of particles uniformly distributed in momentum space." A similar remark has been made by Garrod [58]: for a free particle, the normalization factors needed in path integrals over q can be obtained by formulating path integrals over (q, p) using the product of Liouville measures $\Pi(\mathrm{d}q^\alpha(t_i)\,\mathrm{d}p_\alpha(t_i)/h)$; indeed, setting $q(t_i) = q^i$, $p(t_i) = p_i$, and $t_{i+1} - t_i = \epsilon$, we have for a one dimensional system

$$\int_R \mathrm{d}q^i \int_R \frac{\mathrm{d}p_i}{2\pi\hbar} \exp\frac{\mathrm{i}\epsilon}{\hbar}\left(p_i q^i - \frac{1}{2m}p_i^2\right) = \int_R \mathrm{d}q^i \left(\frac{m}{2\pi\hbar\epsilon}\right)^{1/2} \exp(-\mathrm{i}\pi/4) \exp\frac{\mathrm{i}}{\hbar}\frac{m}{2}(q^i)^2\epsilon.$$

2. Clutton-Brock [25] derived interesting properties of path integrals by means of canonical transformations. But Gervais and Jevicki [62] have shown that the use of canonical transformations in path integrals is not without pitfalls. Their example, however, points out more to the pitfalls of the lattice approximation of path integration than to the shortcomings of canonical transformations. Indeed, their canonical transformation $q \to Q(q)$ introduces a kinetic energy term $g_{\alpha\beta}(Q)\dot{Q}^\alpha\dot{Q}^\beta$ which cannot be treated by the lattice approximation and must be handled by methods suitable for stochastic variables on curved spaces.

3. Faddeev [51] has shown that the phase space formulation of Feynman integrals is very appropriate for systems with constraints. In a recent paper [41] we have developed a method for path integration on phase spaces similar to the method presented in sections 3.2 to 3.6 for path integration on configuration spaces. We present here the main results, as well as new ones, and give an improved discussion of the normalization of the prodistributions. Since in this monograph all equations have been derived from first principles there is no more looseness in determining the normalizations. Path integration in phase space will be used in section 5 for the computation of energy levels and decay rate of bound systems.

The computation of the propagator $\mathscr{K}(B; A)$ in flat space started with the Feynman–Kac formula which, after the change of variable $y \mapsto x$ such that $b + \mu y = q + \mu x$, is a path integral with respect to the Wiener gaussian w_+^{W} on the space X_+ of vector fields x along q vanishing at t_b. It is then reexpressed with respect to a new gaussian w_+ on X_+ which absorbs all quadratic terms in x. Finally it is stated in terms of the gaussian w on X, Leray-related to w_+ on X_+ (eq. 1.31). The gaussians $w_\pm$ and w are elementary kernels of the Jacobi equation. It is possible to express $\mathscr{K}(B; A)$ as a path integral in phase space in terms of gaussians whose covariances are elementary kernels of the Jacobi equation in phase space.

4.2. *The Jacobi equation in phase space**

The action

$$S(q, p) = \int_T [\langle p(t), \dot{q}(t)\rangle - H(p(t), q(t))]\, \mathrm{d}t \tag{4.1}$$

can be expanded around the solution $(\bar{q}, \bar{p})$ of the Hamilton equations by a two parameter variation method similar to the one parameter variation method used in the lagrangian case. Let the configuration space M be an n dimensional riemannian manifold with metric g. The paths (q, p) map T in the cotangent bundle** T^*M. Let U be the interval $[0, 1]$, let $u, v \in U$ and let $\{\bar{\gamma}(u, v)\}$ be a two parameter family of paths:

$$\bar{\gamma}(u, v): T \to T^*M \quad \text{by} \quad \begin{cases} \bar{\alpha}(u): T \to M & \bar{\alpha}(0) = \bar{q}, \quad \bar{\alpha}(1) = q \\ \bar{\beta}(u, v): T \to T^*M & \bar{\beta}(0, 0) = \bar{p}, \quad \bar{\beta}(1, 1) = p. \end{cases}$$

$$\text{Set} \quad \bar{\alpha}(u)(t) = \alpha(u, t) \quad \text{and} \quad \bar{\beta}(u, v)(t) = \beta(u, v, t) \in T^*_{\alpha(u,t)}M. \tag{4.2}$$

We consider first only variations $\bar{\alpha}(u)$ keeping the end points fixed. $\alpha(u, t_a) = a$, $\alpha(u, t_b) = b$ for every $u \in U$. Set

$$\frac{\partial \alpha}{\partial u}(u = 0, t) = x(t) \qquad \text{and} \qquad \frac{\partial \beta}{\partial v}(0, v = 0, t) = y(t). \tag{4.3}$$

(x, y) is a vector field, henceforth called z, along $(\bar{q}, \bar{p})$ such that $x(t_a) = x(t_b) = 0$.

When M is $\mathbf{R}^n$, $\beta(u, v)$ does not depend on u; position and momentum are varied independently. But when M is a riemannian manifold, changing u means changing the fiber $T^*_{\alpha(u,t)}M$ and the momentum $\beta(u, v, t)$ has to be parallel transported accordingly. To define the parallel transport of $\beta(u, v, t)$ when u alone varies we have to choose the path $\alpha(\cdot, t): u \mapsto \alpha(u, t)$. A natural choice is for $\alpha(\cdot, t)$ to be the geodesic generated by exponentiating $x(t)$. Given $\beta(0, v, t)$, $\beta(u, v, t)$ is uniquely defined by the equation

$$\nabla_u \beta = 0. \tag{4.4}$$

*In configuration space the letter q was reserved for a solution of the Euler–Lagrange equation, a letter such as f designating an arbitrary path For simplicity here (q, p) is an arbitrary path, $(\bar{q}, \bar{p})$ is a solution of the Hamilton equation

**Set of cotangent spaces T^*_mM for all $m \in M$ See for instance ref [23] for the definition of bundles

Since $T^*_{\alpha(u,t)}M$ is a linear space, the dependence of $\beta(u, v, t)$ on v can be chosen to be linear:

$$\beta(u, v, t) = \beta(u, 0, t) + v\,\partial\beta(u, v, t)/\partial v\Big|_{v=0} \tag{4.5}$$

The Taylor expansion of the action (4.1) around the classical path can be expressed as an ordinary Taylor expansion with respect to $(u, v) \in \mathbb{R}^2$.

$$S \circ \bar{\gamma}(1, 1) = \sum_{n=0}^{\infty} \frac{1}{n!}(S \circ \bar{\gamma})^{(n)}(0, 0). \tag{4.6}$$

The first variation vanishes for paths satisfying the Hamilton equations. The second variation $(S \circ \bar{\gamma})''(0, 0)$ can, after an integration by parts, be written

$$\left(\frac{\partial^2(S \circ \bar{\gamma})}{\partial u^2} + 2\frac{\partial^2(S \circ \bar{\gamma})}{\partial u\,\partial v} + \frac{\partial^2(S \circ \bar{\gamma})}{\partial v^2}\right)(0, 0) = \int_T (\mathcal{J}(\bar{q}, \bar{p})z(t) \mid z(t))\,\mathrm{d}t \tag{4.7}$$

where z is the $2n$ dimensional vector (n contravariant, n covariant components)

$$z = \begin{pmatrix} x \\ y \end{pmatrix}$$

and $\mathcal{J}(\bar{q}, \bar{p})$ is a $2n \times 2n$ first order linear operator, henceforth called the **Jacobi operator in phase space.**

The second variation is a bilinear form on the space Z of vector fields z and, once again, it can be used to define a gaussian w on Z. Note that Z is the space of vector fields z such that $x(t_a) = x(t_b) = 0$, no condition on $y(t_a)$ or $y(t_b)$. No conditions were imposed on y because no integration by parts were performed on p since S does not depend on p. The uncertainty principle could not have been formulated if the action had been a function of p!

The dual Z' of Z is the space of $2n$ dimensional vector valued measure $\rho = (\mu, \nu)$:

$$\langle \rho, z \rangle = \int_T \mathrm{d}\mu_\alpha(t)x^\alpha(t) + \int_T \mathrm{d}\nu^\alpha(t)y_\alpha(t).$$

The variance W of w is the inverse, in the sense defined in section 1.5, of the second variation. The covariance G of w is the elementary kernel of $\mathcal{J}(\bar{q}, \bar{p})$ with the appropriate boundary conditions for W to be the inverse of $(S \circ \bar{\gamma})''(0, 0)$ (see below). It is sometimes convenient to write

$$W(\rho, \rho) = (\mu_\alpha, \nu^\alpha)\begin{pmatrix} G_1^{\alpha\beta} & G_{2\beta}^{\alpha} \\ G_{\alpha}^{3\beta} & G_{\alpha\beta}^{4} \end{pmatrix}\begin{pmatrix} \mu_\beta \\ \nu^\beta \end{pmatrix}$$

where it is understood that

$$\mu_\alpha G_1^{\alpha\beta}\mu_\beta = \int_T \int_T \mathrm{d}\mu_\alpha(t)\,\mathrm{d}\mu_\beta(s)G_1^{\alpha\beta}(t, s), \quad \text{etc.}.$$

We shall show that G_1 is the covariance defined by the second variation of the lagrangian action $S(q) = \int_T L(q(t), q(t))\,\mathrm{d}t$ and that G_2, G^3, G^4 are completely determined by G_1. Hence the boundary

conditions of G are the boundary conditions of G_1, a result which can be anticipated from the fact that the boundary values of y do not enter eq. (4.7). It is more illuminating to prove these properties first on an example. We shall sketch the general case afterwards.

Example: A free particle on a curved space

$$S(q,p)=\int_T\left[\langle p(t),q(t)\rangle-\frac{1}{2m}(p(t)\,|\,p(t))\right]\mathrm{d}t.$$

The bracket $\langle\ ,\ \rangle$ is used for the duality between $T_{q(t)}M$ and $T^*_{q(t)}M$ and the parentheses $(\,|\,)$ are used for the scalar product on $T^*_{q(t)}M$ defined by the metric g^{-1}. Using the properties of covariant derivatives given in appendix B we obtain readily

$$\left(\frac{\partial^2(S\circ\bar\gamma)}{\partial u^2}+\frac{\partial^2(S\circ\bar\gamma)}{\partial v\,\partial u}+\frac{\partial^2(S\circ\bar\gamma)}{\partial u\,\partial v}+\frac{\partial^2(S\circ\bar\gamma)}{\partial v^2}\right)(0,0)$$

$$=\int_T\mathrm{d}t\left[-\frac{1}{m}\langle\bar p,R(x,g\bar p)x\rangle+\langle y,\nabla_t x\rangle-\langle\nabla_t y,x\rangle-\frac{1}{m}(y\,|\,y)\right] \tag{4.8}$$

and the Jacobi equation*

$$\mathscr{J}(\bar q,\bar p)k(t)=\begin{bmatrix}-\frac{1}{m}R^{\delta}_{\alpha\beta\gamma}g^{\beta\epsilon}\bar p_\epsilon\bar p_\delta & -\delta^\gamma_\alpha\nabla_t\\ \delta^\alpha_\gamma\nabla_t & -\frac{1}{m}g^{\alpha\gamma}\end{bmatrix}\begin{bmatrix}h^\gamma(t)\\ J_\gamma(t)\end{bmatrix}=0. \tag{4.9}$$

This system of coupled equations is readily shown to be equivalent to the equation of geodetic deviation:

$$\nabla_t^2h^\alpha+R^\alpha_{\delta\gamma\beta}q^\delta h^\gamma\dot q^\beta=0. \tag{4.10}$$

The components G_1, G_2, G^3, G^4 of the elementary kernel G satisfy two systems of two coupled vector valued equations:

$$\mathscr{J}_r(\bar q,\bar p)G(r,s)=1\delta_s. \tag{4.11}$$

By elimination and substitution these equations can be reexpressed as follows:

$$\begin{aligned}&-m^2\nabla_r^2G_1^{\alpha\eta}(r,s)-g^{\alpha\rho}g^{\beta\epsilon}R^\delta_{\rho\beta\gamma}p_\epsilon p_\delta G_1^{\gamma\eta}(r,s)=mg^{\alpha\eta}\delta_s(r),\\ &G_\alpha^{3\eta}(r,s)=mg_{\alpha\gamma}\nabla_rG_1^{\gamma\eta}(r,s),\qquad G^\alpha_{2\eta}(r,s)=mg_{\eta\gamma}\nabla_sG_1^{\alpha\gamma}(r,s),\\ &G^4_{\alpha\eta}(r,s)=m^2g_{\alpha\gamma}g_{\eta\delta}\nabla_r\nabla_sG_1^{\gamma\delta}(r,s)-mg_{\alpha\eta}\delta_s(r).\end{aligned} \tag{4.12}$$

Thus G_1 is an elementary kernel of the equation of geodetic deviation and the three other functions G^3, G_2, G^4 are fully determined** by and readily obtained from G_1. For instance let G_1 be the

*As before we give a distinctive label to a Jacobi field, here $k=(h,J)$

**Note that for a free particle in flat space $G_{\alpha\beta}(r,s)=0$ and $G^\alpha_\beta(r,s)$ is not uniquely determined by $G^{\alpha\beta}$ from the first set of equations It is uniquely determined if one treats the flat space solutions as the limit of the curved space solutions, or if one uses the symmetry properties of the covariance $G^\alpha_\beta(r,s)=G^\alpha_\beta(s,r)$

covariance over the space X of vector fields x vanishing on the boundary (eq. B14), then, abbreviating $g(\bar{q}(r))$ to $g(r)$, we obtain

$$G^3(r,s) = mg(r)(\theta(s-r)\tilde{K}(r,t_a)M(t_a,t_b)J(t_b,s) - \theta(r-s)\tilde{K}(r,t_b)M(t_b,t_a)J(t_a,s)).$$

G_2 is obtained from G^3 by the symmetry relation $G^\beta_\alpha(r,s) = G^\beta_\alpha(s,r)$.

$$G^4(r,s) = m^2 g(r)(\theta(s-r)\tilde{K}(r,t_a)M(t_a,t_b)\tilde{K}(t_b,s) - \theta(r-s)\tilde{K}(r,t_b)M(t_b,t_a)\tilde{K}(t_a,s))g(s) - mg(r)\delta(r-s).$$

Example. Wiener covariances in phase space. The Wiener covariances in phase space are the Green functions of the Jacobi operator

$$\mathcal{J}(\bar{q},\bar{p}) = \begin{pmatrix} 0 & -\nabla_t \\ \nabla_t & -1 \end{pmatrix}.$$

$\mathcal{J}(\bar{q},\bar{p})$, like $\mathcal{J}(\bar{q})$, is obtained from the action of a free particle of mass 1. We record below the covariances for the action of a free particle of mass m. One must remember to set $m = 1$ when using the Wiener covariances.

$$G(r,s) = \begin{pmatrix} \theta(s-r)(r-t_a)(t_a-t_b)^{-1}(t_b-s) & -m(\theta(s-r)(r-t_a)(t_a-t_b)^{-1} \\ \quad -\theta(r-s)(r-t_b)(t_b-t_a)^{-1}(t_a-s) & \quad -\theta(r-s)(t-t_b)(t_b-t_a)^{-1}) \\ m(\theta(s-r)(t_a-t_b)^{-1}(t_b-s) & m^2(t_b-t_a)^{-1} \\ \quad -\theta(r-s)(t_b-t_a)^{-1}(t_a-s)) & \end{pmatrix}, \tag{4.13}$$

$$G_+(r,s) = \begin{pmatrix} \theta(s-r)(t_b-s)+\theta(r-s)(t_b-r) & -m\theta(s-r) \\ -m\theta(r-s) & 0 \end{pmatrix},$$

$$G_-(r,s) = \begin{pmatrix} \theta(s-r)(t_a-r)+\theta(r-s)(t_a-s) & -m\theta(r-s) \\ -m\theta(s-r) & 0 \end{pmatrix}. \tag{4.14}$$

We now return to the calculation of the second variation in the general case. It remains simple if one uses covariant derivatives throughout. The hamiltonian H is a function of scalars. Since $\nabla_u\beta = 0$, $\nabla_u\nabla_u\alpha = 0$ and $\partial^2\beta/\partial v^2 = 0$, the variations of H come automatically in their desired form as multilinear forms of x and y. $\partial H/\partial u$ is a linear form of $\partial\alpha/\partial u$, and $\partial H/\partial v$ is a linear form of $\partial\beta/\partial v$ which we shall write

$$\partial H/\partial u = \langle \mathrm{D}H/\partial\alpha, \partial\alpha/\partial u\rangle, \qquad \text{and} \quad \partial H/\partial v = \langle \partial\beta/\partial v, \mathrm{D}H/\partial\beta\rangle$$

These expressions define uniquely $\mathrm{D}H/\partial\alpha$ and $\mathrm{D}H/\partial\beta$. It is convenient to define similarly $\mathrm{D}^2H/\partial\alpha^2$, $\mathrm{D}^2H/\partial\alpha\partial\beta$, etc.... by

$$\frac{\partial^2 H}{\partial u^2} + \frac{\partial^2 H}{\partial v\,\partial u} + \frac{\partial^2 H}{\partial u\,\partial v} + \frac{\partial^2 H}{\partial v^2} = (\partial\alpha/\partial u, \partial\beta/\partial v)\begin{pmatrix} \mathrm{D}^2H/\partial\alpha^2 & \mathrm{D}^2H/\partial\alpha\partial\beta \\ \mathrm{D}^2H/\partial\beta\partial\alpha & \mathrm{D}^2H/\partial\beta^2 \end{pmatrix}\begin{pmatrix} \partial\alpha/\partial u \\ \partial\beta/\partial v \end{pmatrix}.$$

When the Legendre matrix $A_{\alpha\beta}(t) = \partial^2 L/\partial\dot{\bar{q}}^\beta(t)\partial\dot{\bar{q}}^\alpha(t)$ is nonsingular, $\partial^2 H/\partial\bar{p}\partial\bar{p} = A^{-1}(t)$.

Set $R(p)$ the matrix defined by $R_{\alpha\beta}(p) = R^\delta_{\alpha\gamma\beta\epsilon}g^{\gamma\epsilon}p_\epsilon p_\delta$. The covariance is given by the coupled equations

$$(-R(p) - \mathrm{D}^2H/\partial p\partial q)(r)G_1(r,s) - (\nabla_r + \mathrm{D}^2H/\partial q\partial p)(r)G^3(r,s) = \delta_s(r) \tag{4.15a}$$

$$(\nabla_r - \mathrm{D}^2H/\partial p\partial q)(r)G_1(r,s) - (\partial^2 H/\partial\bar{p}\partial\bar{p})(r)G^3(r,s) = 0 \tag{4.15b}$$

$$(-R(p) - \mathrm{D}^2H/\partial q\partial q)(r)G_2(r,s) - (\nabla_r + \mathrm{D}^2H/\partial q\partial p)(r)G^4(r,s) = 0 \tag{4.15c}$$

$$(\nabla_r - \mathrm{D}^2H/\partial p\partial q)(r)G_2(r,s) - (\partial^2 H/\partial\bar{p}\partial\bar{p})(r)G^4(r,s) = \delta_s(r). \tag{4.15d}$$

Equation (4.15b) can be solved for G^3 in terms of G_1. Then this expression for G^3 is substituted into (4.15a) giving a differential equation for G_1 which can be shown to be the Jacobi equation of the Lagrangian formulation. The symmetry property $G^3(r,s) = G_2(s,r)$ is used to determine G_2 in terms of G_1. Finally one uses eq (4.15d) to obtain G^4 in terms of G_1.

We shall label $G_\pm$, G the covariances of the gaussians on the spaces $Z_\pm$, Z of paths $z = (x, y)$ defined by the following conditions:

Z_+:	$x(t_b) = 0$	no restrictions on $x(t_a)$, $y(t_a)$, $y(t_b)$
Z_-:	$x(t_a) = 0$	no restrictions on $x(t_b)$, $y(t_a)$, $y(t_b)$
Z:	$x(t_a) = x(t_b) = 0$	no restrictions on $y(t_a)$, $y(t_b)$.

The fact that the set of eqs. (4.15) define covariances whose G_1 component is the covariance in configuration space has been proved by Bryce DeWitt for the covariances G on Z (Feynman–Green function) using a different approach. Mizrahi [109] has worked out the covariances of the gaussian prodistributions for arbitrary time dependent quadratic hamiltonians.

4.3. Normalization in phase space

Let w_+ on Z_+ be the normalized gaussian of covariance G_+, the Leray-related gaussian w on Z is normalized to

$$w(Z) = \int_{Z_+} \delta(\mu x(t_a))\,\mathrm{d}w_+(z).$$

$w(Z)$ is a cylindrical integral and can be expressed as an integral over $\mathbb{R}^{2n}$ where n is the dimension of the configuration space. Indeed let $P: Z_+ \to \mathbb{R}^{2n}$ by $u^\alpha = \langle \delta^\alpha_{t_a}, x\rangle$, $v_\alpha = \langle \delta_{t\alpha}, y\rangle$ for an arbitrary $t \neq t_a$, then

$$w(Z) = \int_{R^{2n}} \mu^{-n}\delta(u)\,\mathrm{d}u\,\mathrm{d}v(2\pi\mathrm{i})^{-n}(\det \mathcal{W}^{-1})^{1/2}\exp(\tfrac{1}{2}\mathrm{i}\mathcal{W}^{-1}(u,v)(u,v))$$

where $\mathcal{W}^{-1}$ is the inverse of

$$\mathcal{W} = \begin{pmatrix} G_{1+}(t_a,t_a) & G_{2+}(t_a,\theta) \\ G^{3\beta}_{+\alpha}(\theta,t_a) & G^4_{+\alpha\beta}(\theta,\theta) \end{pmatrix}$$

and $\mathcal{W}^{-1}(u,v)(u,v)$ the bilinear form constructed with $\mathcal{W}^{-1}$. Since

$$\delta(u)\exp\{\tfrac{1}{2}\mathrm{i}\mathcal{W}^{-1}(u,v)(u,v)\} = \delta(u)\exp\{\tfrac{1}{2}\mathrm{i}G^{\alpha\beta}_{1+}(t_a,t_a)v_\alpha v_\beta/\det\mathcal{W}\}$$

we obtain

$$w(Z) = (2\pi\mathrm{i}\mu^2)^{-n/2}(\det G^{\alpha\beta}_{1+}(t_a,t_a))^{1/2}. \tag{4.16}$$

Lemma. The normalization of w on Z is equal to the normalization of the corresponding gaussian on X (i.e. gaussian on X Leray-related to the gaussian on X_+ of covariance G_{1+})*

Note that the integrations on p-space and q-space *cannot be performed independently of one another.* Here the integrand did not depend on y, nevertheless we had to integrate with respect to y and this was accomplished via the matrix $\mathscr{W}^{-1}$ which couples the x and the y integration. In the papers on phase space path integration based on Feynman's original definition, one often reads the prescription "perform the 'p' integration before the 'q' integration". This procedure introduces undefined terms proportional to $\delta(0)$ which are either discarded or shown to cancel other undefined terms.

4.4. Physical interpretation of the covariance in phase space

Proceeding as in the previous section, we can show that

$$\mu^2 \int_Z x(t)x(s)\,\mathrm{d}w(z)/w(Z) = \mathrm{i}\hbar G_1(t, s)/m$$

$$\mu^2 \int_Z x(t)y(s)\,\mathrm{d}w(z)/w(Z) = \mathrm{i}\hbar G_2(t, s)/m = \mathrm{i}\hbar G^3(s, t)/m.$$

$$\mu^2 \int y(t)y(s)\,\mathrm{d}w(z)/w(Z) = \mathrm{i}\hbar G^4(t, s)/m.$$

Note that G_2 and G^3 are discontinuous at $t = s$ Their discontinuity is a manifestation of the uncertainty principle. For instance let S be a free particle; then

$$\int_Z [q^\alpha(s^+)p_\beta(s) - q^\alpha(s^-)p_\beta(s)]\,\mathrm{d}w(z)/w(Z) = \mathrm{i}\hbar\delta^\beta_\alpha$$

G^4 is continuous at $r = s$. For a free particle $G^4_{\alpha\beta}(r, s) = g_{\alpha\beta}/(t_b - t_a)$; it does not depend on r or s.

4.5. The Liouville measure

It has often been conjectured that the "measure" for phase space path integration is an "infinite dimensional Liouville measure". We shall compute the propagator $\mathscr{K}(B; A)$ for a free particle in flat space and give a precise meaning to this conjecture:

$$\mathscr{K}(B; A) = \exp\{\mathrm{i}S(\bar{q}, \bar{p})/\hbar\}I$$

$$I = \int_{Z_+} \mathrm{d}w_+(z)\delta(\mu x(t_a))$$

*In ref [41] the gaussians on $X_\pm$ are not normalized to 1, the normalization of $w(Z)$ is modified accordingly At one time, it had seemed simpler to choose the normalization of the gaussians on $X_\pm$ such that it absorbs the determinants introduced by the Cameron–Martin formula The derivations presented here start from first principles and lead via product integrals and the Feynman–Kac formula to gaussians on $X_\pm$ normalized to unity

where w_+ is the gaussian on Z_+ of covariance G_+ given by eq. (4.14).

Let us consider a particle at rest at the origin, $\bar{q}(t) = 0$, $\bar{p}(t) = 0$, then $S(\bar{q}, \bar{p}) = 0$, $\mu x = q$ and $\mu y = p$. Let $t_a = t_0 < t_1 \cdots < t_{p+1} = t_b$ and $t_k < \theta_k < t_{k+1}$. Let $P : Z_+ \to \mathbb{R}^{2(p+1)}$ by

$$u^k = \langle \mu^k, x\rangle = \langle \delta_{t_{k+1}} - \delta_{t_k}, x\rangle = x(t_{k+1}) - x(t_k) \equiv x^{k+1} - x^k$$

with $x(t_a)$ arbitrary and $x(t_b) = 0$. Let

$$v_k = \langle \nu_k, y\rangle = \langle \delta_{\theta_k}, y\rangle = y(\theta_k) = y_k.$$

Since p is discontinuous at the partition times t_k, θ_k has been chosen so that p is evaluated at points θ_k where it is continuous. Regardless of how fine the division is, there will always be a point θ_k between two points t_{k+1} and t_k. Under the mapping P,

$$I = \int_{R^{2(p+1)}} \delta(\mu x^0) \prod_{k=0}^{p} ((2\pi i)^{-1}\, du^k\, dv_k)(\det \mathcal{W}^{-1})^{1/2} \exp\{\tfrac{1}{2} i \mathcal{W}^{-1}(u, v)(u, v)\}$$

where

$$\mathcal{W} = \begin{pmatrix} W_1(\mu^i, \mu^j) & W_2(\mu^i, \nu_j) \\ W^3(\nu_i, \mu^j) & W^4(\nu_i, \nu_j) \end{pmatrix} \qquad i, j = 1, \ldots p+1$$

$$W_1(\mu^k, \mu^k) = t_{k+1} - t_k, \qquad W_2(\mu^k, \nu_k) = W^3(\nu_k, \mu^k) = m.$$

All the other components vanish and the matrix is easy to invert:

$$\tfrac{1}{2}\mathcal{W}^{-1}(u, v)(u, v) = \sum \frac{1}{m}(x^{k+1} - x^k) y_k - \frac{1}{2m^2}(t_{k+1} - t_k) y_k^2$$

$$= \hbar^{-1} \sum (q^{k+1} - q^k) p_k - (2m)^{-1}(t_{k+1} - t_k) p_k^2,$$

$$\prod_{k=0}^{p} ((2\pi i)^{-1}\, du^k\, dv_k)(\det \mathcal{W}^{-1})^{1/2} = \prod_{k=0}^{p} dq^k\, dp_k/h$$

and*

$$I = \int_{R^{2(p+1)}} \delta(q^0) \prod_{k=0}^{p} (dq^k\, dp_k/h) \exp \frac{i}{\hbar} \sum ((q^{k+1} - q^k) p_k - \frac{1}{2m}(t_{k+1} - t_k) p_k^2).$$

Note that $dq^k\, dp_k = dq(t_k)\, dp(\theta_k)$ with $t_k < \theta_k$. $dq^k\, dp_k/h$ is a "directed" Liouville measure when t_k tends to θ_k from below. If we had worked with the space Z_- of vector fields characterized by $x(t_a) = 0$, no other restrictions, we would have been led to a directed Liouville measure which tends to the Liouville measure when t_k tends to θ_k from above [e.g. 41]. In conclusion, the propagator for a free particle at rest at the origin is

$$\mathcal{K}(B; A) = \lim_{p=\infty} \int_{R^{2(p+1)}} \delta(q^0) \prod_{k=0}^{p} (dq^k\, dp_k/h) \exp \frac{i}{\hbar} \sum ((q^{k+1} - q^k) p_k - \frac{1}{2m}(t_{k+1} - t_k) p_k^2) = \int_Z dw(z). \tag{4.17}$$

*In the previous line i from the determinant combine with i explicitly written to give a real quantity

We have established

Proposition. The "infinite directed Liouville measure from below"

$$\lim_{p=\infty} \prod_{k=0}^{p} (\mathrm{d}q^k\, \mathrm{d}p_k/h) \text{ multiplied by } \exp\frac{\mathrm{i}}{\hbar}\int_T \left(pq - \frac{1}{2m}p^2\right)\mathrm{d}t$$

is the normalized prodistribution w_+ on Z_+ of covariance G_+ (eq. 4.14) *obtained from the Wiener prodistribution w_{1+} on X_+* (example 5, p. 264). *A similar proposition holds for the directed Liouville measure "from above".*

4.6. *Path integration in phase space*

We shall proceed* as in sections 3.2 and 3.4, and treat only the flat case. Now the Feynman–Kac formula reads

$$\mathscr{K}(B; A) = \int_{Z_+} \mathrm{d}w_+^{\mathrm{W}}(z) \exp\left\{\frac{-1}{\mu^2 m}\int_T V(b + \mu x(t), m\mu y(t))\,\mathrm{d}t\right\}\delta(b + \mu x(t_a) - a).$$

Let $(\bar{q}, \bar{p})$ be the classical path such that

$$\dot{\bar{q}}^\alpha(t) = g^{\alpha\beta}\bar{p}_\beta(t)/m + \partial V/\partial p^\alpha(t), \qquad \dot{\bar{p}}_\alpha(t) = -\partial V/\partial q^\alpha(t), \qquad \bar{q}(t_a) = a, \qquad \bar{q}(t_b) = b$$

Make the change of variable

$$b + \mu x = \bar{q} + \mu X, \qquad m\mu y = \bar{p} + m\mu Y.$$

Then $\langle y, x\rangle - (y \mid y)/2$ becomes $(\langle \bar{p}, \dot{\bar{q}}\rangle - (\bar{p} \mid \bar{p})/2m)/\hbar + \langle \bar{p}/m\mu, X\rangle + \mu^{-1}\langle Y, \partial V/\partial \bar{p}\rangle + \langle Y, X\rangle - (Y \mid Y)$. The first two terms will contribute to the classical action, the last two terms will be "included" in the new gaussian $w_+^{\mathrm{W}}(Z)$ where $Z = (X, Y)$. Integrate by parts:

$$\int_T \langle \bar{p}/m\mu, \dot{X}\rangle\,\mathrm{d}t = -\langle \bar{p}(t_a)/m\mu, X(t_a)\rangle + \frac{1}{m\mu}\int_T \langle \nabla V(q(t)), X(t)\rangle\,\mathrm{d}t.$$

Expand $V(\bar{q} + \mu X, \bar{p} + m\mu Y)$ in powers of μ:

$$V(\bar{q} + \mu X, \bar{p} + m\mu Y) = V(\bar{q}, \bar{p}) + \mu(\partial V/\partial \bar{q})X + \mu m(\partial V/\partial \bar{p})Y + \mu^2 \mathscr{V}(\bar{q}, \bar{p})ZZ + \mu^2 \Omega(\bar{q}, \mu X)$$

where

$$\mathscr{V}(\bar{q}, \bar{p})ZZ = \frac{\partial^2 V}{\partial \bar{q}^\alpha \partial \bar{q}^\beta} X^\alpha X^\beta + m\frac{\partial^2 V}{\partial \bar{q}^\alpha \partial \bar{p}_\beta} X^\alpha Y_\beta + m\frac{\partial^2 V}{\partial \bar{p}_\alpha \partial \bar{q}^\beta} Y_\alpha X^\beta + m^2 \frac{\partial^2 V}{\partial \bar{p}_\alpha \partial \bar{p}_\beta} Y_\alpha Y_\beta.$$

It is assumed that the third derivatives of $V(q, p)$ do not depend on p. Then

*A minor change of notation is introduced, whereas in section 3.2 the first step is a change of variable $b + \mu y \mapsto q + \mu x$ here the first step is a change of variable $(b + \mu x \mapsto \bar{q} + \mu X,\ m\mu y \mapsto \bar{p} + m\mu Y)$

$$\mathcal{K}(B;A) = \exp\{iS(\bar{q},\bar{p})/\hbar\} \int_{Z_+} dw_+^{w}(Z) \exp\left\{-\frac{i}{2m}\int_I dt[V(\bar{q}(t),\bar{p}(t))Z(t)Z(t) + \Omega(\bar{q}(t),\mu X(t))]\right\}\delta(\mu X(t_a)).$$

By an argument similar to the one developed in section 1.5 one can make a linear change of variable of integration such that the covariance of the new gaussian w_+ is the Green function of the Jacobi operator satisfying the boundary conditions appropriate to Z_+. This change of variable of integration introduces a determinant which can be shown to be equal to $(\det K(t_b,t_a)/\det K(t_a,t_a))^{-1/2}$ as before (eq. 1.17). Finally one can introduce the gaussian w on Z, Leray related to w_+ on Z_+. Its normalization has been computed in section 4.3 and found equal to the normalization of the corresponding gaussian in configuration space. Then

$$\mathcal{K}(B;A) = \mathcal{K}_{\mathrm{WKB}}(B;A)\int_Z \exp\left\{\frac{-i\mu}{2m}\int_T \Omega(\bar{q}(t),\mu X(t))\,dt\right\} dw(Z)/w(Z)$$

$$\mathcal{K}_{\mathrm{WKB}}(B;A) = \exp\{iS(\bar{q},\bar{p})/\hbar\}(m/2\pi i\hbar)^{n/2}(\det M(t_b,t_a))^{1/2}.$$

It has been shown in sections 4.3 and 4.5 how to carry on integrals over Z. Here nothing has been gained by working in phase space. We shall see in the next section, however, that, for bound systems, it is preferable to work in phase space than in configuration space.

5. Bound states, stable and unstable

5.1. Introduction

Some insight in the path integral formalism is gained by examining it in the broader context of dynamical systems. Indeed the role played by classical paths in the study of quantum systems is analogous to the role played by equilibrium points in the study of classical dynamical systems: Consider a classical dynamical system $dx(t)/dt = f(x(t))$, for example

$$\begin{cases} dq(t)/dt = v(t) & q: T \to M \\ dv(t)/dt = -\mathrm{grad}\ V(q(t)). \end{cases} \tag{5.1}$$

An equilibrium point x_0 of the system is a particular "motion" of the system which satisfies $f(x_0) = 0$. The nature of an equilibrium point is determined by the longtime behavior of the nearby motions. This, in turn, is determined to a great extent* by the nature of the eigenvalues of the derivative $f'(x_0)$ of f at the equilibrium point x_0, complex or real with positive or negative real parts [e.g. 68, p. 92–97]. In the given example the equilibrium point ($q_0 \in M$, v_0 is a critical point of the potential function V, grad $V(q_0) = 0$. Its nature and the longtime behavior of nearby motions are determined by the hessian $-\partial^2 V/\partial q_0^\alpha \partial q_0^\beta$ of V at $q_0 \in M$.

The path integral formalism of quantum physics has brought out a similar pattern. Consider the quantum dynamical system

$$\partial\psi(x,t)/\partial t = -iH\psi(x,t)/\hbar \tag{5.2}$$

*See for instance ref [143] p 412, the effects of the higher order derivatives

corresponding to the classical system given above. Consider the classical flow $\mathscr{C}_t : M \to M$ given by $a \mapsto q(t, a, v_a)$. It has been shown (p. 299) that in the limit $\hbar = 0$ the probability of finding in $\Omega \subset M$ at time t the system, known to be in $\mathscr{C}_t^{-1}\Omega$ at time t_a, is unity. Thus in the limit $\hbar = 0$, the probability of finding the system at $b \in M$ at time t_b is peaked along the classical path $q(t, a, v_a)$ such that $q(t_b, a, v_a) = b$. The classical path q can be considered as an "equilibrium point" in the space of paths going from (a, t_a) to (b, t_b), reached by the system when $S(f)/\hbar$ tends to infinity. q is the critical point of the action $S'(q) = 0$ and the qualitative features of the quantum system whose limit is q are determined by the second variation of the action $S''(q)xx$.

In this section we shall investigate the quantum systems whose limit q is a periodic orbit. The presence and the qualitative features of other classical periodic and quasi-periodic orbits in the neighborhood of a chosen periodic orbit is felt by the quantum system and many of its properties can be obtained from the properties of the neighboring families of classical orbits.

The relation between the periodic orbits of a classical system and the energy levels of the corresponding quantum system was first discovered [e.g. 147, p. 6, 7] by Einstein, Bohr and Sommerfeld. The extent to which the "Old Quantum Theory" was successful is magnificently preserved by Born's book, *the Mechanics of the Atom*, whose preface to the German edition begins by these words: "The title *Atommechanik* given to these lectures which I delivered in Göttingen during the session 1923–24 was chosen to correspond to the designation *Himmelsmechanik*... I have called the present book 'Vol. I'; the second volume is to contain a closer approximation to the 'final' mechanics of the atom. I know that the promise of such a second volume is bold, for at present we have only a few hazy indications as to the departures which must be made from the classical mechanics to explain atomic phenomena." The year was 1924. When the second volume [12] appeared the birth of Quantum Mechanics had relegated the *Mechanics of the Atom* to a work of historical interest.

Much later Keller (1958) [79] obtained a generalization of the Bohr–Sommerfeld quantum condition by requiring the wave function to be single valued, and Gutzwiller (1971) in trail blazing articles [64; 65, p. 351] introduced the Morse index and the characteristic exponents of celestial mechanics in the WKB quantizations. But he made some unwarranted simplifications and his final expression is not correct. Voros [142] obtained the correct result by an entirely different approach using geometric quantization and the Maslov method. Miller [104] showed how the Gutzwiller procedure should be corrected to obtain the right formula for systems with classical periodic orbits.

The path integral formalism of quantum mechanics incorporates naturally the characteristic exponents and the Morse index in the determination of the bound state energy spectrum and provides a simple proof of the Gutzwiller–Voros result. Dashen, Hasslacher and Neveu [33] derived similar formulae in model field theories. Conjectures they made for systems with n degrees of freedom are justified and factors left undetermined in their expressions are obtained explicitly.

We first turn to Poincaré to learn the properties of families of stationary paths (i.e. solutions of Hamilton's equations) in the neighborhood of a periodic orbit. Some new results (lemmas 1, 2, 3 and 4) of interest for path integration are direct applications of Poincaré's work.

5.2. *Characteristic exponents, alias stability angles*

The Jacobi fields along periodic orbits have been analyzed by Poincaré in a beautiful chapter* of "Les Méthodes Nouvelles de la Mécanique Céleste". The Jacobi equation defined by equations (4.7),

*"Les exposants caractéristiques" [120, p 176] See also ref [143] p 397 and ref [103]

(4.9) and (4.15)

$$\mathscr{J}(\bar{q},\bar{p})k(t)=\begin{pmatrix}-\partial^2 H/\partial\bar{q}^\alpha\bar{q}^\beta & -\nabla_t-\partial^2 H/\partial\bar{q}^\alpha\partial\bar{p}_\beta\\ \nabla_t-\partial^2 H/\partial\bar{p}_\alpha\partial\bar{q}^\beta & -\partial^2 H/\partial\bar{p}_\alpha\partial\bar{p}_\beta\end{pmatrix}\begin{pmatrix}h^\beta(t)\\ j_\beta(t)\end{pmatrix}=0 \tag{5.3}$$

is written by Poincaré in the following form

$$(\nabla_t\mathbf{1}-\mathscr{H}(\bar{q},\bar{p}))k(t)=\left(\begin{pmatrix}\nabla_t & 0\\ 0 & \nabla_t\end{pmatrix}+\begin{pmatrix}-\partial^2 H/\partial\bar{p}_\alpha\partial\bar{p}^\beta & -\partial^2 H/\partial\bar{p}_\alpha\partial\bar{p}_\beta\\ \partial^2 H/\partial\bar{q}^\alpha\partial\bar{q}^\beta & \partial^2 H/\partial\bar{q}^\alpha\partial\bar{p}_\beta\end{pmatrix}\right)\begin{pmatrix}h^\beta(t)\\ j_\beta(t)\end{pmatrix}=0 \tag{5.4}$$

which defines $\mathscr{H}(\bar{q},\bar{p})$.

Let G be the Green functions of $\mathscr{J}(\bar{q},\bar{p})$ and $G_{\mathscr{H}}$ be the Green functions of $(\nabla_t\mathbf{1}-\mathscr{H}(\bar{q},\bar{p}))$, then

$$G=\begin{pmatrix}G_1 & G_2\\ G^3 & G^4\end{pmatrix}\quad\Leftrightarrow\quad G_{\mathscr{H}}=\begin{pmatrix}G_2 & -G_1\\ G^4 & -G^3\end{pmatrix}. \tag{5.5}$$

The systems (5.3) or (5.4) of $2n$ first order linear coupled differential equations with periodic coefficients of period τ admits in general [120, p. 67] $2n$ linearly independent solutions of the form

$$k_k(t)=\exp(\alpha_k t)S_k(t),\qquad k=\pm1,\ldots\pm n \tag{5.6}$$

where the functions $\{S_k(t)\}$ are periodic in t with period τ and the α_k are $2n$ constants called the **characteristic exponents** or the **stability angles.**

If two characteristic exponents are equal, say $\alpha_1=\alpha_{-1}$, then

$$k_1(t)=\exp(\alpha_1 t)S_1(t)$$

$$k_{-1}(t)=\exp(\alpha_1 t)(tS_1(t)+T(t)),\quad S_1 \text{ and } T \text{ periodic of period } \tau, \tag{5.7}$$

are solutions of the Jacobi equation. Similarly if n exponents are equal the corresponding solutions of the Jacobi equation are of the form $\exp(\alpha t)$ multiplied by polynomials in t with periodic coefficients. k_1 is called a **fundamental solution of first kind**, the polynomial solutions such as k_{-1} are called **fundamental solutions of second kind.**

Poincaré called **stable** a solution $(\bar{q},\bar{p})$ such that all its Jacobi fields are bounded $\|k(t)\|<\infty$. The **Poincaré stability** is also called **linear stability** because equations (5.3) or (5.4) are the equations of a linear flow.

Poincaré Stability Lemma. A solution is linearly stable if and only if all its characteristic exponents are purely imaginary.

If some α_k have a real part $\|k(t)\|$ tends to infinity for either $t=+\infty$ or $t=-\infty$. Future [past] stability is possible only if $\mathrm{Re}\,\alpha_k\leqslant 0$ [if $\mathrm{Re}\,\alpha_k\geqslant 0$]. We shall see later that characteristic exponents come in pairs (α, and its complex conjugate $\bar{\alpha}$) and $(\alpha,-\alpha)$. It follows that the future and the past stability conditions become identical, namely a solution is stable if and only if $\{\mathrm{Re}\,\alpha_k=0 \text{ for all } k\}$. ■

Under a small perturbation, a stable periodic orbit becomes quasiperiodic, its characteristic exponents being the normal modes of oscillation about the periodic orbit.

The Poincaré map, also called the **fundamental matrix**, is the $2n \times 2n$ matrix $R(\tau)$ defined by

$$k(t+\tau) = R(\tau)k(t). \tag{5.8}$$

It gives the deviation from a periodic orbit $(\bar{q}, \bar{p})$ after a period has elapsed.

Lemma. The eigenvalues of the Poincaré map are $\{\exp \alpha_k \tau; k = \pm 1, \ldots, \pm n\}$. *The fundamental solutions of first kind of the Jacobi equation are eigenfunctions of the Poincaré map.*

Proof. The fundamental solutions of first kind satisfy the equation

$$k_1(t+\tau) = \exp(\alpha_1 \tau) k_1(t). \qquad \blacksquare$$

The eigenvalues of the Poincaré map are often called the **characteristic roots** or the **characteristic multipliers** of the solution $(\bar{q}, \bar{p})$. Note that fundamental solutions of second kind are not eigenfunctions.

Lemma The Poincaré map is volume preserving.

Proof. Since $R(\tau)$ is real, the characteristic exponents come in pairs $(\alpha_k, \bar{\alpha}_k)$. Poincaré has proved [120, p. 193] that for a hamiltonian system they come also in pairs $(\alpha_k, -\alpha_k)$. This property follows after some arguments from the fact that $\Sigma_{\alpha=1}^{n} h_k^{\alpha}(t) j_{l\alpha}(t) - j_{k\alpha}(t) h_l^{\alpha}(t) = \text{constant} \propto \exp(\alpha_k + \alpha_l)t$. $\Sigma\, \alpha_k = 0$ implies $\det R(\tau) = 1$, hence the Poincaré map is volume preserving. $\blacksquare$

Remark. When α vanishes, a pair of characteristic exponents vanish and one (only one) of the two corresponding fundamental solutions is periodic.

Lemma 1. *The eigenvalues of* $\int_0^{\tau} \mathscr{H}(\bar{q}(s), \bar{p}(s))\, \mathrm{d}s$ *are* $\{\alpha_k \tau\}$ *where* $\{\alpha_k\}$ *are the characteristic exponents of the solution* $(\bar{q}, \bar{p})$.

Proof. It follows from eq. (5.4) and from the definition of the Poincaré map that

$$k(t + t_a) = \prod_{t_a}^{t_a + t} \exp\{\mathscr{H}(\bar{q}(s), \bar{p}(s))\, \mathrm{d}s\} k(t_a) \tag{5.9}$$

$$R(\tau) = \prod_{0}^{\tau} \exp \mathscr{H}(\bar{q}(s), \bar{p}(s))\, \mathrm{d}s \tag{5.10}$$

$$\nabla_{\tau} R(\tau) = \mathscr{H}(\bar{q}(\tau), \bar{p}(\tau)) R(\tau). \tag{5.11}$$

Let all the exponents be distinct, then $\mathscr{H}(\bar{q}, \bar{p})$ can be diagonalized by a similarity transformation. Set $\hat{\mathscr{H}}$ the diagonal form of $\mathscr{H}$ and $\hat{R}(\tau)$ the product integral of $\hat{\mathscr{H}}$,

$$\hat{R}(\tau) = \exp \int_0^{\tau} \hat{\mathscr{H}}(\bar{q}(s), \bar{p}(s))\, \mathrm{d}s. \tag{5 12}$$

The proof when all the exponents are not distinct is more elaborate. $\blacksquare$

Lemma 2. The eigenfunctions and eigenvalues of* $\nabla_t 1 - \mathscr{H}(\bar{q}, \bar{p})$ *are*

$$\psi_{k\nu}(t) = k_k(t) \exp(-\alpha_k t + 2\pi i \nu t/\tau), \quad k = \pm 1, \ldots \pm n, \qquad \nu = \pm 1, \pm 2, \ldots$$
$$\lambda_{k\nu} = -\alpha_k + 2\pi i \nu/\tau \tag{5.13}$$

where k_k *are the fundamental solutions of* $(\nabla_t 1 - \mathscr{H}(\bar{q}, \bar{p}))k_k(t) = 0$ *and* α_k *are the characteristic exponents.*

The null subspace of the Jacobi operator. We recall that the null subspace of the Jacobi operator $\mathscr{J}(\bar{q})$ where $\bar{q}$ is a stationary path from (a, t_a) to (b, t_b) is spanned by the nonvanishing Jacobi fields h such that $h(t_a) = h(t_b) = 0$. The number of such linearly independent Jacobi fields is called the nullity of the Jacobi operator. It is equal to the multiplicity of the conjugate points a and b along $\bar{q}$ - the multiplicity being zero if a and b are not conjugate. The null subspace of the Jacobi operator $\nabla_t 1 - \mathscr{H}(\bar{q}, \bar{p})$ where $(\bar{q}, \bar{p})$ is a periodic orbit of period τ will play the same role in the study of bound states as the null subspace of $\mathscr{J}(\bar{q})$ in scattering states. The periodic orbits, like the conjugate points, are not generic. But their importances far outweigh their numbers: Without conjugate points, many optical instruments could not be built, and without periodic orbits many bound states would not exist.

Lemma 3. The nullity of $\nabla_t 1 - \mathscr{H}(\bar{q}, \bar{p})$ *and of* $\mathscr{J}(\bar{q}, \bar{p})$ *is equal to the number of periodic Jacobi fields.*

Proof. The equations $(\nabla_t 1 - \mathscr{H}(\bar{q}, \bar{p}))\psi_{k\nu}(t) = 0$ and $\mathscr{J}(\bar{q}, \bar{p})\psi_{k\nu}(t) = 0$ have the same solutions, namely $\psi_{k\nu}(t) = k_k(t)$ where $k_k(t)$ are the fundamental solutions which correspond to zero characteristic exponents since $\lambda_{k\nu} = 0$ implies $\alpha_k \tau = 2\pi i \nu$. ■

*Properties of the characteristic exponents for systems which possess constants of integration***

$$F_j(\bar{q}(t), \bar{p}(t) = \text{constant}, \qquad j = 1, \ldots p \leq 2n$$

Theorem. If a system admits p constants of integration and if all Poisson brackets $[F_j, F_k] = 0$, *then either* $2p$ *characteristic exponents vanish*
or the $(p \times 2n)$ *matrix* $(\partial F_j/\partial \bar{q}^\alpha(t), \partial F_j/\partial \bar{p}_\alpha(t))$ *is of rank less than p.*

Proof: First a quick proof for time independent hamiltonians. If $(\bar{q}(t), \bar{p}(t))$ is a solution so is $(\bar{q}(t + t_0), \bar{p}(t + t_0))$, hence $(h(t) = \partial \bar{q}(t + t_0)/\partial t_0, j(t) = \partial \bar{p}(t + t_0)/\partial t_0)$ is a Jacobi field. Since $(\bar{q}, \bar{p})$ is periodic so is its derivative (h, j). The Jacobi field (h, j) is a fundamental solution corresponding to a zero characteristic exponent.

The general proof rests on the fact that if there is a constant of integration for a hamiltonisn system, there is a corresponding constant of integration for its Jacobi fields, namely

$$\frac{\partial F_j}{\partial \bar{q}(t)} h(t) + \frac{\partial F_j}{\partial \bar{p}(t)} j(t) = \text{constant}.$$

*These eigenfunctions were obtained in ref [33], p 3440, by requiring $\psi_{k\nu}(t)$ to be periodic

**Poincaré labels the constants of integration (intégrales du mouvement) as follows no label for the hamiltonian, $j = 1$, $p - 1$ for the remaining ones

Hence

$$h_j(t) = \partial F_j/\partial \bar{p}(t), \qquad j_j(t) = -\partial F_j/\partial \bar{q}(t) \tag{5.14}$$

is a Jacobi field. It is a periodic Jacobi field, hence $\alpha_j = 0$ There are np linearly independent pairs $(h_j^\alpha, j_{j\alpha})$ solution of the system (5.14) unless the $p \times 2n$ matrix

$$(\partial F_j/\partial \bar{q}^\alpha(t),\ \partial F_j/\partial \bar{p}_\alpha(t))$$

is of rank less than p. ■

See Poincaré for a discussion of the case in which all the Poisson brackets $[F_j, F_k]$ do not vanish.

Since constants of integration express conservation laws, and since conservation laws are related via Noether's theorem to invariance of the system under group of transformations, i.e. to symmetries of the system, this theorm is of great practical value as will be seen for instance (p. 342) when the hamiltonian is a constant of the motion.

Consider a family of periodic orbits $\bar{z}(t, z_0(\lambda))$ which can be parametrized by their periods $\tau(\lambda)$ Let

$$\bar{z}(t + \tau(\lambda), z_0(\lambda)) = \bar{z}(t, z_0(\lambda))$$
$$\bar{z}(0, z_0(\lambda)) = z_0(\lambda)$$
$$\bar{z}(\cdot, z_0(0)) = (\bar{q}, \bar{p}).$$

There is an interesting relationship, given by the following lemma, between the variation of the initial point $\mathrm{d}z_0(\lambda)/\mathrm{d}\tau(\lambda)|_{\lambda=0}$ and the velocity along the basic orbit at the initial time.

*Broucke Lemma**

$$(\mathbf{1} - R(\tau(0)))\,\mathrm{d}z_0(\lambda)/\mathrm{d}\tau(\lambda)\Big|_{\lambda=0} = \partial\bar{z}(t, z_0(0))/\partial t\Big|_{t=0} \tag{5.15}$$

Proof. Expand $\bar{z}(t + \tau(\lambda), z_0(\lambda))$ in powers $\tau(\lambda) - \tau(0)$ and $z_0(\lambda) - z_0(0)$, set $t = 0$:

$$\bar{z}(\tau(\lambda), z_0(\lambda)) = \bar{z}(\tau(0), z_0(0)) + (\tau(\lambda) - \tau(0))\partial\bar{z}/\partial t\Big|_{t=0} + (z_0(\lambda) - z_0(0))\partial\bar{z}/\partial z_0(0) + \cdot$$

Since $\{\partial\bar{z}^\alpha/\partial z_0^\beta(0);\ \beta \text{ fixed}, \alpha = 1, \ldots 2n\}$ is a Jacobi field along $(\bar{q}, \bar{p})$ and since R is a matrix whose columns are the Jacobi fields along $(\bar{q}, \bar{p})$,

$$(z_0(\lambda) - z_0(0))(\mathbf{1} - R) = (\tau(\lambda) - \tau(0))\partial\bar{z}/\partial t\Big|_{t=0} + \cdot\cdot$$

Take the limit $\lambda = 0$ and the lemma is proved. ■

The operator $1 - R(\tau)$ appears in the density of energy states (eqs. 5.37 and 5.46).

There is at least one periodic Jacobi field along a periodic orbit and the determinant of $R - \mathbf{1}$ vanishes. This corresponds to the fact that any point along an orbit can be used as the initial point z_0. Let the characteristic exponents be $(0, 0, \alpha_{\pm 2}, \ldots \alpha_{\pm n})$, then $\mathbf{1} - R$ is either of rank $2n - 1$ or $2n - 2$ according to whether the Jordan canonical form of $1 - R$ is nondiagonal or diagonal. It is in general nondiagonal and there is a one-parameter family of periodic orbits in the neighborhood of $(\bar{q}, \bar{p})$

*R Broucke, unpublished Lecture Notes, Department of Aerospace Science and Engineering Mechanics, University of Texas at Austin

If there is more than one pair of vanishing characteristic exponents there is in general more than one one-parameter family of periodic orbits. Thus the characteristic exponents of a periodic solution are important because they give information not only on the stability of the orbit but also on the structure of the manifold of periodic solutions. Broucke has made numerical experiments with eq. (5.15) and has discovered bifurcation points for the families of solutions of the spring-pendulum system.

Other properties of the characteristic exponents and their explicit calculation for the three body problem have been developed by Poincaré and can be found in treatises of Celestial Mechanics and Analytical Dynamics.*

The characteristic exponents have been called "the dynamical generalization of the normal mode frequencies" [104, p. 998]. Indeed, the role played by classical closed periodic orbits is analogous to the role played by equilibrium points in the study of classical dynamical systems.** Consider a classical dynamical system whose time evolution is governed by the dynamical equation $\mathrm{d}X(t)/\mathrm{d}t = f(X(t))$. For example

$$\mathrm{d}q(t)/\mathrm{d}t = v(t), \qquad \mathrm{d}v(t)/\mathrm{d}t = -\mathrm{grad}\, V(q(t)).$$

An equilibrium point $\bar{X} = (q_0, v_0)$ of the system is a particular "motion" which satisfies the equation $\mathrm{d}\bar{X}/\mathrm{d}t = f(\bar{X}) = 0$. The small displacements $x(t) = q(t) - q_0$ from equilibrium are obtained from a lagrangian $L = \frac{1}{2}\Sigma(m_{\alpha\beta}x^\alpha\dot{x}^\beta - k_{\alpha\beta}x^\alpha x^\beta)$ whose diagonal form $L = \frac{1}{2}\Sigma(\dot{Q}_\alpha^2 - \omega_\alpha^2 Q_\alpha^2)$ is called the normal form.† The normal coordinates Q_α execute simple periodic motions $Q_\alpha(t) = \exp(\pm i\omega_\alpha t)$. The normal mode frequencies ω_α are the solutions of the equation $\det|k_{\alpha\beta} - \omega^2 m_{\alpha\beta}| = 0$.

A similar pattern appears in the study of classical paths around a closed orbit $(\bar{q}_0, \bar{p}_0)$. Let $(\bar{q}, \bar{p})$ be a nearby classical orbit; the small deviation $(\bar{q} - q_0, \bar{p} - p_0)$ is a Jacobi field. The $2n$ Jacobi fields along $(\bar{q}_0, \bar{p}_0)$ form the column of the matrix $R(t)$ whose value for $t = \tau$ is the Poincaré map (eq. (5.11)). The diagonal form of $R(t)$ is obtained from eq. (5.12):

$$\hat{R}(t) = \exp \int_0^t \hat{\mathscr{H}}(\bar{q}_0(s), \bar{p}_0(s))\, \mathrm{d}s.$$

$\hat{\mathscr{H}}$ is the diagonal form of $\mathscr{H}$ which in the case of a particle of mass m in a potential V reads††

$$\mathscr{H}(\bar{q}(s), \bar{p}(s)) = \begin{pmatrix} 0 & -\delta^{\alpha\beta}m^{-1} \\ \partial_\alpha\partial_\beta V(\bar{q}(s)) & 0 \end{pmatrix}.$$

If the closed orbit reduces to an equilibrium point (q_0, p_0), the periodic function $\mathscr{H}$ reduces to a constant, and the elements of the diagonal matrix $\hat{R}(t)$ are $\hat{R}_{kk}(t) = \exp \alpha_k t$ where the eigenvalues $\{\alpha_k\}$ of $\mathscr{H}$ are the solutions of the equation $\det|\partial_\alpha\partial_\beta V + \alpha^2 m\delta_{\alpha\beta}| = 0$. Thus when $\mathscr{H}$ is constant, the characteristic exponents are precisely§ the normal mode frequencies. The reader may enjoy the portraits of families of classical paths drawn by Hirsch and Smale [68] when $\mathscr{H}$ is constant.

*In particular refs [143], [129] and [115]

**On page 331 we discuss the role of the classical paths in the study of quantum systems Here we discuss the role of a closed orbit in a family of classical quasiperiodic orbits

†See for instance ref [85] p 66, the normal mode analysis of small oscillations around an equilibrium point

††The argument applies also to a many particle system

§Modulo a factor i depending on conventions Here $\alpha = \pm i\omega$

5.3. Density of energy states

To set up the stage we recall [e.g. 10] briefly how the density of energy states of a bound system

$$\rho(E) = \sum_n \delta(E - E_n)$$

can be obtained from the trace of the propagator $\mathcal{K}(b, t_b; a, t_a)$. Consider a time independent* hamiltonian whose discrete eigenstates can be used to form a complete** orthogonal basis for the wave functions:

$$H\phi_n(x) = E_n\phi_n(x), \qquad \int_M \phi_n^*(x)\phi_m(x)\,dx = \delta_{nm}, \qquad \sum_{n=1}^{\infty} \phi_n(x)\phi_n^*(y) = \delta(x - y)$$
$$\psi(x, t) = \sum_n c_n \exp\left(\frac{-i}{\hbar}E_n t\right)\phi_n(x). \tag{5.16}$$

Feynman [56, p. 88] has shown that

$$\mathcal{K}(b, t_b; a, t_a) = \theta(t) \sum_n \phi_n(b)\phi_n^*(a) \exp(-iE_n t/\hbar) \qquad \text{with} \quad t = t_b - t_a$$

Assuming that it exists, let tr $\mathcal{K}$ be the function of t defined by

$$\operatorname{tr} \mathcal{K}(t) = \int_M da\, \mathcal{K}(a, t_b; a, t_a) = \theta(t) \sum_n \exp(-iE_n t/\hbar), \tag{5.17}$$

and let $\mathcal{G}$ be the function of E defined by the Fourier transform† $\mathcal{F}$ tr $\mathcal{K}$ of tr $\mathcal{K}$ as follows

$$\mathcal{G}(E) = (i\hbar)^{-1}(\mathcal{F} \operatorname{tr} \mathcal{K})(-E/\hbar) = (i\hbar)^{-1} \sum_n (\mathcal{F}\theta)((E_n - E)/\hbar). \tag{5.18}$$

$\mathcal{G}(E)$ is often written formally

$$\mathcal{G}(E) = (i\hbar)^{-1} \int_R dt\, \theta(t) \sum_n \exp i(E - E_n)t/\hbar.$$

This equation is meaningless because the Fourier transform of the step function cannot be defined in the sense of function but only in the sense of distribution. If one treats $\mathcal{F}\theta$ as a function one is forced to introduce $\pm i\epsilon$ to give meaning to otherwise meaningless expressions; if one treats $\mathcal{F}\theta$ as a distribution all factors are automatically and unambiguously determined. Let P stand for principal value

$$\mathcal{G}(E) = \sum_n (\mathrm{P}(E - E_n)^{-1} - i\pi\delta(E - E_n)). \tag{5.19}$$

It is convenient sometimes to write

*To analyze the case of time dependent hamiltonians, start for instance with Poincaré [120] or with Whittaker [143] pp 386–399

**n may be a multi-index

†See appendix C for the normalization convention To see quickly how different conventions for the Fourier transform change $\mathcal{F}\theta$ see for instance the derivation of $\mathcal{F}\theta$ in ref [23] p 452

$$\mathcal{G}(E) = \sum_n (E - E_n + i\epsilon)^{-1} = (i\hbar)^{-1} \int_0^\infty dt \exp \frac{i}{\hbar}(E - E_n + i\epsilon)t. \tag{5.20}$$

The density of energy states can thus be obtained from $\mathcal{G}(E)$,

$$\rho(E) = \sum_n \delta(E - E_n) = i\pi^{-1}\Big(\mathcal{G}(E) - \sum \mathrm{P}(E - E_n)^{-1}\Big). \tag{5.21}$$

Alternatively if we introduce *another* function $\mathcal{G}_\epsilon$ defined by $\mathcal{G}_\epsilon(E + i\epsilon) = \Sigma_n (E - E_n + i\epsilon)^{-1}$ we can write

$$\rho(E) = (-2i\pi)^{-1}(\mathcal{G}_\epsilon(E + i\epsilon) - \mathcal{G}_\epsilon(E - i\epsilon)). \tag{5.22}$$

If the operation Fourier transform and trace commute, then it is convenient to compute first the Fourier transform of $\mathcal{K}(b, t_a + t; a, t_a)$. Formally*

$$\mathcal{G}(b, a, E) = (i\hbar)^{-1} \int_R dt \exp(iEt/h)\mathcal{K}(b, t_a + t; a, t_a). \tag{5.23}$$

The WKB approximation of $\mathcal{G}(b, a, E)$ is

$$\mathcal{G}_{\mathrm{WKB}}(b, a, E) = (i\hbar)^{-1} \int_R dt \exp(iEt/\hbar)(2\pi i\hbar)^{-n/2} \times \sum_j |\det \partial^2 \bar{S}_j/\partial b^\alpha \partial a^\beta|^{1/2} \exp \frac{i}{\hbar}(\bar{S}_j(b, t_a + t; a, t_a) - h\lambda_j/4) \tag{5.24}$$

where the sum over j is the sum over all stationary paths $\bar{q}_j$ from (a, t_a) to $(b, t_a + t)$, λ_j is the Morse index of $\bar{q}_j$, $\bar{S}_j(b, t_a + t; a, t_a)$ is the integral of the lagrangian for $\bar{q}_j$. It is consistent with the WKB approximation to compute (5.24) by the stationary phase method. Let τ be the value of t that minimizes the exponent in (5.24), i.e. let τ be the function of b, a and E solution of

$$\partial \bar{S}(b, t_a + t; a, t_a)/\partial t \Big|_{t=\tau} + E = 0 \tag{5.25}$$

then

$$\mathcal{G}_{\mathrm{WKB}}(b, a, E) = 2\pi(2\pi i\hbar)^{-(n+1)/2} \sum_j |D_{\bar{W}_j}(b, a, E)|^{1/2} \exp \frac{i}{\hbar}(\bar{W}_j(b, a, E) - h(\lambda_j + p_j)/4) \tag{5.26}$$

where

$$\bar{W}_j(b, a, E) = \bar{S}_j(b, t_a + \bar{\tau}_j(b, a, E); a, t_a) + E\bar{\tau}_j(b, a, E) = \int_{\bar{q}_j} p_\alpha(\bar{q}(s), E)\, d\bar{q}^\alpha(s) \tag{5.27}$$

the integral being evaluated along the classical path $\bar{q}$ from a to b traversed in time $\bar{\tau}(b, a, E)$,

$$D_{\bar{W}}(b, a, E) = \det \begin{pmatrix} \partial^2 \bar{W}/\partial a^\alpha \partial b^\beta & \partial^2 \bar{W}/\partial a^\alpha \partial E \\ \partial^2 \bar{W}/\partial E \partial b & \partial^2 \bar{W}/\partial E^2 \end{pmatrix} \tag{5.28}$$

p_j are the number of "turning points" [e.g. 87, p. 158] or "libration points" [147, p. 49] defined below.

*The correct meaning is as given by eq (5.18)

Proof of eq. (5.26). Since (5.26) is the stationary phase value of (5.25)

$$D_{\bar{W}}(b,a,E)=\det(\partial^2\bar{S}(b,t_a+t;a,t_a)/\partial b^\alpha\partial a^\beta)(\partial^2\bar{S}(b,t_a+t;a,t_a)/\partial t^2)^{-1}\Big|_{t=\bar{\tau}(b,a,E)}. \tag{5.29}$$

It follows from eqs. (5.27) and (5.25) that

$$\begin{aligned}&\partial\bar{W}/\partial E=((\partial\bar{S}/\partial\bar{\tau})+E)\,\partial\bar{\tau}/\partial E+\bar{\tau}\\&\partial\bar{W}(b,a,E)/\partial E=\bar{\tau}(b,a,E).\end{aligned} \tag{5.30}$$

It follows from eqs. (5.30) and (5.25) that $\partial^2\bar{W}/\partial E^2=\partial\bar{\tau}/\partial E$ and $(\partial^2\bar{S}/\partial\bar{\tau}^2)\partial\bar{\tau}/\partial E+1=0$, hence

$$\partial^2\bar{S}(b,t_a+\bar{\tau}(b,a,E);a,t_a)/\partial\bar{\tau}^2=-(\partial^2\bar{W}(b,a,E)/\partial E^2)^{-1} \tag{5.31}$$

Let b' be a point on $\bar{q}$ between a and b, $\mathcal{G}_{\mathrm{WKB}}(b',a,E)$ loses a phase equal to $1\pi/2$ each time $\partial^2\bar{W}(b',a,E)/\partial E^2$ changes sign (p. 319). $\partial^2\bar{W}(b',a,E)/\partial E^2$ changes sign each time $(\partial^2\bar{W}(b,a,E)/\partial E^2)^{-1}$ vanishes, i.e. at the so-called **turning points** or **libration points**. For example, [e.g. 87, p. 142], let the system be a particle of mass m in a potential V

$$\bar{W}(b,a,E)=\pm\int_{\bar{q}}(2m(E-V(\bar{q}(s))))^{1/2}\|\mathrm{d}\bar{q}(s)\|$$

$(\partial^2\bar{W}/\partial E^2)^{-1}$ vanishes when $V(\bar{q}(s))=E$. Finally we have to compute the other second derivatives of $\bar{W}(b,a,E)$ using eqs. (5 27) and (5.25):

$$\frac{\partial^2\bar{W}}{\partial b\,\partial a}=\frac{\partial^2\bar{S}}{\partial b\partial a}+\frac{\partial^2\bar{S}}{\partial\bar{\tau}\partial a}\frac{\partial\bar{\tau}}{\partial b}=\frac{\partial^2\bar{S}}{\partial b\partial a}-\frac{\partial^2\bar{S}}{\partial\bar{\tau}\partial a}\frac{\partial^2\bar{S}}{\partial b\partial\bar{\tau}}\Big/\frac{\partial^2\bar{S}}{\partial\bar{\tau}^2},$$

$$\frac{\partial^2\bar{W}}{\partial E\partial a}=\frac{\partial^2\bar{S}}{\partial\bar{\tau}\partial a}\frac{\partial\bar{\tau}}{\partial E},\qquad\frac{\partial^2\bar{W}}{\partial E\partial b}=\frac{\partial^2\bar{S}}{\partial\bar{\tau}\partial b}\frac{\partial\bar{\tau}}{\partial E}.$$

Hence

$$\frac{\partial^2\bar{S}}{\partial b\partial a}=\frac{\partial^2\bar{W}}{\partial b\partial a}-\frac{\partial^2\bar{W}}{\partial E\partial a}\frac{\partial^2\bar{W}}{\partial E\partial b}\Big/\frac{\partial^2 W}{\partial E^2}$$

and it follows, after some easy algebraic manipulations, that eq. (5.29) is equal to (5.28). ■

Equation (5.26) suggests that there exists a path integral representation of $\mathcal{G}(b,a,E)$. We shall return to this point in section 5.5.

A deeper insight into the phase gain of the action at a turning point can be obtained by examining [83] the following example: Consider the reflection of a particle of mass m by the potential $V(x)=E(x_0/x)^2$. The equation of motion of the particle is $x(t)=(x_0^2+2Et^2/m)^{1/2}$. The particle reaches a minimum distance x_0 from the origin at time $t=0$. Its total energy is E. The action along the path from a to b which bounces off the potential barrier is

$$\bar{S}(b,t_b;a,t_a)=m(b+a)^2(t_b-t_a)^{-1}-2E\int_{t_a}^{t_b}(\Delta t)^2(4t^2+(\Delta t)^2)^{-1}\,\mathrm{d}t,\qquad\Delta t=x_0(2m/E)^{1/2}$$

As the potential is made increasingly more abrupt, the action tends to

$$\lim_{x_0=0} \bar{S}(b, t_b; a, t_a) = m(b+a)^2(t_b - t_a)^{-1} - \pi E \Delta t.$$

Δt can be considered as the "time of interaction" and according to the uncertainty principle $E\Delta t > \hbar$. Roughly speaking the action is equal to the sum of the action of a free particle from a to $x_0 = 0$, then from x_0 to b, plus a contribution at the turning point due to the fact that we cannot measure simultaneously with infinite precision the energy of the system and the time of interaction. This argument should of course be taken with a grain of salt since the Einstein relation $\Delta E = h\Delta\nu$, together with the purely classical relation $\Delta\nu\,\Delta t \propto 1$, is not a Heisenberg uncertainty relation [e.g. 18].

To complete the calculation of the density of states, we need to compute

$$\mathcal{G}(E) = \int_M \mathcal{G}(b = a, a, E)\, da \tag{5.32}$$

whose WKB approximation can be evaluated like (5.24) by the stationary phase approximation. Let a^* be the value of a that minimizes the exponent in eq. (5.26):

$$0 = (\partial \bar{W}(b, a, E)/\partial a + \partial \bar{W}(b, a, E)/\partial b)\Big|_{a=b=a^*} = -p_{\text{in}}(a^*, E) + p_{\text{fin}}(a^*, E) \tag{5.33}$$

p_{in} and p_{fin} are the initial and final momenta of the stationary path which starts at a^* and ends up at a^*. A closed stationary path which satisfies eq. (5.33) is a periodic orbit. Hence periodic orbits *if they exist* are the only closed stationary paths which contribute to $\mathcal{G}_{\text{WKB}}(E)$.

5.4. Systems with classical periodic orbits

The calculation of $\mathcal{G}_{\text{WKB}}(E)$ requires the evaluation of the action $\bar{W}(E) = \bar{W}(a^*, a^*, E)$ and of the hessian of the action $\bar{W}(b, a, E)$ at $a = b = a^*$ which is related to the Poincaré map $R(\tau)$ by some pretty formulae: The Jacobi fields $k = (h, j)$ can be obtained by variation through stationary paths, thus to first order in (h, j)

$$p(t_a) + j(t_a) = -\partial \bar{W}(b + h(t_b), a + h(t_a), E)/\partial a$$

$$p(t_b) + j(t_b) = \partial \bar{W}(b + h(t_b),\ a + h(t_a), E)/\partial b$$

hence

$$j_\alpha(t_a) = -\frac{\partial^2 \bar{W}}{\partial b^\beta \partial a^\alpha} h^\beta(t_b) - \frac{\partial^2 \bar{W}}{\partial a^\beta \partial a^\alpha} h^\beta(t_a), \qquad j_\alpha(t_b) = \frac{\partial^2 \bar{W}}{\partial b^\beta \partial b^\alpha} h^\beta(t_b) + \frac{\partial^2 \bar{W}}{\partial a^\beta \partial b^\alpha} h^\beta(t_a). \tag{5.34}$$

If now $a = b = a^*$, the system (5.34) of $2n$ linear equations can be rewritten in the form

$$\begin{pmatrix} h^\alpha(t_a + \tau) \\ j_\alpha(t_a + \tau) \end{pmatrix} = R(\tau) \begin{pmatrix} h^\alpha(t_a) \\ j_\alpha(t_a) \end{pmatrix}. \tag{5.35}$$

If (5.34) were invertible, comparison of (5.34) and (5.35) would yield

$$-\det(\partial^2 \bar{W}/\partial b^\alpha \partial a^\beta)\Big|_{a=b=a^*} = \det R(\tau) = 1 \tag{5.36}$$

$$\det\left(\frac{\partial^2\bar{W}}{\partial b^\alpha \partial b^\beta}+\frac{\partial^2\bar{W}}{\partial b^\alpha \partial a^\beta}+\frac{\partial^2\bar{W}}{\partial a^\alpha \partial b^\beta}+\frac{\partial^2\bar{W}}{\partial a^\alpha \partial a^\beta}\right)\Bigg|_{a=b=a^*}=\det(R(\tau)-\mathbf{1}). \tag{5.37}$$

Equations (5.36) and (5.37) are easily checked in one dimension, the proof is a more involved piece of linear algebra for systems with more than one degree of freedom. We shall show that (5.34) is not invertible, but the hessian of the action can be block diagonalized into a vanishing matrix and a non-vanishing matrix and equations (5.36) and (5.37) become

$$-\widehat{\det}\,\partial^2\bar{W}/\partial b^\alpha \partial a^\beta\Big|_{a=b=a^*}=\det R(\tau)=1 \tag{5.38}$$

$$\widehat{\det}\left(\frac{\partial^2\bar{W}}{\partial b^\alpha \partial b^\beta}+\frac{\partial^2\bar{W}}{\partial b^\alpha \partial a^\beta}+\frac{\partial^2\bar{W}}{\partial a^\alpha \partial b^\beta}+\frac{\partial^2\bar{W}}{\partial a^\alpha \partial a^\beta}\right)\Bigg|_{a=b=a^*}=\widehat{\det}(R(\tau)-1) \tag{5.39}$$

where $\widehat{\det}$ means the determinant of the nonvanishing matrix.

Equation (5.34) is not invertible because the system has at least one constant of the motion, namely the hamiltonian. Indeed take the derivatives of the two Hamilton-Jacobi equations

$$H(-\partial\bar{W}(b,a,E)/\partial a,a)=E,\qquad H(\partial\bar{W}(b,a,E)/\partial b,b)=E \tag{5.40}$$

with respect to b^α and a^α and use Hamilton's equations

$$-\bar{q}^\beta(t_a)\frac{\partial^2\bar{W}}{\partial b^\alpha \partial a^\beta}=0,\qquad -\bar{q}^\beta(t_a)\frac{\partial^2\bar{W}}{\partial a^\alpha \partial a^\beta}-\bar{p}_\alpha(t_a)=0,$$

$$\dot{\bar{q}}^\beta(t_b)\frac{\partial^2\bar{W}}{\partial a^\alpha \partial b^\beta}=0,\qquad \bar{q}^\beta(t_b)\frac{\partial^2\bar{W}}{\partial b^\alpha \partial b^\beta}-\bar{p}_\alpha(t_b)=0.$$

It follows that the determinants on the left hand side of (5.36) and (5.37) vanish. Choose an atlas* on M such that in every coordinate patch the components of $\dot{\bar{q}}(t)$ are $(\|\dot{\bar{q}}(t)\|,0,\ldots 0)$ then

$$\partial^2\bar{W}/\partial b^\alpha \partial a^1=\partial^2\bar{W}/\partial a^\alpha \partial b^1=0 \tag{5.41}$$

$$\partial^2\bar{W}/\partial a^\alpha \partial a^1=-\dot{\bar{p}}_\alpha(t_a)/\|\dot{\bar{q}}(t_a)\|,\qquad \partial^2\bar{W}/\partial b^\alpha \partial b^1=\dot{\bar{p}}_\alpha(t_b)/\|\dot{\bar{q}}(t_b)\|. \tag{5.42}$$

On the other hand because the hamiltonian is a constant of the motion, there is at least one periodic Jacobi field, namely $(\dot{\bar{q}},\dot{\bar{p}})$, and one pair of vanishing characteristic exponents. Set $k_1=(\dot{\bar{q}},\dot{\bar{p}})$, then $\alpha_1=\alpha_{-1}=0$. If there are no other constants of integration eqs. (5.38) and (5.39) are satisfied with the determinants being taken with respect to $\alpha,\beta=2,\ldots n$ in the chosen system of coordinates, or with respect to the nonvanishing characteristic exponents.

If there are $j>1$ constants of the motion

$$F_{j'}(\bar{q}(t),\bar{p}(t))=\text{constant}\qquad j'=1,\ldots j$$

then there are j periodic Jacobi fields given by equation (5.14) and j pairs of vanishing characteristic exponents. Choose an atlas on M such that in every coordinate patch $h^{j'}(t)$ has only one nonvanishing component along the j'-axis equal to its norm. By an argument similar to the previous one we see that eqs. (5.38) and (5.39) are satisfied with the determinants taken with respect to $\alpha,\beta=j+1,\ldots n$ or with respect to the nonvanishing characteristic exponents.

*If this requires a change of coordinate system, see for instance ref [23] p 149 how to construct the coordinate system such that a given field has only one nonvanishing component

We shall complete the calculation of $\mathcal{G}_{\mathrm{WKB}}(E)$ assuming that the hamiltonian is the only constant of the motion.* We assume also that the characteristic exponents are all distinct and different from $2\pi/\mathrm{i}\tau$ (mod $4\pi/\mathrm{i}\tau$). The elements of the null subspace of the Jacobi operator have components only along $(\dot{\bar{q}}(t), \dot{\bar{p}}(H))$. In the chosen system of coordinates, the integration over $\mathrm{d}a^2 \ldots \mathrm{d}a^n$ is readily obtained by the stationary phase approximation, the integration over $\mathrm{d}a^1 = \mathrm{d}a^*$ has to be done explicitly.

We first evaluate $D_{\bar{W}}(a^*, a^*, E)$. Take the derivatives of (5.40) with respect to E and use Hamilton's equations. It gives in the chosen system of coordinates $\partial^2 \bar{W}/\partial E \partial b^1 = \|\dot{\bar{q}}(t_b)\|^{-1}$, $\partial^2 \bar{W}/\partial a^1 \partial E = -\|\dot{\bar{q}}(t_a)\|^{-1}$. It follows from eqs. (5.28) and (5.41) that

$$D_{\bar{W}}(b, a, E) = -\|\dot{\bar{q}}(t)\|^{-2} \det \partial^2 \bar{W}(b, a, E)/\partial b^j \partial a^k \qquad \text{with} \quad j, k = 2, \ldots n \tag{5.43}$$

which together with (5.38) gives

$$D_{\bar{W}}(a^*, a^*, E) = \|\dot{\bar{q}}(t)\|^{-2}$$

where t is the time such that $\bar{q}(t) = a^*$.

The integration over $\mathrm{d}a^2 \ldots \mathrm{d}a^n$ introduces the following factors (see eq. (5.39))

$$(2\pi \mathrm{i}\hbar)^{(n-1)/2} (\det(R(\tau) - \mathbf{1}))^{-1/2} \exp(-\mathrm{i}k\pi/2) \tag{5.44}$$

where k is the number of negative eigenvalues of $R(\tau) - \mathbf{1}$. It will be convenient to reexpress the determinant as follows.

$$\widehat{\det}(R(\tau) - \mathbf{1}) = \prod_{k=\pm 2}^{\pm n} (\exp(\alpha_k \tau) - 1) = \prod_{k=2}^{n} 4 \sin^2 \mathrm{i}\alpha_k \tau/2$$

$$(\widehat{\det}(R(\tau) - 1))^{-1/2} = \prod_{k=2}^{n} \sum_{m=0}^{\infty} \exp(m_k + \tfrac{1}{2})\alpha_k \tau$$

$$= \sum_{m_2=0}^{\infty} \sum_{m_n=0}^{\infty} \exp \sum_{k=2}^{n} (m_k + \tfrac{1}{2})\alpha_k \tau. \tag{5.45}$$

The integration over $\mathrm{d}a^1$ reduces to $\oint_{\bar{q}} \|\dot{\bar{q}}(t)\|^{-1} \mathrm{d}a^* = \tau$ whether the periodic motion is a rotation or a libration [e.g. 12]. Finally

$$\mathcal{G}_{\mathrm{WKB}}(E) = (\mathrm{i}\hbar)^{-1} \sum_{\substack{\text{periodic} \\ \text{orbits}}} \tau_j |\widehat{\det}(R(\tau) - 1)|^{-1/2} \exp\left(\frac{\mathrm{i}}{\hbar} \bar{W}_j(E) - h(\lambda_j + p_j + k_j)/4\right) \tag{5.46}$$

$$\mathcal{G}_{\mathrm{WKB}}(E) = (\mathrm{i}\hbar)^{-1} \sum_{\substack{\text{periodic} \\ \text{orbits}}} \tau_j(E) \sum_{m_2=0}^{\infty} \cdots \sum_{m_n=0}^{\infty} \exp \frac{\mathrm{i}}{\hbar} \hat{\bar{W}}_j(E, m_2 \ldots m_n) \tag{5.47}$$

where

$$\hat{\bar{W}}_j(E, m_2 \ldots m_n) = \bar{W}_j(E) - h((\lambda_j + p_j + k_j)/4 - \mathrm{i} \sum_{k=2}^{n} (m_k + \tfrac{1}{2})\alpha_k(E)\tau_j(E)/2\pi). \tag{5.48}$$

The sum over the periodic orbits consists of an infinite sum over the multiple traverses of a basic orbit and a finite sum over basic orbits. Recall that in eq. (5.47), $\tau_j(E)$ came from $\int_M \mathcal{G}(b = a, a, E)\,\mathrm{d}a$, i.e. from an integral over the configuration space, whereas $\bar{W}_j(E)$ came from a time integral

*For the use of collective coordinate methods when a system has continuous symmetries see refs [61] and [63]

$\int (\langle \bar{p}, \dot{\bar{q}} \rangle - H(\bar{q}, \bar{p}))\, dt$, hence

$$\mathcal{G}_{\mathrm{WKB}}(E) = (i\hbar)^{-1} \sum_{\substack{\text{basic}\\ \text{orbits}}} \tau_J(E) \sum_{n=1}^{\infty} \sum_{m_2=0}^{\infty} \cdots \sum_{m_n=0}^{\infty} \exp \frac{1n}{\hbar} \hat{\bar{W}}_J(E, m_2, \ldots m_n)$$

$$= (i\hbar)^{-1} \sum_{\substack{\text{basic}\\ \text{orbits}}} \tau_J(E) \sum_{m_2=0}^{\infty} \cdots \sum_{m_n=0}^{\infty} \exp \frac{i}{\hbar} \hat{\bar{W}}(E, m_2 \ldots m_n) \Big/ \Big(1 - \exp \frac{1}{\hbar} \hat{\bar{W}}_J(E.\ m_2 \ldots m_n)\Big). \tag{5.49}$$

The poles of $\mathcal{G}(E)$ are the energy eigenvalues of the system; they occur for $\hat{\bar{W}}_J(E, m_2, \ldots m_n) = hn$, i.e. for

$$\bar{W}(E) = \oint_{\bar{q}} \bar{p}_\alpha(\bar{q}, E)\, d\bar{q}^\alpha = h\Big(n + (\lambda + p + k)/4 + i \sum_{k=2}^{n} (m_k + \tfrac{1}{2}) \alpha_k(E) \tau(E)/2\pi\Big). \tag{5.50}$$

This is the generalized Bohr–Sommerfeld quantization condition.*
Two cases: 1. Each α_k is purely imaginary, the system is stable, the energy is real. 2. Some α_k are complex, the system is unstable, the energy is complex, the wave function (5.16) has a decaying term whose decay rate is given by the imaginary part of the energy. The characteristic exponents are, of course, only partly responsible for the line breadths. The primary reason for the decay of bound states is the interaction of the electrons with the electromagnetic field.

Remark. Liapunov has shown that the norm is not the only function on the Jacobi fields which can be used to define stability. The second variation of the action is certainly a good candidate to investigate stability in the sense of Liapunov

Remark on complex classical paths. We started with the real classical energies and real classical paths. The characteristic exponents have introduced complex valued classical trajectories and complex energies in the Bohr–Sommerfeld condition. Complex valued classical trajectories were first introduced by Keller [78] in his "geometrical theory of diffraction". With McLaughlin he has shown [80] how the classical paths of all types – including the classical diffracted paths – enter the WKB approximation. Balian and Bloch [6, 7] have systematically investigated the complex Hamilton–Jacobi equation when the potential is analytic and developed quantum mechanics in terms of complex classical paths. Balian, Parisi and Voros [8] have shown in an example how asymptotic expansions can fail if the classical complex trajectories are not included in the WKB approximation.

In conclusion, the WKB approximation of the energy spectrum is obtained from the closed orbits of the system, if any, and the nearby family of quasiperiodic** orbits†. the characteristic exponents of a closed orbit $(\bar{q}, \bar{p})$ are obtained from the Poincaré map $R(\tau)$ where the matrix $R(t)$ consists of the Jacobi fields along $\bar{q}$, $\bar{p}$, and the Jacobi fields are obtained by $2n$ parameter variations of the classical paths which can be deformed continuously into $(\bar{q}, \bar{p})$.

If the system does not admit periodic orbits, then $\mathcal{K}(a, t_a + t; a, t_a)$ cannot be computed by the WKB approximation and some other method has to be investigated If the system admits

*See ref [33] for the case in which the energy is not the only constant of motion

A vector valued function is said to **quasiperiodic or **multiply periodic** if its components can be represented by a series of the form $\Sigma_k C_k \exp i(k \mid \omega)$ where $(k \mid \omega) = \Sigma_{\alpha=1}^{n} k_\alpha \omega^\alpha$ with $\omega \in R^n$ and $k \in Z^n$ (integer components) $\Sigma_k C^k$ is assumed to be convergent

†The objection made by Berry and Tabor that the Gutzwiller–Voros result rests on the assumption that the closed orbits are isolated is not sustained

quasiperiodic orbits, Berry and Tabor [11] have proposed that the action be written in terms of action-angle variables (I, θ) rather than in the natural phase space coordinates (q, p). The paths are closed in the (I, θ) space and the computation proceeds basically as before. The Berry–Tabor result is justified by the fact that, according to Carruthers and Nieto [22], canonical transformations do not affect WKB approximations.

Little is known about generic nonintegrable systems and their quantum properties. It is hoped that new insight into quantum properties will come from the recent studies of classical dynamical systems. As we have seen in this section, the bridge constructed between quantum and classical mechanics by Wentzel, Kramers and Brillouin is very beneficial to quantum mechanics.*

5.5. *On the existence of path integral representations of $\mathcal{G}(b, a, E)$ and $\mathcal{G}(E)$*

$i\hbar\mathcal{G}(b, a, E)$ has been defined as the Fourier transform of $\mathcal{K}(b, t_a + t; a, t_a)$ and $i\hbar\mathcal{G}_{\mathrm{WKB}}$ is the stationary phase approximation of the Fourier transform of $\mathcal{K}_{\mathrm{WKB}}$. The result, written for a and b within focal distance

$$i\hbar\mathcal{G}_{\mathrm{WKB}}(b, a, E) = (2\pi i\hbar)^{-(n-1)/2}(D_{\bar{W}}(b, a, E))^{1/2}\exp\left(\frac{1}{\hbar}\bar{W}(b, a, E)\right) \tag{5.51}$$

is very striking. It is the WKB approximation one would have formally written down for

$$\mathcal{G}(b, a, E) = \int_{\mathsf{E}} \exp\left(\frac{\mathrm{i}}{\hbar}W(q, E)\right)\mathcal{D}q \quad \text{(formally)}, \tag{5.52}$$

where

$$W(q, E) = \int_a^b (2m(E - V(q)))^{1/2}\left(\sum g_{\alpha\beta}\,\mathrm{d}q^\alpha\,\mathrm{d}q^\beta\right)^{1/2},$$

and where E is the space of paths from a to b with *average* energy

$$E = \tau^{-1}\int_{t_a}^{t_a+\tau} (m\|q(t)\|^2/2 + V(q(t)))\,\mathrm{d}t$$

$$q(t_a) = a, \quad q(t_a + \tau) = b. \tag{5.53}$$

Indeed, let $\bar{q}$ be the classical path from a to b with *constant* energy E. Then $\bar{W}(b, a, E) = W(\bar{q}, E)$. We now show that $D_{\bar{W}}(b, a, E)$ is the Van Vleck determinant of $\bar{W}(b, a, E)$. Let us parametrize the classical path $\bar{q}$ by one of its co-ordinates, say $\bar{q}^1$. Then $\bar{W}(b, a, E) = \int_{a^1}^{b^1} L_E(\bar{q}^1, \bar{q}^j(\bar{q}^1), \dot{\bar{q}}^j(\bar{q}^1))\,\mathrm{d}\bar{q}^1$, $j = 2, \ldots, n$. The Van Vleck determinant of $\bar{W}(b^j, b^1; a^j, a^1)$ is $\det \partial^2\bar{W}/\partial b^j\partial a^k$. On the other hand in the system of co-ordinates where $\bar{q}^1(t) = \|\bar{q}(t)\|$, $D_{\bar{W}}(b, a, E)$ is given by eq. (5.43). In the $\bar{q}^1$ parametrization where $\dot{\bar{q}}^1(\bar{q}^1) = 1$, it reads

$$D_{\bar{W}}(b, a, E) = \det \partial^2\bar{W}/\partial b^j\,\mathrm{d}a^k. \qquad \blacksquare$$

Whereas the path integral representation of $\mathcal{K}(b, t_b; a, t_a)$ is over the space of paths going from a to

*It should also be beneficial to classical mechanics since classical mechanics is the limit of quantum mechanics But this is another story

b in a given amount of time $t_b - t_a$, the formal path integral representation of $\mathcal{G}(b, a, E)$ is over the space of paths going from a to b with a given amount of average energy E. The action $W(q, E)$ is the action of a free particle on a curved space M with metric

$$\mathrm{d}l^2 = 2m(E - V(q))g_{\alpha\beta}\,\mathrm{d}q^\alpha\,\mathrm{d}q^\beta. \tag{5.54}$$

Can we define a prodistribution w^E on E such that

$$\mathcal{G}(b, a, E) = \int_{\mathrm{E}} \mathrm{d}w^E(q)?$$

The best we can hope for, at the present time, is an implicit definition. Two approaches suggest themselves, both very difficult:

1. A prodistribution on the space of paths from a to b constrained on the Riemannian manifold M can be defined implicitly, via the development mapping, from a prodistribution on the tangent space at one end point, T_aM or T_bM.

2. It may be possible to define implicitly w^E by a random process $\{q(t)\}$ on $\mathbf{R}^n$. Recall that the Wiener gaussian w_-^{W} on X_- was first known, not explicitly as the normalized gaussian of covariance $\inf(t - t_a, s - t_a)$, but implicitly as the gaussian such that the random process $\{x(t)\}$ is brownian (see example 6, p 266; and appendix D). The prodistribution w^E on E must be such that it defines a random process $\{q(t)\}$ with the following characteristics:

$$q(t_a) = a, \qquad q(t_a + \tau) = b$$

τ is a stochastic variable such that eq. (5.53) is satisfied.

$$\int_{\mathrm{E}} (\|q(t_k) - q(t_{k-1})\|^2 - 2m(E - V(q(t_{k-1})))(t_k - t_{k-1})^2)\,\mathrm{d}w_{\mathrm{E}}(q) = 0. \tag{5.55}$$

Note that the last condition says that E is the average energy along the path. Indeed, since q is not differentiable, we cannot write $\|\mathrm{d}q(t)\|^2 - 2m(E - V(q(t)))\,\mathrm{d}t^2 = 0$, but we can write that the expectation value of the left-hand side vanishes. This situation was recognized by Garrod [58, p. 488] and Gutzwiller [64, p. 1984] who wrote down a formal path integral representation of $\mathcal{G}(b, a, E)$ using spaces of paths with given average energy and computed $\mathcal{G}_{\mathrm{WKB}}(b, a, E)$.

We do not know if the conditions (5.55) given for the random process $\{q(t)\}$ are sufficient to determine a prodistribution w^E on E. The fact that a random process with brownian motion characteristics *does* determine a promeasure w_- on X_- is not a trivial result but a great achievement of Wiener. It does not seem that random processes of type (5.55) have been studied, nothing can be said about the existence of a promeasure they might define, let alone the existence of a prodistribution.

The WKB approximation of $\mathcal{G}(E)$ is also very striking and similar considerations can be made on the possible existence of a path integral representation of $\mathcal{G}(E)$.

Conclusion

The world is global and stochastic and physical laws are local and deterministic. The beautiful thing is that these complementary descriptions of nature can be brought together: A path integral is a global and stochastic expression, it is also the solution of a local and deterministic partial differential equation.

In this monograph we have computed path integrals in terms of solutions of ordinary differential equations, and thereby produced solutions of partial differential equations of parabolic type with Cauchy data. The corner-stones have been

1. The Fourier transform of the gaussian w_-^{W} on X_- exists (a source of delight for mathematicians) and is known explicitly (a source of delight for physicists)

$$\mathcal{F}w_-^{\mathrm{W}}(\mu) = \exp\Big(-\tfrac{1}{2}\mathrm{i}\int_T \mathrm{d}\mu(t)\int_T \mathrm{d}\mu(s)\inf(t-t_a, s-t_a)\Big).$$

2. Linear mappings of spaces of paths introduce gaussians whose covariance are elementary kernels of the Jacobi equation. So much is known about the Jacobi equation from many branches of physics and mathematics that the prodistribution formalism can borrow a wealth of results derived by Jacobi, Sturm, Liouville, Poincaré, to name but a few.

Many more problems can be investigated with the methods developed here. Some of them we had hoped to incorporate, some others came to our attention when this monograph was in the last stages of completion. We shall use the size limitation of Physics Reports as an excuse to stop here for the time being.

Appendix A. Some differences between integration on $\mathbf{R}^n$ and functional integration

"Physical intuition often borders on wishful thinking"*

Theorem 1. On a finite dimensional space, linearity implies continuity; not so on an infinite dimensional space.

Theorem 2. The compact subsets of $\mathbf{R}^n$ *are the closed bounded subsets of* $\mathbf{R}^n$. *A closed bounded subset, with nonempty interior, of an infinite dimensional normed space is never compact under the norm topology.* (Roughly speaking a compact set has no interior.)

Theorem 3. Let X be an infinite dimensional normed space. Any continuous function(al) on X with compact support is identically zero.

Theorem 4. There is no measure invariant under translation on a Hilbert space H such that the measure of every bounded open ball, $\|x\| < \rho$, *is finite.*

*"When dealing with less simple and concrete equations, physical intuition is less reliable and often borders on wishful thinking" [N G Van Kampen]

These striking differences between finite and infinite dimensional spaces are an indication of the pitfalls into which our intuition, based on the properties of $\mathbb{R}^n$, can lead us.

Before discussing these theorems, recall some definitions. A subset $A \subseteq X$ is said to be **compact** if every covering of A by open sets has a finite subcovering. Note that a compact subspace of a Hausdorff space is necessarily closed.

The **interior** of a set A is the largest open set contained in A

The **boundary** ∂A is the set of all points contained both in the closure of A and in the closure of the complement of A:

$$\partial A \overset{\text{def}}{=} \bar{A} \cap \overline{CA}.$$

These definitions generalize to topological spaces the familiar notion on $\mathbb{R}^n$; to see why they imply different properties on $\mathbb{R}^n$ and on infinite dimensional spaces we shall consider some simple examples.

One of the simplest generalizations of $\mathbb{R}^n$ is the space H of sequences $\{x^i; i = 1, \ldots\}$ such that $\Sigma_1^\infty (x^i)^2$ is finite, together with the topology induced by the metric

$$d(x, y) = \left(\sum_1^\infty (x^i - y^i)^2 \right)^{1/2}.$$

In $\mathbb{R}^n$ a closed unit ball is a compact set with nonempty interior. A compact set in $\mathbf{R}^n$ with empty interior is for instance a closed subset of $\mathbb{R}^{n-1}$. If we try to construct in H a compact set with nonempty interior we succeed in constructing either a noncompact set (example 1), or a set which does not belong to H (example 2), or a set with empty interior (example 3).

Example 1. The obvious generalization of the closed unit ball in $\mathbb{R}^n$ is the set of points $\{x^i\} \in H$ such that $\Sigma (x^i)^2 \leqslant 1$. Its interior $\Sigma (x^i)^2 < 1$ is nonempty. We shall show that this set is not compact: If the ball were compact, any infinite sequence of points in the ball would have an accumulation point in the ball. Consider the sequence of points $a_\alpha \in H$ such that $a_\alpha^i = \delta_\alpha^i$. This sequence is in the closed unit ball, no subsequence converges to anything, the ball is not compact.

Example 2. Consider the unit cube in $\mathbb{R} \times \mathbb{R} \times \cdots$, i.e the set of points whose coordinates $0 \leqslant x^i \leqslant 1$. This set is compact in the space $\mathbb{R} \times \mathbb{R} \times \cdots$ with its usual infinite product topology (Tychonoff topology). But all the points of the cube are not in H. The corner point $\{1, 1, \ldots\}$ is not square summable.

Example 3. Consider the Hilbert cube in H. This is the set of sequences $\{x^i\}$ such that $0 \leqslant x^i \leqslant 1/i$, i.e. the parallelepiped whose edges have length 1, 1/2, 1/3, ... The Hilbert cube is compact because it is the infinite product of compact sets with a metric topology that is equivalent to the Tychonoff topology. But the Hilbert cube has an empty interior: it contains no open set.

Proof. The open balls in H form a basis for the topology induced by the metric d on H. Let $B_\epsilon(x_0)$ be the open ball of radius 2ϵ centered at x_0. For any $x_0 \in H$ and any $\epsilon > 0$ there is a point $y \in B_\epsilon(x_0)$ which is not in the Hilbert cube. Indeed, let $n > 1/\epsilon$. The point $y = \{x_0^1, \ldots x_0^{n-1}, x_0^n + \epsilon, x_0^{n+1}\}$ is in $B_\epsilon(x_0)$ but is not in the Hilbert cube. The Hilbert cube is too cramped to put any open set inside it. ■

These examples explain the contents of theorem 2: A compact subset of an infinite dimensional space X is all boundary, like a closed subset of $\mathbb{R}^{n-1}$ in $\mathbb{R}^n$.

We shall now use theorem 2 to prove theorem 3. Consider a continuous function(al) on X which is zero outside a compact set. The set of $x \in X$ with $f(x) \neq 0$ is open and is contained in a compact set and is hence void. Thus $f(x) = 0$ for all x. ■

We would expect any measure on X to have the usual reasonable properties of measures on R^n. Theorem 4 shows that no such measure exists.

Proof of Theorem 4. Let a be the measure of the unit ball, let b be the measure of balls of radius $\epsilon < 1$. Let $\{e_n\}$ be an orthonormal infinite subset in H. Let $x_n = \lambda e_n$ and consider the balls $\{x; \|x - x_n\| < \epsilon\}$ They are included in the unit ball if $\lambda + \epsilon < 1$. They are disjoint if $\lambda\sqrt{2} > 2\epsilon$. There is an infinite number of disjoint balls of measure b included in the unit ball, therefore additivity would imply that the measure of the unit ball be infinite.

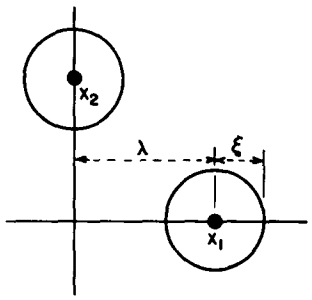


Fig 10

Remark. The expression "invariant" measure is also used in a different sense from theorem 4. A measure μ on X is said to be **invariant** under a transformation $T: X \to X$ if the sets of measure zero are the same for μ and for its image under T.

Appendix B. Jacobi fields and related topics

When the covariance of a gaussian prodistribution is identified as the elementary kernel of a Jacobi equation, the work is in a very advanced stage of completion: the properties of the Jacobi equation have been investigated, under different names, in various branches of physics and mechanics and many theorems can be used for computing path integrals with respect to gaussian prodistributions with such covariances.

Some other names for the Jacobi equation are: **variational equation** [e.g. 143, p. 268], **équation aux variations** [120, p. 163], **small disturbance equation** [37, p. 165] and, in the context of Riemannian spaces, **equation of geodetic deviation.**

An elementary kernel is often called a Green function, although, strictly speaking, a Green function is an elementary kernel satisfying a particular set of properties. Many properties derived in this appendix apply obviously to the elementary kernels of any homogeneous second-order linear differential operator.

Consider a lagrangian system S. Its action

$$S(f) = \int_T L(f(t), \dot{f}(t))\, dt, \qquad T = [t_a, t_b]$$

can be expanded around a classical path

$$S(f) = S(q) + \tfrac{1}{2}S''(q)xx + \Omega(q, x). \tag{B1}$$

If $f: T \to \mathbf{R}^n$, then $x = f - q$. The simplest method to compute the expansion (B1) is the one-parameter variation method [40, 41, 105]. It is valid when $f: T \to M$ where M is a Riemannian manifold with metric g equal to the *Legendre matrix**, assumed here to be invertible

$$g_{\alpha\beta}(q(t)) = m^{-1}\,\partial^2 L/\partial q^\alpha(t)\partial q^\beta(t). \tag{B2}$$

Let U be the interval $[0, 1]$, let $u \in U$, and let $\{\bar\alpha(u);\, u \in U\}$ be a one parameter family of paths

$$\bar\alpha(u): T \to M \text{ such that } \bar\alpha(0) = q \qquad \text{and} \quad \bar\alpha(1) = f.$$

Set

$$\bar\alpha(u)(t) = \alpha(u, t), \qquad \partial\alpha(u, t)/\partial u = \bar\alpha'(u)(t) \qquad \text{and } \bar\alpha'(0) = x.$$

The function $\alpha: U \times T \to M$ defines a parametrized two dimensional surface. We use primes for covariant derivatives along the curves $\alpha(\cdot, t): U \to M$ and dots for covariant derivatives along the curves $\alpha(u, \cdot): T \to M$. We use either of the following notations according to typographical convenience:

$$\nabla_u\alpha(u, t) = \partial\alpha(u, t)/\partial u = \partial_u\alpha(u, t) = \alpha'(u, t)$$

$$\nabla_t\alpha(u, t) = \partial\alpha(u, t)/\partial t = \partial_t\alpha(u, t) = \dot\alpha(u, t).$$

Note that $\alpha'(u, t) = \nabla_u\nabla_t\alpha(u, t) = \nabla_t\nabla_u\alpha(u, t)$.
Let V be a vector field on the parametrized surface α; the Riemann tensor R is defined by

$$(\nabla_u\nabla_t - \nabla_t\nabla_u)V = R(\partial_u\alpha, \partial_t\alpha)V.$$

The expansion (B1) is easily computed as a Taylor expansion with respect to the parameter u:

$$S(f) = S\circ\bar\alpha(1) = \sum_{n=0}^{\infty}(1/n!)(S\circ\alpha)^{(n)}(0) \tag{B3}$$

$$(S\circ\bar\alpha)'(u) = S'(\bar\alpha(u))\bar\alpha'(u)$$

$$(S\circ\bar\alpha)''(u) = S''(\bar\alpha(u))\bar\alpha'(u)\bar\alpha'(u) + S'(\bar\alpha(u))\bar\alpha''(u), \quad \text{etc.}$$

Since $S\circ\bar\alpha$ is a function with values in $\mathbf{R}$, its derivatives can be understood as ordinary derivatives or as covariant derivatives. They are considered here to be covariant derivatives for simplicity and convenience, and so are the derivatives on the right hand side.

The first variation is

$$(S\circ\bar\alpha)'(u) = \int_T \left(L_1 - \frac{\mathrm{d}}{\mathrm{d}t}L_2\right)\alpha'(u, t)\,\mathrm{d}t + L_2\alpha'(u, t)\Big|_{t=t_a}^{t_b} \tag{B4}$$

where L_1 and L_2 are the derivatives of L with respect to its first and second argument, understood to

*The Legendre matrix is, most often, defined to be $A_{\alpha\beta}(q(t)) = -\partial^2 L/\partial q^\alpha(t)\partial q^\beta(t)$. For this reason, in previous papers, we have sometimes used $g_{\alpha\beta} = A_{\alpha\beta}/\hbar$. The choice (B2) is preferable because it gives $g_{\alpha\beta} = \delta_{\alpha\beta}$ in flat space. Moreover, it brings out explicitly the dependence of the wave function on $\hbar$ and on $\mu = (\hbar/m)^{1/2}$.

be $\alpha(u, t)$ and $\dot{\alpha}(u, t)$ respectively. Set

$$\mathscr{L}q(t) = L_1(q(t), q(t)) - \frac{\mathrm{d}}{\mathrm{d}t} L_2(q(t), q(t)).$$

The **Euler–Lagrange equation** is

$$\mathscr{L}q(t) = 0.$$

The term $S''(\bar{\alpha}(u))$ in the second variation is a symmetric bilinear form* on the space of vector fields along $\bar{\alpha}(u)$, which after integration by parts, reads

$$S''(\bar{\alpha}(u))\bar{\alpha}'(u)\bar{\alpha}'(u) = \int_T \{\mathscr{J}(\bar{\alpha}(u))\alpha'(u, t)\}\alpha'(u, t)\,\mathrm{d}t + \left\{\left(L_{21} - \frac{1}{2}\frac{\mathrm{d}L_{22}}{\mathrm{d}t}\right)\alpha'(u, t)\alpha'(u, t) + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(L_{22}\alpha'(u, t)\alpha'(u, t))\right\}\Big|_{t_a}^{t_b}$$

where L_{21} and L_{22} are the derivatives of L_2 with respect to its first and second argument, more precisely $L_{21}^{\mu\nu} = \partial^2 L/\partial\dot{\alpha}^\nu(u, t)\partial\alpha^\mu(u, t) \neq L_{12}^{\mu\nu}$, and where

$$\mathscr{J}(\bar{\alpha}(u)) = -L_{22}\frac{\mathrm{d}^2}{\mathrm{d}t^2} + (L_{12} - L_{21} - \mathrm{d}L_{22}/\mathrm{d}t)\frac{\mathrm{d}}{\mathrm{d}t} + (L_{11} - \mathrm{d}L_{21}/\mathrm{d}t).$$

The **Jacobi equation** is

$$\mathscr{J}(\bar{\alpha}(u))\alpha'(u, t) = 0. \tag{B5}$$

A solution of the Jacobi equation is called a **Jacobi field** along $\bar{\alpha}(u)$. In general we shall set:

$$\alpha'(0, t) = h(t) \quad \text{if } h \text{ is a Jacobi field along } q.$$

Jacobi matrices and related matrices. The mapping $J_\beta^\alpha(t, t_a): T_aM \to T_{q(t)}M$ such that

$$\begin{cases} J_\beta^\alpha(t, t_a)v^\beta = h^\alpha(t) & \text{is the } \alpha\text{-component of a Jacobi field along } q \\ h^\alpha(t_a) = 0, \qquad \nabla_{t_a}h^\alpha(t_a) = v^\alpha, & \text{for any } v \in T_aM \end{cases} \tag{B6}$$

defines a matrix $J_\beta^\alpha(t, t_a)$, called a **Jacobi matrix**; each column of $J_\beta^\alpha(t, t_a)$ consists of the components $h_{(\beta)}^\alpha$ of the Jacobi field $h_{(\beta)}$ vanishing at t_a and whose derivatives $\dot{h}_{(\beta)}^\alpha(t_a) = \delta_\beta^\alpha$.
The mapping $K_\beta^\alpha(t, t_a): T_aM \to T_{q(t)}M$ such that

$$\begin{cases} K_\beta^\alpha(t, t_a)v^\beta = h^\alpha(t) & \text{is the } \alpha\text{-component of a Jacobi field along } q \\ h^\alpha(t_a) = v^\alpha, \qquad \nabla_{t_a}h^\alpha(t_a) = 0, & \text{for any } v \in T_aM \end{cases} \tag{B7}$$

defines a matrix $K_\beta^\alpha(t, t_a)$, called a **Jacobi matrix**; each column of $K_\beta^\alpha(t, t_a)$ consists of the components $h_{(\beta)}^\alpha$ of the Jacobi field $h_{(\beta)}$, whose derivative vanishes at t_a and such that $h_{(\beta)}^\alpha(t_a) = \delta_\beta^\alpha$.

The Jacobi matrices $J(t, t_a)$ and $K(t, t_a)$ are known respectively as the **commutator function** and the **Hadamard function**. We shall show that J is indeed the commutator function (modulo $-m^{-1}$). Namely

$$-m^{-1}J^{\alpha\beta}(t, s) = \frac{\partial q^\alpha(t)}{\partial a^\gamma}\frac{\partial q^\beta(s)}{\partial p_{a_\gamma}} - \frac{\partial q^\beta(s)}{\partial a^\gamma}\frac{\partial q^\alpha(t)}{\partial p_{a_\gamma}},$$

*Often called the **hessian** of S at $\bar{\alpha}(u)$

where $q(t)$ is the stationary* path $q(t, a, p_a)$ defined by its initial position $q(t_a) = a$ and initial momentum p_a.

*Proof.*** The derivatives of q with respect to a and p_a are Jacobi fields.† Set $s = t_a$ in the above equation, it turns out that

$$m^{-1} J^{\alpha\beta}(t, t_a) = \partial q^{\alpha}(t) / \partial p_{a\beta}.$$

Thus $J(t, t_a)$ defined by the Poisson bracket (modulo $-m^{-1}$) satisfies the same equation and the same boundary conditions as the Jacobi matrix defined by (B6). Note $m^{-1} J^{\alpha\beta}(t_b, t) = -\partial q^{\beta}(t) / \partial p_{b\alpha}$.

Definition. Let $\bar{S}(a, t_a; b, t_b) = S(q)$ be the action function for the stationary path q such that $q(t_a) = a$ and $q(t_b) = b$. The off diagonal block of the hessian of $\bar{S}$ is called the **Van Vleck** matrix.

$$\text{Van Vleck matrix} = \partial^2 \bar{S} / \partial a^{\alpha} \partial b^{\beta}. \tag{B8}$$

Lemma. The inverse of the Jacobi matrix J defined by

$$M_{\alpha\beta}(t_a, t_b) J^{\beta\gamma}(t_b, t_a) = \delta_{\alpha}^{\gamma} \tag{B9}$$

is equal to the Van Vleck matrix, modulo m^{-1}

$$M_{\alpha\beta}(t_a, t_b) = -m^{-1} \partial^2 \bar{S}(a, t_a; b, t_b) / \partial a^{\alpha} \partial b^{\beta}.$$

Proof † The inverse of the Poisson bracket is the Lagrange bracket, hence $M(t_a, t)$ is the Lagrange bracket, modulo $-m$,

$$-m M_{\alpha\beta}(t_a, t_b) = -\partial p_{b\beta} / \partial a^{\alpha} = \partial^2 \bar{S} / \partial a^{\alpha} \partial b^{\beta}. \qquad \blacksquare$$

The **advanced** and **retarded Green functions** are, respectively, $G^{\text{adv}}(t, s) = -\theta(s - t) J(t, s)$, $G^{\text{ret}}(t, s) = \theta(t - s) J(t, s)$. The advanced and retarded Green functions are often labelled $G^{\pm}$ and not to be confused with the same symbols used here for the covariances.

The Jacobi matrix J is obviously antisymmetric since it is equal to the commutation function

$$J^{\alpha\beta}(t, s) = -J^{\beta\alpha}(s, t).$$

So is the Van Vleck matrix. The other Jacobi matrix, K, does not have, in general, any symmetry property. We shall label $\tilde{K}(t_a, t)$ the matrix with entries

$$\tilde{K}^{\alpha\beta}(t_a, t) = K^{\beta\alpha}(t, t_a).$$

We shall label N and $\tilde{N}$ the inverses of K and $\tilde{K}$, respectively,

$$N_{\alpha\beta}(t_a, t) K^{\beta\gamma}(t, t_a) = \delta_{\alpha}^{\gamma}, \qquad \tilde{K}^{\gamma\beta}(t_a, t) \tilde{N}_{\beta\alpha}(t, t_a) = \delta_{\alpha}^{\gamma}. \tag{B10}$$

*We use the expression "stationary path" to refer to a solution of the Euler–Lagrange equation, usually reserving the term "classical path" for a solution which minimizes the action

**These simple proofs are due to Mizrahi [107] See other properties of the Jacobi matrices in [108] More elaborate proofs and other results can be found in ref [40] p 373 See also ref [128]

†See next paragraph a detailed analysis of one-parameter variations through classical paths

One-parameter variations through stationary paths. The dimension of the configuration space being n, there are at most $2n$ *linearly independent Jacobi fields along* q. They are easily computed if one knows the general solution of the Euler–Lagrange equation. Indeed [73, 40] the set of derivatives of the general solution of the Euler–Lagrange equation with respect to its $2n$ constants of integration is a complete set of Jacobi fields. Thus one way of obtaining a Jacobi field is to make what is known as a "**one-parameter variation through solutions of the Euler–Lagrange equation**"; i.e. a variation $\bar{\alpha}(u)$ such that $\mathscr{L}\alpha(u, t) = 0$.

If this variation keeps one end fixed, say $\alpha(u, t_a) = a$ for every $u \in U$, then $\partial\alpha(u = 0, \cdot)/\partial u$ is a Jacobi field along q vanishing at t_a. The condition that the family of paths $\{\mathscr{L}\alpha(u, \cdot);\ u \in U\}$ has a fixed end point $\alpha(u, t_a) = a$ determines n of the $2n$ constants of integration of the general solution of the Euler–Lagrange equation, leaving n undetermined constants which can be varied to obtain n Jacobi fields vanishing at t_a. These n Jacobi fields are the columns of the Jacobi matrix $J(t, t_a)$.

Remark. This construction of $J^{\alpha\beta}(t_b, t_a)$ provides a very simple method for computing the Van Vleck determinant.

In flat space one can obtain the remaining n Jacobi fields by making n one-parameter variations through families of stationary paths with the same initial velocity. If one thinks of such a family as a family of stationary paths with initial velocities perpendicular to a given plane $0 = S_0(a) = g_{\alpha\beta}a^\alpha v^\beta$, one can generalize this construction to curved spaces: Let $S_0(a) = 0$ be an initial wave front, for instance $S_0(a)$ can be the initial value of a solution of the Hamilton–Jacobi equation, or $\exp(iS_0(a)/\hbar)T(a)$ can be the initial wave function of a system (section 3.2). Let $S_0(a)$ have first order contact with its tangent space at $q(t_a)$

$$\nabla_\alpha \nabla_\beta S_0(q(t_a)) = 0$$

where the covariant derivative $\nabla_\alpha = D/\partial q^\alpha(t_a)$. Consider a family of stationary paths $\{\bar{\alpha}(u)\}$ with initial velocities $\dot{\alpha}^\alpha(u, t_a) = \nabla^\alpha S_0(\alpha(u, t_a))$. Then the Jacobi field h along $\bar{\alpha}(u)$ such that

$$h(t_a) = \partial_u \alpha(u, t_a)\Big|_{u=0} \quad \text{and} \quad \dot{h}(t_a) = 0$$

is obtained by making n one-parameter variations through the family $\{\bar{\alpha}(u)\}$. Indeed

$$\dot{h}(t_a) = \nabla_{t_a}\partial_u \alpha(u, t_a)\Big|_{u=0} = \nabla_u \alpha(u, t_a)\Big|_{u=0} = g^{\alpha\beta}\nabla_\gamma \nabla_\beta S_0(q(t_a))h^\gamma(t_a) = 0. \qquad \blacksquare$$

Caustics and conjugate points. We shall give three equivalent definitions of a caustic.

1. It can happen that an n-parameter family of stationary paths has an envelope. The envelope is the **caustic** with respect to the n initial data which define the family.

2. It can happen that there are k nonzero Jacobi fields along q with vanishing boundary conditions at $q(t_a) = a$ and $q(t_b) = b$. The two points a and b are then said to be **conjugate along** q with **multiplicity** k. A **caustic** is a set of conjugate points.

The vanishing boundary conditions can be either Dirichlet $h(t_a) = h(t_b) = 0$, or von Neuman conditions $\dot{h}(t_a) = \dot{h}(t_b) = 0$, or a mixture of both ($k$ components of $h(t_a)$ and $n - k$ components of $\dot{h}(t_b)$ vanishing). A Jacobi field with vanishing Cauchy data is always identically null (see below).

3. It can happen that there are fewer than $2n$ linearly independent Jacobi fields defined by

boundary conditions at t_a and t_b. If there are $2n-k$ linearly independent Jacobi fields, a and b are said to be **conjugate along** q with **multiplicity** k.

The equivalence of these three definitions is proved in ref. [40, p. 375]. Milnor [105, Th 18.1, p. 98] gives still another equivalent definition in the case of geodesics. We shall only make a few comments to indicate how one definition is related to the others.

1. Recall that two curves f_1 and f_2 have an intersection of order k at t if $f_1(t) = f_2(t)$ as well as their first k derivatives. An envelope is the limit of the intersections of a family of "infinitesimally close" curves. In the limit these intersections are of order $k \geq 1$. Hence the Jacobi field along q obtained by a one parameter variation of stationary paths vanishes when q touches its caustic. And a caustic defined as an envelope is indeed a set of conjugate points with respect to the initial conditions which define the family of stationary paths

Note that if two stationary paths with common origin have an intersection of order $k = 0$, then the intersection is not a conjugate point of the origin.

2. Let a and b be conjugate along q and let h_1 be a nonzero Jacobi field such that $h_1(t_a) = h_1(t_b) = 0$, then if h_2 is a Jacobi field defined by its values at t_a and t_b, h_2 and $h_1 + h_2$ are two different Jacobi fields satisfying the same boundary conditions It follows that definition 2 implies definition 3.

Criterion for identifying conjugate points. Consider a family of stationary paths emanating from a fixed point. $q(t)$ *is conjugate to* $q(t_a)$ *if and only if* $\det J(t, t_a) = 0$

*Consider a family of stationary paths with equal initial velocities.** $q(t)$ *is conjugate to* $q(t_a)$ *if and only if* $\det K(t, t_a) = 0$. This criterion follows immediately from the third definition.

*Example. Surface area of a soap film held by two loops.*** The properties of caustics and their relationship to catastrophes can be displayed in the following example, often used in the calculus of variations.

Dip two loops of radius r and R in a soap solution. Remove them. Assume that the loops, originally concentric, are gradually pulled apart so that their planes remain perpendicular to the axis joining their centres. The soap film forms a surface of revolution of minimum area and eventually breaks into two circular discs held by the loops. When does the film break?

Answer: The area of the surface of revolution generated by the curve f is

$$S(f) = 2\pi \int_{t_a}^{t_b} f(t)(1 + \dot{f}^2(t))^{1/2}\, dt.$$

Here $t_b - t_a$ is the distance between the two loops. $S(f)$ is minimum for q such that $S'(q) = 0$. The Euler–Lagrange equation and the Jacobi equation are, respectively,

$$\mathscr{L}q(t) = -q(t)q(t) + \dot{q}^2(t) + 1 = 0,$$

$$\mathscr{J}(q)h(t) = (1 + \dot{q}^2(t))^{-3/2}(-q(t)h(t) + 2\dot{q}(t)h(t) - \dot{q}(t)h(t)) = 0.$$

*See p 353 for the meaning to be given to this phrase when the configuration space is a riemannian manifold

**DeWitt-Morette and Tschumi in ref [133]

The general solution of the Euler–Lagrange equation is the two-parameter family of catenaries

$$\alpha(u, v, t) = u \cosh((t - v)/u), \qquad u, v > 0.$$

The derivatives of α with respect to u and with respect to v are Jacobi fields. The most general Jacobi field along $\bar{\alpha}(u, v)$ is thus

$$h(u, v, t) = \lambda \partial\alpha/\partial u + \mu \partial\alpha/\partial v,$$

where λ and μ are two constants of integration.

The family of catenaries keeping one end fixed is a one-parameter family of catenaries defined by $r = \alpha(u, v, t_a) = u \cosh(v/u)$. This equation determines either v as a function of u or u as a function of v. Say $v(u)$. The Jacobi field along $\alpha(u, v(u), t)$ is $h(u, t) = \lambda(\partial\alpha/\partial u + (\partial\alpha/\partial v)(\partial v/\partial u))$. It vanishes at $t = t_a$ since $\alpha(u, v(u), t_a) =$ constant for all u's

On the other hand, the envelope of the one-parameter family of catenaries $\{\alpha(u, v(u)\}$ is by definition the set of points on $\{\alpha(u, v(u), t)\}$ such that $\partial\alpha/\partial u + (\partial\alpha/\partial v)(\partial v/\partial u) = 0$ (limit of the intersection of infinitesimally close curves of order $k > 1$). The Jacobi field $h(u, t)$ is a nonzero Jacobi field vanishing at the origin and on the envelope of $\{\bar{\alpha}(u, v(y)\}$. The point where $\alpha(u, v(u), t)$ touches the envelope of $\{\bar{\alpha}(u, v(u))\}$ is conjugate to $\alpha(u, v(u), t_a)$: the envelope is the caustic defined as the set of conjugate points of $\alpha(u, v(u), t_a) = r$.

The Jacobi matrices J and K have only one entry. Along the curve $\alpha(u, v(u), t)$ they are, respectively,

$$J(t, t_a) = \sinh\frac{t - t_a}{u} + \frac{t - t_a}{u} \sinh\frac{t - v(u)}{u} \sinh\frac{t_a - v(u)}{u},$$

$$K(t, t_a) = \frac{1}{u} \cosh\frac{t_a - v(u)}{u}\left(\cosh\frac{t - v(u)}{u} - \frac{t - t_a}{u} \sinh\frac{t - v(u)}{u}\right).$$

Note that $J(t, t_a)$ is not function of $(t - t_a)$. But $J(t, t_a) = -J(t_a, t)$. The Jacobi matrix $K(t, t_a)$ has no symmetry property.

The condition $J(t, t_a) = 0$ determines the caustic with respect to a fixed initial value $\alpha(u, v, t_a) =$ constant. The condition $K(t, t_a) = 0$ determines the caustic with respect to a fixed initial slope $\partial\alpha(u, v, t_a)/\partial t_a =$ constant.

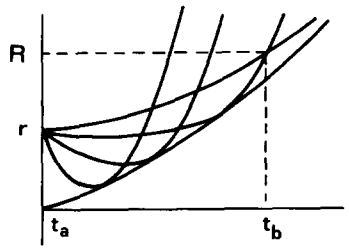


Fig 11 A family of catenary with fixed origin

Given r, R, T there are two solutions, or one solution, or no solution, depending on whether (R, t_b) is above, on or below the envelope. Assuming R fixed, the bubble breaks when t_b is such that (R, t_b) is on the caustics.

Example. The equation of geodetic deviation.

Consider a free particle in curved space, $L(f(t)) = \frac{1}{2}\|\dot{f}(t)\|^2$.

$$S \circ \bar{\alpha}(u) = \int_T \tfrac{1}{2}(\alpha(u,t) \mid \alpha(u,t))\,\mathrm{d}t$$

$$(S \circ \bar{\alpha})'(u) = \int_T (\alpha(u,t) \mid \nabla_t \partial_u \alpha(u,t))\,\mathrm{d}t = (\alpha(u,t) \mid \alpha'(u,t))\Big|_{t_a}^{t_b} - \int_T (\nabla_t \nabla_t \alpha(u,t) \mid \alpha'(u,t))\,\mathrm{d}t$$

$$(S \circ \bar{\alpha})''(u) = (\nabla_t \partial_u \alpha(u,t) \mid \alpha'(u,t))\Big|_{t_a}^{t_b} + (\alpha(u,t) \mid \nabla_u \alpha'(u,t))\Big|_{t_b}^{t_a}$$
$$- \int_T (\nabla_t \nabla_t \alpha'(u,t) + R(\alpha'(u,t), \alpha(u,t))\dot{\alpha}(u,t)) \mid \alpha'(u,t))\,\mathrm{d}t$$
$$- \int_T (\nabla_t \nabla_t \alpha(u,t) \mid \nabla_u \alpha'(u,t))\,\mathrm{d}t.$$

This example shows how one can work entirely with covariant derivatives. In practise, one is interested either in a variation $\{\bar{\alpha}(u)\}$ keeping the end points fixed, or keeping one end point fixed, or keeping the initial, or final, velocity (covariantly) constant, and the above expressions simplify accordingly.

The Jacobi equation is

$$\nabla_t \nabla_t h(t) + R(h(t)\dot{q}(t))\dot{q}(t) = 0 \tag{B11}$$

known as the equation of geodetic deviation.

Construction of Jacobi fields by variation through geodesics:

a) Geodesics emanating from a point.

In flat space $J^\alpha{}_\beta(t, t_a) = \delta^\alpha_\beta(t - t_a)$. In general $J^\alpha{}_\beta(t, t_a)$ tells how a family of geodesics emanating from a point a at t_a diverge.

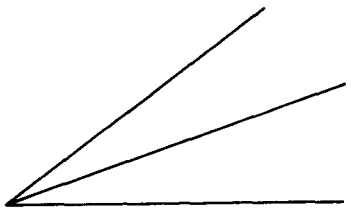


Fig 12

b) Geodesics with equal velocities.

In flat space $K^\alpha{}_\beta(t, t_a) = \delta^\alpha_\beta$. In general one can use the construction described previously (p. 353) to build a family of geodesics with "equal" initial velocities. $K^\alpha{}_\beta(t, t_a)$ tells how such a family of geodesics diverge.

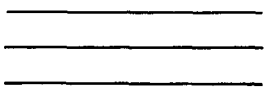


Fig 13

Elementary kernels. The elementary kernels of the Jacobi operator are the natural covariances for lagrangian and hamiltonian systems. They are easily constructed [40] in terms of the Jacobi matrices.

All the elementary kernels are symmetric; $G^{\alpha\beta}(t, s) = G^{\beta\alpha}(s, t)$.

$$\begin{cases} G_+(t = t_b, s) = 0 \\ \nabla_t G_+(t = t_a, s) = 0 \end{cases} \quad \begin{cases} G_-(t = t_a, s) = 0 \\ \nabla_t G_-(t = t_b, s) = 0 \end{cases} \quad \begin{cases} G(t = t_a, s) = 0 \\ G(t = t_b, s) = 0. \end{cases}$$

$G(t, s)$ is known as the Feynman Green function.

$$G_+(r, s) = \theta(s - r)K(r, t_a)N(t_a, t_b)J(t_b, s) - \theta(r - s)J(r, t_b)\tilde{N}(t_b, t_a)\tilde{K}(t_a, s), \tag{B12}$$

$$G_-(r, s) = \theta(s - r)J(r, t_a)\tilde{N}(t_a, t_b)\tilde{K}(t_b, s) - \theta(r - s)K(r, t_b)N(t_b, t_a)J(t_a, s), \tag{B13}$$

$$G(r, s) = \theta(s - r)J(r, t_a)M(t_a, t_b)J(t_b, s) - \theta(r - s)J(r, t_b)M(t_b, t_a)J(t_a, s). \tag{B14}$$

See note III added in proof for the boundary conditions of K when the potential is velocity dependent.

Examples.

1. The covariances of the Wiener gaussians are elementary kernels of $-\mathrm{d}^2/\mathrm{d}t^2$. They are constructed from $J^{\alpha\beta}(t, t_a) = g^{\alpha\beta}(t - t_a)$ and $K^{\alpha\beta}(t, t_a) = g^{\alpha\beta}$. (B15)
2. The covariances of the Ornstein–Uhlenbeck gaussians are elementary kernels of $-\mathrm{d}^2/\mathrm{d}t^2 + \omega^2$. See note III added in proof.

$J^{\alpha\beta}(t, t_a)$ is always antisymmetric. In general $K^{\alpha\beta}(t, t_a)$ is not symmetric.

Some properties of the covariances most often needed in path integration.*

1. If the potential does not depend on the velocity, the Van Vleck matrix for a short time interval is

$$M_{\alpha\beta}(t_b, t_a) = (g_{\alpha\beta}/(t_b - t_a))(1 + \mathrm{O}((t_b - t_a)^2)). \tag{B16}$$

Proof: If the potential does not depend on the velocity, $\mathscr{J}_t$ is of the form $\mathscr{J}_t = -\nabla_t^2 + R(t)$. The Taylor expansion of $J(t, s)$ is

$$\begin{aligned} J(t, s) &= J(s, s) + (t - s)\nabla_t J(t = s, s) + \tfrac{1}{2}(t - s)^2\nabla_t^2 J(t = s, s) + \cdots \\ &= (t - s)g^{-1}(s) + \mathrm{O}(t - s)^3, \end{aligned}$$

where we have used $\nabla_t^2 J(t = s, s) = R(s)J(s, s) = 0$. Equation (B16) follows. Equation (B16) is no longer true for velocity dependent potentials as can easily be seen from the action function of a particle in a constant magnetic field [56, p. 64]. ■

2. Let $\{t_1, \ldots t_p\}$ define a p division of $T = [t_a, t_b]$

$$t_a = t_0 < t_1 < \cdots < t_p < t_{p+1} = t_b.$$

*For other properties also used in path integration and for the calculations and proofs of the results quoted in sections 2 to 4 see ref [40] pp 389–393 and p 373

The image of the gaussians of covariances G, $G_\pm$ under the mappings $P: X \to R^{pn}$, $P_\pm: X_\pm \to R^{(p+1)n}$ by

$$P: x \mapsto \{u^{i\alpha} = x^\alpha(t_i);\ i = 1, \dots p\}, \qquad P_+: x \mapsto \{u^{i\alpha} = x^\alpha(t_i);\ i = 0, \dots p\},$$
$$P_-: x \mapsto \{u^{i\alpha} = x^\alpha(t_i);\ i = 1, \dots p+1\}$$

are respectively the gaussians on $\mathbb{R}^{pn}$ and $\mathbb{R}^{(p+1)n}$ of covariances $\mathcal{W}^{i\alpha j\beta} = G^{\alpha\beta}(t_i, t_j)$, $\mathcal{W}_\pm^{i\alpha i\beta} = G_\pm^{\alpha\beta}(t_i, t_j)$. To complete the computation of an integral whose integrator is a gaussian known by its covariance $\mathcal{W}$, or $\mathcal{W}_\pm$, one needs the inverse matrices $\mathcal{W}^{-1}$, $\mathcal{W}_\pm^{-1}$ and their determinants. They can be computed from G, $G_\pm$ using the properties of the Jacobi fields, they are given in [40, pp. 391, 392]. The determinants are needed for the computation of the Fredholm determinants in section 1.5:

$$\det \mathcal{W}^{-1} = \det M(t_b, t_p) \det M(t_p, t_{p-1}) \dots \det M(t_1, t_a)/\det M(t_b, t_a),$$
$$\det \mathcal{W}_+^{-1} = \det M(t_b, t_p) \dots \det M(t_1, t_a)/\det K(t_a, t_a) \det N(t_a, t_b),$$
$$\det \mathcal{W}_-^{-1} = \det M(t_b, t_p) \dots \det M(t_1, t_a)/\det K(t_b, t_b) \det N(t_b, t_a). \tag{B17}$$

3. In section 1.5, it has been established that the Fredholm determinant of the linear mapping $M: Y \to X$, where Y and X are spaces of $L^{2,1}$ paths vanishing either at t_b or at t_a is

$$(\operatorname{Det} M^{-1})^2 = \operatorname{Det} G_B(r, s)/\operatorname{Det} G_A(r, s).$$

G_B is the covariance of the gaussian w_B on Y, image under M^{-1} of an arbitrarily chosen gaussian w_A on X of covariance G_A. Let $\mathcal{W}_B^{i\alpha j\beta} = G_B^{\alpha\beta}(t_i, t_j)$ and $\mathcal{W}_A^{i\alpha j\beta} = G_A^{\alpha\beta}(t_i, t_j)$

$$\operatorname{Det} G_B(r, s)/\operatorname{Det} G_A(r, s) = \lim_{p=\infty} \det \mathcal{W}_B^{i\alpha j\beta}/\det \mathcal{W}_A^{i\alpha j\beta}.$$

Since* for a short time interval $M_B(t_k, t_{k-1}) = M_A(t_k, t_{k-1}) + O(t_k - t_{k-1})^2)$ one obtains

$$(\operatorname{Det} M_-^{-1})^2 = \det K_A(t_a, t_b)/\det K_B(t_a, t_b), \qquad (\operatorname{Det} M_+^{-1})^2 = \det K_A(t_b, t_a)/\det K_B(t_b, t_a). \tag{B18}$$

4. A Jacobi field h can be specified by its Dirichlet data $\{h(t_a), h(t_b)\}$, its Cauchy data $\{h(t_a), \dot{h}(t_a)\}$ or $\{h(t_b), \dot{h}(t_b)\}$ or its von Neumann data $\{h(t_a), \dot{h}(t_b)\}$ or $\{\dot{h}(t_a), h(t_b)\}$:

$$h(t) = -J(t, t_a)M(t_a, t_b)h(t_b) - J(t, t_b)M(t_b, t_a)h(t_a) \tag{B19}$$
$$h(t) = K(t, t_a)g(q(t_a))\dot{h}(t_a) + K(t, t_a)g(q(t_a))h(t_a) \tag{B20}$$

and three other similar equations. From these five equations one obtains many linear relationships between $J(t, t_a)$, $J(t, t_b)$, $K(t, t_a)$, and $K(t, t_b)$. Taking derivatives of these relationships leads to other relationships, in particular for velocity independent potentials**

$$\nabla_t J(t, t_a) = \tilde{K}(t, t_a) \quad \text{where} \quad \tilde{K}^{\alpha\beta}(t, t_a) = K^{\beta\alpha}(t_a, t). \tag{B21}$$

Note that $\dot{h}(t_a) = h(t_a) = 0$ implies $h(t) = 0$ (eq. B20), but $h(t_b) = h(t_a) = 0$ does not imply $h(t) = 0$ since $M(t_a, t_b)$ can be infinite.

In this appendix we have constructed Jacobi fields by taking derivatives of the stationary paths with respect to constants of integration. Conversely, it is sometimes convenient to solve the classical boundary

*Although (B16) is not true for velocity dependent potentials, (B18) remains true B Sheeks, private communication

**See note III added in proof for velocity dependent potentials

value problem in terms of the Jacobi matrices J and K. Indeed, the classical path $q(t, a, b)$ such that $q(t_a) = a$, $q(t_b) = b$ can be obtained as the average path over the space of paths from (a, t_a) to (b, t_b). Mizrahi [108]* has derived several formulae which solve the boundary value problem and give convenient expressions for $\bar{S}(a, t_a; b, t_b)$.

Appendix C. Index of sign conventions and basic formulae

1. *Fourier transforms.* The normalization of the Fourier transform is chosen so that $\mathcal{F}(\delta * A) = (\mathcal{F}\delta)(\mathcal{F}A) = \mathcal{F}A$. The sign convention is:

$$(\mathcal{F}f)(y) = \int_{R^n} \exp(-i\langle y, x\rangle) f(x)\, dx,$$

$$(\mathcal{F}^{-1}g)(x) = \frac{1}{(2\pi)^n} \int_{R^n} \exp(i\langle y, x\rangle) g(y)\, dy.$$

Note that if $(\mathcal{F}f)(y)$ is defined to be $\int_{R^n} \exp(i\langle y, x\rangle) f(x)\, dx$ then the roles of the lower- and upper-half complex planes are reversed.

2. *Riemann curvature tensor.* The definition of the curvature tensor is the same as of ref. [67]. The sign is the same as that of ref. [67] and the opposite of that of ref. [105]. Thus if $Y(t, \mu)$ is a surface parametrized by t and μ and Z is a vector in the surface, then the commutator of covariant derivatives is

$$\nabla_t \nabla_\mu Z - \nabla_\mu \nabla_t Z = R(\partial Y/\partial t, \partial Y/\partial \mu) Z.$$

In component form

$$Z^\alpha{}_{,\delta\gamma} - Z^\alpha{}_{,\gamma\delta} = R^\alpha{}_{\beta\gamma\delta} Z^\beta.$$

3. *The Jacobi operator.* For a lagrangian $L = \frac{1}{2}m\|\dot{Z}(t)\|^2 - V(Z(t))$, the Jacobi operator along a solution $\bar{Z}(t)$ of the Euler–Lagrange equations is

$$-m\nabla_t^2 - g^{-1}(\bar{Z}(t))\nabla\nabla V(\bar{Z}(t)) + (R(\cdot, \dot{\bar{Z}}(t)), \cdot\, |\dot{\bar{Z}}(y)).$$

4. *Jacobi matrices.* Unless otherwise stated, the Jacobi matrices are solutions of

$$\mathcal{J}_t J(t, s) = 0, \qquad \mathcal{J}_t K(t, s) = 0$$

with the boundary conditions

$$\nabla_t J(t = s, s) = g^{-1}(s), \qquad J(t = s, s) = 0, \qquad \nabla_t K(t = s, s) = 0, \qquad K(t = s, s) = g^{-1}(s).$$

Their inverses are M and N:

$$J(t, s)M(s, t) = 1, \qquad K(t, s)M(s, t) = 1.$$

(These signs differ from ref. [40].)

If the Jacobi equation is the small disturbance equation of a classical mechanical system, then M is

*[108] pp 63 and 74 See also p 75 – a criterion for the non-existence of a classical path

the Van Vleck matrix of the system:

$$M^{\alpha\beta}(t_a, t_b) = -m^{-1}\,\partial^2\bar{S}/\partial a^\alpha \partial b^\beta$$

where $\bar{S}$ is the classical action from (a, t_a) to (b, t_b).

5. *Elementary kernels of the Jacobi operator*

$$\mathscr{J}_t G_\pm(t, s) = \delta(t-s)g^{-1}(s).$$

All of the elementary kernels are symmetric: $G^{\alpha\beta}(t, s) = G^{\beta\alpha}(s, t)$. On configuration space, the boundary conditions, unless otherwise stated, are:

$$\begin{cases} G_+(t = t_b, s) = 0 \\ \nabla_t G_+(t = t_a, s) = 0 \end{cases} \qquad \begin{cases} G_-(t = t_a, s) = 0 \\ \nabla_t G_-(t = t_b, s) = 0 \end{cases} \qquad \begin{cases} G(t = t_a, s) = 0 \\ G(t = t_b, s) = 0. \end{cases}$$

$G(t, s)$ is known as the **Feynman–Green** function. The elementary kernels on configuration space can be expressed in terms of the Jacobi matrices:

$$G_+(r, s) = \theta(s-r)K(r, t_a)N(t_a, t_b)J(t_b, s) - \theta(r-s)J(r, t_b)\tilde{N}(t_b, t_a)\tilde{K}(t_a, s),$$

$$G_-(r, s) = \theta(s-r)J(r, t_a)\tilde{N}(t_a, t_b)\tilde{K}(t_b, s) - \theta(r-s)K(r, t_b)N(t_b, t_a)J(t_a, s),$$

$$G(r, s) = \theta(s-r)J(r, t_a)M(t_a, t_b)J(t_b, s) - \theta(r-s)J(r, t_b)M(t_b, t_a)J(t_a, s).$$

For a free particle on flat space, $\mathscr{J}_t = -g(t)\nabla_t^2$ and

$$G_+(r, s) = \inf(t_b - r, t_b - s),$$

$$G_-(r, s) = \inf(r - t_a, s - t_a),$$

$$G(r, s) = \theta(s-r)(r-t_a)(t_b-t_a)^{-1}(t_b-s) + \theta(r-s)(t_b-r)(t_b-t_a)^{-1}(s-t_a).$$

On phase space, the blocks of the elementary kernels are obtained from the elementary kernel on configuration space. For a free particle

$$\mathscr{J}_t = \begin{pmatrix} 0 & -\nabla_t \\ \nabla_t & -\dfrac{1}{m}g^{-1} \end{pmatrix}$$

$$G_-(r, s) = \begin{pmatrix} G_-^{\alpha\beta}(r, s) & G_-{}^{\alpha}{}_{\beta}(r, s) \\ G_{-\alpha}{}^{\beta}(r, s) & G_{-\alpha\beta}(r, s) \end{pmatrix}$$

where $G_-^{\alpha\beta}(r, s)$ is the elementary kernel of the free particle on configuration space, and:

$$G_-{}^{\alpha}{}_{\beta}(r, s) = m\nabla_s G_-^{\alpha\gamma}(r, s)g_{\alpha\beta}(s) = -m\delta^{\alpha}{}_{\beta}\theta(r-s)$$

$$G_{-\alpha}{}^{\beta}(r, s) = mg_{\alpha\gamma}(r)\nabla_r G^{\alpha\beta}(r, s) = -m\delta_{\alpha}{}^{\beta}\theta(s-r)$$

$$G_{-\alpha\beta}(r, s) = m^2 g_{\alpha\gamma}(r)\nabla_r\nabla_s G_-^{\gamma\delta}(r, s)g_{\delta\beta}(s) - mg_{\alpha\beta}(r)\delta(r-s) = 0.$$

Thus, in cartesian coordinates,

$$G_-(r, s) = \begin{pmatrix} \delta^{\alpha\beta}(\theta(s-r)(r-t_a) + \theta(r-s)(s-t_a)) & -m\delta^{\alpha}{}_{\beta}\theta(r-s) \\ -m\delta_{\alpha}{}^{\beta}\theta(r-s) & 0 \end{pmatrix}.$$

Similarly,

$$G_+(r,s)=\begin{pmatrix}\delta^{\alpha\beta}(\theta(s-r)(t_b-s)+\theta(r-s)(t_b-r)) & -m\delta^{\alpha}{}_{\beta}\theta(s-r)\\ -m\delta_{\alpha}{}^{\beta}\theta(r-s) & 0\end{pmatrix}.$$

6. *The Cameron–Martin transformations, their inverses, and their determinants.*

$M_-^{-1}: X_- \to Y_-$ by $x(t)\mapsto y(t)$

$$y(t)=x(t)-\int_T \theta(t-s)K(t,t_b)\dot{N}(t_b,s)x(s)\,\mathrm{d}s;$$

$M_-: Y_- \to X_-$ by $y(t)\mapsto x(t)$

$$x(t)=y(t)-\int_T \theta(t-r)\dot{K}(r,t_b)N(t_b,r)y(r)\,\mathrm{d}r;$$

$\operatorname{Det} M_-^{-1}=(\det K(t_b,t_b)/\det K(t_a,t_b))^{1/2}$.

$M_+^{-1}: X_+ \to Y_+$ by $x(t)\vdash y(t)$

$$y(t)=x(t)+\int_T \theta(s-t)K(t,t_a)\dot{N}(t_a,s)x(s)\,\mathrm{d}s;$$

$M_+: Y_+ \to X_+$ by $y(t)\mapsto x(t)$

$$x(t)=y(t)+\int_T \theta(r-t)\dot{K}(r,t_a)N(t_a,r)y(r)\,\mathrm{d}r;$$

$\operatorname{Det} M_+^{-1}=(\det K(t_a,t_a)/\det K(t_b,t_a))^{1/2}$.

7. *The Feynman–Kac formula* is

$$\psi(b,t_b)=\int_{X_+}\mathrm{d}w_+^{\mathrm{w}}(x)\exp\left(\frac{-\mathrm{i}}{\mu^2 m}\int_T V(\mathrm{Dev}_b(\mu x)(t))\,\mathrm{d}t\right)\phi(\mathrm{Dev}_b(\mu x)(t_a)).$$

In flat space

$$\mathrm{Dev}_b(\mu x)=b+\mu x.$$

8. *Normalized complex gaussians on* $\mathbf{R}^n$ *and their Fourier transforms*

$$\mathrm{d}w_n(v)=(2\pi\mathrm{i})^{-n/2}|\det(\mathcal{W}^{-1})_{ij}|^{1/2}\exp(\tfrac{1}{2}\mathrm{i}(\mathcal{W}^{-1})_{ij}v^iv^j)\,\mathrm{d}v^1\ldots\mathrm{d}v^n,$$

$$(\mathcal{F}w_n)(y)=\exp(\tfrac{1}{2}\mathrm{i}\mathcal{W}^{ij}y_iy_j).$$

Appendix D.* The Itô integral and the Stratonovitch integral

The art of time slicing has been perfected by physicists while the science of random variables indexed by time has been developed by probabilists. Physicists have discovered that different prescriptions for discretizing a path lead to different path integrals. For instance the path integrals constructed with the discretized action

$$\sum_k L\left(x(t_k), \frac{x(t_{k+1})-x(t_k)}{t_{k+1}-t_k}\right)(t_{k+1}-t_k) \tag{D1}$$

and with the discretized action

$$\sum_k L\left(x\left(\frac{t_{k+1}+t_k}{2}\right), \frac{x(t_{k+1})-x(t_k)}{t_{k+1}-t_k}\right)(t_{k+1}-t_k) \tag{D2}$$

are not, in general, equal. They are solutions of different Schrodinger equations. Mizrahi [110] has established the general correspondence between time slicing prescriptions in path integration and factor ordering prescriptions in the Schrödinger equation.

Probabilists, on the other hand, have derived many important results on the statistical properties of $x(t)$ when x is not a smooth path. Since their language and their script is not usually familiar to physicists, we shall introduce the concept of a family of random variables indexed by time. First we give a few definitions [e.g. 57], with the probabilists' notation

Definitions· A **probability space** consists of a triple $(\Omega, \mathcal{F}, P)$ where

i) Ω is a space of points ω, called the **sample space** and the **sample points.**

ii) $\mathcal{F}$ is a σ field of subsets of Ω. These subsets are called **events.**

iii) $P(\cdot)$ is a probability measure on $\mathcal{F}$.

General and abstract properties of random systems follow from this definition. In this appendix we consider the following example.

Let Ω be the space of continuous paths $\omega: T \to \mathbf{R}^d$.

Let $X(t, \cdot): \Omega \to \mathbf{R}^d$; for instance $X(t, \omega) = \omega(t)$ or $X(t, \omega) = (\mathrm{Dev}\ \omega)(t)$ where Dev is the development map defined in section 3.3. Since ω is not a smooth path, $X(s+\epsilon, \omega)$ is not determined by $X(s, \omega)$ for $\epsilon > 0$. The notion of randomness follows from the fact that ω is not differentiable

$X(t, \cdot)$ is called a **random variable** on $(\Omega, \mathcal{F})$ if for every Borel set** B in $\mathbf{R}^d$ the set $\{\omega; X(t, \omega) \in B\} \in \mathcal{F}$. A random variable $X(t, \cdot)$ is usually abbreviated by $X(t)$ or X_t and a set $\{\omega; X(t, \omega) \in B\}$ is abbreviated by $\{X(t) \in B\}$.

Let $\mathcal{F}$ be the smallest σ field generated by the family $\{\mathcal{F}_t; t_a \leq t \leq t_b\}$ where $\mathcal{F}_t$ is generated by the sets

$$\{\omega; X(s, \omega) \in B, \quad s \leq t, \quad B \in \mathcal{B}\}. \tag{D3}$$

It follows from the definition that, if $s \leq t$, $\mathcal{F}_s \subset \mathcal{F}_t$ and $\mathcal{F}_s = \bigcap_{t \geq s} \mathcal{F}_t$. Indeed consider for example the random variable $X(t, \omega) = \omega(t)$. We shall construct a set $F_t \in \mathcal{F}_t$ which is not in $\mathcal{F}_s$:

$F_s \in \mathcal{F}_s \Leftrightarrow \omega \in F_s$ implies $\omega' \in F_s$ whenever $\omega'(\sigma) = \omega(\sigma)$ for all $0 \leq \sigma \leq s$ (and does not imply $\omega'(\sigma) = \omega(\sigma)$ for $\sigma > s$).

*This appendix has been written after the monograph was completed, following the participation of one of us (C DeW) in the 1978 session on Stochastic Differential Equations [24]

**A Borel set of $\mathbf{R}^d$ is an element of a Borel σ field $\mathcal{B}$ of $\mathbf{R}^d$ A Borel σ field of $\mathbf{R}^d$ is the smallest σ-field generated by complementation, and by countable intersections and unions of the open sets of $\mathbf{R}^d$

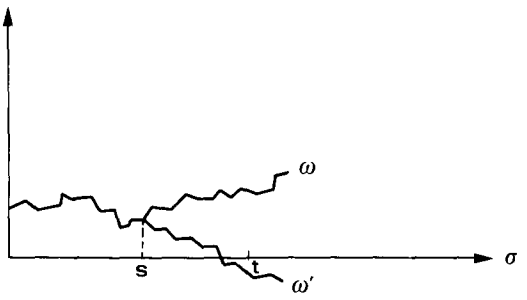


Fig 14

Thus if $s < t$ a set $F_t \in \mathcal{F}_t$ is not in general in $\mathcal{F}_s$ because the sets in $\mathcal{F}_s$ are defined by conditions on $X(\sigma, \omega)$ for $0 \leq \sigma \leq s$ and not by conditions on $X(\sigma, \omega)$ for $0 \leq \sigma \leq t$.

A process is a family of random variables $\{X_t\}$ indexed by t. A process is said to be adapted to an increasing family $\{\mathcal{F}_t\}$ if X_t is $\mathcal{F}_t$ measurable, i.e. $\{X_t(\omega) \in B\} \in \mathcal{F}_t$.

The probability measure P on Ω defines the properties of the random variable $X(t)$; for example, the expectation value of $X(t)$ is

$$E(X(t)) = \int_{\Omega} X(t, \omega)\, \mathrm{d}P(\omega). \tag{D4}$$

Alternative notations are $\int X(t)\, \mathrm{d}P$, $\int X(t, \omega) P(\mathrm{d}\omega)$.

Example: Let P be the Wiener measure, let $X(t, \omega) = \omega(t)$, with $\omega(0) = 0$, let $0 = t_0 < t_1 \cdots < t_n < t_{n+1} = t_b$. The random variables $\{X(t_1),\ X(t_2) - X(t_1), \ldots,\ X(t_b) - X(t_n)\}$ are independent for the probability P for any time partition. $X(t_k) - X(t_{k-1})$ has a normal (i.e. gaussian) distribution with mean 0 and covariance $|t_k - t_{k-1}|$. Proof (see p. 266).

Let $U : X(\ ) \to \{u', \ldots, u^{n+1}\}$ by $u^k = X(t_k) - X(t_{k-1})$, then

$$\int_{\Omega} \varphi(X(t_1), \ldots, X(t_b) - X(t_n))\, \mathrm{d}P(X) = \int_{R^{n+1}} \varphi(u^1, \ldots, u^{n+1})\, \mathrm{d}\gamma_1(u^1) \ldots \mathrm{d}\gamma_{n+1}(u^{n+1})$$

where $\mathrm{d}\gamma_k(u^k) = (2\pi)^{-1/2} \exp(-(u^k)^2/2(t_k - t_{k-1}))\, \mathrm{d}u^k$.

The process $\{X(t);\ t \geq 0\}$ defined by the Wiener measure is called the normalized Brownian motion.

In this monograph we have exploited the consequences of linear mappings U on Ω and computed the images under U of the probability measures P. Probabilists have investigated a different – but in some cases related – problem. Given the d-dimensional Brownian motion $\{\beta(t);\ t \geq 0\}$, define a new process $\{\xi(t);\ t \geq 0\}$ by the stochastic differential equation,

$$\begin{cases} \mathrm{d}\xi(t, \omega) = \sigma(t, \xi(t, \omega))\, \mathrm{d}\beta(t, \omega) + b(t, \xi(t, \omega))\, \mathrm{d}t, & t \geq s, \\ \xi(s, \omega) = x, \end{cases} \tag{D5}$$

where $\mathrm{d}\xi(t, \omega)$ denotes the infinitesimal increment in ξ during the time interval $[t, t + \mathrm{d}t]$ and $\mathrm{d}\beta(t, \omega)$ denotes the corresponding increment in β. We know that the conditional probability $P(a, t_a; b, t_b)$ of finding a Brownian particle at (b, t_b) knowing that it was at a, at t_a is the solution of the diffusion

equation* $\partial P/\partial t_b - \Delta_b P = 0$. What is the diffusion equation of the particle whose random motion is given by eq. (D5)?

Many powerful theorems are derived from this interplay between stochastic differential equations and partial differential equations both for diffusion equations and eigenvalue problems of elliptic equations. We wish we had learned this subject before writing this monograph.

When dealing with stochastic differential equations, one of the first questions which arises is "Since $\beta(t, \omega)$ is nowhere differentiable, can one attach a meaning to $\int_s^t \sigma(u, \xi(u, \omega))\, \mathrm{d}\beta(u, \omega)$ given some continuity condition on σ?" The following definition has been proposed by Itô. Set $s < u_1 < \cdots < u_n < t$,

$$\int_s^t \sigma(u, \xi(u, \cdot))\, \mathrm{d}\beta(u, \cdot) = \lim \sum_k \sigma(u_k, \xi(u_k, \cdot))(\beta(u_k, \cdot) - \beta(u_{k-1}, \cdot)).$$

The following example gives one of the basic rules of the Itô calculus:

$$\text{Compute } I = \int_T 2\beta(t)\, \mathrm{d}\beta(t) \quad \text{where } \beta \text{ is the Brownian process of mean 0.}$$

If $\beta(t)$ is differentiable, ordinary calculus can be used and $I = \beta^2(t_b) - \beta^2(t_a)$. If $\beta(t)$ is not differentiable we can use Itô calculus. Set $\beta(t_k) = \beta_k$, then

$$I = \lim \sum_k 2\beta_k(\beta_{k+1} - \beta_k) = \lim \sum_k (\beta_{k+1}^2 - \beta_k^2 - (\beta_{k+1} - \beta_k)^2).$$

The expectation value $E(\beta_{k+1} - \beta_k)^2 = t_{k+1} - t_k$. Hence

$$E \int_T 2\beta(t)\, \mathrm{d}\beta(t) = E(\beta^2(t_b) - \beta^2(t_a) - (t_b - t_a)).$$

This equation is written in Itô calculus $\mathrm{d}\beta^2(t) = 2\beta(t)\, \mathrm{d}\beta(t) + \mathrm{d}t$.

Itô calculus proceeds to defining the differential of $f(\xi(t), t)$. It is noted that $\mathrm{d}f(\xi(t), t)$ is expressed in terms of first and second derivatives of f with respect to its first argument and first derivative with respect to its second argument together with the "Itô rules": $\mathrm{d}t\, \mathrm{d}t = 0$, $\mathrm{d}\beta(t)\, \mathrm{d}t = 0$, $\mathrm{d}\beta(t)\, \mathrm{d}\beta(t) = \mathrm{d}t$.

Itô calculus was built to compute integrals where the integrand is non-anticipative

$$\int_T f(t, \beta(t))\, \mathrm{d}\beta(t) = \sum_k f(t_k, \beta(t_k))(\beta(t_{k+1}) - \beta(t_k)).$$

*In general $\mathcal{F}$ is generated by the sets (D3) and this forces probabilists to work with the Wiener covariance $G_-(t, s) = \inf(t - t_a, s - t_a)$ even in problems where it would be simpler to work with $G_+(t, s)$. This explains comments on "$-t$ parabolic equation", "forward Cauchy data", "backward equation" etc.

At time t_k we know $\beta(t_k)$ and the stochastic properties of $\beta(t_{k+1})-\beta(t_k)$. We do not know $\beta((t_k+t_{k+1})/2)$.

Stratonovitch [132] remarked that the rules of ordinary calculus could be applied to stochastic integrals if one defined the integrand at the mid-point. A rule which is precisely [59] the rule that had been used by Feynman all along. Schulman [5] has given interesting arguments for justifying Feynman's heuristic rules. Probabilists however, prefer to work with the Itô calculus, since the Stratonovitch calculus can be shown to be only a particular case of the Itô calculus.

In this monograph, we encountered briefly stochastic integrals in the integration by parts which enter the calculation of the Feynmann–Kac formula (sections 3.2, 3.3, 3.4) and proceeded according to the rules of ordinary calculus, i.e. we treated our integrals as Stratonovitch integrals. It follows that with our rules the determinant of the linear mapping $y \mapsto x$ such that $x(t) = y(t) + \int_{t_a}^{t} y(s)\,ds$ is $\exp\frac{1}{2}(t_b - t_a)$. If we had worked with Ito calculus, the determinant of this mapping would have been one*. The final results would have been the same.

The difference between the probabilists' approach and the methods followed here can be summarized by noting that probabilists work with probability spaces $(\Omega, \mathcal{F}, P)$, the careful elaboration of the σ field $\mathcal{F}$ makes it possible for them to define a probability measure P. Alternatively but less frequently, they consider P as a projective family of measures on the projective system $\mathcal{Q}$ of Ω and work with $(\Omega, \mathcal{Q}, P)$. We started from promeasures i.e. from $(\Omega, \mathcal{Q}, P)$ to introduce prodistributions and develop a scheme which can include Feynman path integrals. The central object has been $(\Omega, \mathcal{Q}, w)$ where Ω is the space of paths with values in the configuration space or in the phase space of the system and w a prodistribution with covariance adapted to the lagrangian or hamiltonian nature of the system. We have put various structures on Ω (space of paths with values in multiply connected riemannian manifolds) and have used linear maps on Ω to induce prodistributions adapted to the given problem.

Acknowledgments

It all began when Y. Choquet-Bruhat suggested to one of us (C. DeW.) to read Bourbaki's Chapter IX. She knew of her interest in Feynman path integrals and C. DeW. knew that under her guidance she would make progress. A NATO grant made it possible for them to meet several times over a period of three years (1971–1973). Prodistributions owe their existence to this collaboration. An NSF grant** (1977–1978) provided the means to develop prodistributions beyond the embryonic stage and work with them until they have become a quantitative versatile tool. The first draft of this monograph was written in Bangalore during the Summer of 1977, thanks to a travel grant from the Arts and Sciences Foundation of the University of Texas awarded to one of us (C. DeW.).

The treatment of path integration on curved spaces is so rooted in Elworthy's unpublished work that there is no way we can give him appropriate thanks. We shall remain indebted (literally) to him for sharing freely his results before the publication of the Eells–Elworthy monograph, delayed only by their desire to present a well polished tool.

Three Centers have given us the opportunity of collaborating and have provided excellent working conditions, each with a different flavor, and together the best we needed: The Center for Relativity of the University of Texas in Austin; The Center for Theoretical Studies of the Indian Institute of

*K D Elworthy, private communication

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Science, Bangalore (1977); The International Center for Theoretical Physics, Trieste (1978).

We have enjoyed the discussion with our referee, H. Grosse, and appreciated the policy of *Physics Reports* where referees are not anonymous *gendarmes* but colleagues appointed to make sure that the publication meets the criteria set by the Magazine.

Notes added in proof

I. (To be inserted p 291 line 9 from bottom.) In both cases, however, the result is the wave function at time t_b knowing the wave function at time $t_a < t_b$. In the S-matrix theory, we need also the wave function at time t_a knowing what it is at time t_b. The "earlier" wave function is a solution of the $(-t)$-Schrödinger equation

$$\partial\psi/\partial t = \frac{1}{\hbar}(\hat{H}_0 + \hat{V}(x))\psi(t, x)$$

and the corresponding Feynman and Kac formulae are respectively

$$\psi(t_a, x) = \int_{Y_-} \mathrm{d}w_-^{W^*}(y) \exp\left(+\frac{1}{\hbar}\int_{t_a}^{t_b} V(x + \mu y(t))\,\mathrm{d}t\right)\phi(x + \mu y(t_b)) \qquad \text{(Feynman)}$$

$$\psi(t_a, x) = \int_{Y_+} \mathrm{d}w_+^{W^*}(z) \exp\left(+\frac{1}{\hbar}\int_{t_a}^{t_b} V(x + \mu z(t))\,\mathrm{d}t\right)\phi(x + \mu z(t_a)). \qquad \text{(Kac)}$$

We call "Feynman formula" the one which translates immediately into mathematical terms, the "sum over all paths" idea: the probability amplitude of finding at (x, t_a) the system known to be in the state ϕ at t_b is given by the sum over all paths which are at x at t_a; the condition satisfied by the paths at t_b is inferred from the function ϕ. The prodistributions $(w_\pm^W)^*$ are defined by

$$(\mathcal{F}w^*)(\xi) = (\mathcal{F}w)^*(-\xi) = (\mathcal{F}w)^*(\xi).$$

II. (To be inserted p. 293 before "Non Relativistic Quantum Mechanics".) The S-matrix can be constructed in terms of the Møller wave operators*. Let ϕ_{in} and ϕ_{fin} be two eigenstates of $\hat{H}_0$ with the same energy E_0 Let

$$\psi_{in}(t_0, x) = W_+^{t_0}\phi_{in}(x) \qquad \text{and} \qquad \psi_{fin}(t_0, x) = W_-^{t_0}\phi_{fin}(x)$$

where

$$W_+^{t_0} = \lim_{t_a = -\infty} \exp(-i(t_0 - t_a)\hat{H}/\hbar)\exp(i(t_0 - t_a)\hat{H}_0/\hbar),$$

$$W_-^{t_0} = \lim_{t_b = +\infty} \exp(i(t_b - t_a)\hat{H}/\hbar)\exp(-i(t_b - t_0)\hat{H}_0/\hbar).$$

Contrary to usual practice we do not set $t_0 = 0$. Note that in the definition of $W_\pm^t$ on p. 292, t_0 is set equal to zero, and the superscript t refers to t_a or t_b.

*See for instance [149, pp 173–215, in particular eqs 142, 149, 159] or preferably [151, pp 112–115]

By definition*, the S-matrix is

$$\langle\phi_{\text{fin}}|S|\phi_{\text{in}}\rangle = \int_M (\psi_{\text{fin}}(t_0, x) \mid \psi_{\text{in}}(t_0, x))\, \mathrm{d}x$$

$$= \int_M (\psi_{\text{fin}}(t_0, x))^*\, \psi_{\text{in}}(t_0, x)\, \mathrm{d}x = \langle\phi_{\text{fin}}|(W_-^{t_0})^*\, W_+^{t_0}|\phi_{\text{in}}\rangle$$

$$= \lim_{t_a=-\infty,\, t_b=\infty} \langle\phi_{\text{fin}}|\exp(\mathrm{i}(t_b - t_0)\hat{H}_0/\hbar)\exp(-\mathrm{i}(t_b - t_a)\hat{H}/\hbar)\exp(\mathrm{i}(t_0 - t_a)\hat{H}_0/\hbar)|\phi_{\text{in}}\rangle.$$

We shall assume $\phi_{\text{in}}(x)$ and $\phi_{\text{fin}}(x)$ to be plane waves of momentum p_{i} and p_{f} respectively,

$$\phi_{\text{in}}(x) = \langle x|\phi_{\text{in}}\rangle = \exp(\mathrm{i}\langle p_{\text{i}}, x\rangle/\hbar),$$

$$\phi^*_{\text{fin}}(x) = \langle\phi_{\text{in}}|x\rangle = \exp(-\mathrm{i}\langle p_{\text{f}}, x\rangle/\hbar).$$

The path integral representation of the S-matrix is then readily obtained from the path integral representation of the Møller wave operator by setting $a(p) = \delta(p - p_{\text{i}})$ and $a(p) = \delta(p - p_{\text{f}})$ in the initial and final wave function respectively. Moreover, set $Y = Y_+ \oplus Y_-$ the space of paths g such that

$$g(t - t_0) = \theta(t_0 - t)\, y(t - t_0) + \theta(t - t_0)\, z(t - t_0).$$

The prodistribution w^{W} on Y defined by w_+^{W} on Y_+ and w_-^{W} on Y_- is characterized by

$$\mathcal{F}w^{\text{W}}(\xi) = \mathcal{F}w_+^{\text{W}}(\xi_+)\, \mathcal{F}w_-^{\text{W}}(\xi_-),$$

where ξ_+ and ξ_- are elements in the duals of Y_+ and Y_-, respectively. w^{W} is a normalized gaussian of covariance

$$G^{\text{W}}(t, s) = \theta(t_0 - t)\, \theta(t_0 - s)\, (\theta(t - s)\, (t_0 - t) + \theta(s - t)\, (t_0 - s)) + \theta(t - t_0)\, \theta(s - t_0)\, (\theta(t - s)\, (s - t_0) + \theta(s - t)\, (t - t_a)).$$

It follows from $S = (W_-^{t_0})^*\, W_+^{t_0}$ that

$$\langle\phi_{\text{fin}}|S|\phi_{\text{in}}\rangle = \int_Y \mathrm{d}w^{\text{W}}(g) \int_R \exp\left(-\frac{\mathrm{i}}{\hbar}\langle p_{\text{f}} - p_{\text{i}}, x\rangle\right) \mathrm{d}x$$

$$\times \exp\left(-\frac{\mathrm{i}}{\hbar}\int_R V(x + \theta(t_0 - t)\, p_{\text{i}}(t - t_0)/m + \theta(t - t_0)\, p_{\text{f}}(t - t_0)/m + \mu g(t - t_0)\right) \mathrm{d}t.$$

Albeverio and Høegh-Krøhn have proved that path integrals over Y are valid for potentials $V(x)$ which tend to zero faster than $|x|^{-1-\epsilon}$ for some positive ϵ.

Campbell, Finkler, Jones and Misheloff [148] have obtained a lattice approximation for the phase space path integral representation of the S-matrix valid for the same class of potentials. It is worth mentioning here an interesting feature of their calculation: They make the change of variable $(Q(t), P(t)) \mapsto (q(t), p(t))$ defined by

$$\begin{cases} q(t) = Q(t) - P(t)\, t/m \\ p(t) = P(t) \end{cases}$$

*This is the S-matrix of the interaction picture

and note that the new classical equations of motion can be derived from the variation of

$$S(q,p) = -\int (V(q(t) + p(t)\, t/m) + \langle q(t), \dot{p}(t)\rangle)\, \mathrm{d}t$$

keeping the values of p constant at the end points. $S(q,p)$ is precisely the action which appears in their path integral. They call the new variables $(q(t), p(t))$ the "classical interaction picture variables". They note that for potentials which fall off faster than $1/r$, not only $\lim_{t=\pm\infty} p(t) =$ constant but also $\lim_{t=\pm\infty} q(t) =$ constant. Thus the classical interaction picture variables give immediately the "asymptotic constants" of the motion introduced by Thirring* in his beautiful presentation of the Møller operators and S-matrix. In our derivation of the Møller operator, p. 292, we made a change of variable $y \mapsto z$ such that $\mu z(t) = \mu y(t) - pt/m$. This change of variable generalizes to arbitrary paths $y \in Y_+$ or $y \in Y_-$ the change of variable made by Campbell et al. for the classical path $Q(t)$, so that we could call z an "interaction variable" of integration. Expressing the path integral representation of the Møller operators in terms of the interaction variable showed immediately that the oscillatory terms cancel and that the Møller wave operators exist when a system approaches an integrable system asymptotically.

Under the change of variable $y \mapsto z$, the argument of the potential changed from $x + \mu y(t)$ to $x + pt/m + \mu z(t)$. Both the integral over y and the integral over z are computed with respect to the same prodistribution. Thus the change to the interaction variable can be loosely said to be a change from $x \mapsto x + pt/m$. The variables of integration in a path integral correspond to operators in the operator formalism of quantum mechanics. We recognize in the change $x \mapsto x + pt/m$ the change from the position operator x in the Schrödinger picture to the position $x(t)$ in the interaction picture, where

$$x(t) = \exp(\mathrm{i}H_0 t/\hbar)x \exp(-\mathrm{i}H_0 t/\hbar) = x + pt/m.$$

Of course this remark is not to be construed as a prescription for constructing "path integrals with interaction variables", it is simply a comment to contrast the argument of the potential in the S-matrix with the argument of the potential in the Feynman–Kac formula.

III. (To be inserted p. 357.) If the potential depends linearly on the velocity

$$V(q) = \mathcal{V}(q) + \langle A(q), \dot{q}\rangle$$

it is convenient to work with the following Jacobi matrices:

$J(t, t_a)$ defined as before (eq. B6),

$K(t, t_a)$ defined as before (eq. B7) but with new boundary conditions; namely

$$h^\alpha(t_a) = v^\alpha, \qquad \dot{h}^\alpha(t_a) = \tfrac{1}{2} g^{\alpha\beta}(A_{\beta,\gamma}(t_a) - A_{\gamma,\beta}(t_a)) V^\gamma.$$

Equations (B12), (B13) and (B14) are valid with the above definition of K. The case of velocity dependent potentials is being investigated by B. Nelson and B. Sheeks and will be published elsewhere.

Example: The Ornstein–Uhlenbeck velocity process v with initial velocity $v_0 = 0$ can be obtained from the Brownian process x by a linear map

*See [151, p 112] for the precise statement for the existence of the Møller wave operators

$$v(t) = \gamma x(t) - \beta \int_0^t \exp(-\beta(t-t_b)) \exp(\beta(s-t_b))\ \gamma x(s)\, ds$$

$$= \gamma x(t) - \int_0^t K(t, t_b)\, \dot{N}(t_b, s)\, \gamma x(s)\, ds$$

where K is a solution of

$$(-d^2/dt^2 + \beta^2)\, K(t, t_b) = 0$$

$$K(t_b, t_b) = 0, \qquad \nabla_t K(t, t_b)\Big|_{t=t_b} = -\beta.$$

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