

RC 13964 (#62683) 8/29/88
Mathematics 21 pages

Research Report

A Feynman Path Integral Formalism for General Evolution Equations

Willard L. Miranker and Andrew Winkler

IBM Research Division
T.J. Watson Research Center
Yorktown Heights, N.Y. 10598

89A000187

LIMITED DISTRIBUTION NOTICE: This report has been submitted for publication outside of IBM and will probably be copyrighted if accepted for publication. It has been issued as a Research Report for early dissemination of its contents and will be distributed outside of IBM up to one year after the IBM publication date. In view of the transfer of copyright to the outside publisher, its distribution outside of IBM prior to publication should be limited to peer communications and specific requests. After outside publication, requests should be filled only by reprints or legally obtained copies of the article (e.g., payment of royalties).

IBM Research Division
Almaden • Yorktown • Zurich

A Feynman Path Integral Formalism for General Evolution Equations

Willard L. Miranker and Andrew Winkler
Department of Mathematical Sciences
IBM Thomas J. Watson Research Center
P.O. Box 218
Yorktown Heights, NY 10598

Typed by: Barbara J. White

Abstract: Recourse to phase space allows the introduction of a path integral formalism valid for a broad class of Hamiltonians. Application of this phase space integral is made to the Dirac equation. The roles of geometry and physics in path integral formalisms are clarified.

1. Introduction

Feynman's idea of realizing the propagator for the Schrödinger equation as an integral over all paths of a phase function, with phase proportional to the classical action, has served as a philosophical starting point for understanding and constructing modern field and particle theories. In contrast to classical mechanics, which has meaningful content for an arbitrary choice of Hamiltonian, the path integral of Feynman does not successfully generalize to even the simplest modifications of the Schrödinger equation. It is shown here how recourse to phase space allows the introduction of a path integral formalism which is valid for a broad class of Hamiltonians, including matrix valued ones such as the Dirac operator. Like the version of Feynman, the phase for the phase space path integral introduced here is the classical action, but now expressed in Hamiltonian form.

After presenting the general formalism, we illustrate it by verifying that it applies to the Dirac equation. We also note that the generality of the formalism shows that the path integral idea has purely geometric content and relates to any Hermitian differential operator. In particular, it does not single out any one equation. Since it does not isolate the physically relevant equations, the path integral idea has no specifically physical content. Moreover, some light is shed on the nature of the Legendre transform relation between the Lagrangian and Hamiltonian approaches to classical mechanics.

We include two appendices. In the first, we exhibit the fundamental difficulties which the attempt to generalize the Feynman approach in configuration space encounters. In the second appendix, we include a demonstration that the configuration space path integral (of Feynman) for the Schrödinger equation has the correct small time behavior; this is worth comparing with the far simpler corresponding demonstration for the phase space path integral in Section 2.

2. A path integral in phase space

Feynman [1] observed that a formal propagator kernel for the Schrödinger equation $i\psi_t = \left(-\frac{\Delta}{2m} + V\right)\psi$ may be derived from the classical Lagrangian $L = \frac{mv^2}{2} - V$ in the following fashion. He considers the expression

$$k(x, y, t) = \int_{\substack{\text{paths} \\ \sigma(0)=y \\ \sigma(t)=x}} e^{i \int_{\sigma} L dt}$$

with respect to an unspecified measure and notices that formally $k(x, y, t)$ is the distribution kernel of a semigroup of operators, which has for infinitesimal generator the Schrödinger operator $\left(-\frac{\Delta}{2m} + V\right)$. This is seen by interpreting the integral over paths as an integral over polygonal paths of n segments

$$\int_{\substack{\text{paths} \\ \sigma(0)=y \\ \sigma(t)=x}} e^{i \int_{\sigma} L dt} = \lim_{n \rightarrow \infty} \int \dots \int e^{i \left[\frac{m}{2} \frac{(x_1 - y)^2}{t/n} + \dots + \frac{m}{2} \frac{(x - x_{n-1})^2}{t/n} - V(x_1) \frac{t}{n} - \dots - V(x) \frac{t}{n} \right]} dx_1 \dots dx_{n-1}$$

and evaluating the small t asymptotics of the resulting integral by the method of stationary phase (a rigorous version of this being the subject of Appendix 2 of this work). He also observes that in the limit as $\hbar \rightarrow 0$, when this constant is suitably incorporated into the system of units, that the path integral should have a dominant asymptotic contribution at the path satisfying $\delta \int_{\sigma} L dt = 0$, which is just the Lagrangian form of Newton's laws.

If we replace the Schrödinger equation by the corresponding diffusion equation, then this framework can be interpreted in terms of Wiener integrals [2], and the limit in the formula above can be evaluated using a generalization of the Lie product formula [3] due to Kac [3], which, in fact, is a special case of the celebrated equivalence theorem of Iax [4].

Because the expression for $k(x, y, t)$ represents, at least formally, a semigroup for quite general choices of L , one is tempted to generalize this formula.

There is an obvious way to generalize this methodology. To begin, notice that, for any wave function ψ , we have the Fourier inversion formula

$$\psi(x) = \iint e^{2\pi i p(x-y)} \psi(y) dy dp,$$

and that hence,

$$\begin{aligned} \mathcal{H}\psi(x) &\equiv \left(-\frac{\hbar^2 \Delta}{2m} + V \right) \psi(x) \\ &= \left(-\frac{\hbar^2 \Delta}{2m} + V \right) \iint e^{2\pi i p \frac{(x-y)}{\hbar}} \psi(y) \frac{dy dp}{h} \\ &= \iint \left(\frac{p^2}{2m} + V(x) \right) e^{2\pi i p \frac{(x-y)}{\hbar}} \psi(y) \frac{dy dp}{h} \\ &\equiv \int H(x, p) e^{2\pi i p \frac{(x-y)}{\hbar}} \psi(y) \frac{dy dp}{h}. \end{aligned}$$

\mathcal{H} is the quantum Hamiltonian and H is the classical Hamiltonian. H is called the *symbol* of \mathcal{H} . The expression $L = \frac{mv^2}{2} - V(x)$ is then simply the Legendre transform, defined as the minimum over p of $(v, p) - H(x, p) = (v, p) - \left(\frac{p^2}{2m} + V(x) \right) = \frac{1}{2m} (p - mv)^2 + \frac{mv^2}{2} - V(x)$ which is achieved when $p = mv$, and is just $\frac{mv^2}{2} - V(x)$. Notice that this Legendre transform is effected by simply completing the square. The significance of this will become apparent later.

Now to generalize Feynman's methodology, begin with a quantum Hamiltonian \mathcal{H} and compute its symbol $H(x, p)$ using the Fourier inversion formula. Then compute the Lagrangian L as the Legendre transform of H . Now insert L into the Feynman path integral formula.

However, in the simplest nontrivial cases where one knows explicitly the form of the Legendre transform, the small t asymptotics of the corresponding formal integral produces an expansion including fractional powers of t . Hence, this expression does not produce an infinitesimal generator, and thus cannot produce a sensible semigroup of operators [6]. (In Appendix I, we consider a case in point, namely, the Hamiltonian $\frac{1}{\beta} |p|^\beta$, which has Legendre transform $\frac{1}{\alpha} |v|^\alpha$ with $\frac{1}{\alpha} + \frac{1}{\beta} = 1$.)

Even so, Hörmander's theorem on the propagation of singularities [7] suggests that it is not unreasonable to look for close connections between a general differential operator, or even "pseudo differential operator", and H , the corresponding "classical mechanical system", whose Hamiltonian is the symbol of that differential operator. This connection is found by ignoring the Legendre transform and formulating the construction in phase space.

To proceed we review the notion of the symbol attached to any differential operator, $D = \Sigma a_\alpha(x) D^\alpha$. The action of D can be expressed in terms of the Fourier transform using the inversion formula:

$$\begin{aligned} D\psi(x) &= \Sigma a_\alpha(x) D^\alpha \psi = \Sigma a_\alpha(x) D^\alpha \int \hat{\psi}(p) e^{2\pi i p x} dp \\ &= \Sigma a_\alpha(x) \int \hat{\psi}(p) (D^\alpha e^{2\pi i p x}) dp = \Sigma a_\alpha(x) \int \hat{\psi}(p) (2\pi i p)^\alpha e^{2\pi i p x} dp \\ &= \int \psi(y) e^{2\pi i p(x-y)} dy [\Sigma a_\alpha(x) (2\pi i p)^\alpha] dp. \end{aligned}$$

Definition: The function $\sigma_D(x, p)$ given by $\Sigma a_\alpha(x) (2\pi i p)^\alpha$ is called the symbol of D .

Thus

$$D\psi(x) = \iint e^{2\pi i p(x-y)} \sigma_D(x, p) \psi(y) dy dp.$$

We seek to solve the equation $\psi_t = -2\pi i D\psi$, that is, to generate $\exp(-2\pi i t D)$. We define

$$W(t)\psi(x) = \iint e^{2\pi i p(x-y)} e^{-2\pi i t \sigma_D(x, p)} \psi(y) dy dp,$$

which we assume for the moment to be meaningful (as it certainly is if ψ is smooth and rapidly decaying). We shall see that this expression is meaningful for all relevant wave functions ψ .

Then for small t ,

$$\begin{aligned}
 W(t)\psi(x) &= \iint e^{2\pi i p(x-y)} [1 - 2\pi i t \sigma_D(x, p) + O(t^2)] \psi(y) dy dp \\
 &= \psi(x) - 2\pi i t D\psi(x) + O(t^2).
 \end{aligned}$$

Thus formally

$$[W(\frac{t}{n})]^n = [1 - \frac{2\pi i t D}{n} + O(\frac{1}{n^2})]^n \rightarrow \exp(-2\pi i t D).$$

Compare the ease of this verification with the corresponding verification for the (Feynman) configuration space path integral found in Appendix 2. Before we turn to clarifying the meaning of this, let us point out the connection with path integrals.

$$\begin{aligned}
 [W(t/n)]^n \psi(x) &= \\
 &\int \dots \int e^{2\pi i p_n(x_n - x_{n-1})} e^{-2\pi i \frac{t}{n} \sigma_D(x, p_n)} \dots \\
 &e^{2\pi i p_2(x_2 - x_1)} e^{-2\pi i \frac{t}{n} \sigma_D(x_2, p_2)} e^{2\pi i p_1(x_1 - y)} e^{-2\pi i \frac{t}{n} \sigma_D(x, p_1)} \psi(y) dy dp_1 dx_1 dp_2 \dots dx_{n-1} dp_n.
 \end{aligned}$$

If the symbol is scalar, then these exponential terms combine to give

$$\int \dots \int e^{2\pi i [p_1(x_1 - y) + \dots + p_n(x_n - x_{n-1}) - \frac{t}{n} \sigma_D(x_1, p_1) - \dots - \frac{t}{n} \sigma_D(x, p_n)]} \psi(y) dy dp_1 \dots dx_{n-1} dp_n.$$

This is of the form of a path integral over n -segment polygonal paths in phase space. In the limit as $n \rightarrow \infty$, we formally obtain

$$\iint_{\substack{\text{paths in phase space} \\ \pi\sigma(0)=y \\ \pi\sigma(t)=x}} e^{2\pi i \int (p dx - \sigma_D dt)} \psi(y) dy,$$

that is, a phase space path integral. Here $\pi\sigma(t)$ denotes the spatial component of $\sigma(t)$. $p dx$ is the canonical one form on phase space (which is the cotangent bundle of configuration space) and $\int p dx - \sigma dt$ is the action integral for the Hamiltonian σ .

To connect this phase space path integral with the original path integral of Feynman, consider the relevant case $\sigma = \frac{p^2}{2m} + V(x)$. Now complete the square, in terms of p , in the exponential and integrate out all of the p terms (Gaussian integrals). In this manner, we recover the original formulation of the path integral of Feynman.

The development here suggests that, infinitesimally, $W(t)$ acts like $\exp(-2\pi i t D)$. We may formalize this conclusion by means of the equivalence theorem of Lax [5], a standard tool in the analysis of convergence of finite difference schemes.

Theorem: $W^n\left(\frac{t}{n}\right) \rightarrow \exp(-2\pi i t D)$ if and only if

$$i) \quad \|W^n(t/n)\| \leq C(T), \quad \text{for } 0 \leq t \leq T,$$

and

$$ii) \quad \left\| \frac{W(s) - I + 2\pi i s D}{s} e^{-2\pi i t D} u \right\| \rightarrow 0$$

as $s \rightarrow 0$, uniformly for $0 \leq t \leq T$ for some constant $C(T)$ and for all u in some dense set of vectors.

Property (i) is referred to as 'stability', while (ii) is referred to as 'consistency' (of $W(t)$). A study of the behavior of $W(t)$ for small t is required to be able to invoke the theorem. Examples of such a study are found in [8].

3. The phase space path integral for the Dirac equation

Now we consider the Dirac equation in this framework. Let V be a quadratic vector space with metric Q , and let $\mathcal{C}(V)$ be the Clifford algebra [9] of V . Let W be a Clifford module. For any linear map $\theta: V \rightarrow W$, there is a bilinear map $(v, u) \mapsto v\theta(u)$, where v acts as an element of $\mathcal{C}(V)$ on the element $\theta(u)$ of W . Then we can consider the element $q(\theta)$ of W which is the image of the metric (viewed as an element of $V \otimes V$) under the induced map.

If ψ is a function from V to W , then at any point of V , $d\psi$ is a linear map from V to W . The free particle Dirac equation asks that $q(d\psi) = m\psi$.

If A is a 1-form defined on V , then $A \otimes w$ is a 1-form on V valued in W . The interacting Dirac equation is then $q(id\psi + 2\pi A\psi) = m\psi$. Let

$$\sigma_0 = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

Let

$$\Sigma_0 = \begin{pmatrix} 0 & \sigma_0 \\ -\sigma_0 & 0 \end{pmatrix}, \Sigma_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}.$$

Then

$$\begin{aligned} \Sigma_i \Sigma_j + \Sigma_j \Sigma_i &= \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \\ &= \begin{pmatrix} \sigma_i \sigma_j + \sigma_j \sigma_i & 0 \\ 0 & \sigma_i \sigma_j + \sigma_j \sigma_i \end{pmatrix} = -2\delta_{ij} \\ \Sigma_0 \Sigma_i + \Sigma_i \Sigma_0 &= \begin{pmatrix} 0 & \sigma_0 \\ -\sigma_0 & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_0 \\ -\sigma_0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \sigma_0 \sigma_i - \sigma_i \sigma_0 & 0 \\ 0 & -\sigma_0 \sigma_i + \sigma_i \sigma_0 \end{pmatrix} = 0. \\ 2\Sigma_0^2 &= 2 \begin{pmatrix} -\sigma_0^2 & 0 \\ 0 & -\sigma_0^2 \end{pmatrix} = 2. \end{aligned}$$

Therefore $\Sigma_0, \Sigma_1, \Sigma_2, \Sigma_3$ are the basis of a Clifford algebra corresponding to an orthonormal frame where the metric takes the form

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

Moreover let (φ, A_1, A_2, A_3) be the components of A in this frame. Then the Dirac equation is

$$-\Sigma_0 \left(i \frac{\partial \psi}{\partial t} + 2\pi \phi \psi \right) + \Sigma_1 \left(i \frac{\partial \psi}{\partial x} + 2\pi A_1 \psi \right) + \Sigma_2 \left(i \frac{\partial \psi}{\partial y} + 2\pi A_2 \psi \right) + \Sigma_3 \left(i \frac{\partial \psi}{\partial z} + 2\pi A_3 \psi \right) = m\psi.$$

Multiplying this equation by Σ_0 , the Dirac equation becomes

$$\begin{aligned} i \frac{\partial \psi}{\partial t} &= -m\Sigma_0\psi - 2\pi\phi\psi + \Sigma_0\Sigma_1 \left(i \frac{\partial \psi}{\partial x} + 2\pi A_1 \psi \right) + \Sigma_0\Sigma_2 \left(i \frac{\partial \psi}{\partial y} + 2\pi A_2 \psi \right) \\ &\quad + \Sigma_0\Sigma_3 \left(i \frac{\partial \psi}{\partial z} + 2\pi A_3 \psi \right) \\ &= 2\pi \left(-\frac{m}{2\pi} \Sigma_0\psi - \phi\psi + \Sigma_0\Sigma_1 A_1\psi + \Sigma_0\Sigma_2 A_2\psi + \Sigma_0\Sigma_3 A_3\psi \right. \\ &\quad \left. - \Sigma_0\Sigma_1 \left(\frac{1}{2\pi i} \frac{\partial \psi}{\partial x} \right) - \Sigma_0\Sigma_2 \left(\frac{1}{2\pi i} \frac{\partial \psi}{\partial y} \right) - \Sigma_0\Sigma_3 \left(\frac{1}{2\pi i} \frac{\partial \psi}{\partial z} \right) \right). \end{aligned}$$

Then the symbol corresponding to this operator is

$$\begin{aligned} \sigma_D &= \left(-\frac{m}{2\pi} \Sigma_0 - \phi + \Sigma_0\Sigma_1 A_1 + \Sigma_0\Sigma_2 A_2 + \Sigma_0\Sigma_3 A_3 \right) \\ &\quad - \Sigma_0\Sigma_1 p_1 - \Sigma_0\Sigma_2 p_2 - \Sigma_0\Sigma_3 p_3. \end{aligned}$$

Since $\Sigma_0, \Sigma_0\Sigma_l$ are all Hermitian, σ_D is a Hermitian matrix valued function. Hence we can construct a phase space path integral as the large n limit of $W\left(\frac{t}{n}\right)^n$, where

$$\begin{aligned} W(t)\psi(x) &= \iint e^{2\pi i p(x-y)} e^{-2\pi i t \left(-\frac{m}{2\pi} \Sigma_0 - \phi(x) + \Sigma_0\Sigma_1 A_1(x) + \Sigma_0\Sigma_2 A_2(x) + \Sigma_0\Sigma_3 A_3(x) \right)} \\ &\quad e^{2\pi i t (\Sigma_0\Sigma_1 p_1 + \Sigma_0\Sigma_2 p_2 + \Sigma_0\Sigma_3 p_3)} \psi(y) dy dp \end{aligned}$$

For any matrices A and B , $e^{tA} e^{tB} = e^{t(A+B)}$ in the small t limit. Then since for small t , $W(t)$ is asymptotically the same as

$$\iint e^{2\pi i p(x-y)} e^{-2\pi i t \left(\frac{m}{2\pi} \Sigma_0 - \phi(x) + \Sigma_0\Sigma_1 A_1(x) + \Sigma_0\Sigma_2 A_2(x) + \Sigma_0\Sigma_3 A_3(x) - \Sigma_0\Sigma_1 p_1 - \Sigma_0\Sigma_2 p_2 - \Sigma_0\Sigma_3 p_3 \right)} \psi(y) dy dp.$$

Notice that the argument of $e^{-2\pi i t}$ here is the symbol of the spatial Dirac operator, so that the consistency is clear. Stability follows from the fact that

$$\begin{aligned} \|W(t)\psi(x)\| &= \left\| \int \int e^{2\pi i p(x-y)} e^{2\pi i t(\Sigma_0 \Sigma_1 p_1 + \Sigma_0 \Sigma_2 p_2 + \Sigma_0 \Sigma_3 p_3)} \psi(y) dy dp \right\| \\ &= \left\| \int \int e^{-2\pi i p y} \psi(y) dy \right\| = \|\psi(y)\|. \end{aligned}$$

To apply the Lax equivalence theorem requires now only the usual (hard) estimates which establish this Dirac operator to be Hermitian.

Conclusions

There is a formal path integral propagator defined on phase space for any Schrödinger equation whose Hamiltonian is a square matrix of pseudo-differential operators. In contrast to the impression given by the Feynman integral which is closely tailored to the standard Schrödinger operator, $-\frac{\Delta}{2m} + V$, the phase space path integral concept considered here favors no particular class of Hamiltonian.

There is not such a path integral propagator, in general, defined on configuration space. The Lagrangian - Hamiltonian connection existing in classical dynamics via the Legendre transform has no quantum analogue; quantum mechanics, as defined by path integrals, in general requires the Hamiltonian phase space formulation. In the very special case where the Hamiltonian is quadratic, the Legendre transform is the much more basic duality that arises from completing the square, and apparently nothing more.

One possible objection is that the isolation of time in the Dirac equation is unrelativistic. One should note that any direction, spatial or temporal, could be isolated as a path integral. On the other hand, one can solve the equation

$$\begin{aligned} i \frac{\partial \psi}{\partial s} &= -\Sigma_0 \left(i \frac{\partial}{\partial t} + \varphi \right) \psi + \Sigma_1 \left(i \frac{\partial}{\partial x} + A_1 \right) \psi \\ &\quad + \Sigma_2 \left(i \frac{\partial}{\partial y} + A_2 \right) \psi + \Sigma_3 \left(i \frac{\partial}{\partial z} + A_3 \right) \psi \end{aligned}$$

and then the stationary states are the solutions of the Dirac equation, while the mass is the frequency. This is reasonable because the mass cannot be measured with perfect accuracy in finite time.

References

1. Feynman, R.P., Rev. Mod. Phys. 20 367 (1948).
2. Schulman, L.S., Techniques and Applications of Path Integration, Wiley and Sons, 1981.
3. Varadarajan, V.S., Lie Groups, Lie Algebras, and their representations, Springer-Verlag, 1984.
4. Durrett, R., Brownian Motion and Martingales in Analysis, Wadsworth, 1984.
5. Richtmeyer, R.D., Difference methods for Initial-value Problems, Interscience Publishers, 1967.
6. Hille, E., Functional Analysis and Semigroups, AMS 1948.
7. Hörmander, L., The Analysis of Linear Partial Differential Operators, Springer-Verlag, 1984.
8. Miranker, W.L. and Winkler, A., "Path Integral Numerical Methods for Evolution Equations", IBM RC XXXXX, 1988.
9. Chevalley, C., Theory of Lie Groups, Princeton University Press, 1946.

Appendix 1. The configuration space path integral

In this appendix, we calculate the simplest case other than the classical Schrödinger equation of a configuration space path integral and show that it confronts fundamental difficulties as a solution operator.

Let σ_D be the symbol of a differential operator D . We suppose that the Legendre transform L defined as $L(x, v) = \max_p (p, v) - \sigma_D(x, p)$ exists. For this it is sufficient that $\sigma(x, p)$ be $\Omega(p)$ as $p \rightarrow \infty$, since σ is continuous.

We construct a path integral as a large n limit of an expression

$$\int \dots \int e^{i \left[\frac{t}{n} L(x_0, \frac{x_1 - x_0}{t/n}) + \dots + \frac{t}{n} L(x_{n-1}, \frac{x_n - x_{n-1}}{t/n}) \right]} \phi(x_n) dx_1 \dots dx_n,$$

and note that if the expression is meaningful, it defines a semigroup. This is so because any path on the interval from 0 to $t_1 + t_2$ can be considered as a combination of paths from 0 to t_1 , and from 0 to t_2 . Moreover, since L has no explicit t dependence, $\int_0^{t_1+t_2} L(\sigma(t), \dot{\sigma}(t)) dt = \int_0^{t_1} L(\sigma(t), \dot{\sigma}(t)) dt + \int_{t_1}^{t_1+t_2} L(\sigma(t), \dot{\sigma}(t)) dt = \int_0^{t_1} L(\sigma(t), \dot{\sigma}(t)) dt + \int_0^{t_2} L(\sigma(t), \dot{\sigma}(t)) dt$, while the composition of integral kernels is such that all of the pieces match up.

Hence we are motivated to look for an infinitesimal generator, for having found it, the new path integral would furnish a solution operator for a differential equation involving this generator.

Recall that if $A(t)$ is a semigroup having for small t an asymptotic expansion $A(t) \sim I + tA + o(t)$ then A is the infinitesimal generator.

Let $\frac{1}{\alpha} + \frac{1}{\beta} = 1$. Then corresponding to $H = \frac{1}{\beta} |p|^\beta$, we have $L = \frac{1}{\alpha} |v|^\alpha$. To see this, let $L(v) \equiv \max_p \{(v, p) - H(p)\} = \max_p \{(v, p) - \frac{1}{\beta} |p|^\beta\}$. As long as $\beta > 1$, the expression whose maximum is sought decays with increasing $|p|$. Hence, the maximum is actually assumed. Moreover, the expression is smooth for $p \neq 0$, so the maximum is assumed at a critical point.

We calculate the critical points:

$$\begin{aligned}
 0 &= d \left[(v, p) - \frac{1}{\beta} |p|^\beta \right] = d \left(v_j p^j - \frac{1}{\beta} (\sqrt{g_{ij} p^i p^j})^\beta \right) \\
 &= v_j dp^j - (\sqrt{g_{ij} p^i p^j})^{\beta-1} \left(\frac{g_{ij} p^i dp^j}{\sqrt{g_{ij} p^i p^j}} \right).
 \end{aligned}$$

Then at the critical points,

$$v_j = \left(\sqrt{g_{ij} p^i p^j} \right)^{\beta-2} g_{ij} p^i.$$

Equivalently p is proportional to the dual of v , and moreover $|p| = |v|^{1/\beta-1}$. Then for $L(v)$ we obtain

$$\begin{aligned}
 (v, p) - \frac{1}{\beta} |p|^\beta &= |v|^{1/\beta-1} \cdot |v| - \frac{1}{\beta} |v|^{1/\beta-1} |v|^\beta \\
 &= \left(1 - \frac{1}{\beta} \right) |v|^{1/\beta-1} |v| = \frac{1}{\alpha} |v|^\alpha.
 \end{aligned}$$

Thus we consider

$$\int_{\substack{\text{paths} \\ \sigma(0)=x \\ \sigma(x)=y}} e^{i \int_\sigma \frac{1}{\alpha} |v|^\alpha dt} \psi(x)$$

which we interpret as the large n limit of

$$\begin{aligned}
 &\int \dots \int e^{i \left[\frac{1}{\alpha} \left| \frac{x_0 - x_1}{t/n} \right|^\alpha \frac{t}{n} + \dots + \frac{1}{\alpha} \left| \frac{x_{n-1} - x_n}{t/n} \right|^\alpha \frac{t}{n} \right]} \psi(x_0) dx_0 \dots dx_{n-1} \\
 &= \int \dots \int e^{i(t/n)^{1-\alpha} \left[\frac{|x_0 - x_1|^\alpha}{\alpha} + \dots + \frac{|x_{n-1} - x_n|^\alpha}{\alpha} \right]} \psi(x_0) dx_0 \dots dx_{n-1}.
 \end{aligned}$$

In the one-dimensional case we can evaluate this integral explicitly, as we now show. Expanding $\psi(x_0) = \psi(x_1) + \psi'(x_1)(x_0 - x_1) + \frac{1}{2} \psi''(x_1)(x_0 - x_1)^2 + \dots$, $\lambda = \left(\frac{t}{n}\right)^{1-\alpha}$, the last expression becomes

$$\begin{aligned}
 & \int \dots \int e^{i\lambda \left[\frac{|x_0 - x_1|^\alpha}{\alpha} + \dots + \frac{|x_{n-1} - x_n|^\alpha}{\alpha} \right]} [\psi(x_1) + \psi'(x_1)(x_0 - x_1) + \dots] dx_0 \dots x_{n-1} \\
 &= \int \dots \int e^{i\lambda \left[\frac{|x_1 - x_2|^\alpha}{\alpha} + \dots + \frac{|x_{n-1} - x_n|^\alpha}{\alpha} \right]} dx_1 \dots dx_{n-1} \sum \frac{1}{k!} \psi^k(x_1) \int e^{i\lambda \frac{|x_0 - x_1|^\alpha}{\alpha}} (x_0 - x_1)^k dx_0 \\
 &= \int \dots \int e^{i\lambda \left[\frac{|x_1 - x_2|^\alpha}{\alpha} + \dots + \frac{|x_{n-1} - x_n|^\alpha}{\alpha} \right]} dx_1 \dots dx_{n-1} \sum \frac{1}{k!} \psi^k(x_1) \int e^{i\lambda |x_0|^\alpha} x_0^k dx_0 \\
 &= \int \dots \int e^{i\lambda \left[\frac{|x_1 - x_2|^\alpha}{\alpha} + \dots + \frac{|x_{n-1} - x_n|^\alpha}{\alpha} \right]} dx_1 \dots dx_{n-1} \sum \frac{1}{(2k)!} \psi^{2k}(x_1) \left[2 \frac{1}{\alpha} (-i\lambda)^{-\frac{2k+1}{\alpha}} \Gamma\left(\frac{2k+1}{\alpha}\right) \right] \\
 &= \dots = \sum \frac{1}{(2k_1)!} \dots \frac{1}{(2k_n)!} \psi^{(2k_1 + \dots + 2k_n)}(x_n) \prod \left[2 \frac{1}{\alpha} (-i\lambda)^{-\frac{(2k_j+1)}{\alpha}} \Gamma\left(\frac{2k_j+1}{\alpha}\right) \right] \\
 &= \sum \frac{1}{(2k_1)!} \dots \frac{1}{(2k_n)!} 2^n \frac{1}{\alpha^n} \prod \Gamma\left(\frac{2k_j+1}{\alpha}\right) \left(\frac{-i}{n^{1-\alpha}}\right)^{-\frac{(2k_j+1)}{\alpha}} \psi^{(2k_1 + \dots + 2k_n)}(x_n) t^{-\frac{(1-\alpha)}{\alpha} \sum (2k_j+1)} \\
 &= \frac{2^n}{\alpha^n} \left(\frac{-i}{n^{1-\alpha}}\right)^{-\frac{n}{\alpha}} t^{\frac{n}{\beta}} \sum_{\ell} \sum_{2k_1 + \dots + 2k_n = 2\ell} \prod_{1 \leq j \leq n} \Gamma\left(\frac{2k_j+1}{\alpha}\right) \left(\frac{-i}{n^{1-\alpha}}\right)^{-\frac{2k_j}{\alpha}} \psi^{2\ell}(x_n) t^{\frac{2\ell}{\beta}}.
 \end{aligned}$$

The terms are all of the form $t^{\sum(2k_j+1)/\beta}$. Now the $t^{n/\beta}$ is, of course, part of the normalization, so we are left with terms $t^{2\sum k_j/\beta}$. There is a linear term precisely when β is an even integer, and then we need terms $0 < 2\sum k_j < \beta$ to vanish. Thus we let $\beta = 2m$, and set

$$\left[\sum_{2k_1 + \dots + 2k_n = 2\ell} \prod_{1 \leq j \leq n} \Gamma\left(\frac{2k_j+1}{\alpha}\right) \left(\frac{-i}{n^{1-\alpha}}\right)^{-\frac{2k_j}{\alpha}} \right] \psi^{2\ell}(x_n) = 0$$

for $1 \leq \ell < m$. Combining terms, this becomes

$$\left[\sum_{2k_1 + \dots + 2k_n = 2\ell} \prod \Gamma\left(\frac{2k_j + 1}{\alpha}\right) \right] \left(\frac{-i}{n^{1-\alpha}} \right)^{-\frac{2\ell}{\alpha}} \psi^{2\ell}(x_n) = 0.$$

Unless, $\psi^{2\ell}(x) = 0$ (i.e. ψ is a linear function), we are forced to conclude that

$$\sum_{k_1 + \dots + k_n = \ell} \left(\prod \Gamma\left(\frac{2k_j + 1}{\alpha}\right) \right) = 0.$$

However, the left member here is a sum of positive terms. It is clear then that the configuration space version of the path integral can succeed only in the most exceptional circumstances.

Appendix 2. The stationary phase approach

This appendix, for purposes of comparison with our easily obtained result for the phase space path integral, produces the verification that the configuration space path integral for the classical Schrödinger equation has the correct small time behavior. We can apply the method of stationary phase to finding the small time asymptotics, and thus the infinitesimal generator, of the path integral. Let

$$\int \dots \int e^{\frac{i}{\hbar} \left[\frac{m}{2} \frac{(x_0 - x_1)^2}{t/n} + \frac{(x_1 - x_2)^2}{t/n} + \dots + \frac{(x_{n-1} - x_n)^2}{t/n} - V(x_0) \frac{t}{n} - \dots - V(x_{n-1}) \frac{t}{n} \right]} \psi(x_n) dx_1 \dots dx_n$$

$$= \int e^{i\phi/\hbar} e^{iV/\omega},$$

where

$$\phi(x_0, \dots, x_n) \equiv \frac{mn}{2\hbar} [(x_0 - x_1)^2 + \dots + (x_{n-1} - x_n)^2],$$

$$V(x_0, \dots, x_n) \equiv \frac{1}{n\hbar} [V(x_0) + \dots + V(x_{n-1})].$$

and

$$\omega \equiv \psi(x_n) dx_1 \dots dx_n.$$

Then

$$\begin{aligned} \int e^{i\phi/\hbar} e^{iV/\omega} &= \int e^{i\phi/\hbar} \left[\sum_{m \geq 0} \frac{(-itV)^m}{m!} \right] \omega \\ &= \sum_{m \geq 0} \frac{(-it)^m}{m!} \int e^{i\phi/\hbar} V^m \omega \\ &\sim \sum_p \left[\sum_{m \geq 0} \frac{(-it)^m}{m!} \sum_{k \geq 0} \frac{(it)^k}{k!} \square^k (V^m \omega) \Big|_p \right] t^{\frac{n}{2}} (2\pi)^{\frac{n}{2}} e^{\frac{i\phi(p)}{t}} e^{\frac{\pi i}{4} (2r_p - n)}. \end{aligned}$$

Therefore $r_p = n$, and we seek a coordinate change so that

$$(x_1 \dots x_n) \mapsto (x_1 - x_0, \dots, x_n - x_0) \xrightarrow{A} (\xi_1 \dots \xi_n),$$

which takes the metric tensor Q into the identity. Since

$$\begin{aligned} (x_1 - x_0, \dots, x_n - x_0) Q \begin{pmatrix} x_1 - x_0 \\ \vdots \\ x_n - x_0 \end{pmatrix} &= (x_1 - x_0, \dots, x_n - x_0) A^T A^{-T} Q A^{-1} A \begin{pmatrix} x_1 - x_0 \\ \vdots \\ x_n - x_0 \end{pmatrix} \\ &= (\xi_1 \dots \xi_n) A^{-T} Q A^{-1} \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix}, \end{aligned}$$

we see that A is determined by the condition $A^{-T} Q A^{-1} = I$, or $Q = A^T A$. Now

$$\begin{aligned} \square^k (V^m \omega)_p &= \left[\frac{1}{2} \left(\frac{\partial^2}{\partial \xi_1^2} + \dots + \frac{\partial^2}{\partial \xi_n^2} \right) \right]^k \left[V^m \left(A^{-1} \xi + \begin{pmatrix} x_0 \\ \vdots \\ x_0 \end{pmatrix} \right) \frac{\psi \left(A^{-1} \xi + \begin{pmatrix} x_0 \\ \vdots \\ x_0 \end{pmatrix} \right)}{\det A} \right]_{\xi=0} \\ &= \frac{1}{\det A} \left[\frac{1}{2} \left(\frac{\partial^2}{\partial \xi_1^2} + \dots + \frac{\partial^2}{\partial \xi_n^2} \right) \right]^k [V^m (A^{-1} \xi) \psi(A^{-1} \xi)]_{\xi=A \begin{pmatrix} x_0 \\ \vdots \\ x_0 \end{pmatrix}} \end{aligned}$$

by translation invariance of the Laplace operator.

Note that $(\det A)^2 = \det Q = \left(\frac{mn}{h} \right)^n$. Then the expansion becomes

$$\left[\sum_{m \geq 0} \frac{(-it)^m}{m!} \sum_{k \geq 0} \frac{(it)^k}{k!} \left[\frac{1}{2} \left(\frac{\partial^2}{\partial \xi_1^2} + \dots + \frac{\partial^2}{\partial \xi_n^2} \right) \right]^k [V^m (A^{-1} \xi) \psi(A^{-1} \xi)]_{\xi=A \begin{pmatrix} x_0 \\ \vdots \\ x_0 \end{pmatrix}} \right]$$

$$= \frac{n/2}{(2\pi)^{n/2}} e^{\frac{\pi i n}{4}} \left(\frac{mn}{h} \right)^{-\frac{n}{2}}.$$

Here

$$A^T A = \frac{mn}{\hbar} \begin{bmatrix} 2 & -1 & & & & & & & \\ & -1 & 2 & & & & & & \\ & & & \ddots & & & & & \\ & & & & \ddots & & & & \\ & & & & & 2 & -1 & & \\ & & & & & -1 & 1 & & \end{bmatrix}, \quad V(x_0 \dots x_n) = \frac{1}{n\hbar} [V(x_0) + \dots + V(x_{n-1})].$$

We can combine terms in the overall constant to get $\left(\frac{2n\hbar t}{mn}\right)^{\frac{n}{2}}$, the quantity to divide the integral by to normalize, so that the constant term in the expansion is $\psi(x_0)$.

The linear term is

$$\begin{aligned} & -it \left[\frac{1}{n\hbar} \right] [V(x_0) + \dots + V(x_0)] \psi(x_0) + \frac{it}{2} \left[\frac{\partial^2}{\partial \xi_1^2} + \dots + \frac{\partial^2}{\partial \xi_n^2} \right] \psi(A^{-1} \xi)_{\xi=A \begin{pmatrix} x_0 \\ \vdots \\ x_0 \end{pmatrix}} \\ & = -\frac{it}{\hbar} \left[V(x_0) \psi(x_0) - \frac{\hbar}{2} \left[\frac{\partial^2}{\partial \xi_1^2} + \dots + \frac{\partial^2}{\partial \xi_n^2} \right] \psi(A^{-1} \xi)_{\xi=A \begin{pmatrix} x_0 \\ \vdots \\ x_0 \end{pmatrix}} \right]. \end{aligned}$$

We introduce matrices U and D , so that $U^T D U = Q$, as follows

$$\begin{bmatrix} 1 & 0 \\ -1/2 & 1 \\ & & \ddots & \\ & & & -\frac{n-2}{n-1} & 1 \end{bmatrix} \begin{bmatrix} 2/1 & & & & \\ & 3/2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & \frac{n}{n-1} \end{bmatrix} \begin{bmatrix} 1 & -1/2 & & & \\ & 1 & -2/3 & & \\ & & \ddots & \ddots & \\ & & & \ddots & -\frac{n-2}{n-1} \\ & & & & 1 \end{bmatrix} = \begin{bmatrix} 2 & & & & \\ -1 & 3/2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ -1 & & & & \frac{n}{n-1} \end{bmatrix}$$

$U^T \qquad \qquad \qquad D \qquad \qquad \qquad U$

$$= \begin{bmatrix} 2 & & & & \\ -1 & 3/2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ -1 & & & & \frac{n}{n-1} \end{bmatrix} \begin{bmatrix} 1 & -1/2 & & & \\ & 1 & -2/3 & & \\ & & \ddots & \ddots & \\ & & & \ddots & -\frac{n}{n-1} \\ & & & & 1 \end{bmatrix} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & & & \\ & & \ddots & \ddots & \\ & & & \ddots & -\frac{n}{n-1} \\ & & & & 2 \end{bmatrix}$$

For future reference we record U^{-1} :

$$\begin{matrix}
 \begin{bmatrix} 1 & -1/2 & & & & \\ & 1 & -2/3 & & & \\ & & & \ddots & & \\ & & & & -\frac{n-2}{n-1} & \\ & & & & & 1 \end{bmatrix} & \begin{bmatrix} 1 & 1/2 & 1/3 & & & \\ 0 & 1 & 2/3 & & & \\ & & & \ddots & & \\ & & & & \frac{2}{n-1} & \\ & & & & & \frac{n-2}{n-1} \\ & & & & & & 1 \end{bmatrix} & = & \begin{bmatrix} 1 & 0 & & & & \\ 0 & 1 & & & & \\ & & \ddots & & & \\ & & & & & \\ & & & & & \\ & & & & & & 1 \end{bmatrix} \\
 U & U^{-1} & & & & I
 \end{matrix}$$

Choosing $A = \sqrt{D} U$ is consistent with $A^T A = Q$. Then, in particular, $A^{-1} = U^{-1} \sqrt{D^{-1}}$.

Now the matrix bordering relation

$$\begin{bmatrix} U & UQ^{-1}q \\ 0 & 1 \end{bmatrix}^T \begin{bmatrix} D & 0 \\ 0 & \delta - q^T Q^{-1}q \end{bmatrix} \begin{bmatrix} U & UQ^{-1}q \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} Q & q \\ q^T & \delta \end{bmatrix}$$

is an identity since $U^T D U = Q$, while

$$\begin{bmatrix} U & UQ^{-1}q \\ 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} U^{-1} & -Q^{-1}q \\ 0 & 1 \end{bmatrix}$$

is an identity in U , Q^{-1} and q . Now

$$\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & & & & \\ & & \ddots & & & \\ & & & -1 & & \\ & & & & \ddots & \\ & & & & & -1 & 2 \\ & & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} -\frac{1}{n} \\ \vdots \\ -\frac{n-1}{n} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ -1 \end{bmatrix}$$

so

$$Q^{-1}q = \begin{bmatrix} -\frac{1}{n} \\ \cdot \\ \cdot \\ \cdot \\ -\frac{n-1}{n} \end{bmatrix},$$

and

$$q^T Q^{-1}q = \frac{n-1}{n}.$$

Hence

$$\delta - q^T Q^{-1}q = 1 - \frac{n-1}{n} = \frac{1}{n}.$$

$$A^{-1} = U^{-1}\sqrt{D^{-1}}$$

$$= \begin{bmatrix} 1 & 1/2 & 1/3 & \frac{1}{n-1} & \frac{1}{n} \\ 0 & 1 & & \cdot & \cdot \\ & & & \cdot & \cdot \\ & & & \frac{n-2}{n-1} & \frac{n-1}{n} \\ & & & 1 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{\sqrt{2}}{\sqrt{3}} & & & \\ & & & & \\ & & & & \\ & & & & \\ \frac{\sqrt{n-1}}{\sqrt{n}} & & & & \sqrt{n} \end{bmatrix}$$

together with the scale factor $\left(\frac{mn}{h}\right)^{-1/2}$.

$$\psi(A^{-1}\xi) = \psi(\text{the } n\text{th coordinate of } A^{-1}\xi)$$

$$= \psi\left((0, \dots, 0, 1) \begin{bmatrix} 1 & 1/2 & 1/3 & \frac{1}{n} \\ 0 & 1 & & \cdot \\ & & & \cdot \\ & & & \frac{n-1}{n} \\ & & & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{\sqrt{2}}{\sqrt{3}} & & & \\ & & & & \\ & & & & \\ & & & & \\ \frac{\sqrt{n-1}}{\sqrt{n}} & & & & \sqrt{n} \end{bmatrix} \left(\frac{mn}{h}\right)^{1/2} \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix} \right)$$

$$\begin{aligned}
 &= \psi \left(\sqrt{n} \left(\frac{\hbar}{m} \right)^{1/2} \sqrt{n}^{-1} \xi_n \right) \\
 &= \psi \left(\left(\frac{\hbar}{m} \right)^{1/2} \xi_n \right).
 \end{aligned}$$

Thus

$$\left(\frac{\partial^2}{\partial \xi_1^2} + \dots + \frac{\partial^2}{\partial \xi_n^2} \right) \psi \left(\left(\frac{\hbar}{m} \right)^{1/2} \xi_n \right)_{\xi=A \begin{pmatrix} x_0 \\ \vdots \\ x_0 \end{pmatrix}} = \frac{\hbar}{m} \Delta \psi(x_0).$$

Therefore, the linear term is $-\frac{i\hbar}{\hbar} \left[V(x_0)\psi(x_0) - \frac{\hbar^2}{2m} \Delta \psi(x_0) \right]$, and we have recovered the Schrödinger equation.