

Determinants of Quantum Operators

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Introduction. Justin Sumner has elected to attempt to develop a thesis from material that he encountered in a recent issue of AJP.¹ The paper concerns the evaluation of the “functional determinants” that appear as “preexponential” factors when Feynman’s “sum-over-paths” formalism is used to construct quantum mechanical propagators, and that occur also in some other closely related contexts. The authors may be technically correct when they assert that “the prerequisites for this analysis involve only introductory courses in ordinary differential equations and complex variables,” but neglect to mention that the work is certain to seem entirely unmotivated to readers whose (quantum mechanical) experience happens not to have exposed them to certain fairly arcane issues/problems. Here my primary objective will be to motivate the subject, to place it in an intelligible physical/mathematical context. Initially I will be content to wander about on the periphery of the subject, reminding myself of issues/methods that seem to be of some remote relevance.

Free particle propagator.² The equation

$$\frac{\partial}{\partial t}\psi = a\mathbf{D}^2\psi \quad : \quad \mathbf{D} \equiv \frac{\partial}{\partial x} \quad (1)$$

becomes (*i*) the **free particle Schrödinger equation** if we set

$$a = i \frac{\hbar}{2m}$$

¹ Klaus Kirsten & Paul Loya, “Calculation of determinants using contour integrals,” AJP **76**, 60–64 (2008).

² Here I borrow from the opening paragraphs of my RESEARCH NOTES: *Theory and physical applications of the Appell transform* (1976). That work was inspired by material I encountered in D. V. Widder’s *The Heat Equation* (1975).

and interpret $\psi(x, t)$ to be a probability amplitude; (ii) the **diffusion equation** if we set

$$a = \text{diffusion coefficient}$$

and consider ψ to provide a description of the relevant density; (iii) the Fourier **heat equation** if we set

$$a = \frac{\text{thermal conductivity}}{(\text{specific heat})(\text{density})}$$

Formally, we expect—whatever the interpretation—to have

$$\psi_t(x) = e^{at\mathbf{D}^2} \psi_0(x) \quad (2)$$

Familiarly, one has the Gaussian integral formula

$$\int_{-\infty}^{+\infty} e^{-(\alpha x^2 + \beta x)} dx = \sqrt{\pi/\alpha} \cdot e^{\beta^2/4\alpha} \quad : \quad \Re(\alpha) > 0 \quad (3.1)$$

of which (send $\alpha \mapsto 1/4a$)

$$e^{a\beta^2} = \frac{1}{\sqrt{4\pi a}} \int_{-\infty}^{+\infty} e^{-\frac{1}{4}a^{-1}x^2 - \beta x} dx \quad (3.2)$$

is a notational variant—of present interest because the expression on the right can be considered to provide an integral representation of the expression on the left. We proceed on the tentative assumption that it makes formal sense to write

$$e^{at\mathbf{D}^2} = \frac{1}{\sqrt{4\pi at}} \int_{-\infty}^{+\infty} e^{-\frac{1}{4at}\xi^2 - \xi\mathbf{D}} d\xi \quad : \quad \Re\left(\frac{1}{4at}\right) > 0 \quad (4)$$

—the point here being that the operator \mathbf{D} , which appears squared on the left, appears unsquared on the right. By Taylor's theorem we have (within some unstated radius of convergence)

$$e^{-\xi\mathbf{D}} f(x) = f(x - \xi)$$

so we expect to have

$$\begin{aligned} \psi_t(x) &= \frac{1}{\sqrt{4\pi at}} \int_{-\infty}^{+\infty} e^{-\frac{1}{4at}\xi^2} \psi_0(x - \xi) d\xi \\ &= \int_{-\infty}^{+\infty} g_t(\xi) \psi_0(x - \xi) d\xi \end{aligned}$$

where

$$g_t(x) \equiv \frac{1}{\sqrt{4\pi at}} e^{-\frac{1}{4at}x^2} \quad (5)$$

A final change of variables $\xi \mapsto y = x - \xi$ gives

$$\psi_t(x) = \int_{-\infty}^{+\infty} g_t(x-y) \psi_0(y) dy \quad (6)$$

The function $\psi_t(x)$ thus produced satisfies (1) because each member of the y -parameterized family of functions $g_t(x-y)$ does:

$$\frac{\partial}{\partial t} g_t(x-y) = a \mathbf{D}^2 g_t(x-y) \quad (7.1)$$

And

$$\lim_{t \downarrow 0} \psi_t(x) = g_0(x) \quad \text{because} \quad \lim_{t \downarrow 0} g_t(x-y) = \delta(x-y) = \delta(y-x) \quad (7.2)$$

The functions $g_t(x-y)$ are the so-called “fundamental solutions” of the linear partial differential equation (1). We might write

$$g_{t-t_0}(x-x_0) = G(x, t; x_0, t_0)$$

to cast (6) into the form

$$\psi_t(x) = \int_{-\infty}^{+\infty} G(x, t; x_0, t_0) \psi_0(x_0) dx_0 \quad (8)$$

to emphasize that the fundamental solution is precisely the Green’s function of the differential equation in question.

The prefactor

$$\frac{1}{\sqrt{4\pi at}}$$

provides a trivial instance of the kind of object that the theory of functional determinants has been designed to evaluate.

Higher-dimensional generalization. Let \mathbf{D}^2 be interpreted now to mean

$$\mathbf{D}^2 = \nabla \cdot \mathbb{A} \nabla \quad \text{where} \quad \nabla \equiv \begin{pmatrix} \partial_1 \\ \partial_2 \\ \vdots \\ \partial_n \end{pmatrix} \quad \text{with} \quad \partial_i \equiv \frac{\partial}{\partial x_i}$$

and where \mathbb{A} is a real symmetric $n \times n$ matrix (additional properties yet to be specified). In the case $\mathbb{A} = \mathbb{I}$ the second-order differential operator \mathbf{D}^2 reduces to the familiar Laplacian: $\nabla^2 \equiv \nabla \cdot \nabla$. Now, in straightforward generalization of (3)—*i.e.*, of

$$\int_{-\infty}^{+\infty} e^{-\alpha x^2 \pm \beta x} dx = \sqrt{\frac{\pi}{\alpha}} \exp \left\{ \frac{1}{4} \beta \alpha^{-1} \beta \right\}$$

—one has³

$$\iint \dots \int_{-\infty}^{+\infty} e^{-x^i A_{ij} x^j \pm b_i x^i} d^n x = \sqrt{\frac{\pi^n}{\det \|A_{ij}\|}} e^{\frac{1}{4} b_i A^{ij} b_j}$$

where $\|A^{ij}\| \equiv \|A_{ij}\|^{-1}$ and summation on repeated indices is understood, and to assure convergence we have had to assume that all the (necessarily real) eigenvalues of \mathbb{A} are positive. More neatly,

$$\iint \dots \int_{-\infty}^{+\infty} e^{-\mathbf{x} \cdot \mathbb{A} \mathbf{x} \pm \mathbf{b} \cdot \mathbf{x}} d^n x = \sqrt{\frac{\pi^n}{\det \mathbb{A}}} e^{\frac{1}{4} \mathbf{b} \cdot \mathbb{A}^{-1} \mathbf{b}} \quad (9)$$

or again (send $\mathbb{A} \mapsto \frac{1}{4} \mathbb{B}^{-1}$)

$$e^{\mathbf{b} \cdot \mathbb{B} \mathbf{b}} = \frac{1}{\sqrt{(4\pi)^n \det \mathbb{B}}} \iint \dots \int_{-\infty}^{+\infty} e^{-\frac{1}{4} \mathbf{x} \cdot \mathbb{B}^{-1} \mathbf{x} \pm \mathbf{b} \cdot \mathbf{x}} d^n x$$

on which basis we expect to have (at least formally)

$$e^{t \nabla \cdot \mathbb{A} \nabla} = \frac{1}{\sqrt{(4\pi t)^n \det \mathbb{A}}} \iint \dots \int_{-\infty}^{+\infty} e^{-\frac{1}{4t} \boldsymbol{\xi} \cdot \mathbb{A}^{-1} \boldsymbol{\xi} - \boldsymbol{\xi} \cdot \nabla} d^n \boldsymbol{\xi} \quad (10)$$

from which we recover (4) in the one-dimensional case. The multi-variable Taylor theorem provides (again within some unstated radius of convergence)

$$e^{-\boldsymbol{\xi} \cdot \nabla} f(\mathbf{x}) = f(\mathbf{x} - \boldsymbol{\xi})$$

so we expect the solution of

$$\partial_t \psi(\mathbf{x}, t) = (\nabla \cdot \mathbb{A} \nabla) \psi(\mathbf{x}, t) \quad : \quad \psi(\mathbf{x}, 0) = \psi_0(\mathbf{x})$$

to be expressible

$$\begin{aligned} \psi(\mathbf{x}, t) &= e^{t \nabla \cdot \mathbb{A} \nabla} \psi(\mathbf{x}, 0) \\ &= \iint \dots \int_{-\infty}^{+\infty} g_t(\boldsymbol{\xi}) \psi_0(\mathbf{x} - \boldsymbol{\xi}) d\xi_1 \dots d\xi_n \end{aligned} \quad (12)$$

where now

$$g_t(\mathbf{x}) \equiv \frac{1}{\sqrt{(4\pi t)^n \det \mathbb{A}}} e^{-\frac{1}{4t} \mathbf{x} \cdot \mathbb{A}^{-1} \mathbf{x}} \quad (13)$$

³ See page 32 in my QUANTUM MECHANICS (1967/68), or (for example)

http://en.wikipedia.org/wiki/Gaussian_integral

If \mathbb{A} were diagonal

$$\mathbb{A} = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_n \end{pmatrix}$$

—which can in principle always be achieved by a rotational change of variables—then (13) assumes the especially transparent form

$$g_t(\mathbf{x}) = \prod_{i=1}^n \frac{1}{\sqrt{4\pi a_i t}} e^{-x_i(4a_i t)^{-1} x_i}$$

In such cases, the n -dimensional problem resolves into what are essentially n copies of the one-dimensional problem.⁴

Problems that arise when n is very large. When n is very large (and especially in the limit $n \rightarrow \infty$) and spectral information is absent, the use of (13) presents two closely related problems:

- 1) the definition of $\det \mathbb{A}$ (which involves a sum over signed permutations) becomes unworkable, and
- 2) so also (for similar reason) does the matrix-theoretic construction of \mathbb{A} .

Looking first to the former problem, we if we were in position to write

$$\mathbb{A} = \exp \mathbb{L}$$

then we would have

$$\det \mathbb{A} = \exp \{ \text{tr } \mathbb{L} \} \tag{14}$$

which, if one commands (say) `L=RandomReal[{0,1},{5,5}]` to construct a random 5×5 with random elements drawn from the interval $\{0, 1\}$, is readily verified by calculation. The identity (14) presents this advantage: evaluation of $\text{tr } \mathbb{L}$ involves no permutational combinatorics—is straightforward whatever the dimension of \mathbb{L} .

If spectral information *were* available, one would have

$$\det \mathbb{A} = \prod_i a_i$$

whence

$$\log \det \mathbb{A} = \sum_i \log a_i$$

⁴ My “essentially” becomes “literally” when and only when the initial value of $\psi(\mathbf{x}, t)$ factors:

$$\psi(\mathbf{x}, t) = \prod_{i=1}^n f_i(x_i)$$

Now the non-obvious step which Kirsten & Loya¹ take in the introduction to their paper, and which appears to be entirely characteristic of work in this field: trivially $a^{-s} = e^{-s \log a}$, so

$$\begin{aligned} \frac{d}{ds} a^{-s} &= -e^{-s \log a} \log a \\ &\downarrow \\ &= -\log a \quad \text{at } s = 0 \end{aligned}$$

and we have

$$\begin{aligned} \log \det \mathbb{A} &= -\left\{ -\sum_i \log a_i \right\} \\ &= -\frac{d}{ds} \sum_i a_i^{-s} \Big|_{s=0} \end{aligned}$$

Enlarging upon the definition of the Riemann ζ -function

$$\zeta_{\text{Riemann}}(s) \equiv \sum_{n=1}^{\infty} n^{-s}$$

we define

$$\zeta_{\mathbb{A}}(s) \equiv \sum_{i=1}^{\infty} a_i^{-s} \tag{15}$$

which gives back $\zeta_{\text{Riemann}}(s)$ in the special case $a_i = i$: ($i = 1, 2, 3, \dots$). In this notation

$$\begin{aligned} \log \det \mathbb{A} &= -\frac{d}{ds} \zeta_{\mathbb{A}}(s) \Big|_{s=0} \\ &= -\zeta'_{\mathbb{A}}(0) \\ &\updownarrow \\ \det \mathbb{A} &= \exp \left\{ -\zeta'_{\mathbb{A}}(0) \right\} \end{aligned} \tag{16}$$

Comparison with (14) supplies $-\zeta'_{\mathbb{A}}(0) = \text{tr} \log \mathbb{A}$. These equations are pretty, but become useful only if one is in position to speak *without knowledge of the \mathbb{A} -spectrum* about relevant properties of the function $\zeta_{\mathbb{A}}(s)$.

The preceding remarks have nothing *per se* to do with quantum mechanics, but do have quantum mechanical applications, and it is in the latter context that—for the reason just stated—one acquires interest in the general theory of quantum ζ -functions.⁵

⁵ Richard Crandall, in “On the quantum zeta function,” J. Phys. A: Math. Gen. **29**, 6795–6816 (1996), draws attention to the remarkable fact that

$$Z(s) = \sum_i E_i^{-s}$$

can sometimes be evaluated exactly even though not a single eigenvalue E_i is known. He himself concentrates on cases in which s assumes (not arbitrary complex, but) integral values.

Basic notions. The dynamical evolution of an arbitrary quantum state $|\psi\rangle$ is accomplished by action

$$|\psi\rangle_{t_0} \longmapsto |\psi\rangle_{t_1} = \mathbf{U}(t_1, t_0)|\psi\rangle_{t_0}$$

of a unitary operator of which these are fundamental properties:

$$\mathbf{U}(t_0, t_0) = \mathbf{I} \quad (17.1)$$

$$\mathbf{U}(t_2, t_0) = \mathbf{U}(t_2, t_1)\mathbf{U}(t_1, t_0) \quad (17.2)$$

Differentiation of the unitarity condition $\mathbf{U}(t, t_0)\mathbf{U}^\dagger(t, t_0) = \mathbf{I}$ establishes that necessarily $\mathbf{U}(t, t_0)$ satisfies a differential equation of the form

$$i\hbar\frac{\partial}{\partial t}\mathbf{U} = \mathbf{H}\mathbf{U} \quad : \quad \mathbf{H} \text{ hermitian, with } [\mathbf{H}] = \text{ENERGY} \quad (18)$$

of which the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle_t = \mathbf{H}|\psi\rangle_t$$

is an immediate corollary. If the operator \mathbf{H} (physically, the “Hamiltonian”) is time-independent, one has

$$\mathbf{U}(t, t_0) = e^{\beta(t-t_0)\mathbf{H}} \quad : \quad \beta \equiv -i/\hbar \quad (19)$$

In the x -representation we have

$$(x|\psi\rangle_t = \int (x|\mathbf{U}(t, t_0)|x_0)dx_0(x_0|\psi_0)$$

which differs only notationally from (8), and supplies a description of the Green’s function $G(x, t; x_0, t_0)$ (or “propagator” $K(x, t; x_0, t_0)$ as it is usually called/denoted in the quantum literature):

$$K(x, t; x_0, t_0) = (x|\mathbf{U}(t, t_0)|x_0) \quad (20)$$

The composition law (17.2) permits one to write

$$\begin{aligned} K(x, t; x_0, t_0) &= \int (x|\mathbf{U}(t, t_1)|x_1)dx_1(x_1|\mathbf{U}(t_1, t_0)|x_0) \quad : \quad t > t_1 > t_0 \\ &= \int K(x, t; x_1, t_1)dx_1K(x_1, t_1; x_0, t_0) \end{aligned} \quad (21)$$

In continuation of this basic refinement process, we resolve the interval $\{t, t_0\}$ into $N + 1$ subintervals, each of duration

$$\tau = \frac{t - t_0}{N + 1}$$

$$t_0 < t_1 = t_0 + \tau < \cdots < t_n = t_0 + n\tau < \cdots < t_N = t_0 + N\tau < t_{N+1} \equiv t$$

and as a generalization of (21) have

$$\begin{aligned} &K(x, t; x_0, t_0) \quad (22) \\ &= \underbrace{\int \cdots \int}_{N\text{-fold}} K_\tau(x, x_N)dx_N \cdots dx_{n+1}K_\tau(x_{n+1}, x_n)dx_n \cdots dx_1K_\tau(x_1, x_0) \end{aligned}$$

where the functions $K_\tau(x, y)$ are *short-time* propagators:

$$K_\tau(x, y) = K(x, \tau; y, 0) = (x|e^{\beta\tau\mathbf{H}}|y) \quad (23)$$

At cost of a complication of the form $\int \mapsto \iint \cdots \int$ we have placed ourselves in position to make use of the fact (which Dirac was the first to notice, and Feynman was the first to exploit) that the quantum object $K_\tau(x, y)$ can be assembled from material provided by *classical* mechanics.⁶

Look to the case

$$\mathbf{H}_{\text{free particle}} = \frac{1}{2m} \mathbf{p}^2 \quad (24)$$

Drawing upon the completeness of the \mathbf{p} -eigenfunctions $|p\rangle$

$$\int |p\rangle dp \langle p| = \mathbf{I}$$

we have⁷

$$\begin{aligned} (x|e^{\beta\tau\mathbf{H}}|y) &= \int (x|e^{\beta\tau\mathbf{H}}|p\rangle dp \langle p|y) \\ &= \int e^{(\beta\tau/2m)p^2} (x|p\rangle dp \langle p|y) \\ &= \frac{1}{h} \int e^{(\beta\tau/2m)p^2} e^{\beta(x-y)p} dp \end{aligned}$$

which by formal appeal⁸ to the Gaussian integral formula (3.1) gives

$$= \sqrt{\frac{m}{i\hbar\tau}} \exp\left\{\frac{i}{\hbar} \frac{m}{2} \frac{(x-y)^2}{\tau}\right\} \quad (25)$$

⁶ The sense in which quantum mechanics becomes classical in the limit $\hbar \downarrow 0$ was recognized/stated almost immediately after publication of the Schrödinger equation, by Wentzel, Kramers and Brillouin—independent co-inventors of the WKB “semi-classical approximation” (1926), the analytical essence of which was recognized later to have been introduced into the mathematical literature by Liouville and Green as early as 1837. That

quantum mechanics becomes classical in the short term

was recognized only later (Dirac/Feynman).

⁷ Use $(x|p\rangle = \frac{1}{\sqrt{h}} e^{\frac{i}{\hbar} px}$, which are orthonormal in the sense

$$(p|q) = \int (p|x) dx (x|q) = \delta(p - q)$$

⁸ The substitution $\alpha \mapsto i\tau/\hbar 2m$ places one in violation of the condition $\Re(\alpha) > 0$. Feynman addressed this problem by sending $\frac{1}{\hbar} \mapsto \frac{1}{\hbar} - i\epsilon$ and setting $\epsilon \downarrow 0$ at the end of the calculation. The generally preferred practice today is to complexify time $t \mapsto t' = -i\theta$, and to obtain real-time results by analytic continuation.

As a first step toward the implementation of (22) we compute

$$\begin{aligned}
& \int (x|e^{\beta\tau\mathbf{H}}|\xi)d\xi(\xi|e^{\beta\tau\mathbf{H}}|y) \\
&= \left(\sqrt{\frac{m}{i\hbar\tau}}\right)^2 \int \exp\left\{\frac{i}{\hbar}\frac{m}{2}\frac{(x-\xi)^2 + (\xi-y)^2}{\tau}\right\} d\xi \\
&= \left(\sqrt{\frac{m}{i\hbar\tau}}\right)^2 \sqrt{\frac{i\hbar\tau}{2m}} \exp\left\{\frac{i}{\hbar}\frac{m}{2}\frac{(x-y)^2}{2\tau}\right\} \\
&= \sqrt{\frac{m}{i\hbar 2\tau}} \exp\left\{\frac{i}{\hbar}\frac{m}{2}\frac{(x-y)^2}{2\tau}\right\} \\
&= (x|e^{\beta 2\tau\mathbf{H}}|y)
\end{aligned} \tag{26.1}$$

More generally

$$\begin{aligned}
& \int (x|e^{\beta t_1\mathbf{H}}|\xi)d\xi(\xi|e^{\beta t_2\mathbf{H}}|y) \\
&= \sqrt{\frac{m}{i\hbar t_1}} \sqrt{\frac{m}{i\hbar t_2}} \int \exp\left\{\frac{i}{\hbar}\frac{m}{2}\left[\frac{(x-\xi)^2}{t_1} + \frac{(\xi-y)^2}{t_2}\right]\right\} d\xi \\
&= \sqrt{\frac{m}{i\hbar t_1}} \sqrt{\frac{m}{i\hbar t_2}} \sqrt{\frac{i\hbar t_1 t_2}{m(t_1+t_2)}} \exp\left\{\frac{i}{\hbar}\frac{m}{2}\frac{(x-y)^2}{t_1+t_2}\right\} \\
&= \sqrt{\frac{m}{i\hbar(t_1+t_2)}} \exp\left\{\frac{i}{\hbar}\frac{m}{2}\frac{(x-y)^2}{t_1+t_2}\right\} \\
&= (x|e^{\beta(t_1+t_2)\mathbf{H}}|y)
\end{aligned} \tag{26.2}$$

Equations (26) display a “structural persistence” property which is not at all typical of Hamiltonians-in-general, and in the case $\mathbf{H}_{\text{free particle}}$ renders the complicated

$$\lim_{N \uparrow \infty} \iint \cdots \int$$

process called for on the right side of (22) superfluous: immediately

$$K(x, t; x_0, t_0) = K_{t-t_0}(x, x_0) = \sqrt{\frac{m}{i\hbar(t-t_0)}} \exp\left\{\frac{i}{\hbar}\frac{m}{2}\frac{(x-x_0)^2}{t-t_0}\right\} \tag{27}$$

This conforms precisely to the result obtained at (6), where we in effect had

$$K(x, t, y, 0) = \frac{1}{\sqrt{4\pi at}} e^{-\frac{1}{4at}(x-y)^2} \Big|_{a=i\hbar/2m}$$

Suppose we were ignorant of the exceptional free particle circumstance just noted, determined to proceed as (22) asks us to. At stage $N = 5$ we would—by

$$(x - \xi_5)^2 + \sum_{k=1}^5 (\xi_{k+1} - \xi_k)^2 + (\xi_1 - y)^2 = x^2 + y^2 + \boldsymbol{\xi} \cdot \mathbb{A} \boldsymbol{\xi} - \mathbf{b} \cdot \boldsymbol{\xi}$$

$$\boldsymbol{\xi} = \begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \\ \xi_5 \end{pmatrix}, \quad \mathbb{A} = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 2y \\ 0 \\ 0 \\ 0 \\ 2x \end{pmatrix}$$

—be looking at

$$\mathcal{K}_6 \equiv \left(\sqrt{\frac{m}{i\hbar\tau}} \right)^6 e^{-\alpha(x^2 + y^2)} \cdot \iiint\iiint e^{-\alpha(\boldsymbol{\xi} \cdot \mathbb{A} \boldsymbol{\xi} - \mathbf{b} \cdot \boldsymbol{\xi})} d\xi_1 \dots d\xi_5$$

where $\tau = \frac{1}{6}t$ and $\alpha = -(i/\hbar)(m/2\tau) = \pi(m/i\hbar\tau)$. Drawing upon the Gaussian integral formula (9) we have

$$\iiint\iiint e^{-\alpha(\boldsymbol{\xi} \cdot \mathbb{A} \boldsymbol{\xi} - \mathbf{b} \cdot \boldsymbol{\xi})} d\xi_1 \dots d\xi_5 = \sqrt{\frac{\pi^5}{\det(\alpha\mathbb{A})}} e^{\frac{1}{4}(\alpha\mathbf{b}) \cdot (\alpha\mathbb{A})^{-1}(\alpha\mathbf{b})}$$

So special is the structure of \mathbf{b} that we need compute only the corner elements of

$$(\alpha\mathbb{A})^{-1} = \alpha^{-1} \begin{pmatrix} \frac{5}{6} & \bullet & \bullet & \bullet & \frac{1}{6} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \frac{1}{6} & \bullet & \bullet & \bullet & \frac{5}{6} \end{pmatrix}$$

Also

$$\det(\alpha\mathbb{A}) = 6\alpha^5$$

The results now in hand supply

$$\begin{aligned} \mathcal{K}_6 &= (\sqrt{\alpha/\pi})^6 e^{-\alpha(x^2 + y^2)} \sqrt{\frac{\pi^5}{6\alpha^5}} e^{\frac{1}{6}\alpha(5x^2 + 3xy + 5y^2)} \\ &= \sqrt{\alpha/6\pi} e^{-(\alpha/6)(x-y)^2} \\ &= \sqrt{\frac{m}{i\hbar 6\tau}} \exp \left\{ \frac{i}{\hbar} \frac{m}{2} \frac{(x-y)^2}{6\tau} \right\} \Big|_{\tau=\frac{1}{6}t} \end{aligned}$$

To evaluate \mathcal{K}_N one needs to know that (as follow from some simple recursion relations: see my QUANTUM MECHANICS (1967/68), pages 33–42)

$$(\alpha\mathbb{A})^{-1} = \alpha^{-1} \begin{pmatrix} \frac{N-1}{N} & \bullet & \bullet & \bullet & \frac{1}{N} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \frac{1}{N} & \bullet & \bullet & \bullet & \frac{N-1}{N} \end{pmatrix} : (N-1) \times (N-1)$$

$$\det(\alpha\mathbb{A}) = N\alpha^{N-1}$$

The argument proceeds along otherwise identical lines, and leads to an identical result.

The preceding demonstration that the free particle propagator—which can be obtained by the simplest of means—can also be obtained by relatively complicated means would, on its face, hardly seem to constitute progress. But when one looks to systems more complicated/interesting than $\mathbf{H}_{\text{free}} = \frac{1}{2m} \mathbf{p}^2$ the simplest modes of argument generally fail, and the relatively robust “complicated modes of argument” acquire fresh interest.

Propagators of quantum motion in the presence of a potential. I review several alternative ways of constructing the propagator when $\mathbf{H} = H(\mathbf{p}, \mathbf{x})$ and when, more particularly, the Hamiltonian has the commonly encountered form

$$\mathbf{H} = \frac{1}{2m} \mathbf{p}^2 + V(\mathbf{x})$$

Suppose first of all that one has solved the time-independent eigenvalue problem:

$$\mathbf{H}|n\rangle = E_n|n\rangle \quad (28)$$

Then

$$\mathbf{U}(t) = e^{\beta t \mathbf{H}} = \sum_m \sum_n |m\rangle \langle m| e^{\beta t \mathbf{H}} |n\rangle \langle n| = \sum_n |n\rangle e^{\beta t E_n} \langle n|$$

supplies

$$\begin{aligned} K(x, t; y, 0) &= \langle x | \mathbf{U}(t) | y \rangle = \sum_n \psi_n^*(x) e^{\beta t E_n} \psi_n(y) \\ &= \sum_n \psi_n^*(x) e^{-i \omega_n t} \psi_n(y) \end{aligned} \quad (29)$$

where $\psi_n(y) \equiv \langle n | y \rangle$ and $\omega_n \equiv E_n/\hbar$. The spectral representation (29) of the propagator sees important service in a great variety of applications, but presumes that one possesses all of the detailed spectral information (28).

I sketch now a relatively little known second line of attack that takes us closer to my intended objective. Suppose we were in possession of a function $\mathcal{H}(x, p)$ with the property that it permits us to present the operator $e^{-(i/\hbar) \mathbf{H} \tau}$ in $\mathbf{x} \mathbf{p}$ -ordered⁹ form:

$$e^{-(i/\hbar) \mathbf{H} \tau} = {}_{\mathbf{x}} \left[e^{-(i/\hbar) \mathcal{H}(x, p) \tau} \right]_{\mathbf{p}}$$

⁹ To illustrate both the concept and the way it will be notated, we have

$$\begin{aligned} (\mathbf{x} + \mathbf{p})^2 &= \mathbf{x}^2 + \mathbf{x} \mathbf{p} + \mathbf{p} \mathbf{x} + \mathbf{p}^2 \\ {}_{\mathbf{x}} \left[(\mathbf{x} + \mathbf{p})^2 \right]_{\mathbf{p}} &= \mathbf{x}^2 + 2 \mathbf{x} \mathbf{p} + \mathbf{p}^2 \\ &\neq {}_{\mathbf{p}} \left[(\mathbf{x} + \mathbf{p})^2 \right]_{\mathbf{x}} \end{aligned}$$

We would then be in position to write

$$\begin{aligned}
 K_\tau(x, y) &= \int (x|_x [e^{-(i/\hbar)\mathcal{H}(x,p)\tau}]_p |p) dp(p|y) \\
 &= \int e^{-(i/\hbar)\mathcal{H}(x,p)\tau} (x|p) dp(p|y) \\
 &= \frac{1}{\hbar} \int e^{-(i/\hbar)\mathcal{H}(x,p)\tau} e^{(i/\hbar)(x-y)p} dp \\
 &= \frac{1}{\hbar} \int \exp \left\{ \frac{i}{\hbar} \left[p \frac{x-y}{\tau} - \mathcal{H}(x, p) \right] \tau \right\} dp \tag{30}
 \end{aligned}$$

The expression [etc.] is tantalizingly suggestive of the construction $p\dot{x} - H(x, p)$ that, in conjunction with $\dot{x} = \partial H / \partial p$, serves in classical mechanics to produce the Lagrangian $L(x, \dot{x})$. Lending concrete substance to that observation turns out, however, to be a non-trivial undertaking.¹⁰ It is easier to approach the seeming implication of (30) from another angle:

Let \mathbb{A} and \mathbb{B} be $n \times n$ matrices. Then

$$e^{\mathbb{A}+\mathbb{B}} \neq e^{\mathbb{A}} \cdot e^{\mathbb{B}} \quad \text{unless } \mathbb{A} \text{ and } \mathbb{B} \text{ commute}$$

The **Lie product formula** asserts that

$$e^{\mathbb{A}+\mathbb{B}} = \lim_{N \uparrow \infty} \left(e^{\mathbb{A}/N} \cdot e^{\mathbb{B}/N} \right)^N$$

Ask *Mathematica* to test the accuracy of this statement with random matrices; you will find that it checks out, but that the convergence is typically very slow. H. F. Trotter (1959) and T. Kato (1978) showed that the Lie formula pertains also to a broad class of linear operators, in which context it is known as the **Trotter product formula**¹¹

$$e^{\mathbf{A}+\mathbf{B}} = \lim_{N \uparrow \infty} \left(e^{\mathbf{A}/N} \cdot e^{\mathbf{B}/N} \right)^N$$

Feynman wrote his thesis in 1942, and published in 1948, so was obliged to proceed in ignorance of the Trotter product formula,¹² which is now recognized to provide the most effective mathematical foundation of the “sum-over-paths” formalism. Assume the Hamiltonian to have the form $\mathbf{H} = \mathbf{T} + \mathbf{V}$. Then

¹⁰ See pages 49–50 in Chapter I of my *ADVANCED QUANTUM TOPICS* (2000).

¹¹ See L. S. Schulman, *Techniques and Applications of Path Integration* (1981), pages 9–12; http://en.wikipedia.org/wiki/Lie_product_formula.

¹² Both Feynman and Trotter were at Princeton when they did the work in question, but Trotter wrote in the manner of a pure mathematician with no evident interest in applications, and made no reference to Feynman.

$$\begin{aligned}
K(x, t; y, 0) &= \langle x | e^{\beta(\mathbf{T} + \mathbf{V})t} | y \rangle \\
&= \lim_{N \uparrow \infty} \langle x | [e^{\beta \mathbf{T} \tau} \cdot e^{\beta \mathbf{V} \tau}]^N | y \rangle \quad : \quad \tau = t/N \\
&= \lim_{N \uparrow \infty} \int dx_1 \cdots dx_{N-1} \prod_{k=0}^{N-1} \langle x_{k+1} | e^{\beta \mathbf{T} \tau} \cdot e^{\beta \mathbf{V} \tau} | x_k \rangle \quad (31)
\end{aligned}$$

where it is understood that $|x_0\rangle \equiv |y\rangle$ and $|x_N\rangle \equiv |x\rangle$. Assume, moreover, that $\mathbf{T} = T(\mathbf{p}) = \frac{1}{2m} \mathbf{p}^2$, $\mathbf{V} = V(\mathbf{x})$ and use the mixed representation trick to obtain

$$\begin{aligned}
\langle x_{k+1} | e^{\beta \mathbf{T} \tau} \cdot e^{\beta \mathbf{V} \tau} | x_k \rangle &= \int \langle x_{k+1} | e^{\beta T(\mathbf{p})\tau} | p \rangle dp \langle p | e^{\beta V(\mathbf{x})\tau} | x_k \rangle \\
&= \int e^{\beta T(\mathbf{p})\tau} \langle x_{k+1} | p \rangle \langle p | x_k \rangle dp \cdot e^{\beta V(x_k)\tau} \\
&= \frac{1}{h} \int e^{\beta \frac{1}{2m} p^2 \tau + \beta p(x_{k+1} - x_k)} dp \cdot e^{\beta V(x_k)\tau} \\
&= \sqrt{\frac{m}{i\hbar\tau}} \exp \left\{ \frac{i}{\hbar} \left[\frac{m}{2} \left(\frac{x_{k+1} - x_k}{\tau} \right)^2 - V(x_k) \right] \tau \right\}
\end{aligned}$$

where at the last step we have looked to (25) for evaluation of the Gaussian integral. Returning with this information to (31), we get

$$\begin{aligned}
K(x, t; y, 0) &= \lim_{N \uparrow \infty} \left(\frac{m}{i\hbar\tau} \right)^{\frac{N}{2}} \int dx_1 \cdots dx_{N-1} \quad (32) \\
&\quad \exp \left\{ \frac{i}{\hbar} \sum_{k=0}^{N-1} \left[\frac{m}{2} \left(\frac{x_{k+1} - x_k}{\tau} \right)^2 - V(x_k) \right] \tau \right\}
\end{aligned}$$

The expression $\sum_k [etc.] \tau$ in the exponent looks like a discrete approximation to the classical action

$$\begin{aligned}
S[x(t)] &= \int_0^t L(\dot{x}(t), x(t)) dt \\
L(\dot{x}, x) &= \frac{1}{2} m \dot{x}^2 - V(x)
\end{aligned}$$

of a path $x(t)$ that passes through the points

$$\{y = x_0, x_1, x_2, \dots, x_k, \dots, x_N = x\}$$

at times

$$\{0 = t_0, t_1, t_2, \dots, t_k, \dots, t_N = t\}$$

Equation (32) appears therefore to speak of a “sum-over-paths,” but since the points x_k range independently on $(-\infty, +\infty)$ almost all of the paths in question

are so kinky as to be (continuous but) nowhere differentiable. It is tempting to introduce the abbreviated notation

$$\begin{aligned} & \int e^{\frac{i}{\hbar}S[x(t)]} \mathcal{D}x(t) \\ & \equiv \lim_{N \uparrow \infty} \int dx_1 \cdots dx_{N-1} \exp \left\{ \frac{i}{\hbar} \sum_{k=0}^{N-1} \left[\frac{m}{2} \left(\frac{x_{k+1} - x_k}{\tau} \right)^2 - V(x_k) \right] \tau \right\} \end{aligned}$$

but the expression on the right cannot have literal stand-alone meaning for, as we saw at (32), it must be multiplied by

$$\left(\frac{m}{i\hbar\tau} N \right)^{\frac{N}{2}}, \text{ which blows up as } N \uparrow \infty$$

if we are to achieve the finite valuation $K(x, t; y, 0)$.

Feynman finessed that awkward point. He interpreted $K(x, t; y, 0)$ to be the *probability amplitude for the transition* $x(t) \leftarrow x(0) \equiv y$, asserted that¹³

$$\text{net probability amplitude} = \sum_{\text{independent paths}} \text{amplitude of each contributory path}$$

and postulated that

$$\text{path amplitude} = A \cdot e^{\frac{i}{\hbar}S[\text{path}]}$$

where A is a normalization factor, which acquires its value from the requirement that

$$\int |K(x, t; y, 0)|^2 dx = 1$$

A is precisely the “preexponential factor” to the evaluation of which Kirsten & Loya devote their paper.¹

Exploring the neighborhood of a classical path. We write

$$x(t) = x_{\text{cl}}(t) + \eta(t) \quad : \quad \eta(0) = \eta(t) = 0$$

to describe variants of the classical path $x_{\text{cl}}(t)$ —of which there may be more than one—that proceeds from $(x_0, t_0) \equiv (y, 0)$ to $(x_1, t_1) \equiv (x, t)$. Immediately,

$$S[x_{\text{cl}}(t) + \eta(t)] = \int_{t_0}^{t_1} L(x_{\text{cl}}(t) + \eta(t), \dot{x}_{\text{cl}}(t) + \dot{\eta}(t)) dt$$

¹³ This, by probability = |probability amplitude|², is seen to be “the square root of the familiar statement that the probabilities (here: probability amplitudes) of independent events add.”

$$\begin{aligned}
&= \int_{t_0}^{t_1} \left\{ L(x_{\text{cl}}, \dot{x}_{\text{cl}}) + [L_x(x_{\text{cl}}, \dot{x}_{\text{cl}})\eta + L_{\dot{x}}(x_{\text{cl}}, \dot{x}_{\text{cl}})\dot{\eta}] \right. \\
&\quad \left. + \frac{1}{2} [L_{xx}(x_{\text{cl}}, \dot{x}_{\text{cl}})\eta\eta + 2L_{x\dot{x}}(x_{\text{cl}}, \dot{x}_{\text{cl}})\eta\dot{\eta} + L_{\dot{x}\dot{x}}(x_{\text{cl}}, \dot{x}_{\text{cl}})\dot{\eta}\dot{\eta}] + \dots \right\} dt
\end{aligned} \tag{33}$$

The 0th-order term becomes $S[x_{\text{cl}}]$. The 1st-order term can, after an integration by parts, be written

$$\int_{t_0}^{t_1} \left\{ L_x(x_{\text{cl}}, \dot{x}_{\text{cl}}) - \frac{d}{dt} L_{\dot{x}}(x_{\text{cl}}, \dot{x}_{\text{cl}}) \right\} \eta dt + L_{\dot{x}}(x_{\text{cl}}, \dot{x}_{\text{cl}})\eta(t) \Big|_{t_0}^{t_1}$$

and is seen therefore to vanish: the first term vanishes because $x_{\text{cl}}(t)$ is a solution of Lagrange's equation of motion; the second term is killed by the endpoint conditions $\eta(t_0) = \eta(t_1) = 0$. To simplify discussion of the higher-order contributions to (33) I assume the Lagrangian to be of the form

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

in which case we have

$$\begin{aligned}
S[x_{\text{cl}}(t) + \eta(t)] &= S[x_{\text{cl}}(t)] + \int_{t_0}^{t_1} \left\{ \frac{1}{2} [m\dot{\eta}\dot{\eta} - V''(x_{\text{cl}}(t))\eta\eta] \right. \\
&\quad \left. - \frac{1}{3!} V'''(x_{\text{cl}}(t))\eta\eta\eta + \dots \right\} dt
\end{aligned}$$

It is difficult to imagine a case in which the terms of order $n \geq 3$ do not serve to make the integration problem impossibly complicated. Let us suppose, therefore, that such terms are absent:

$$V(x) = \alpha + \beta x + \frac{1}{2}m\omega^2 x^2$$

The problem then is to evaluate

$$\frac{m}{2} \int_{t_0}^{t_1} [\dot{\eta}\dot{\eta} - \omega^2\eta\eta] dt = \frac{m}{2} \int_{t_0}^{t_1} \left[\frac{d}{dt}(\eta\dot{\eta}) - \eta\ddot{\eta} - \omega^2\eta\eta \right] dt$$

The endpoint conditions $\eta(t_0) = \eta(t_1) = 0$ serve to kill the first term on the right, and we are left with

$$= -\frac{m}{2} \int_{t_0}^{t_1} \eta(t) [\partial_t^2 + \omega^2] \eta(t) dt \tag{34}$$

where $\partial_t \equiv \frac{d}{dt}$. Returning this problem to the context from which it sprang, we

have

$$\begin{aligned} K(x_1, t_1; x_0, t_0) &= A \cdot \int e^{\frac{i}{\hbar} S[x(t)]} \mathcal{D}x(t) \\ &= A \exp \left\{ \frac{i}{\hbar} S[x_{\text{cl}}(t)] \right\} \cdot \int \exp \left\{ \frac{i}{\hbar} \int_{t_0}^{t_1} \frac{m}{2} [\dot{\eta}\dot{\eta} - \omega^2 \eta\eta] dt \right\} \mathcal{D}\eta(t) \end{aligned} \quad (35)$$

which appears as equation (3.13) on page 46 of Ashok Das' *Field Theory: A Path Integral Approach* (1993).

In his §§3.2–3 (pages 47–62) Das evaluates the expression on the right side of (35) by two different methods. Das' second method is too familiar to be interesting: he slices the time interval $t_0 \leq t \leq t_1$ into intervals of duration τ (*a la* Feynman), notices that $[\dot{\eta}\dot{\eta} - \omega^2 \eta\eta]$ can be rendered as a quadratic form in the discrete values that $\eta(t)$ assumes at the ends of those intervals, solves the resulting many-variable Gaussian integration problem. Das' first method is more interesting: he writes

$$\eta(t) = \sum_{n=1}^{\infty} a_n \sin \left(n\pi \frac{t - t_0}{t_1 - t_0} \right) \quad : \quad \text{endpoint conditions automatic}$$

and obtains

$$\int_{t_0}^{t_1} [\dot{\eta}\dot{\eta} - \omega^2 \eta\eta] dt = \frac{t_1 - t_0}{2} \sum_{n=1}^{\infty} \left[\left(\frac{n\pi}{t_1 - t_0} \right)^2 - \omega^2 \right] a_n^2$$

The Fourier coefficients a_n are the “coordinates” that serve to identify the individual elements $\eta(t)$ of η -space. The process $\int \mathcal{D}\eta(t)$ is understood now to mean $\int \int \cdots \int da_1 da_2 \cdots = \prod_n \int da_n$, so we once again confront an infinite product of Gaussian integrals, which—after the dust has settled—gives¹⁴

$$K_{\text{osc}}(x_1, t_1; x_0, t_0) = A_{\text{osc}} \sqrt{\frac{\omega(t_1 - t_0)}{\sin[\omega(t_1 - t_0)]}} \cdot \exp \left\{ \frac{i}{\hbar} S_{\text{osc}}[x_{\text{cl}}(t)] \right\} \quad (36)$$

To fix the value of A —which remains still indeterminate—Das imposes the requirement that

$$\lim_{\omega \downarrow 0} K_{\text{osc}}(x_1, t_1; x_0, t_0) = K_{\text{free}}(x_1, t_1; x_0, t_0)$$

It is easy to see that

$$\lim_{\omega \downarrow 0} S_{\text{osc}}[x_{\text{cl}}(t)] = S_{\text{free}}[x_{\text{cl}}(t)]$$

¹⁴ Critical use is made of the identity

$$\prod_{n=1}^{\infty} \left[1 - \left(\frac{z}{n\pi} \right)^2 \right] = \frac{\sin z}{z}$$

and that

$$\lim_{\omega \downarrow 0} \sqrt{\frac{\omega(t_1 - t_0)}{\sin[\omega(t_1 - t_0)]}} = 1$$

Das argues on this basis that necessarily

$$A_{\text{osc}} = A_{\text{free}}$$

though he is in fact in position to argue only that

$$A_{\text{osc}} = A_{\text{free}} \cdot (\text{function of } \omega \text{ and } t \text{ that goes to unity as } \omega \downarrow 0)$$

Feynman's normalization requirement is free from this defect.¹⁵

Enter: the “functional determinant”. We have made repeated use of the multi-variable Gaussian integral formula (9), which in the case $\mathbf{b} = \mathbf{0}$ reads

$$\iint \dots \int_{-\infty}^{+\infty} e^{-\mathbf{x} \cdot \mathbb{A} \mathbf{x}} d^n x = \sqrt{\frac{\pi^n}{\det \mathbb{A}}} \quad (37.1)$$

—the assumption there being that the square matrix \mathbb{A} was real & symmetric (therefore hermitian) and positive definite (all eigenvalues real and strictly positive). By formal extension⁸ we therefore have

$$\iint \dots \int_{-\infty}^{+\infty} e^{i\mathbf{x} \cdot \mathbb{A} \mathbf{x}} d^n x = \sqrt{\frac{(i\pi)^n}{\det \mathbb{A}}} \quad (37.2)$$

I have remarked in reference to (35), in connection with Das' “uninteresting first method,” that we expect to be able to write¹⁶

$$\int \exp \left\{ i \alpha \int_{t_0}^{t_1} [\dot{\eta} \dot{\eta} - \omega^2 \eta \eta] dt \right\} \mathcal{D}\eta(t) = \lim_{N \uparrow \infty} \iint \dots \int_{-\infty}^{+\infty} e^{i\boldsymbol{\eta} \cdot \mathbb{A} \boldsymbol{\eta}} d^n \boldsymbol{\eta} \quad (38)$$

for some suitably designed matrix \mathbb{A} (constructed along the lines of the \mathbb{A} on page 10). Using (34) to reformulate the expression on the left side of (38), and using (37) to evaluate the expression on the right, we are led to write

$$\int \exp \left\{ -i \alpha \int_{t_0}^{t_1} \eta (\partial_t^2 + \omega^2) \eta dt \right\} \mathcal{D}\eta(t) = \mathcal{N} \frac{1}{\sqrt{\det(\partial_t^2 + \omega^2)}} \quad (39)$$

where the α has been absorbed into the as-yet-undetermined normalization constant \mathcal{N} . Das asserts (his page 72) that we can, on the basis of this result,

¹⁵ So also are the arguments that serve to relate the prefactor A to the VanVleck determinant (of which Das nowhere makes any use).

¹⁶ Here $\alpha = m/2\hbar$.

expect to be able more generally to write

$$\int \exp \left\{ i \int_{t_0}^{t_1} \eta(t) \mathcal{O}(t) \eta(t) dt \right\} \mathcal{D}\eta(t) = \mathcal{N} \frac{1}{\sqrt{\det \mathcal{O}(t)}} \quad (40)$$

How much more generally (for *what class* of operators $\mathcal{O}(t)$?) is a question that at this point remains to be determined—a question that will be settled by mathematical requirements that will emerge when we look more closely into meaning of (40).

We have

$$K_{\text{osc}}(x_1, t_1; x_0, t_0) = A \int \exp \left\{ i \alpha \int_{t_0}^{t_1} (\dot{\eta}\dot{\eta} - \omega^2 \eta\eta) dt \right\} \mathcal{D}\eta(t) \cdot e^{\frac{i}{\hbar} S_{\text{osc}}[x_{\text{cl}}(t)]}$$

and Das has already evaluated the prefactor by two distinct methods: his “matrix method,” which involves Feynmanesque time-slicing carried to the limit $N \uparrow \infty$, and his “Fourier transform method,” which proceeds from writing

$$\eta(t) = \sum_n a_n \sin \left(n\pi \frac{t - t_0}{t_1 - t_0} \right)$$

and interpreting $\mathcal{D}\eta(t)$ to mean $\prod_n da_n$.¹⁷ To those two he on pages 76–77 adds a third which has a much more “operator theoretic” flavor.¹⁸ It proceeds from

$$\int \exp \left\{ i \alpha \int_{t_0}^{t_1} (\dot{\eta}\dot{\eta} - \omega^2 \eta\eta) dt \right\} \mathcal{D}\eta(t) = \int \exp \left\{ -i \alpha \int_{t_0}^{t_1} \eta (\partial_t^2 + \omega^2) \eta dt \right\} \mathcal{D}\eta(t)$$

Das proposes to obtain the value of the expression on the right by analytic continuation of

$$\int \exp \left\{ -\alpha \int_{\tau_0}^{\tau_1} \eta(\tau) (-\partial_\tau^2 + \omega^2) \eta(\tau) d\tau \right\} \mathcal{D}\eta(\tau) \quad : \quad \tau = it$$

—the point here being that

$$(-\partial_\tau^2 + \omega^2) \eta(\tau) = \lambda \cdot \eta(\tau) \quad : \quad \eta(\tau_0) = \eta(\tau_1) = 0$$

presents a tractable eigenvalue problem. If, for the moment, we suspend the condition $\eta(\tau_1) = 0$ we get

$$\eta(\tau) \sim \sin \left(\sqrt{\lambda - \omega^2} (\tau - \tau_0) \right)$$

The suspended condition now requires λ to be a solution of

$$\sin \left(\sqrt{\lambda - \omega^2} (\tau_1 - \tau_0) \right) = 0 \quad (41)$$

¹⁷ Das passes over in silence the fact that his two methods assign two distinct meanings to the “space of paths.”

¹⁸ To those three methods Kirsten & Loya¹, in their §III, add yet a fourth.

so λ must assume one or another of the (eigen)values

$$\lambda_n = \left(\frac{n\pi}{\tau_1 - \tau_0} \right)^2 + \omega^2 \quad : \quad n = 1, 2, 3, \dots \quad (42)$$

The corresponding eigenfunctions (of which in the present context we have actually no need) are

$$\eta_n(\tau) = A_n \sin \left(n\pi \frac{\tau - \tau_0}{\tau_1 - \tau_0} \right)$$

Orthogonality is automatic, and normalization requires that we set

$$A_n = \sqrt{\frac{2}{\tau_1 - \tau_0}} \quad : \quad \text{all } n$$

For finite-dimensional matrices \mathbb{A} one can always write

$$\det \mathbb{A} = \prod_n \lambda_n$$

so Das writes

$$\begin{aligned} \det(-\partial_\tau^2 + \omega^2) &= \prod_{n=1}^{\infty} \left[\left(\frac{n\pi}{\tau_1 - \tau_0} \right)^2 + \omega^2 \right] \\ &= \underbrace{\prod_{n=1}^{\infty} \left(\frac{n\pi}{\tau_1 - \tau_0} \right)^2}_{?} \cdot \underbrace{\prod_{n=1}^{\infty} \left[1 + \left(\frac{\omega(\tau_1 - \tau_0)}{n\pi} \right)^2 \right]}_{\frac{\sinh \omega(\tau_1 - \tau_0)}{\omega(\tau_1 - \tau_0)}} \\ &\quad \downarrow \\ \det(\partial_t^2 + \omega^2) &= B \cdot \frac{\sin \omega(t_1 - t_0)}{\omega(t_1 - t_0)} \end{aligned} \quad (43)$$

The problematic factor is the ∞ -valued B , to which Das is prepared to assign whatever value is required in order to achieve

$$\lim_{t_1 \downarrow t_0} K(x_1, t_1; x_0, t_0) = \delta(x_1 - x_0)$$

This procedure would, however, be unavailable if the problem of assigning value to $\det(\partial_t^2 + \omega^2)$ had arisen as a free-standing problem, detached from any reference to the Feynman path-integral formalism.

Note that the problem just touched upon can be circumvented if one takes motivation from

$$\lim_{\omega \downarrow 0} \frac{\sin \omega(t_1 - t_0)}{\omega(t_1 - t_0)} = 1 \quad \text{and the } \omega\text{-independence of } B \equiv \prod_{n=1}^{\infty} \left(\frac{n\pi}{i(t_1 - t_0)} \right)^2$$

to look not to $\det(\partial_t^2 + \omega^2)$ itself but to the following *ratio* of functional determinants

$$\frac{\det(\partial_t^2 + \omega^2)}{\det(\partial_t^2)} = \frac{\sin \omega(t_1 - t_0)}{\omega(t_1 - t_0)} \quad (44)$$

Introduction to the contour integral method. It is—for a reason now evident—with *ratios* of functional determinants that Kristen and collaborators¹⁹ mainly concern themselves, as also does the anonymous author of the Wikipedia article on functional determinants²⁰ (though the latter neglects to mention the contour integral method, and does not cite Kristen).

Let $F(\lambda)$ be an entire function of the complex variable λ , and let it be the case that the zeros λ_n of $F(\lambda)$ are real/simple/non-negative. The associated zeta function is

$$\zeta_F(s) = \sum_n \lambda_n^{-s} = \frac{1}{2\pi i} \oint_{\mathcal{C}} \lambda^{-s} \left\{ \sum_n \frac{1}{\lambda - \lambda_n} \right\} d\lambda$$

where \mathcal{C} is any contour that envelopes all the zeros. Notice that expansion of $F(\lambda)$ around λ_n gives

$$\begin{aligned} F(\lambda) &= (\lambda - \lambda_n)F'(\lambda_n) + \frac{1}{2}(\lambda - \lambda_n)^2 F''(\lambda_n) + \dots \\ \frac{1}{F(\lambda)} &= \frac{1}{(\lambda - \lambda_n)F'(\lambda_n)} - \frac{F''(\lambda_n)}{2[F'(\lambda_n)]^2} + \mathcal{O}((\lambda - \lambda_n)^{-1}) \\ \frac{F'(\lambda)}{F(\lambda)} &= \frac{1}{(\lambda - \lambda_n)} + \frac{F''(\lambda_n)}{2F'(\lambda_n)} + \mathcal{O}((\lambda - \lambda_n)^{-1}) \end{aligned}$$

from which we learn that the function

$$\frac{d}{d\lambda} \log F(\lambda) = \frac{F'(\lambda)}{F(\lambda)}$$

has simple poles at the zeros of $F(\lambda)$. We are in position now to write

$$\zeta_F(s) = \sum_n \lambda_n^{-s} = \frac{1}{2\pi i} \oint_{\mathcal{C}} \lambda^{-s} \frac{d}{d\lambda} \log F(\lambda) d\lambda \quad (45)$$

which, as Kristen & Loya emphasize, may prove useful *even in situations where the zeros of $F(\lambda)$ remain unknown*.

¹⁹ His initial/principal collaborator appears to have been A. J. McKane: see “Functional determinants by contour integral methods,” *Ann. Phys.* **308**, 502–527 (2003) and “Functional determinants for general Sturm-Liouville problems,” *J. Phys. A* **37**, 4649–4670 (2004). It is interesting that neither paper makes explicit reference (in its title, at least) to the Feynman formalism.

²⁰ http://en.wikipedia.org/wiki/Functional_determinant

To illustrate the application of their method, Kristen & Loya look to the evaluation of the expression $\det(\partial_t^2 + \omega^2)$ that appears on the right side of (39), which was motivated by an equation

$$K_{\text{osc}}(x_1, t_1; x_0, t_0) = A \int \exp \left\{ -i \alpha \int_{t_0}^{t_1} \eta(\partial_t^2 + \omega^2) \eta dt \right\} \mathcal{D}\eta(t) \cdot e^{\frac{i}{\hbar} S_{\text{osc}}[x_{\text{cl}}(t)]}$$

produced in course of an application of the Feynman formalism to the oscillator problem.²¹ In their §2 they look to the evaluation of $\det(\partial_t^2)$,²² which in their §3 they look to the ratio (44). I follow their example:

FREE PARTICLE Borrowing now some equations from page 18 (in which I have set $\omega = 0$) we have

$$\begin{aligned} -\partial_\tau^2 \eta(\tau) &= \lambda \cdot \eta(\tau) & : & \quad \eta(\tau_0) = \eta(\tau_1) = 0 \\ \eta(\tau) &\sim \sin(\sqrt{\lambda}(\tau - \tau_0)) \end{aligned}$$

where λ is fixed by the condition

$$\sin(\sqrt{\lambda}T) = 0 \quad : \quad T \equiv \tau_1 - \tau_0$$

Evidently $\sqrt{\lambda} = n\pi/T$: $n = 0, 1, 2, \dots$ and the associated eigenfunctions are $\eta_n(\tau) \sim \sin(n\pi(\tau - \tau_0)/T)$. But $\eta_0(\tau)$ vanishes identically, so we must exclude the case $n = 0$. This Kristen & Loya do by identifying the eigenvalues λ_n with the zeros of

$$F(\lambda) \equiv \frac{\sin(\sqrt{\lambda}T)}{\sqrt{\lambda}T} = \frac{e^{i\sqrt{\lambda}T} - e^{-i\sqrt{\lambda}T}}{2i\sqrt{\lambda}T}$$

Introducing

$$f(\lambda) \equiv \frac{d}{d\lambda} \log F(\lambda) = \frac{T \cot \sqrt{\lambda}T}{2\sqrt{\lambda}} - \frac{1}{2\lambda}$$

into (45), we have

$$\zeta_F(s) = \frac{1}{2\pi i} \oint_{\mathcal{C}} \left\{ \lambda^{-(s+\frac{1}{2})} \cdot \frac{1}{2} T \cot \sqrt{\lambda}T - \frac{1}{2} \lambda^{-(s+1)} \right\} d\lambda$$

and see that to insure convergence of such integrals we must have $\frac{1}{2} < \Re(s)$. Relatedly, expansion about the origin gives

$$\lambda^{-s} f(\lambda) = -\frac{1}{6} T^2 \lambda^{-s} - \frac{1}{90} T^4 \lambda^{1-s} - \frac{1}{945} T^6 \lambda^{2-s} - \dots \quad (46)$$

so if we are (after we have deformed the contour—see below) to avoid picking up a residue at the origin we must have $\frac{1}{2} < \Re(s) < 1$.

²¹ Kristen & Loya mention the Feynman formalism in their abstract, but do not attempt to indicate how one gets from Feynman formalism to the class of problems they address.

²² An oscillator with $\omega = 0$ is, of course, simply a free particle.

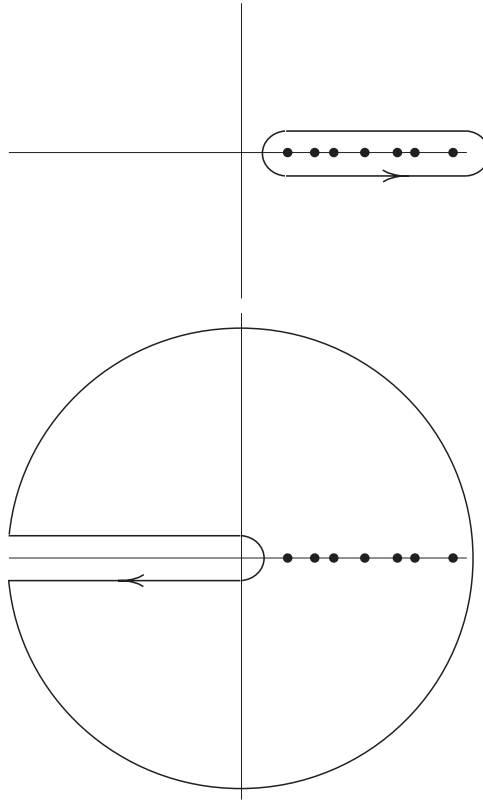


FIGURE 1: *The contours \mathcal{C} and \mathcal{C}' employed by Kristen & Loya.*

Kristen & Loya now exercise their established right to deform the contour: $\mathcal{C} \rightarrow \mathcal{C}'$. The integral of interest resolves into three components:

$$\begin{aligned}
 \frac{1}{2\pi i} \oint_{\mathcal{C}'} \lambda^{-s} f(\lambda) d\lambda &= \frac{1}{2\pi i} \int_{-\infty}^0 (\xi + i\varepsilon)^{-s} f(\xi + i\varepsilon) d(\xi + i\varepsilon) \\
 &+ \frac{1}{2\pi i} \int_{\pi/2}^{-\pi/2} (\varepsilon e^{i\theta})^{-s} f(\varepsilon e^{i\theta}) \varepsilon i d\theta \\
 &+ \frac{1}{2\pi i} \int_0^{-\infty} (\xi - i\varepsilon)^{-s} f(\xi - i\varepsilon) d(\xi - i\varepsilon)
 \end{aligned} \tag{47}$$

The second term is (by (46)) readily seen to vanish in the limit $\varepsilon \downarrow 0$. Looking to the first and third terms, we observe that $(\xi + i\varepsilon)$ has a branch cut that extends along the negative half of the real axis: as one passes \downarrow across the negative real axis the phase jumps from $+\pi$ to $-\pi$.²³ We therefore have

²³ To see this, command `Plot3D[Evaluate[Arg[ComplexExpand[x+iy]]], {x,-5,5}, {y,-5,5}, PlotRange->{-π,π}]`

$$\lim_{\varepsilon \downarrow 0} (-x + i\varepsilon)^{-s} = x e^{-i\pi s}$$

$$\lim_{\varepsilon \downarrow 0} (-x - i\varepsilon)^{-s} = x e^{+i\pi s}$$

The phase of $f(\xi + i\varepsilon) d(\xi + i\varepsilon)$ is, on the other hand, found to be zero on the negative real axis, and to display no such phase discontinuity. So the first and third of the terms on the right side of (47) can be written

$$\begin{aligned} & \frac{e^{-i\pi s}}{2\pi i} \int_{\infty}^0 x^{-s} \frac{d}{dx} \log F(-x) dx + \frac{e^{+i\pi s}}{2\pi i} \int_0^{\infty} x^{-s} \frac{d}{dx} \log F(-x) dx \\ &= \frac{\sin \pi s}{\pi} \int_0^{\infty} x^{-s} \frac{d}{dx} \log F(-x) dx \\ &= \frac{\sin \pi s}{\pi} \int_0^{\infty} x^{-s} \frac{d}{dx} \log \frac{\sinh \sqrt{x} T}{\sqrt{x} T} dx \end{aligned} \quad (48)$$

If that were indeed a correct description of $\zeta_F(s)$ it would immediately follow that

$$\zeta'_F(0) = \int_0^{\infty} \frac{d}{dx} \log \frac{\sinh \sqrt{x} T}{\sqrt{x} T} dx = \log \frac{\sinh \sqrt{x} T}{\sqrt{x} T} \Big|_0^{\infty} = \infty - 0$$

but $s \downarrow 0$ has placed us in violation of the condition $\frac{1}{2} < \Re(s) < 1$, and has led to an absurd result. Kristen & Loya remind us that the condition $\frac{1}{2} < \Re(s)$ was introduced to temper an integrand in the limit $x \uparrow \infty$. Returning to (48), they write

$$\int_0^{\infty} = \int_0^1 + \int_1^{\infty}$$

and in the latter integral use

$$\log \frac{\sinh \sqrt{x} T}{\sqrt{x} T} = \log e^{T\sqrt{x}} - \log T\sqrt{x} + \log (1 - e^{-2T\sqrt{x}})$$

to obtain

$$\begin{aligned} & \int_1^{\infty} x^{-s} \frac{d}{dx} \log \frac{\sinh \sqrt{x} T}{\sqrt{x} T} dx \\ &= \int_1^{\infty} \left\{ \frac{1}{2} T x^{-s-\frac{1}{2}} - \frac{1}{2} x^{-s-1} + x^{-s} \frac{d}{dt} \log (1 - e^{-2T\sqrt{x}}) \right\} dx \\ &= T \frac{1}{2s-1} - \frac{1}{2s} + \int_1^{\infty} x^{-s} \frac{d}{dt} \log (1 - e^{-2T\sqrt{x}}) dx \end{aligned}$$

giving

$$\begin{aligned} \zeta_F(s) &= T \frac{\sin \pi s}{(2s-1)\pi} - \frac{\sin \pi s}{2\pi s} + \frac{\sin \pi s}{\pi} \int_1^{\infty} x^{-s} \frac{d}{dx} \log (1 - e^{-2T\sqrt{x}}) dx \\ &\quad + \frac{\sin \pi s}{\pi} \int_0^1 x^{-s} \frac{d}{dx} \log \frac{\sinh \sqrt{x} T}{\sqrt{x} T} dx \end{aligned}$$

where the leading term shows the origin of the $\frac{1}{2} < \Re(s)$ requirement. Now apply $\lim_{s \downarrow 0} \frac{d}{ds}$, get²⁴

$$\begin{aligned}
\zeta'_F(0) &= -T - 0 + \left\{ \log \left(1 - e^{-2T\sqrt{x}} \right) \right\} \Big|_1^\infty \\
&\quad + \left\{ \log e^{T\sqrt{x}} + \log \left(\frac{1 - e^{-2T\sqrt{x}}}{T\sqrt{x}} \right) \right\} \Big|_0^1 \\
&= -T - 0 + \{ 0 - \log(1 - e^{-2T}) \} \\
&\quad + \{ T + \log(1 - e^{-2T}) - \log T \} \\
&\quad - \log \left(\frac{\sinh T\sqrt{x}}{T\sqrt{x}} \right) \Big|_0 \\
&= -\log T - \left\{ \log 2 + \frac{2}{3}T^2x - \frac{4}{45}T^6x^3x^2 + \frac{64}{2835}T^6x^3 - \dots \right\} \Big|_0 \\
&= -\log 2T
\end{aligned} \tag{49}$$

To recapitulate: standard quantum mechanics leads naturally to the spectral representation of the propagator, which in the case of a free particle (see again page 8) reads

$$\begin{aligned}
K_{\text{free}}(x_1, t_1; x_0, t_0) &= \int (x_1|p) e^{-\frac{i}{\hbar} \frac{1}{2m} p^2 (t_1 - t_0)} (p|x_0) \\
&= \sqrt{\frac{m}{i\hbar(t_1 - t_0)}} \cdot \exp \left\{ \frac{i}{\hbar} S_{\text{classical free}}(x_1, t_1; t_0, t_0) \right\}
\end{aligned}$$

where

$$S_{\text{classical free}}(x_1, t_1; t_0, t_0) = \frac{m}{2} \frac{(x_1 - x_0)^2}{t_1 - t_0}$$

We were, on the other hand, led (at (35)) by Feynman formalism to write

$$\begin{aligned}
K_{\text{free}}(x_1, t_1; x_0, t_0) &= A \int \exp \left\{ \frac{i}{\hbar} \int_{t_0}^{t_1} \frac{m}{2} [\dot{\eta}\dot{\eta}] dt \right\} \mathcal{D}\eta(t) \\
&\quad \cdot \exp \left\{ \frac{i}{\hbar} S_{\text{classical free}}(x_1, t_1; t_0, t_0) \right\}
\end{aligned}$$

and looked therefore to the evaluation of

$$\begin{aligned}
\int \exp \left\{ \frac{i}{\hbar} \int_{t_0}^{t_1} \frac{m}{2} [\dot{\eta}\dot{\eta}] dt \right\} \mathcal{D}\eta(t) &= \int \exp \left\{ -i\alpha \int_{t_0}^{t_1} \eta (\partial_t^2) \eta dt \right\} \mathcal{D}\eta(t) \\
&= \int \exp \left\{ -\alpha \int_{\tau_0}^{\tau_1} \eta (-\partial_\tau^2) \eta d\tau \right\} \mathcal{D}\eta(\tau)
\end{aligned}$$

²⁴ Use

$$\frac{\sin \pi s}{2\pi s} = \frac{1}{2} - \frac{1}{12}(\pi s)^2 + \frac{1}{240}(\pi s)^4 \dots$$

In the final step of the argument we will again use Taylor expansion to clarify the meaning of a seemingly improper limit.

where $\alpha = m/2\hbar$ and $\tau = it$. We found it expedient to set $\alpha = 1$ and, proceeding in formal imitation of (37.1), wrote

$$\begin{aligned} \int \exp \left\{ - \int_{\tau_0}^{\tau_1} \eta (-\partial_\tau^2) \eta d\tau \right\} \mathcal{D}\eta(\tau) &\sim \frac{1}{\sqrt{\det(-\partial_\tau^2)}} \\ &= \frac{1}{\sqrt{\det(\prod_n \lambda_n)}} \end{aligned}$$

where the λ_n are defined by the equations

$$(-\partial_\tau^2)\eta(\tau) = \lambda \cdot \eta(\tau) \quad : \quad \eta(\tau_0) = \eta(\tau_1) = 0$$

and were found to comprise the zeros of

$$F(\lambda) = \frac{\sin(\sqrt{\lambda}(\tau_1 - \tau_0))}{\sqrt{\lambda}(\tau_1 - \tau_0)}$$

We introduced

$$\zeta_F(s) = \sum_n \lambda_n^{-s}$$

in terms of which we were able to write

$$\det(-\partial_\tau^2) = \exp \{ -\zeta'_F(0) \}$$

We used Kristen & Loya's contour integration technique to obtain

$$\zeta'_F(0) = -\log[2(\tau_1 - \tau_0)]$$

whence

$$\begin{aligned} \det(-\partial_\tau^2) &= 2(\tau_1 - \tau_0) \\ \int \exp \left\{ - \int_{\tau_0}^{\tau_1} \eta (-\partial_\tau^2) \eta d\tau \right\} \mathcal{D}\eta(\tau) &\sim \frac{1}{\sqrt{2(\tau_1 - \tau_0)}} \\ &= \frac{1}{\sqrt{2i(t_1 - t_0)}} \end{aligned}$$

To relax the $\alpha = 1$ assumption we have only to rescale τ :

$$\begin{aligned} \int \exp \left\{ - \int_{\tau_0}^{\tau_1} \eta (-\partial_\tau^2) \eta d\tau \right\} \mathcal{D}\eta(\tau) &= \int \exp \left\{ - \alpha \int_{\tau_0/\alpha}^{\tau_1/\alpha} \eta (-\partial_{\alpha\tau}^2) \eta d(\alpha\tau) \right\} \mathcal{D}\eta(\tau) \\ &\sim \sqrt{\frac{\alpha}{2(\tau_1 - \tau_0)}} \\ &= \sqrt{\frac{m\pi}{i\hbar(t_1 - t_0)}} \end{aligned}$$

So to achieve

$$\lim_{t_1 \downarrow t_0} K_{\text{free}}(x_1, t_1; x_0, t_0) = \delta(x_1 - x_0)$$

we have to set $A = \sqrt{1/\pi}$.

OSCILLATOR The functional integral of interest now reads

$$\int \exp \left\{ - \int_{\tau_0}^{\tau_1} \eta (-\partial_\tau^2 + \omega^2) \eta d\tau \right\} \mathcal{D}\eta(\tau) \sim \frac{1}{\sqrt{\det(-\partial_\tau^2 + \omega^2)}}$$

The equations

$$(-\partial_\tau^2 + \omega^2)\eta(\tau) = \lambda \cdot \eta(\tau) \quad : \quad \eta(\tau_0) = \eta(\tau_1) = 0$$

lead to eigenvalues that are the zeros of

$$G(\lambda) = \frac{\sin(\sqrt{\lambda - \omega^2}(\tau_1 - \tau_0))}{\sqrt{\lambda - \omega^2}(\tau_1 - \tau_0)}$$

Kirsten & Loya elect to look to the ratio

$$\frac{\det(-\partial_\tau^2 + \omega^2)}{\det(-\partial_\tau^2)} = \frac{\exp\{-\zeta'_G(0)\}}{\exp\{-\zeta'_F(0)\}} = \exp\{-\zeta'_G(0) + \zeta'_F(0)\}$$

Reading from (45), we have

$$\begin{aligned} \zeta'_G(s) - \zeta'_F(s) &= \frac{1}{2\pi i} \oint_{\mathcal{C}} \lambda^{-s} \frac{d}{d\lambda} \log \frac{G(\lambda)}{F(\lambda)} d\lambda \\ &= \frac{1}{2\pi i} \oint_{\mathcal{C}} \lambda^{-s} \frac{d}{d\lambda} \log \left[\frac{\sin(T\sqrt{\lambda - \omega^2})}{\sqrt{\lambda - \omega^2}} \frac{\sqrt{\lambda}}{\sin(T\sqrt{\lambda})} \right] d\lambda \end{aligned}$$

where (as before) $T = (\tau_1 - \tau_0)$. Deformation of the contour supplies

$$= \frac{\sin \pi s}{\pi s} \int_0^\infty x^{-s} \frac{d}{dx} \log \left[\frac{\sinh(T\sqrt{x + \omega^2})}{\sqrt{x + \omega^2}} \frac{\sqrt{x}}{\sinh(T\sqrt{x})} \right] dx$$

From here the argument proceeds as before (but without the intrusion of nasty singularities) to

$$\log \frac{\det(-\partial_\tau^2 + \omega^2)}{\det(-\partial_\tau^2)} = -\zeta'_G(0) + \zeta'_F(0) = \log \frac{\sinh \omega(\tau_1 - \tau_0)}{\omega(\tau_1 - \tau_0)}$$

from which we could easily extract a description of

$$\frac{K_{\text{osc}}(x_1, t_1; x_0, t_0)}{K_{\text{free}}(x_1, t_1; x_0, t_0)}$$

if reason could be discovered to have interest in such a ratio.