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CALCULUS OF FUNCTIONALS

Introduction. In classical mechanics one has interest in functions x(t) of a single variable, while in field theory one's interest shifts to functions $\varphi(t, x)$ of several variables, but the ordinary calculus of functions of several variables would appear to be as adequate to the mathematical needs of the latter subject as it is to the former. And so, in large part, it is. But the "variational principles of mechanics" do typically reach a little beyond the bounds of the ordinary calculus. We had occasion already on p. 16 to remark in passing that $S[\varphi] = \int \mathcal{L}(\varphi, \partial \varphi) dx$ is by nature a "number-valued function of a function," and to speak therefore not of an "action function" but of the action functional; it was, in fact, to emphasize precisely that distinction that we wrote not $S(\varphi)$ but $S[\varphi]$. When one speaks—as Hamilton's principle asks us to do—of the variational properties of such an object one is venturing into the "calculus of functionals," but only a little way. Statements of the (frequently very useful) type $\delta f(x) = 0$ touch implicitly upon the concept of differentiation, but scarcely hint at the elaborate structure which is the calculus itself. Similarly, statements of the (also often useful) type $\delta S[\varphi] = 0$, though they exhaust the subject matter of the "calculus of variations," scarcely hint at the elaborate (if relatively little known) structure which I have in the present chapter undertaken to review. Concerning my motivation:

At (60) in Chapter I we had occasion to speak of the "Poisson bracket" of a pair of functionals $A = \int \mathcal{A}(\pi, \varphi, \nabla \pi, \nabla \varphi) dx$ and $B = \int \mathcal{B}(\pi, \varphi, \nabla \pi, \nabla \varphi) dx$, and this—since in mechanics the Poisson bracket of observables A(p,q) and B(p,q) is defined

$$[A,B] \equiv \sum_{k=1}^{n} \left\{ \frac{\partial A}{\partial q^{k}} \frac{\partial B}{\partial p_{k}} - \frac{\partial B}{\partial q^{k}} \frac{\partial A}{\partial p_{k}} \right\}$$

—would appear (as noted already on p. 49) to entail that be we in position to attach meaning to the "derivative" of a functional. One of my initial objectives

will be to show how this is done. We will learn how to compute functional derivatives to all orders, and will discover that such constructions draw in an essential way upon the theory of distributions—a subject which, in fact, belongs properly not to the theory of functions but to the theory of functionals.¹ We will find ourselves then in position to construct the functional analogs of Taylor series. Our practical interest in the integral aspects of the functional calculus we owe ultimately to Richard Feynman; we have seen that the Schrödinger equation provides—interpretive matters aside—a wonderful instance of a classical field, and it was Feynman who first noticed (or, at least, who first drew attention to the importance of the observation) that the Schrödinger equation describes a property of a certain functional integral. We will want to see how this comes about. Methods thus acquired become indispensible when one takes up the quantization of classical field theory; they are, in short, dominant in quantum field theory. Which, however, is not our present concern. Here our objective will be simply to put ourselves in position to recognize certain moderately subtle distinctions, to go about our field-theoretic business with greater precision, to express ourselves with greater notational economy.

Construction of the functional derivative. By way of preparation, let $F(\varphi)$ be a number-valued function of the finite-dimensional vector φ . What shall we mean by the "derivative of $F(\varphi)$?" The key observation here is that we can mean many things, depending on the direction in which we propose to move while monitoring rate of change; the better question therefore is "What shall me mean by the directional derivative of $F(\varphi)$?" And here the answer is immediate: take λ to be any fixed vector and form

$$\mathbf{D}_{[\boldsymbol{\lambda}]}F(\boldsymbol{\varphi}) \equiv \lim_{\epsilon \to 0} \frac{F(\boldsymbol{\varphi} + \epsilon \boldsymbol{\lambda}) - F(\boldsymbol{\varphi})}{\epsilon}$$
(1.1)

$$=\sum_{i}\frac{\partial F(\varphi)}{\partial \varphi^{i}}\lambda^{i}$$
(1.2)

 \equiv derivative of $F(\boldsymbol{\varphi})$ "in the direction $\boldsymbol{\lambda}$ "

We might write

$$\mathbf{D}_{[\boldsymbol{\lambda}]}F(\boldsymbol{\varphi}) \equiv F[\boldsymbol{\varphi};\boldsymbol{\lambda}]$$

to underscore the fact that $\mathbf{D}_{[\lambda]}F(\varphi)$ is a *bifunctional*. From (1.2) it is plain that $F[\varphi; \lambda]$ is, so far as concerns its λ -dependence, a *linear* functional:

$$F[\boldsymbol{\varphi}; c_1 \boldsymbol{\lambda}_1 + c_2 \boldsymbol{\lambda}_2] = c_1 F[\boldsymbol{\varphi}; \boldsymbol{\lambda}_1] + c_2 F[\boldsymbol{\varphi}; \boldsymbol{\lambda}_2]$$

I have now to describe the close relationship between "linear functionals" on the one hand, and "inner products" on the other. Suppose $\boldsymbol{\alpha} = \sum \alpha^{i} \mathbf{e}_{i}$ and $\boldsymbol{\lambda} = \sum \lambda^{i} \mathbf{e}_{i}$ are elements of an inner product space. Then $(\boldsymbol{\alpha}, \boldsymbol{\lambda})$ is, by one

¹ See J. Lützen's wonderful little book, The Prehistory of the Theory of Distributions, (1982).

Functional differentiation

of the defining properties of the inner product, a bilinear functional. It is, in particular, a linear functional of λ —call it $A[\lambda]$ —and can be described

$$(\boldsymbol{\alpha}, \boldsymbol{\lambda}) = A[\boldsymbol{\lambda}] = \sum_{i} \alpha_i \lambda^i \quad \text{with} \quad \alpha_i = \sum_{j} (\mathbf{e}_i, \mathbf{e}_j) \alpha^j$$

The so-called *Riesz-Frechet Theorem* runs in the opposite direction; it asserts² that if $A[\boldsymbol{\lambda}]$ is a linear functional defined on an inner product space, then there exists an $\boldsymbol{\alpha}$ such that $A[\boldsymbol{\lambda}]$ can be represented $A[\boldsymbol{\lambda}] = (\boldsymbol{\alpha}, \boldsymbol{\lambda})$. Returning in the light of this fundamental result to (1), we can say that (1.1) defines a linear functional of $\boldsymbol{\lambda}$, therefore there exists an $\boldsymbol{\alpha}$ such that

$$\mathbf{D}_{[\boldsymbol{\lambda}]}F(\boldsymbol{\varphi}) = (\boldsymbol{\alpha},\boldsymbol{\lambda}) = \sum_i \alpha_i \lambda^i$$

and that we have found it convenient/natural in place of α_i to write $\frac{\partial F(\varphi)}{\partial \varphi^i}$.

It is by direct (infinite-dimensional) imitation of the preceeding line of argument that we construct what might be (but isn't) called the "directional derivative of a functional $F[\varphi(x)]$." We note that

$$\mathbf{D}_{[\lambda(x)]}F[\varphi(x)] \equiv \lim_{\epsilon \to 0} \frac{F[\varphi(x) + \epsilon\lambda(x)] - F[\varphi(x)]}{\epsilon}$$
(2.1)

is a linear functional of $\lambda(x)$, and admits therefore of the representation

$$= \int \alpha(x')\lambda(x')\,dx' \tag{2.2}$$

And we agree, as a matter simply of notation (more specifically, as a reminder that $\alpha(x)$ came into being as the result of a differentiation process applied to the functional $F[\varphi(x)]$), to write

$$\alpha(x) = \frac{\delta F[\varphi]}{\delta \varphi(x)} = \int \alpha(x') \,\delta(x' - x) \,dx' \tag{3}$$

Evidently $\frac{\delta F[\varphi]}{\delta \varphi(x)}$ itself can be construed to describe the result of differentiating $F[\varphi]$ in the "direction" of the δ -function which is singular at the point x. If, in particular, $F[\varphi]$ has the structure

$$F[\varphi] = \int f(\varphi(x)) dx \tag{4.1}$$

then the construction (2.1) gives

$$\mathbf{D}_{[\lambda]}F[\varphi] = \int \lambda(x) \frac{\partial}{\partial \varphi} f(\varphi(x)) \, dx$$

² For a proof see F. Riesz & B. Sz.Nagy, *Functional Analysis* (1955), p. 61.

whence

$$\frac{\delta F[\varphi]}{\delta \varphi(x)} = \frac{\partial}{\partial \varphi} f(\varphi(x)) \tag{4.2}$$

And if, more generally,

$$F[\varphi] = \int f(\varphi(x), \varphi_x(x)) \, dx \tag{5.1}$$

then by a familiar argument

$$\mathbf{D}_{[\lambda]}F[\varphi] = \int \lambda(x) \left\{ \frac{\partial}{\partial \varphi} - \frac{\partial}{\partial x} \frac{\partial}{\partial \varphi_x} \right\} f(\varphi(x), \varphi_x(x)) \, dx$$

and we have

$$\frac{\delta F[\varphi]}{\delta \varphi(x)} = \left\{ \frac{\partial}{\partial \varphi} - \frac{\partial}{\partial x} \frac{\partial}{\partial \varphi_x} \right\} f(\varphi(x), \varphi_x(x))$$
(5.2)

In such cases $\frac{\delta F[\varphi]}{\delta \varphi(x)}$ flourishes in the sunshine, as it has flourished unrecognized in preceeding pages, beginning at about p. 43. But it is in the general case distribution-like, as will presently become quite clear; it popped up, at (2.2), in the shade of an integral sign, and can like a mushroom become dangerous when removed from that protective gloom. There is, in short, some hazard latent in the too-casual use of (3).

It follows readily from (2) that the functional differentiation operator $\mathbf{D}_{[\lambda(x)]}$ acts linearly

$$\mathbf{D}_{[\lambda]} \{ F[\varphi] + G[\varphi] \} = \mathbf{D}_{[\lambda]} F[\varphi] + \mathbf{D}_{[\lambda]} G[\varphi]$$
(6.1)

and acts on products by the familiar rule

$$\mathbf{D}_{[\lambda]}\left\{F[\varphi] \cdot G[\varphi]\right\} = \left\{\mathbf{D}_{[\lambda]}F[\varphi]\right\} \cdot G[\varphi] + F[\varphi] \cdot \left\{\mathbf{D}_{[\lambda]}G[\varphi]\right\}$$
(6.2)

In the shade of an implied integral sign we therefore have

$$\frac{\delta}{\delta\varphi(x)} \Big\{ F[\varphi] + G[\varphi] \Big\} = \frac{\delta}{\delta\varphi(x)} F[\varphi] + \frac{\delta}{\delta\varphi(x)} G[\varphi]$$
(7.1)

and

$$\frac{\delta}{\delta\varphi(x)} \Big\{ F[\varphi] \cdot G[\varphi] \Big\} = \Big\{ \frac{\delta}{\delta\varphi(x)} F[\varphi] \Big\} \cdot G[\varphi] + F[\varphi] \cdot \Big\{ \frac{\delta}{\delta\varphi(x)} G[\varphi] \Big\}$$
(7.2)

In connection with the product rule it is, however, important not to confuse $F[\varphi] \cdot G[\varphi] = \int f dx' \cdot \int g dx''$ with $F[\varphi] * G[\varphi] = \int (f \cdot g) dx$.

A second φ -differentiation of the linear bifunctional

$$F[\varphi;\lambda_1] = \mathbf{D}_{[\lambda_1]}F[\varphi] = \int \frac{\delta F[\varphi]}{\delta \varphi(x')} \lambda_1(x') \, dx'$$

Volterra series

yields a bilinear trifunctional

$$F[\varphi;\lambda_1,\lambda_2] = \mathbf{D}_{[\lambda_2]}F[\varphi;\lambda_1] = \mathbf{D}_{[\lambda_2]}\mathbf{D}_{[\lambda_1]}F[\varphi]$$
$$= \int \int \frac{\delta^2 F[\varphi]}{\delta\varphi(x')\delta\varphi(x'')}\lambda_1(x')\lambda_2(x'')\,dx'dx'' \tag{8}$$

In general we expect to have (and will explicitly assume that)

$$\mathbf{D}_{[\lambda_2]}\mathbf{D}_{[\lambda_1]}F[\varphi] = \mathbf{D}_{[\lambda_1]}\mathbf{D}_{[\lambda_2]}F[\varphi]$$

which entails that

$$\frac{\delta^2 F[\varphi]}{\delta \varphi(x') \delta \varphi(x'')} \quad \text{is a symmetric function of } x' \text{ and } x''$$

By natural extension we construct φ -derivatives of all orders:

$$\begin{split} \mathbf{D}_{[\lambda_n]} \cdots \mathbf{D}_{[\lambda_2]} \mathbf{D}_{[\lambda_1]} F[\varphi] &= F[\varphi; \lambda_1, \lambda_2, \dots, \lambda_n] \\ &= \iint \cdots \int \underbrace{\frac{\delta^n F[\varphi]}{\delta\varphi(x^1)\delta\varphi(x^2) \cdots \delta\varphi(x^n)}}_{\text{totally symmetric in } x^1, x^2, \dots, x^n} \end{split}$$

Functional analog of Taylor's series. In the ordinary calculus of functions, derivatives of ascending order are most commonly encountered in connection with the theory of Taylor series; one writes

$$f(x+a) = \exp\left\{a\frac{d}{dx}\right\}f(x) = \sum_{n}\frac{1}{n!}\frac{d^{n}f(x)}{dx^{n}}a^{n}$$
(9)

which is justified by the observation that, for all n,

$$\lim_{a \to 0} \left(\frac{d}{da}\right)^n (\text{lefthand side}) = \lim_{a \to 0} \left(\frac{d}{da}\right)^n (\text{righthand side})$$

Similarly

$$\begin{aligned} f(x+a,y+b) &= \exp\left\{a\frac{\partial}{\partial x} + b\frac{\partial}{\partial y}\right\}f(x) \\ &= f(x,y) + \left\{af_x(x,y) + bf_y(x,y)\right\} \\ &+ \frac{1}{2!}\left\{a^2f_{xx}(x,y) + 2abf_{xy}(x,y) + b^2f_{yy}(x,y)\right\} + \cdots \end{aligned}$$

No mystery attaches now to the sense in which (and why) it becomes possible (if we revert to the notation of p.74) to write

$$F(\varphi + \lambda) = \exp\left\{\sum \lambda^{i} \frac{\partial}{\partial \varphi^{i}}\right\} F(\varphi)$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left\{\sum_{i_{1}} \sum_{i_{2}} \cdots \sum_{i_{n}} F_{i_{1}i_{2}\cdots i_{n}}(\varphi) \lambda^{i_{1}} \lambda^{i_{2}} \cdots \lambda^{i_{n}}\right\}$$

with $F_{i_1i_2\cdots i_n}(\boldsymbol{\varphi}) \equiv \partial_{i_1}\partial_{i_2}\cdots \partial_{i_n}F(\boldsymbol{\varphi})$ where $\partial_i \equiv \frac{\partial}{\partial \varphi^i}$. Passing finally to the continuous limit, we obtain

$$F[\varphi + \lambda] = \exp\left\{\mathbf{D}_{[\lambda]}\right\} F[\varphi]$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left\{ \iint \cdots \int F(x^1, x^2, \dots, x^n; \varphi) \lambda(x^1) \lambda(x^2) \cdots \lambda(x^n) dx^1 dx^2 \cdots dx^n \right\}$$
(10)

with $F(x^1, x^2, ..., x^n; \varphi) \equiv \delta^n F[\varphi] / \delta \varphi(x^1) \delta \varphi(x^2) \cdots \delta \varphi(x^n)$. The right side of (10) displays $F[\varphi + \lambda]$ as a "Volterra series"—the functional counterpart of a Taylor series.³ Taylor's formula (11) embodies an idea

function of interest =
$$\sum$$
 elementary functions

which is well known to lie at the heart of analysis (i.e., of the theory of functions).⁴ We are encouraged by the abstractly identical structure and intent of Volterra's formula (12) to hope that this obvious variant

functional of interest = \sum elementary functionals

$$f(a+x) = \sum_{n} \frac{1}{n!} f_n x^n \quad \text{with} \quad f_n = \frac{d^n f(a)}{da^n} \tag{11}$$

Similarly, (10) upon interchange $\varphi \leftrightarrows \lambda$ and subsequent notational adjustment $\lambda \to \alpha$ becomes

$$F[\alpha + \varphi] = \sum_{n=0}^{\infty} \frac{1}{n!} \left\{ \iint \cdots \int F(x^1, x^2, \dots, x^n) \cdot \\ \cdot \varphi(x^1)\varphi(x^2) \cdots \varphi(x^n) dx^1 dx^2 \cdots dx^n \right\}$$
(12)

with $F(x^1, x^2, \dots, x^n) \equiv \delta^n F[\alpha] / \delta \alpha(x^1) \delta \alpha(x^2) \cdots \delta \alpha(x^n).$

⁴ To Kronecker's "God made the integers; all else is the work of man" his contemporary Weierstrass is said to have rejoined "God made *power series*; all else is the work of man." It becomes interesting in this connection to recall that E. T. Bell, in his *Men of Mathematics*, introduces his Weierstrass chapter with these words: "The theory that has had the greatest development in recent times is without any doubt the theory of functions." And that those words were written by Vito Volterra—father of the functional calculus.

³ Set $a = \delta x$ in (9), or $\lambda = \delta \varphi$ in (10), and you will appreciate that I had the calculus of variations in the back of my mind when I wrote out the preceeding material. The results achieved seem, however, "backwards" from another point of view; we standardly seek to "expand f(a + x) in powers of x about the point a," not the reverse. A version of (9) which is less offensive to the eye of an "expansion theorist" can be achieved by simple interchange $x \leftrightarrows a$:

Volterra series

of that same idea will lead with similar force and efficiency to a theory of functionals (or functional analysis).

Simple examples serve to alert us the fact that surprises await the person who adventures down such a path. Look, by way of illustration, to the functional

$$F[\varphi] \equiv \int \varphi^2(x) \, dx \tag{13.1}$$

Evidently we can, if we wish, write

$$= \int \int F(x^1, x^2) \cdot \varphi(x^1)\varphi(x^2) dx^1 dx^2$$
$$F(x^1, x^2) = \delta(x^1 - x^2) \tag{13.2}$$

with

The obvious lesson here is that, while the expansion coefficients
$$f_n$$
 which appear on the right side of Taylor's formula (11) are by nature numbers, the "expansion coefficients" $F(x^1, x^2, \ldots, x^n)$ which enter into the construction (12)

of a "Volterra series" may, even in simple cases, be *distributions*.

Look next to the example

$$F[\varphi] \equiv \int \varphi(x)\varphi_x(x)\,dx \tag{14.1}$$

From $\varphi \varphi_x = \frac{1}{2} (\varphi^2)_x$ we obtain

= boundary terms

Since familiar hypotheses are sufficient to cause boundary terms to vanish, what we have here is a *complicated description of the zero-functional*, the Volterra expansion of which is trivial. One might, alternatively, argue as follows:

$$\begin{split} \varphi_x(x) &= \int \delta(y-x)\varphi_y(y)\,dy\\ &= -\int \delta'(y-x)\varphi(y)\,dy \quad \text{by partial integration} \end{split}$$

Therefore

$$F[\varphi] = -\int \int \delta'(y-x)\varphi(x)\varphi(y)\,dxdy$$

But only the symmetric part of $\delta'(y-x)$ contributes to the double integral, and

$$\delta'(y-x) = \lim_{\epsilon \to 0} \frac{\delta(y-x+\epsilon) - \delta(y-x-\epsilon)}{2\epsilon}$$

is, by the symmetry of $\delta(z)$, clearly antisymmetric. So again we obtain

$$F[\varphi] = 0 \tag{14.2}$$

Look finally to the example

$$F[\varphi] \equiv \int \varphi_x^2(x) \, dx \tag{15.1}$$

From $\varphi_x^2 = -\varphi \varphi_{xx} + (\varphi \varphi_x)_x$ we have $F[\varphi] = -\int \varphi \varphi_{xx} dx$ plus a boundary term which we discard. But

$$\begin{split} \varphi_{xx}(x) &= \int \delta(y-x)\varphi_{yy}(y)\,dy \\ &= -\int \delta'(y-x)\varphi_y(y)\,dy \quad \text{by partial integration} \\ &= +\int \delta''(y-x)\varphi(y)\,dy \quad \text{by a second partial integration} \end{split}$$

and

$$\delta^{\prime\prime}(y-x) = \lim_{\epsilon \to 0} \frac{\delta^{\prime}(y-x+\epsilon) - \delta^{\prime}(y-x-\epsilon)}{2\epsilon}$$

is, by the antisymmetry of $\delta'(z)$, symmetric. So we have

$$F[\varphi] = \int \int F(x^1, x^2) \cdot \varphi(x^1) \varphi(x^2) dx^1 dx^2$$

with

$$F(x^1, x^2) = \delta''(x^1 - x^2)$$
(15.2)

Again, the "expansion coefficient" $F(x^1, x^2)$ is not a number, not a function, but a distribution.

The methods employed in the treatment of the preceeding examples have been straightforward enough, yet somewhat *ad hoc*. Volterra's formula (12) purports to supply a systematic general method for attacking such problems. How does it work? Let $F[\varphi]$ be assumed to have the specialized but frequently encountered form

$$F[\varphi] = \int f(\varphi, \varphi_x) \, dx \tag{16}$$

Our objective is to expand $F[\alpha + \varphi]$ "in powers of φ " (so to speak) and then set $\alpha(x)$ equal to the "zero function" 0(x). Our objective, in short, is to construct the functional analog of a "Maclaurin series:"

$$F[\varphi] = F_0 + F_1[\varphi] + \frac{1}{2}F_2[\varphi] + \cdots$$
 (17)

Trivially $F_0 = \int f(\alpha, \alpha_x) dx \big|_{\alpha=0}$ and familiarly

$$F_{1}[\varphi] = \left[\mathbf{D}_{[\varphi]} \int f(\alpha, \alpha_{x}) dx\right]_{\alpha=0}$$
$$= \int \underbrace{\left[\left\{\frac{\partial}{\partial \alpha} - \frac{d}{dx} \frac{\partial}{\partial \alpha_{x}}\right\} f(\alpha, \alpha_{x})\right]_{\alpha=0}}_{=\frac{\delta F[\alpha]}{\delta \alpha(x)}, \text{ evaluated at } \alpha = 0$$
(18)

Volterra series

But this is as far as we can go on the basis of experience standard to the $(1^{st}$ -order) calculus of variations. We have

$$F_{2}[\varphi] = \left[\mathbf{D}_{[\varphi]} \mathbf{D}_{[\varphi]} \int f(\alpha, \alpha_{x}) dx \right]_{\alpha=0}$$

$$= \left[\mathbf{D}_{[\varphi]} \int \underline{g(\alpha, \alpha_{x}, \alpha_{xx})} \varphi(x) dx \right]_{\alpha=0}$$

$$= \left\{ \frac{\partial}{\partial \alpha} - \frac{d}{dx} \frac{\partial}{\partial \alpha_{x}} \right\} f(\alpha, \alpha_{x}) = \frac{\delta F[\alpha]}{\delta \alpha(x)}$$

$$= \left[\int \frac{\delta^{2} F[\alpha]}{\delta \alpha(x) \delta \alpha(y)} \varphi(x) \varphi(y) dx dy \right]_{\alpha=0}$$
(19)

Our problem is construct explicit descriptions of the 2^{nd} variational derivative $\frac{\delta^2 F[\alpha]}{\delta \alpha(x) \delta \alpha(y)}$ and of its higher-order counterparts. The trick here is to introduce

$$\varphi(x) = \int \delta(x - y)\varphi(y) \, dx \tag{20}$$

into (19) for we then have

$$F_{2}[\varphi] = \int \underbrace{\left[\mathbf{D}_{[\varphi]} \int g(\alpha, \alpha_{x}, \alpha_{xx}) \delta(x - y) \, dx \right]_{\alpha = 0}}_{= \left[\int h(\alpha, \alpha_{x}, \alpha_{xx}, \alpha_{xxx}) \varphi(x) \, dx \right]_{\alpha = 0}} (21.1)$$

with

$$h(\alpha, \alpha_x, \alpha_{xx}, \alpha_{xxx}) = \frac{\delta^2 F[\alpha]}{\delta \alpha(x) \delta \alpha(y)}$$

$$= \left\{ \frac{\partial}{\partial \alpha} - \frac{d}{dx} \frac{\partial}{\partial \alpha_x} + \frac{d^2}{dx^2} \frac{\partial}{\partial \alpha_{xx}} \right\} g(\alpha, \alpha_x, \alpha_{xx}) \delta(x - y)$$
(21.2)

The pattern of the argument should at this point be clear; as one ascends from one order to the next one begins always by invoking (20), with the result that δ -functions and their derivatives stack ever deeper, while the variational derivative operator

$$\left\{\frac{\partial}{\partial\alpha} - \frac{d}{dx}\frac{\partial}{\partial\alpha_x} + \frac{d^2}{dx^2}\frac{\partial}{\partial\alpha_{xx}} + \cdots\right\}$$

acquires at each step one additional term.

In ordinary analysis one can expand f(x) about the point x = a only if a is a "regular point," and the resulting Taylor series $f(x) = \sum \frac{1}{n!} f_n (x-a)^n$ can be expected to make sense only within a certain "radius of convergence." Such details become most transparent when x is allowed to range on the complex

plane. Similar issues—though I certainly do not intend to pursue them here can be expected to figure prominently in any fully developed account of the theory of functionals.

Construction of functional analogs of the Laplacian and Poisson bracket. Now that we possess the rudiments of a theory of functional differentiation, we are in position to contemplate a "theory of functional differential equations." I do not propose to lead an expedition into that vast jungle, which remains (so far as I am aware) still largely unexplored. But I do want to step out of our canoe long enough to draw your attention to one small methodological flower that grows there on the river bank, at the very edge of the jungle. Central to many of the partial differential equations of physics is the Laplacian operator, ∇^2 . Here in the jungle it possess a functional analog. How is such an object to be constructed? The answer is latent in the "sophisticated" answer to a simpler question, which I pose in the notation of p. 74: How does

$$\nabla^2 F(\boldsymbol{\varphi}) = \left\{ \sum_i \left(\frac{\partial}{\partial \varphi^i} \right)^2 \right\} F = \operatorname{tr} \|\partial^2 F / \partial \varphi^i \partial \varphi^j\|$$

come to acquire from $\mathbf{D}_{[\boldsymbol{\lambda}]}F(\boldsymbol{\varphi})$ the status of a "natural object"? Why, in particular, does $\nabla^2 F$ contain no allusion to $\boldsymbol{\lambda}$? We proceed from the observation that

$$\begin{aligned} \mathbf{D}_{[\boldsymbol{\lambda}]} \mathbf{D}_{[\boldsymbol{\lambda}]} F(\boldsymbol{\varphi}) &= \sum \sum \frac{\partial^2 F}{\partial \varphi^i \partial \varphi^j} \lambda^i \lambda^j \\ &= \boldsymbol{\lambda}^{\mathsf{T}} \mathbb{F} \, \boldsymbol{\lambda} \quad \text{where } \mathbb{F} \text{ is the square matrix } \|\partial^2 F / \partial \varphi^i \partial \varphi^j\| \\ &= \operatorname{tr} \mathbb{F} \mathbb{L} \quad \text{where } \mathbb{L} \text{ is the square matrix } \|\lambda^i \lambda^j\| \end{aligned}$$

We note more particularly that $\mathbb{L}^2 = (\boldsymbol{\lambda} \cdot \boldsymbol{\lambda})\mathbb{L}$, so if $\boldsymbol{\lambda}$ is a unit vector $(\boldsymbol{\lambda} \cdot \boldsymbol{\lambda} = 1)$ then \mathbb{L} is a *projection matrix* which in fact projects upon $\boldsymbol{\lambda}$: $\mathbb{L}\mathbf{x} = (\boldsymbol{\lambda} \cdot \mathbf{x})\boldsymbol{\lambda}$. Now let $\{\mathbf{e}_i\}$ refer to some (any) *orthonormal basis*, and let $\{\mathbb{E}_i\}$ denote the associated set of projection matrices. Orthonormality entails $\mathbb{E}_i \mathbb{E}_j = \delta_{ij} \mathbb{E}_i$ while $\sum \mathbb{E}_i = \mathbb{I}$ expresses the presumed *completeness* of the set $\{\mathbf{e}_i\}$. From these elementary observations⁵ it follows that

$$\begin{split} \sum \mathbf{D}_{[\mathbf{e}_i]} \mathbf{D}_{[\mathbf{e}_i]} F(\varphi) &= \sum \operatorname{tr} \mathbb{F} \mathbb{E}_i = \operatorname{tr} \mathbb{F} \\ &= \sum \| \partial^2 F / \partial \varphi^i \partial \varphi^i | \\ &= \nabla^2 F(\varphi) \end{split}$$

Turning now from functions to functionals, we find it quite natural to construct

$$\sum \mathbf{D}_{[e_i]} \mathbf{D}_{[e_i]} F[\varphi] = \sum \int \int \frac{\delta^2 F[\varphi]}{\delta \varphi(x) \delta \varphi(y)} e_i(x) e_i(y) dx dy$$

⁵ The ideas assembled here acquire a striking transparency when formulated in a simplified variant of Dirac's "bra-ket notation." Readers familiar with that notation are encouraged to give it a try.

Functional Laplacian and Poisson bracket

And if we assume the functions $\{e_i(x)\}$ to be orthonormal $\int e_i(x)e_j(x)dx = \delta_{ij}$ and (which is more to the immediate point) complete in function space

$$\sum e_i(x)e_j(y) = \delta(x-y)$$

then we obtain this natural definition of the "Laplacian of a functional":

$$\nabla^2 F[\varphi] \equiv \left\{ \sum \mathbf{D}_{[e_i]} \mathbf{D}_{[e_i]} \right\} F[\varphi] = \int \int \frac{\delta^2 F[\varphi]}{\delta \varphi(x) \delta \varphi(x)} dx$$
(22)

Familiarly, the "partial derivative of a function of several variables" is a concept which arises by straightforward generalization from that of "the (ordinary) derivative of a function of a single variable." The "partial functional derivative" springs with similar naturalness from the theory of "ordinary functional derivatives," as outlined in preceeding paragraphs; the problem one encounters is not conceptual but notational/terminological. Let us agree to write $\mathbf{D}_{[\lambda]/\varphi}F[\ldots,\varphi,\ldots]$ to signify "the partial derivative of $F[\ldots,\varphi,\ldots]$ —a functional of several variables—with respect to $\varphi(x)$ in the direction $\lambda(x)$:

$$\mathbf{D}_{[\lambda]/\varphi}F[\ldots,\varphi,\ldots] = \int \frac{\delta F[\ldots,\varphi,\ldots]}{\delta\varphi(x)}\lambda(x)\,dx$$

I shall not pursue this topic to its tedious conclusion, save to remark that one expects quite generally to have "equality of cross derivatives"

$$\mathbf{D}_{[\lambda_1]/\varphi}\mathbf{D}_{[\lambda_2]/\psi}F[\varphi,\psi] = \mathbf{D}_{[\lambda_2]/\psi}\mathbf{D}_{[\lambda_1]/\varphi}F[\varphi,\psi]$$

since, whether one works from the expression on the left or from that on the right, one encounters $F[\varphi + \lambda_1, \psi + \lambda_2] - F[\varphi + \lambda_1, \psi] - F[\varphi, \psi + \lambda_2] + F[\varphi, \psi]$. Instead I look to one of the problems that, on p. 73, served ostensibly to motivate this entire discussion. Let $A[\varphi, \pi]$ and $B[\varphi, \pi]$ be given functionals of two variables, and construct

$$\begin{aligned} \mathbf{D}_{[\lambda_1]/\varphi} A \cdot \mathbf{D}_{[\lambda_2]/\pi} B - \mathbf{D}_{[\lambda_1]/\varphi} B \cdot \mathbf{D}_{[\lambda_2]/\pi} A \\ &= \int \int \left\{ \frac{\delta A}{\delta\varphi(x)} \frac{\delta B}{\delta\pi(y)} - \frac{\delta B}{\delta\varphi(x)} \frac{\delta A}{\delta\pi(y)} \right\} \lambda_1(x) \lambda_2(y) \, dx dy \end{aligned}$$

Proceeding now in direct imitation of the construction which led us a moment ago to the definition (22) of the functional Laplacian, we write

$$[A, B] \equiv \sum \left\{ \mathbf{D}_{[e_i]/\varphi} A \cdot \mathbf{D}_{[e_i]/\pi} B - \mathbf{D}_{[e_i]/\varphi} B \cdot \mathbf{D}_{[e_i]/\pi} A \right\}$$
$$= \int \int \left\{ \frac{\delta A}{\delta \varphi(x)} \frac{\delta B}{\delta \pi(y)} - \frac{\delta B}{\delta \varphi(x)} \frac{\delta A}{\delta \pi(y)} \right\} \cdot \sum e_i(x) e_i(y) \, dx \, dy$$
$$= \int \left\{ \frac{\delta A}{\delta \varphi(x)} \frac{\delta B}{\delta \pi(x)} - \frac{\delta B}{\delta \varphi(x)} \frac{\delta A}{\delta \pi(x)} \right\} \, dx \qquad (23)$$
$$= \int [\mathcal{A}, \mathcal{B}] \, dx \quad \text{in the notation of (60), Chapter I}$$

At (23) we have achieved our goal; we have shown that the Poisson bracket —a construct fundamental to Hamiltonian field theory—admits of natural description in language supplied by the differential calculus of functionals.

I return at this point to discussion of our "functional Laplacian," partly to develop some results of intrinsic interest, and partly to prepare for subsequent discussion of the integral calculus of functionals. It is a familiar fact—the upshot of a "folk theorem"—that

$$\nabla^2 \varphi(x) \sim \langle \text{average of neighboring values} \rangle - \varphi(x)$$
 (24)

 $\nabla^2 \varphi$ provides, therefore, a natural measure of the "local disequilibration" of the φ -field; in the absence of "disequilibration" ($\nabla^2 \varphi = 0$) the field is said to be "harmonic." I begin with discussion of an approach to the proof of (24) which, though doubtless "well-known" in some circles, occurred to me only recently.⁶ Working initially in two dimensions, let $\varphi(x, y)$ be defined on a neighborhood containing the point (x, y) on the Euclidian plane. At points on the boundary of a disk centered at (x, y) the value of φ is given by

$$\begin{aligned} \varphi(x + r\cos\theta, y + r\sin\theta) &= e^{r\cos\theta \frac{\partial}{\partial x} + r\sin\theta \frac{\partial}{\partial y}} \cdot \varphi(x, y) \\ &= \varphi + r(\varphi_x \cos\theta + \varphi_y \sin\theta) \\ &+ \frac{1}{2}r^2(\varphi_{xx} \cos^2\theta + 2\varphi_{xy} \cos\theta \sin\theta + \varphi_{yy} \sin^2\theta) + \cdots \end{aligned}$$

The average $\langle \varphi \rangle$ of the values assumed by φ on the boundary of the disk is given therefore by

$$\begin{split} \langle \varphi \rangle &= \frac{1}{2\pi r} \int_0^{2\pi} \{ \text{right side of preceeding equation} \} \, r d\theta \\ &= \varphi + 0 + \frac{1}{4} r^2 \{ \varphi_{xx} + \varphi_{yy} \} + \cdots \end{split}$$

from which we obtain

$$\nabla^2 \varphi = \frac{4}{r^2} \left\{ \langle \varphi \rangle - \varphi \right\} + \cdots \quad \text{in the 2-dimensional case}$$
(25)

This can be read as a sharpened instance of (24).⁷ In three dimensions we are motivated to pay closer attention to the notational organization of the

restoring force =
$$k \{ \langle \varphi \rangle - \varphi \}$$

= mass element · acceleration
= $2\pi r^2 \rho \cdot \varphi_{tt}$

and we are led from (25) to an instance of the wave equation:

$$\nabla^2 \varphi = \frac{1}{c^2} \varphi_{tt}$$

with $c^2 = k/8\pi\rho$.

⁶ See the introduction to my notes "Applications of the Theory of Harmonic Polynomials" for the Reed College Math Seminar of 7 March 1996.

 $^{^7}$ If φ refers physically to (say) the displacement of a membrane, then it becomes natural to set

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argument; we write

$$\varphi(\boldsymbol{x}+\boldsymbol{r}) = \varphi(\boldsymbol{x}) + \boldsymbol{r} \cdot \boldsymbol{\nabla}\varphi + \frac{1}{2}\boldsymbol{r} \cdot \begin{pmatrix} \varphi_{11} & \varphi_{12} & \varphi_{13} \\ \varphi_{21} & \varphi_{22} & \varphi_{23} \\ \varphi_{31} & \varphi_{32} & \varphi_{33} \end{pmatrix} \boldsymbol{r} + \cdots$$
(26)

which we want to average over the surface of the sphere $r_1^2 + r_2^2 + r_3^2 = r^2$. It is to that end that I digress now to establish a little LEMMA, which I will phrase with an eye to its dimensional generalization:

Let $\langle x^p \rangle$ denote the result of averaging the values assumed by x^p on the surface of the 3-sphere of radius r. Proceeding in reference to the figure, we have

$$\langle x^p \rangle = \frac{1}{S_3(r)} \int x^p dS \\ dS = S_2(r \sin \theta) \cdot r d\theta$$

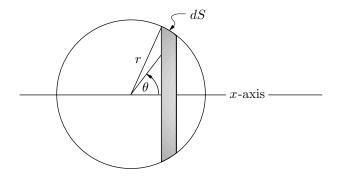


FIGURE 1: Geometrical construction intended to set notation used in proof of the Lemma. The figure pertains fairly literally to the problem of averaging x^p over the surface of a 3-sphere, but serves also to provide schematic illustration of our approach to the problem of averaging x^p over the surface of an N-sphere.

where I have adopted the notation

$$S_N(r) \equiv \text{surface area of } N \text{-sphere of radius } r = \begin{cases} 2\pi r & \text{when } N = 2\\ 4\pi r^2 & \text{when } N = 3\\ \vdots \end{cases}$$

Evidently

$$\begin{aligned} \langle x^p \rangle &= \frac{S_2(r)}{S_3(r)} r^{p+1} \underbrace{\int_0^\pi \cos^p \theta \sin \theta \, d\theta}_{=\int_{-1}^1 u^p \, du} = \begin{cases} \frac{2}{p+1} & \text{for } p \text{ even} \\ 0 & \text{for } p \text{ odd} \end{cases} \end{aligned}$$

which in the cases of particular interest gives

$$\begin{split} \langle x^{0} \rangle &= \frac{S_{2}(r)}{S_{3}(r)} r^{1} \frac{2}{1} = 1 \\ \langle x \rangle &= 0 \\ \langle x^{2} \rangle &= \frac{S_{2}(r)}{S_{3}(r)} r^{3} \frac{2}{3} = \frac{1}{3} r^{2} \end{split}$$

Returning with this information to (26), we rotate to the coordinate system relative to which the $\|\varphi_{ij}\|$ matrix is diagonal

$$\begin{pmatrix} \varphi_{11} & \varphi_{12} & \varphi_{13} \\ \varphi_{21} & \varphi_{22} & \varphi_{23} \\ \varphi_{31} & \varphi_{32} & \varphi_{33} \end{pmatrix} \longrightarrow \begin{pmatrix} \phi_{11} & 0 & 0 \\ 0 & \phi_{22} & 0 \\ 0 & 0 & \phi_{33} \end{pmatrix}$$

and obtain

$$\langle \varphi \rangle = \varphi + 0 + \frac{1}{2} \text{tr} \begin{pmatrix} \phi_{11} & 0 & 0 \\ 0 & \phi_{22} & 0 \\ 0 & 0 & \phi_{33} \end{pmatrix} \cdot \frac{1}{3} r^2$$

But the trace is rotationally invariant, so we have (compare (25))

$$\nabla^2 \varphi = \frac{6}{r^2} \left\{ \langle \varphi \rangle - \varphi \right\} + \cdots \quad \text{in the 3-dimensional case}$$
(27)

Dimensional generalization of this result follows trivially upon dimensional generalization of our LEMMA. If $\langle x^p \rangle$ is taken now to denote the result of averaging the values assumed by x^p on the surface of the *N*-sphere of radius *r*, then—arguing as before—we have

$$\begin{split} \langle x^p \rangle &= \frac{1}{S_N(r)} \int x^p \, dS \\ &dS = S_{N-1}(r \sin \theta) \cdot r d\theta \end{split}$$

A simple scaling argument is sufficient to establish that

$$S_N(r) = r^{N-1} \cdot S_N(1)$$

so we have

$$\langle x^p \rangle = \frac{S_{N-1}(1)}{S_N(1)} r^p \underbrace{\int_0^\pi \cos^p \theta \sin^{N-2} \theta \, d\theta}_{0} \tag{28}$$

and because the integrand is even/odd on the interval $0 \le \theta \le \pi$ we have (for $N = 2, 3, 4, \ldots$; i.e., for $q \equiv N - 2 = 0, 1, 2, \ldots$)

$$= \begin{cases} 0 & \text{when } p \text{ is odd} \\ 2\int_0^{\frac{1}{2}\pi} \cos^p \theta \sin^q \theta \, d\theta & \text{when } p \text{ is even} \end{cases}$$

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The surviving integral is tabulated; we have⁸

$$\int_0^{\frac{1}{2}\pi} \cos^p \theta \sin^q \theta \, d\theta = \frac{1}{2} B\left(\frac{p+1}{2}, \frac{q+1}{2}\right)$$

where

$$B(x,y) \equiv \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$$

Here $\Gamma(x) \equiv \int_0^\infty e^{-t} t^{x-1} dt$ is Euler's gamma function. Familiarly, $\Gamma(1) = 1$ and $\Gamma(x+1) = x\Gamma(x)$ so when x is an integer one has

$$\Gamma(n+1) = n!$$

from which it follows that

$$B(m+1, n+1) = \frac{\Gamma(m+1)\Gamma(n+1)}{\Gamma(m+n+2)}$$
$$= \frac{1}{m+n+1} \cdot \frac{m!n!}{(m+n)!}$$

Just as Euler's gamma function $\Gamma(x)$ is a function with the wonderful property that at non-negative integral points it reproduces the factorial, so does Euler's beta function B(x, y) possess the property that at non-negative lattice points it reproduces (to within a factor) the combinatorial coefficients. From $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ it follows that at half-integral points one has

$$\Gamma(n+\frac{1}{2}) = \frac{(2n-1)!!}{2^n} \sqrt{\pi} = \begin{cases} \frac{1}{2}\sqrt{\pi} & \text{at } n=1\\ \frac{1\cdot3}{2^2}\sqrt{\pi} & \text{at } n=2\\ \frac{1\cdot3\cdot5}{2^3}\sqrt{\pi} & \text{at } n=3\\ \vdots \end{cases}$$

We find ourselves now in position to write

$$\int_0^{\pi} \cos^0 \theta \sin^q \theta \, d\theta = B\left(\frac{1}{2}, \frac{q+1}{2}\right)$$
$$= \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{q+1}{2}\right)}{\Gamma\left(\frac{q}{2}+1\right)}$$
$$= \frac{\sqrt{\pi}\Gamma\left(\frac{q+1}{2}\right)}{\Gamma\left(\frac{q}{2}+1\right)}$$
(29.1)

⁸ See I. Gradshteyn & I. Ryzhik, *Table of Integrals, Series, and Products* (1965), **3.621.5**, p. 369 or W. Gröbner & N. Hofreiter, *Bestimmte Integrale* (1958), **331.21**, p. 95.

and

$$\int_{0}^{\pi} \cos^{2} \theta \sin^{q} \theta d\theta = B\left(\frac{3}{2}, \frac{q+1}{2}\right)$$
$$= \frac{\Gamma(\frac{3}{2})\Gamma(\frac{q+1}{2})}{\Gamma(\frac{q}{2}+2)}$$
$$= \frac{\frac{1}{2}\sqrt{\pi}\Gamma(\frac{q+1}{2})}{(\frac{q}{2}+1)\Gamma(\frac{q}{2}+1)}$$
(29.2)

It can be shown (and will be shown, though I find it convenient to postpone the demonstration) that

$$S_N(r) = \frac{2\pi^{\frac{N}{2}}}{\Gamma(\frac{N}{2})} r^{N-1}$$
(30)

 \mathbf{SO}

$$\frac{S_{N-1}(1)}{S_N(1)} = \frac{\Gamma(\frac{N}{2})}{\sqrt{\pi}\Gamma(\frac{N-1}{2})} \\
= \frac{\Gamma(\frac{q}{2}+1)}{\sqrt{\pi}\Gamma(\frac{q+1}{2})} \quad \text{by } N = q+2$$
(31)

Returning with (29) and (31) to (28) we find, after much cancellation, that $\langle x^0 \rangle = 1$ (which is gratifying) and that

$$\langle x^2 \rangle = \frac{1}{q+2}r^2 = \frac{1}{N}r^2$$

Since (26) responds in an obvious way to dimensional generalization, we obtain at once

$$\nabla^2 \varphi = \frac{2N}{r^2} \{ \langle \varphi \rangle - \varphi \} + \cdots \quad \text{in the } N \text{-dimensional case}$$
(32)

which gives back (25) and (27) as special cases. This is a result of (if we can agree to overlook the labor it cost us) some intrinsic charm. But the point to which I would draw my reader's particular attention is this: equation (32) relates a "local" notion—the Laplacian that appears on the left side of the equality—to what might be called a "locally global" notion, for the construction of $\langle \varphi \rangle$ entails *integration* over a (small) *hypersphere*.⁹ Both the result and the method of its derivation anticipate things to come.

But before I proceed to my main business I digress again, not just to make myself honest (I have promised to discuss the derivation of (30)) but to plant

 $^{^9}$ "Integration over a hypershpere" is a process which echoes, in a curious way, the "sum over elements of a complete orthonormal set" which at p. 80 in Chapter I entered critically into the *definition* of the Laplacian, as at p. 81 it entered also into the construction of the Poisson bracket.

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some more seeds. To describe the volume $V_N({\mathbb R})$ of an $N\text{-sphere of radius }{\mathbb R}$ we we might write

$$V_N(R) = \iint \dots \int_{x_1^2 + x_2^2 + \dots + x_N^2 = R^2} dx_1 dx_2 \dots dx_N = V_N \cdot R^N$$

where $V_N = V_N(1)$ is a certain yet-to-be-determined function of N. Evidently the surface area of such a hypersphere can be described

$$S_N(R) = \frac{d}{dR} V_N(R) = S_N \cdot R^{N-1} \quad \text{with} \quad S_N = NA_N$$

Conversely $V_N(R) = \int_0^R S_N(r) dr$, which is familiar as the "onion construction" of $V_N(R)$. To achieve the evaluation of S_N —whence of A_N —we resort to a famous trick: pulling

$$I \equiv \iint \cdots \int_{-\infty}^{\infty} e^{-(x_1^2 + x_2^2 + \dots + x_N^2)} dx_1 dx_2 \cdots dx_N$$

from our hat, we note that

$$= \begin{cases} \left[\int_{-\infty}^{\infty} e^{-x^2} dx \right]^N & \text{on the one hand} \\ S_N \cdot \int_0^{\infty} e^{-r^2} r^{N-1} dr & \text{on the other} \end{cases}$$

On the one hand we have the N^{th} power of a Gaussian integral, and from $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$ obtain $I = \pi^{N/2}$, while on the other hand we have an integral which by a change of variable (set $r^2 = u$) can be brought to the form $\frac{1}{2} \int_{0}^{\infty} e^{-u} u^{\frac{N}{2}-1} du$ which was seen on p. 85 to define $\Gamma(\frac{N}{2})$. So we have

$$S_N = \frac{2\pi^{\frac{N}{2}}}{\Gamma(\frac{N}{2})}$$

as was asserted at (30), and which entails

$$V_N = \frac{1}{N} S_N = \frac{\pi^{\frac{N}{2}}}{\frac{N}{2}\Gamma(\frac{N}{2})} = \frac{\pi^{\frac{N}{2}}}{\Gamma(\frac{N+2}{2})}$$
(33)

Fairly immediately $V_0 = 1$, $V_1 = 2$ and $V_N = \frac{2\pi}{N}V_{N-2}$ so

$$V_{N=2n} = \frac{\pi^{n}}{n!} V_{N=2n+1} = 2\pi^{n} \frac{2^{n}}{1 \cdot 3 \cdot 5 \cdots (2n+1)}$$
(34)

which reproduce familiar results at N = 2 and N = 3. Note the curious fact that one picks up an additional π -factor only at every second step as one advances through ascending N-values.

First steps toward an integral calculus of functionals: Gaussian integration. Look into any text treating "tensor analysis" and you will find elaborate discussion of various derivative structures (covariant derivatives with respect to prescribed affine connections, intrinsic derivatives, constructs which become "accidentally tensorial" because of certain fortuitious cancellations), and of course every successful differentiation process, when "read backwards," becomes a successful antidifferentiation process. But you will find little that has to do with the construction of *definite* integrals. What little you do find invariably depends critically upon an assumption of "total antisymmetry," and falls into the domain of that elegant subject called the "exterior calculus," where integral relations abound, but all are variants of the same relation—called "Stokes' theorem." Or look into any table of integrals. You will find antiderivatives and definite integrals in stupifying (if never quite sufficient) abundance, but very little that pertains to what might be called the "systematics of multiple integration." What little you do find¹⁰ displays a curious preoccupation with hyperspheres, gamma functions, Gaussians. I interpret these circumstances to be symptoms not of neglect but of deep fact: it becomes *possible* to speak in dimensionally extensible generality of the integral properties of multi-variable objects only in a narrowly delimited set of contexts, only in the presence of some highly restrictive assumptions. It would be the business of an "integral calculus of functionals" to assign meaning to expressions of the type

 $\int_{\text{elements of some "function space"}} F[\varphi] d[\varphi]$

and it is sometimes alleged (mainly by persons who find themselves unable to do things they had naively hoped to do) that this is an "underdeveloped subject in a poor state of repair." It is, admittedly, a relatively new subject,¹¹ but has enjoyed the close attention of legions of mathematicians/physicists of the first rank. My own sense of the situation is that it is not so much lack of technical development as *restrictions inherent in the subject matter* that mainly account for the somewhat claustrophobic feel that tends to attach to the integral calculus of functionals. That said, I turn now to review of a few of the most characteristic ideas in the field.

¹⁰ See Gradshteyn & Ryzhik's §§**4.63–4.64**, which runs to a total of scarcely five pages (and begins with the volume of an *N*-sphere!) or the more extended §**3.3** in A. Prudnikov, Yu. Brychkov & O. Marichev's *Integrals and Series* (1986).

¹¹ N. Wiener was led from the mathematical theory of Brownian motion to the "Wiener integral" only in the 1930s, while R. Feynman's "sum-over-paths formulation of quantum mechanics" dates from the late 1940s.

Gaussian integration

One cannot expect a multiple integral

$$\int \int \cdots \int F(x^1, x^2, \dots, x^N) \, dx^1 dx^2 \cdots dx^N$$

to possess the property of "dimensional extensibility" unless the integrand "separates;" i.e., unless it possesses some variant of the property

$$F(x^{1}, x^{2}, \dots, x^{N}) = F_{1}(x^{1})F_{2}(x^{2})\cdots F_{N}(x^{N})$$

giving

$$\int \int \cdots \int F(x^1, x^2, \dots, x^N) dx^1 dx^2 \cdots dx^N = \prod_{i=1}^N \int F_i(x^i) dx^i$$

If $F(x^1, x^2, ..., x^N) = e^{f(x^1, x^2, ..., x^N)}$ and $f(x^1, x^2, ..., x^N)$ separates in the additive sense $f(x^1, x^2, ..., x^N) = f_1(x^1) + f_2(x^2) + \cdots + f_N(x^N)$ then

$$\int \int \cdots \int e^{f(x^1, x^2, \dots, x^N)} dx^1 dx^2 \cdots dx^N = \prod_{i=1}^N \int e^{f_i(x^i)} dx^i$$

represents a merely notational variant of the same basic idea, while a more radically distinct variation on the same basic theme would result from

$$F(r^1, \theta^1, r^2, \theta^2, \dots, r^N, \theta^N) = \prod_i F_i(r^i, \theta^i)$$

"Separation" is, however, a very fragile property in the sense that it is generally not stable with respect to coordinate transformations $\mathbf{x} \longrightarrow \mathbf{y} = \mathbf{y}(\mathbf{x})$; if $F(\mathbf{x})$ separates then $G(\mathbf{y}) \equiv F(\mathbf{x}(\mathbf{y}))$ does, in general, not separate. Nor is it, in general, easy to discover whether or not $G(\mathbf{y})$ is "separable" in the sense that separation can be achieved by some suitably designed $\mathbf{x} \leftarrow \mathbf{y}$. A weak kind of stability can, however, be achieved if one writes $F(\mathbf{x}) = e^{f(\mathbf{x})}$ and develops $f(\mathbf{x})$ as a multi-variable power series:

$$f(\mathbf{x}) = f_0 + f_1(\mathbf{x}) + \frac{1}{2}f_2(\mathbf{x}) + \dots = \sum \frac{1}{n!}f_n(\mathbf{x})$$

where $f_n(\mathbf{x})$ is a multinomial of degree *n*. For if $\mathbf{x} = \mathbf{x}(\mathbf{y}) \longleftarrow \mathbf{y}$ is *linear*

$$\mathbf{x} = \mathbb{T}\mathbf{y} + \mathbf{t}$$

then $g_n(\mathbf{y}) = f_n(\mathbf{x}(\mathbf{y}))$ contains no terms of degree higher than n, and is itself a multinomial of degree n in the special case $\mathbf{t} = \mathbf{0}$.

Integrals of the type

$$\int \int \cdots \int_{-\infty}^{+\infty} e^{f_0 + f_1(\mathbf{x})} \, dx^1 dx^2 \cdots x^N$$

are divergent, so the conditionally convergent integrals

$$\int \int \cdots \int_{-\infty}^{+\infty} e^{f_0 + f_1(\mathbf{x}) + \frac{1}{2}f_2(\mathbf{x})} dx^1 dx^2 \cdots x^N$$

acquire in this light a kind of "simplest possible" status. The question is: do they possess also the property of "dimensional extensibility"? Do they admit of discussion in terms that depend so weakly upon N that one can contemplate proceeding to the limit $N \longrightarrow \infty$? They do.

Our problem, after some preparatory notational adjustment, is to evaluate

$$I \equiv \int \int \cdots \int_{-\infty}^{+\infty} e^{-\frac{1}{2}(\mathbf{x} \cdot \mathbb{A}\mathbf{x} + 2\mathbf{B} \cdot \mathbf{x} + C)} dx^1 dx^2 \cdots x^N$$

To that end, we introduce new variables \mathbf{y} by $\mathbf{x} = \mathbb{R}\mathbf{y}$ and obtain

$$I = \int \int \cdots \int_{-\infty}^{+\infty} e^{-\frac{1}{2}(\mathbf{y} \cdot \mathbb{R}^{\mathsf{T}} \mathbb{A} \mathbb{R} \mathbf{y} + 2\mathbf{b} \cdot \mathbf{y} + C)} J \, dy^{1} dy^{2} \cdots y^{N}$$

where $\mathbf{b} = \mathbb{R}^{\mathsf{T}} \mathbf{B}$, where the Jacobian $J = \left| \frac{\partial(x^1, x^2, \dots, x^N)}{\partial(y^1, y^2, \dots, y^N)} \right| = \det \mathbb{R}$, and where \mathbb{A} can without loss of generality be assumed to be symmetric. Take \mathbb{R} to be in particular the rotation matrix that diagonalizes \mathbb{A} :

$$\mathbb{R}^{\mathsf{T}} \mathbb{A} \mathbb{R} = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_N \end{pmatrix}$$

The numbers a_i are simply the eigenvalues of \mathbb{A} ; they are necessarily real, and we assume them all to be positive. Noting also that, since \mathbb{R} is a rotation matrix, $J = \det \mathbb{R} = 1$, we have

$$I = e^{-\frac{1}{2}C} \cdot \prod_{i} \underbrace{\int_{-\infty}^{+\infty} e^{-\frac{1}{2}(a_{i}y^{2} + 2b_{i}y)} dy}_{= \sqrt{\frac{2\pi}{a_{i}}} \exp\left\{\frac{1}{2}\left[b_{i} \cdot \frac{1}{a_{i}} \cdot b_{i}\right]\right\}}$$
(35)

$$= e^{-\frac{1}{2}C} \cdot \sqrt{\frac{(2\pi)^N}{a_1 a_2 \cdots a_N}} e^{\frac{1}{2} \mathbf{b} \cdot (\mathbb{R}^{\mathsf{T}} \mathbb{A} \mathbb{R})^{-1} \mathbf{b}}$$
$$= e^{-\frac{1}{2}C} \cdot \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} e^{\frac{1}{2} \mathbf{B} \cdot \mathbb{A}^{-1} \mathbf{B}}$$
(36)

Offhand, I can think of no formula in all of pure/applied mathematics that supports the weight of a greater variety of wonderful applications than does the formula that here—fittingly, it seems to me—wears the equation number

Gaussian integration

 $137 = \hbar c/e^2$. One could easily write at book length about those applications, and still not be done. Here I confine myself to a few essential remarks.

Set $\mathbf{B} = -i\mathbf{p}$, C = 0 and the multi-dimensional Gaussian Integral Formula (36) asserts that the Fourier transform of a Gaussian is Gaussian:

$$\left(\frac{1}{\sqrt{2\pi}}\right)^{N} \int_{-\infty}^{+\infty} e^{i\mathbf{p}\cdot\mathbf{x}} e^{-\frac{1}{2}\mathbf{x}\cdot\mathbb{A}\mathbf{x}} dx^{1} dx^{2} \cdots dx^{N} = \frac{1}{\sqrt{\det \mathbb{A}}} e^{-\frac{1}{2}\mathbf{p}\cdot\mathbb{A}^{-1}\mathbf{p}}$$
(37.1)

of which

$$(\det \mathbb{A})^{\frac{1}{4}} e^{-\frac{1}{2}\mathbf{x} \cdot \mathbb{A}\mathbf{x}} \xrightarrow[]{\text{Fourier transformation}} (\det \mathbb{A}^{-1})^{\frac{1}{4}} e^{-\frac{1}{2}\mathbf{p} \cdot \mathbb{A}^{-1}\mathbf{p}}$$
(37.2)

provides an even more symmetrical formulation. This result is illustrative of the several "closure" properties of Gaussians. Multiplicative closure—in the sense

 $e^{\text{quadratic}} \cdot e^{\text{quadratic}} = e^{\text{quadratic}}$

—is an algebraic triviality, but none the less important for that; it lies at the base of the observation that if

$$G(x-m;\sigma) \equiv \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\left[\frac{x-m}{\sigma}\right]^2\right\}$$

is taken to notate the familiar "normal distribution" then

$$G(x - m'; \sigma') \cdot G(x - m''; \sigma'') = G(m' - m''; \sqrt{\sigma'^2 + \sigma''^2}) \cdot G(x - m; \sigma)$$

where $(1/\sigma)^2 = (1/\sigma')^2 + (1/\sigma'')^2$ is less than the lesser of σ' and σ'' , while $m = m'(\sigma/\sigma')^2 + m''(\sigma/\sigma'')^2$ has a value intermediate between that of m' and m''. In words:

normal distribution \cdot normal distribution =

attenuation factor \cdot skinny normal distribution

This result is absolutely fundamental to statistical mechanics, where it gives one license to make replacements of the type $\langle f(x) \rangle \longrightarrow f(\langle x \rangle)$; it is, in short, the reason there exists such a subject as thermodynamics!

Also elementary (though by no means trivial) is what might be called the "integrative closure" property of Gaussians, which I now explain. We proceed from the observation that

$$Q(x) \equiv \begin{pmatrix} x \\ y \end{pmatrix} \cdot \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + 2 \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} \cdot \begin{pmatrix} x \\ y \end{pmatrix} + C$$

can be notated

$$Q(x) = ax^2 + 2bx + c$$

with

$$\begin{split} a &= A_{11} \\ b &= \frac{1}{2}(A_{12} + A_{21})y + B_1 \\ c &= A_{22}y^2 + 2B_2y + C \end{split}$$

Therefore

$$\int_{-\infty}^{+\infty} e^{-\frac{1}{2}Q(x)} dx = \sqrt{\frac{2\pi}{a}} \exp\left\{\frac{b^2 - ac}{a}\right\}$$

The point is that the result thus achieved has the form

$$= \sqrt{\frac{2\pi}{a}} \, e^{-\frac{1}{2}Q'(y)} \quad \text{with} \quad Q'(y) \equiv a'y^2 + 2b'y + c'$$

so that if one were to undertake a second integration one would confront again an *integral of the original class*.¹² The statement

$$\int_{-\infty}^{+\infty} e^{\text{quadratic in } N \text{ variables}} d(\text{variable}) = e^{\text{quadratic in } N-1 \text{ variables}}$$
(38)

appears to pertain uniquely to quadratics. In evidence I cite the facts that even the most comprehensive handbooks¹³ list very few integrals of the type

$$\int_{-\infty}^{+\infty} e^{\text{non-quadratic polynomial in } x} dx$$

and that in the "next simplest case" one has¹⁴

$$\int_{-\infty}^{+\infty} e^{-\frac{1}{2}(ax^4 + 2bx^2 + c)} dx = \sqrt{\frac{b}{2a}} e^{\frac{1}{2} \left[\frac{b^2 - 2ac}{2a}\right]} K_{\frac{1}{4}} \left(\frac{b^2}{2a}\right)$$

= e^{quartic} !

It is "integrative closure" that permits one to construct multiple integrals by tractable iteration of single integrals. The moral appears to be that if it is

¹² Indeed, if one works out explicit descriptions of a', b' and c' and inserts them into $\int e^{-\frac{1}{2}Q'(y)dy}$ one at length recovers precisely (36), but that would (especially for $N \gg 2$) be "the hard way to go."

 $^{^{13}}$ See, for example, $\S\S{\bf 3.32-3.34}$ in Gradshteyn & Ryzhik and $\S{\bf 2.3.18}$ in Prudnikov, Brychkov & Marichev.

¹⁴ See Gradshteyn & Ryzhik, **3.323.3**. Properties of the functions $K_{\nu}(x)$ —sometimes called "Basset functions"—are summarized in Chapter 51 of An Atlas of Functions by J. Spanier & K. Oldham (1987). They are constructed from Bessel functions of fractional index and imaginary argument.

Gaussian integration

iterability that we want, then it is Gaussians that we are stuck with. And Gaussians are, as will emerge, enough.¹⁵

At the heart of (38) lies the familiar formula

$$\int_{-\infty}^{+\infty} e^{-\frac{1}{2}(ax^2 + 2bx + c)} dx = \sqrt{\frac{2\pi}{a}} e^{\frac{1}{2} \left[\frac{b^2 - ac}{a} \right]}$$
(39)

of which we have already several times made use. And (39) is itself implicit in this special case:

$$\int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi} \tag{40}$$

This is a wonderfully simple result to support the full weight of the integral calculus of functionals! We are motivated to digress for a moment to review the derivation of (40), and details of the mechanism by which (40) gives rise to (39). Standardly, one defines $G \equiv \int e^{-x^2} dx$ and observes that

$$G \cdot G = \int \int_{-\infty}^{+\infty} e^{-(x^2 + y^2)} dx dy$$
$$= \int_0^{2\pi} \int_0^{\infty} e^{-r^2} r dr d\theta$$
$$= 2\pi \cdot \frac{1}{2} \int_0^{\infty} e^{-s} ds$$
$$= \pi$$

from which (40) immediately follows.¹⁶ It is a curious fact that to achieve this result we have had to do a certain amount of "swimming upstream," against the prevailing tide: to evaluate the single integral which lies at the base of our theory of iterative multiple integration we have found it convenient to exploit a change-of-variables trick as it pertains to a certain *double* integral! Concerning

¹⁵ Feynman's "sum-over-paths" is defined by "refinement" $N \longrightarrow \infty$ of just such an iterative scheme. The Gaussians arise there from the circumstance that \dot{x} enters quadratically into the construction of physical Lagrangians. One can readily write out the Lagrangian physics of systems of the hypothetical type $L = \frac{1}{3}\mu\dot{x}^3 - U(x)$. But look at the Hamiltonian: $H = \frac{2}{3}\frac{1}{\sqrt{\mu}}p^{\frac{3}{2}} + U(x)!$ Look at the associated Schrödinger equation!! The utter collapse of the Feynman formalism in such cases, the unavailability of functional methods of analysis, inclines us to dismiss such systems as "impossible."

¹⁶ The introduction of polar coordinates entailed tacit adjustment (square to circle) of the domain of integration, which mathematicians correctly point out requires some justification. This little problem can, however, be circumvented

the production of (39) from (40), we by successive changes of variable have

$$\sqrt{\frac{2\pi}{a}} = \int_{-\infty}^{+\infty} e^{-\frac{1}{2}ax^2} dx$$
$$= \int_{-\infty}^{+\infty} e^{-\frac{1}{2}a(x+\frac{b}{a})^2} dx$$
$$= e^{-\frac{1}{2}\left[\frac{b^2 - ac}{a}\right]} \cdot \int_{-\infty}^{+\infty} e^{-\frac{1}{2}(ax^2 + 2bx + c)} dx$$

What's going on here, up in the exponent, is essentially a "completion of the square." These elementary remarks acquire deeper interest from an observation and a question. Recalling from p. 87 the definition of the gamma function, we observe that

$$\int_{0}^{+\infty} e^{-x^{n}} dx = \frac{1}{n} \int_{0}^{+\infty} e^{-u} u^{\frac{1}{n}-1} du$$
$$= \frac{1}{n} \Gamma(\frac{1}{n})$$

which, by the way, gives back (40) at n = 2. Why can we not use this striking result to construct a general theory of $\int e^{\text{polynomial of degree } n} dx$? Because there exists no cubic, quartic...analog of "completion of the square;"

$$P_n(x) = (x+p)^n + q$$

serves to describe the most general monic polynomial of degree n only in the case n = 2. This little argument provides yet another way (or another face of an old way) to understand that the persistent intrusion of Gaussians into theory of iterative multiple integration (whence into the integral calculus of functionals) is not so much a symptom of "Gaussian chauvinism" as it is a reflection of some essential facts. I have belabored the point, but will henceforth consider it to have been established; we agree to accept, as a fact of life, the thought that if we are to be multiple/functional integrators we are going to have, as a first qualification, to be familiar with all major aspects of Gaussian integration theory. Concerning which some important things remain to be said:

by a trick which I learned from Joe Buhler: write y = ux and obtain

$$G \cdot G = 2^2 \int_0^\infty \int_0^\infty e^{-x^2(1+u^2)} x dx du$$

= $4 \int_0^\infty \int_0^\infty \frac{e^{-v}}{2(1+u^2)} du dv$ where $v = x^2(1+u^2)$
= $2 \int_0^\infty e^{-v} dv \cdot \int_0^\infty \frac{du}{1+u^2}$
= $2 \cdot 1 \cdot \arctan(\infty)$
= π

Gaussian integration

Returning to (39), we note that the integrand $e^{-\frac{1}{2}Q(x)}$ will be maximal when $Q(x) \equiv ax^2 + 2bx + c$ is minimal, and from $\frac{d}{dx}Q(x) = 2(ax + b) = 0$ find that Q(x) is minimal at $x = x_0 \equiv -\frac{b}{a}$, where $Q(x_0) = -\left[\frac{b^2-ac}{a}\right]$. The pretty implication is that (39) can be notated

$$\int_{-\infty}^{+\infty} e^{-\frac{1}{2}Q(x)} dx = \sqrt{\frac{2\pi}{a}} e^{-\frac{1}{2}Q(x_0)}$$
(41)

where

$$Q(x) \equiv ax^2 + 2bx + c$$
 and $x_0 \equiv -a^{-1}b$

But by Taylor expansion (which promptly truncates)

$$= Q(x_0) + a(x - x_0)^2$$

Equation (41) can therefore be rewritten in a couple of interesting ways; we have

$$\int_{-\infty}^{+\infty} e^{-\frac{1}{2}\{Q(x_0) + a(x - x_0)^2\}} dx = \sqrt{\frac{2\pi}{a}} e^{-\frac{1}{2}Q(x_0)}$$
(42.1)

-of which more in a minute—and we have the (clearly equivalent) statement

$$\int_{-\infty}^{+\infty} \left\{ \sqrt{\frac{a}{2\pi}} e^{-\frac{1}{2}a(x-x_0)^2} \right\} \, dx = 1 \quad : \quad \text{all } a \text{ and all } x_0 \tag{42.2}$$

where the integrand is a "normal distribution function," and can in the notation of p. 91 be described $G(x - x_0; a^{-\frac{1}{2}})$. By an identical argument (36) becomes (allow me to write **b** and *c* where formerly I wrote **B** and *C*)

$$\int \int \dots \int_{-\infty}^{+\infty} e^{-\frac{1}{2}Q(\mathbf{x})} dx^1 dx^2 \dots x^N = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} e^{-\frac{1}{2}Q(\mathbf{x}_0)}$$
(43)

where

$$Q(\mathbf{x}) \equiv \mathbf{x} \cdot \mathbb{A}\mathbf{x} + 2\mathbf{b} \cdot \mathbf{x} + c \qquad \text{and} \qquad \mathbf{x}_0 \equiv -\mathbb{A}^{-1}\mathbf{b}$$

By Taylor expansion

$$= Q(\mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0) \cdot \mathbb{A}(\mathbf{x} - \mathbf{x}_0)$$

so we have

$$\int \int \cdots \int_{-\infty}^{+\infty} e^{-\frac{1}{2} \{Q(\mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0) \cdot \mathbb{A}(\mathbf{x} - \mathbf{x}_0)\}} dx^1 dx^2 \cdots x^N = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} e^{-\frac{1}{2}Q(\mathbf{x}_0)}$$

and

$$\int \int \dots \int_{-\infty}^{+\infty} \left\{ \sqrt{\frac{\det \mathbb{A}}{(2\pi)^N}} \ e^{-\frac{1}{2}(\mathbf{x} - \mathbf{x}_0) \cdot \mathbb{A}(\mathbf{x} - \mathbf{x}_0)} \right\} \ dx^1 dx^2 \cdots x^N = 1$$
(44)

The function in braces describes what might be called a "bell-shaped curve in N-space," centered at \mathbf{x}_0 and with width characteristics fixed by the eigenvalues of \mathbb{A} .

Asymptotic evaluation of integrals by Laplace's method. Pierre Laplace gave the preceeding material important work to do when in 1814 he undertook to study the *asymptotic evaluation of integrals* of the general type

$$I(\lambda) = \int_{-\infty}^{+\infty} f(x) e^{-\lambda g(x)} \, dx$$

Assume g(x) to have a minimum at $x = x_0$. One expects then to have (in ever-better approximation as $\lambda \longrightarrow \infty$)

$$I(\lambda) \sim \int_{x_0-\epsilon}^{x_0+\epsilon} f(x)e^{-\lambda g(x)} dx$$

By Taylor expansion $g(x) = g(x_0) + 0 + \frac{1}{2}g''(x_0)(x-x_0)^2 + \cdots$ with $g''(x_0) > 0$. Drawing now upon (42) we obtain

$$I(\lambda) \sim e^{-\lambda g(x_0)} \sqrt{\frac{2\pi}{\lambda g''(x_0)}} \int f(x) \left\{ \sqrt{\frac{\lambda g''(x_0)}{2\pi}} e^{-\frac{1}{2}\lambda g''(x_0)(x-x_0)^2} \right\} dx$$

In a brilliancy which anticipated the official "invention of the δ -function" by more than a century, Laplace observed that the expression in braces nearly vanishes except on a neighborhood of x_0 that becomes ever smaller as λ becomes larger, and arrived thus at the celebrated "Laplace asymptotic evaluation formula"¹⁷

$$I(\lambda) \sim f(x_0) e^{-\lambda g(x_0)} \sqrt{\frac{2\pi}{\lambda g''(x_0)}}$$
(45)

In classic illustration of the practical utility of (45) we recall from p. 87 that ∞

$$\Gamma(n+1) \equiv \int_0^\infty e^{-x} x^n \, dx = n!$$
 for *n* integral

But a change of variables $x \longrightarrow y \equiv x/n$ gives

$$= n^{n+1} \int_0^\infty e^{-n(y - \log y)} \, dy$$

and $g(y) \equiv y - \log y$ is minimal at y = 1, so by application of (45) we have

$$\Gamma(n+1) = n! \sim \sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n}$$

¹⁷ For careful discussion of Laplace's formula and its many wonderful variants see Chapter II of A. Erdélyi, *Asymptotic Expansions* (1956) or N. De Bruijn, *Asymptotic Methods in Analysis* (1958).

Laplace's formula

which is familiar as "Stirling's formula." De Bruijn, in his §4.5, shows how one can, with labor, refine the argument so as to obtain

$$n! \sim \sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n} \cdot \exp\left\{\frac{B_2}{1 \cdot 2n} + \frac{B_4}{3 \cdot 4n^3} + \frac{B_6}{5 \cdot 6n^5} + \cdots\right\}$$
$$= \sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n} \cdot \left\{1 + \frac{1}{12n} + \frac{1}{288n^2} - \frac{139}{51840n^3} - \frac{571}{2488320n^4} + \cdots\right\}$$

where B_2 , B_4 , B_6 , ... are Bernoulli numbers. The pretty particulars of this last result are of less interest than its general implication: Laplace's argument does not simply blurt out its answer and then fall silent; it supports a "refinement strategy" (though this is, to my knowledge, seldom actually used).

I thought I heard some gratuitous coughing during the course of that last paragraph, so hasten to turn now to an "illustration of the practical utility" of Laplace's formula which has a latently more physical feel about it. Let G(p) be the Fourier transform of F(x):

$$F(x) \xrightarrow[\text{Fourier}]{\text{Fourier}} G(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}px} F(x) \, dx$$

Let us, moreover, agree to write $F(x) = \mathcal{F}(x)e^{-\frac{i}{\hbar}f(x)}$ and $G(p) = \mathcal{G}(p)e^{-\frac{i}{\hbar}g(p)}$. The implied relationship

$$\mathcal{G}(p)e^{-\frac{i}{\hbar}g(p)} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathcal{F}(x)e^{-\frac{i}{\hbar}[f(x)-px]} dx$$

between $\{\mathcal{F}(x), f(x)\}$ and $\{\mathcal{G}(p), g(p)\}$ is difficult/impossible to describe usefully in general terms, but in the asymptotic limit $\frac{1}{\hbar} \longrightarrow \infty$ we can draw formally upon (45) to obtain

$$\mathcal{G}(p) \cdot e^{-\frac{i}{\hbar}g(p)} \sim \left. \sqrt{\frac{\hbar}{f''(x)}} \,\mathcal{F}(x) \cdot e^{-\frac{i}{\hbar}[f(x) - px]} \right|_{x \to x(p)} \tag{46}$$

where x(p) is obtained by functional inversion of p = f'(x). The remarkable implication is that g(p) is precisely the *Legendre transform* of f(x)! We have established that, in a manner of speaking,

Fourier transformations $\longrightarrow e^{i \, (\text{Legendre transformations})}$

and in precisely that same manner of speaking it emerges that

$$\begin{array}{ccc} \text{physical optics} & & & \\ \hline c \longrightarrow \infty & e^{-i} \text{ (geometrical optics)} \\ \text{quantum mechanics} & & \\ \hline \hbar^{-1} \longrightarrow \infty & e^{-i} \text{ (classical mechanics)} \\ \text{statistical mechanics} & & \\ \hline k^{-1} \longrightarrow \infty & e^{-(\text{thermodynamics})} \end{array}$$

The physical connections thus sketched comprise, I think we can agree, physics of a high order (indeed, physics of an *asymptotically* high order!). Remarkably, at the heart of each of those many-faceted connections live either Laplace's formula or one of its close relatives (the Riemann–Debye "method of steepest descents," the Stokes–Kelvin "method of stationary phase"). And at the heart of each of those lives a Gaussian integral.¹⁸

Laplace's asymptotic formula admits straightforwardly of N-dimensional generalization. We write

$$I(\lambda) \equiv \int \int \cdots \int_{-\infty}^{+\infty} F(\mathbf{x}) e^{-\lambda g(\mathbf{x})} dx^1 dx^2 \cdots dx^N$$

Assume $g(\mathbf{x})$ to have a minimum at $\mathbf{x} = \mathbf{x}_0$. Then

$$g(\mathbf{x}) = g(\mathbf{x}_0) + 0 + \frac{1}{2}(\mathbf{x} - \mathbf{x}_0) \cdot \mathbb{G}(\mathbf{x} - \mathbf{x}_0) + \cdots$$

where $\mathbb{G} \equiv \|\partial^2 g(\mathbf{x})/\partial x^i \partial x^j\|$ —the matrix of second partials, evaluated at \mathbf{x}_0 —is positive definite. Arguing as before, we obtain

$$I(\lambda) \sim F(\mathbf{x}_0) e^{-\lambda g(\mathbf{x}_0)} \sqrt{\frac{(2\pi/\lambda)^N}{\det \mathbb{G}}}$$
(47)

Physically motivated functional integration. I turn now to discussion of how a theory of functional integration emerges " by refinement" (i.e., in the limit $N \to \infty$) from the interative theory of multiple integration. Both Wiener (in the late 1920's, for reasons characteristic of his approach to the theory of Brownian motion¹⁹) and Feynman (in the early 1940's, for reasons characteristic of his approach to quantum mechanics²⁰) had reason to be interested in what have come universally (if awkwardly) to be called "sum-over-path" processes.

¹⁸ I remarked in the text that (46) was obtained by "formal" application of (45). The adjective alludes to the fact that the Gaussian integral formula (39) holds if an only if $\Re(a) > 0$, which in the present context may not be satisfied. The problem would not have arisen had we been discussing Laplace transforms rather than Fourier transforms, and can frequently be circumvented by one or another of strategies which physicists have been at pains to devise; for example, one might (as Feynman himself suggested: see footnote #13 to his "Space-time approach to non-relativistic quantum mechanics," Rev. Mod. Phys. **20**, 367 (1948)) make the replacement $\hbar \longrightarrow \hbar(1 - i\epsilon)$ and then set $\epsilon \downarrow 0$ at the end of the day. My own practice will be to proceed with formal abandon, trusting to the sensible pattern of our (formal) results, and to the presumption that when we have accumulated results in a sufficient mass we will find both motivation and some elegant means to dot the i's and cross the mathematical t's. ¹⁹ See Chapter I of his Nonlinear Problems in Random Theory (1958).

 $^{^{20}}$ See §4 of the classic paper cited on the previous page, or Chapter II of *Quanatum Mechanics and Path Integrals* by R. Feynman & A. Hibbs (1965).

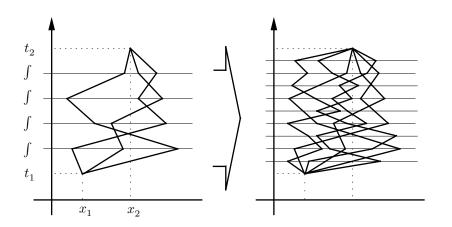


FIGURE 2: Representation of the elementary essentials of the idea from which the Wiener-Feynman "sum-over-paths" construction proceeds.

Each worked in a subject area marked (as it happens) by the natural occurrence —for distinct reasons—of Gaussians, each was led to contemplate expressions of the type

$$\lim_{N \to \infty} \int \cdots \int e^{-(\text{quadratic form in N variables})} d(\text{variables}) \tag{48}$$

and each was protected from disaster by the "integrative closure" property of Gaussians. Each was led to write something like

$$\int_{\text{space of paths } x(t)} F[x(t)]\mathcal{D}x(t)$$
(49)

to describe the result of such a limiting process. Concerning the structure of the "space of paths" over which the functional integral (49) ranges: the figures suggests that the elements x(t) of "path space" are, with rare exceptions, too spiky to permit the construction of $\dot{x}(t)$. It would, however, be a mistake to waste time pondering whether this development is to be regarded as a "physical discovery" or a "formal blemish," for to do so would be to attach to the figure a literalness it is not intended to support. Suppose, for example, we were to write

$$x(t) = x_{\rm nice}(t) + s(t)$$

where $x_{\text{nice}}(t)$ is any (nice or unnice) designated path linking specified spacetime endpoints $(x_1, t_1) \longrightarrow (x_2, t_2)$ and where

$$s(t) \equiv \sum_{n=1}^{\infty} a_n \sin\left\{n\pi \left[\frac{t - t_1}{t_2 - t_1}\right]\right\}$$
(50)

has by design the property that $s(t_1) = s(t_2) = 0$. Individual paths would then be specified not by "the locations of their kinks" but by their Fourier coefficients $\{a_n\}$. Elements of the path space thus constructed can be expected to have differentiability properties quite different from those originally contemplated, and "summing-over-paths" would entail iterated operations of the type $\int da.^{21}$ Applications of the functional integral concept tend, to a remarkable degree, to proceed independently of any precise characterization of path space.

In order to make as concretely clear as possible the issues and methods most characteristic of the applied integral calculus of functionals, I look now to the essential rudiments of the Feynman formalism. By way of preparation, in order to grasp Feynman's train of thought, we remind remind ourselves that in abstract quantum mechanics one has $i\hbar\frac{\partial}{\partial t}|\psi\rangle = \mathbf{H}|\psi\rangle$, giving $|\psi\rangle_t = \exp\{\frac{1}{i\hbar}\mathbf{H}t\}|\psi\rangle_0$. In the *x*-representation²² we have $(x|\psi)_t = \int (x|\exp\{\frac{1}{i\hbar}\mathbf{H}t\}|y)dy(y|\psi)_0$ which is more often written

$$\psi(x,t) = \int K(x,t;y,0)\psi(y,0) \, dy$$

It is from the preceeding equation that the Green's function of the Schrödinger equation—usually called the "propagator"

$$K(x,t;y,0) \equiv (x,t|y,0) = (x|\exp\{\frac{1}{i\hbar}\mathsf{H}t\}|y)$$

—acquires its role as the "fundamental object of quantum dynamics." Three properties of the propagator are of immediate importance. We note first that $K(x,t;\bullet,\bullet)$ is itself a solution of the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}K(x,t;\bullet,\bullet) = \mathsf{H}K(x,t;\bullet,\bullet)$$
(51.1)

From

$$\lim_{t \to 0} K(x,t;y,0) = (x|y) = \delta(x-y)$$
(51.2)

we see that K(x,t;y,0) is in fact the solution that evolved from an initial δ -function. It follows finally from the triviality $e^{\mathsf{H}(a+b)} = e^{\mathsf{H}a} \cdot e^{\mathsf{H}b}$ that

$$K(x,t;z,0) = \int K(x,t;y,\tau) dy K(y,\tau;y,0) \quad \text{for all } t \ge \tau \ge 0$$
(51.3)

It was by an interative refinement procedure based upon the "composition rule" that Feynman was led to the imagery of FIGURE 10. But it was a stroke of

 $^{^{21}}$ For discussion of details relating to this mode of proceeding, see Chapter I, pp. 56–60 of QUANTUM MECHANICS (1967).

²² The "space-time approach..." of Feynman's title reflects his appreciation of the fact that selection of the *x*-representation is an arbitrary act, yet an act basic to the imagery from which his paper proceeds.

Wiener-Feynman "sum-over-path" processes

 $genius^{23}$ which led Feynman to contemplate a formula of the structure

$$K(x_2, t_2; x_1, t_1) = \int e^{\frac{i}{\hbar}S[x(t)]} \mathcal{D}x(t)$$
(52)

Here x(t) is a "path" with the endpoint properties

$$x(t_1) = x_1$$
 and $x(t_2) = x_2$

S[x(t)] is the *classical* action functional associated with that path

$$S[x(t)] = \int_{t_1}^{t_2} L(x(t), \dot{x}(t)) dt$$
(53)

and $\mathcal{D}x(t)$ —for which in some contexts it becomes more natural to write $R[x(t)]\mathcal{D}x(t)$ —alludes implicitly to the as-yet-unspecified "measure-theoretic" properties of path space. Our problem is to assign specific meaning to the functional integral that stands on the right side of (52). To that end, let $L(x,\dot{x}) = \frac{1}{2}m\dot{x}^2 - U(x)$ describe the classical dynamics of some one-dimensional system, let $x_c(t)$ be a solution of the equations of motion that interpolates $(x_1, t_1) \longrightarrow (x_2, t_2)$ between specified endpoints, let s(t) be some given/fixed nice function with the property that $s(t_1) = s(t_2) = 0$ and let

$$x(t) = x_c(t) + \lambda s(t)$$

be the elements of a one-parameter path space generated by s(t). Under such circumstances the action functional (53)—though it remains a functional of s(t)—becomes an ordinary function of the parameter λ (and of the endpoint coordinates). This is the simplification that makes the present discussion²⁴ work. We have

$$\begin{split} L(x_c + \lambda s, \dot{x}_c + \lambda \dot{s}) &= e^{\lambda \left(s \frac{\partial}{\partial x_c} + \dot{s} \frac{\partial}{\partial x_c}\right)} L(x_c, \dot{x}_c) \\ &= \sum_k \frac{1}{k!} \lambda^k L_k(x_c, \dot{x}_c, s, \dot{s}) \end{split}$$

giving

$$S[x(t)] = \sum_{k} \frac{1}{k!} \lambda^{k} \underbrace{S_{k}(x_{2}, t_{2}; x_{1}, t_{1}; s(t))}_{= \int_{t_{1}}^{t_{2}} L_{k}(x_{c}.\dot{x}_{c}, s, \dot{s}) dt$$

 $^{^{23}}$ Dirac's genius, one might argue. See §32 "The action principle," in *The* Principles of Quantum Mechanics (1958) and "The Lagrangian in quantum mechanics," Physik. Zeits. Sowjetunion **3**, 64 (1933), both of which—and little else—are cited by Feynman. The latter paper has been reprinted in J. Schwinger (ed.) Quantum Electrodynamics (1958).

²⁴ It has served my expository purpose to depart here from the historic main line of Feynman's argument; I follow instead in the footsteps of C. W. Kilmister, "A note on summation over Feynman histories," Proc. Camb. Phil. Soc. **54**, 302 (1958).

and notice that

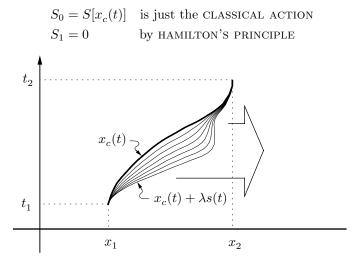


FIGURE 3: λ -parameterized family of paths having $x_c(t)$ as a member, and generated by an arbitrary s(t). The arrow indicates the effect of increasing λ . We are making integral use of what is, in fact, the construction standard to the calculus of variations.

By computation

$$L_0 = \frac{1}{2}m\dot{x}_c^2 - U(x_c)$$

$$L_1 = \text{need not be computed}$$

$$L_2 = -m\dot{s}^2 - U''(x_c)s^2$$

$$\vdots$$

$$L_k = -U^{(k)}(x_c)s^k$$

so within the path space here in question we have 25

$$S[x(t)] = S_{\text{classical}}(x_2, t_2; x_1, t_1) + \frac{1}{2}\lambda^2 \int_{t_1}^{t_2} \left\{ m \dot{s}^2 - U''(x_c) s^2 \right\} dt$$

$$- \sum_{k=3}^{\infty} \frac{1}{k!} \lambda^k \int_{t_1}^{t_2} U^{(k)}(x_c) s^k dt$$
(54)

 25 This is a specialized instance of (see again (9)) the generic Volterra series

$$S[x_{c} + \lambda s] = S[x_{c}] + \lambda \int_{t_{1}}^{t_{2}} \frac{\delta S[x_{c}]}{\delta x_{c}(t)} s(t) dt + \frac{1}{2} \lambda^{2} \int_{t_{1}}^{t_{2}} \int_{t_{1}}^{t_{2}} \frac{\delta^{2} S[x_{c}]}{\delta x_{c}(t') \delta x_{c}(t'')} s(t') s(t'') dt' dt'' + \cdots$$

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It becomes natural at this point to write

$$\int_{\text{paths generated by } s(t)} e^{\frac{i}{\hbar}S[x(t)]} \mathcal{D}x(t) = \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}\{S_0 + \frac{1}{2}\lambda^2 S_2 + \text{higher order terms}\}} d\lambda \qquad (55)$$

In the interests of maximal tractability (always fair in exploratory work) we opt to kill the "higher order terms" by assuming the potential U(x) to depend at most quadratically upon x; we assume, in short, that the Lagrangian $L(x, \dot{x})$ pertains to an oscillator in a gravitational field:

$$U(x) = mgx + \frac{1}{2}m\omega^2 x^2 \tag{56}$$

Equation (54) then truncates:

$$S[x(t)] = \underbrace{S_{\text{classical}}(x_2, t_2; x_1, t_1)}_{S_0} + \frac{1}{2}\lambda^2 \cdot \underbrace{\int_{t_1}^{t_2} m\{\dot{s}^2 - \omega^2 s^2\} dt}_{S_2}$$
(57)

Remarkably, all reference to $x_c(t)$ —and therefore to the variables x_1 and x_2 —has disappeared from the 2nd-order term, about which powerful things of several sorts can be said. We might write

$$S_2 = S_2[s(t)] = \mathbf{D}_{[s]}^2 S[x(t)]$$
(58.1)

to emphasize that S_2 is a functional of s(t) from which all x(t)-dependence has dropped away. And we might write

$$S_2 = S_2(t_2 - t_1) \tag{59.2}$$

to emphasize that S_2 depends upon t_1 and t_2 only through their difference,²⁶ and is (as previously remarked) independent of x_1 and x_2 . If we now return

$$\begin{split} \int_{t_1}^{t_2} F\left(x\left(\frac{t-t_1}{t_2-t_1}\right), \dot{x}\left(\frac{t-t_1}{t_2-t_1}\right)\right) dt &= \int_0^1 F\left(x(\vartheta), \frac{1}{t_2-t_1} \frac{d}{d\vartheta} x(\vartheta)\right) \left(t_2 - t_1\right) d\vartheta \\ &= \text{function of } (t_2 - t_1) \end{split}$$

so one has only to insert (50) into the integral that defines S_2 to achieve the result claimed in the text. One could, however, continue; drawing upon

$$\int_0^1 \sin m\pi\vartheta \sin n\pi\vartheta \, d\vartheta = \int_0^1 \cos m\pi\vartheta \cos n\pi\vartheta \, d\vartheta = \frac{1}{2}\delta_{mn}$$

for $m, n = 1, 2, 3, \cdots$ one can actually do the integral. One obtains at length

$$S_2 = \frac{m}{2T} \sum (\pi n)^2 \left[1 - \left(\frac{\omega T}{\pi n}\right)^2 \right] a_n^2 \quad \text{with} \quad T \equiv t_2 - t_1$$

which is the starting point for the $\int da$ -procedure to which I alluded on p. 99.

 $^{^{26}}$ It is elementary that

with (57) to (55) we obtain

$$\int_{\text{paths generated by } s(t)} e^{\frac{i}{\hbar}S[x(t)]} \mathfrak{D}x(t) = e^{\frac{i}{\hbar}S_0} \cdot \int_{-\infty}^{+\infty} e^{-\frac{1}{2} \cdot \frac{1}{i\hbar}S_2[s(t)] \cdot \lambda^2}$$
(59)

To perform the Gaussian integral is to obtain

$$=e^{\frac{i}{\hbar}S_{0}}\cdot\sqrt{\frac{2\pi i\hbar}{S_{2}[s(t)]}}$$

which, because of its surviving functional dependence upon the arbitrarily selected generator s(t), cannot possibly provide a description of the propagator $(x_2, t_2|x_1, t_1)$. One obvious way to remedy this defect is—consistently with the essential spirit of the Feynman formalism—to sum over all generators; we back up to (59), set $\lambda = 1$, and obtain

$$\begin{split} K(x_2, t_2; x_1, t_1) &= \int_{\text{all paths}} e^{\frac{i}{\hbar} S[x(t)]} \mathcal{D}x(t) \\ &= e^{\frac{i}{\hbar} S_0(x_2, t_2; x_1, t_1)} \cdot \left\{ \int_{\text{all generators}} e^{\frac{i}{\hbar} \frac{1}{2} S_2[s(t)]} \mathcal{D}s(t) \right\} \end{split}$$

We appear to have simply replaced one functional integral by another, but the latter is an object we know something about: it is (since a sum of such functions) a function of $t_2 - t_1$. So we have

$$K(x_2, t_2; x_1, t_1) = A(t_2 - t_1) \cdot e^{\frac{i}{\hbar}S_0(x_2, t_2; x_1, t_1)}$$
(60.1)

with

$$A(t_2 - t_1) = \int_{\text{all generators}} e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_1}^{t_2} \{\dot{s}^2 - \omega^2 s^2\} dt} \mathbb{D}s(t)$$
(60.2)

There are several alternative ways in which we might now proceed. We might roll up our sleeves and undertake (as Feynman did) to *evaluate* the functional integral that defines $A(t_2 - t_1)$. To that end we would write

$$\begin{split} \int_{t_1}^{t_2} \{\dot{s}^2 - \omega^2 s^2\} dt \\ &= \lim_{N \to \infty} \tau \Big\{ \Big(\frac{s_1 - 0}{\tau}\Big)^2 + \Big(\frac{s_2 - s_1}{\tau}\Big)^2 + \dots + \Big(\frac{s_N - s_{N-1}}{\tau}\Big)^2 + \Big(\frac{0 - s_N}{\tau}\Big)^2 \\ &- \omega^2 \Big(s_1^2 + s_2^2 + \dots + s_{N-1}^2 + s_N^2\Big) \Big\} \\ &= \lim_{N \to \infty} \frac{1}{\tau} \mathbf{s} \cdot \mathbb{M} \mathbf{s} \end{split}$$

with $\tau = (t_2 - t_1)/(N+1) = [(t_2 - t_1)/N] \{1 - \frac{1}{N} + \frac{1}{N^2} + \cdots\} \sim (t_2 - t_1)/N$ and

$$\mathbb{M} \equiv \begin{pmatrix} M & -1 & 0 & 0 & & 0 \\ -1 & M & -1 & 0 & & 0 \\ 0 & -1 & M & -1 & & 0 \\ & & \ddots & & & \\ & & & \ddots & & \\ 0 & & & -1 & M & -1 \\ 0 & & & 0 & -1 & M \end{pmatrix} \quad \text{where} \quad M \equiv 2 - (\tau \omega)^2$$

We look to the N-fold integral

$$I_N = \int \cdots \int_{\infty}^{+\infty} e^{-\frac{1}{2}\mathbf{s} \cdot \mathbf{A} \cdot \mathbf{s}} \, ds_1 ds_2 \cdots ds_N$$

where $\mathbb{A}=\beta\mathbb{M}$ and $\beta=m/i\hbar\tau$ and draw upon the multi-dimensional Gaussian integral formula to obtain

$$I_N = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} = \sqrt{\frac{(2\pi/\beta)^N}{\det \mathbb{M}}}$$
(61)

To evaluate $D_N = \det \mathbb{M}$ when \mathbb{M} is $N \times N,$ we look to the sequence of

$$D_1 = (M), \quad D_2 = \begin{pmatrix} M & -1 \\ -1 & M \end{pmatrix}, \quad D_3 = \begin{pmatrix} M & -1 & 0 \\ -1 & M & -1 \\ 0 & -1 & M \end{pmatrix}, \quad \dots$$

of sub-determinants and obtain

$$\begin{array}{l} D_{1} = M \\ D_{2} = M^{2} - 1 \\ D_{3} = M^{3} - 2M \\ \vdots \\ D_{n} = MD_{n-1} - D_{n-2} \end{array}$$

We introduce the "tempered" numbers $\mathcal{D}_n\equiv\omega\tau D_n$ to facilitate passage to the limit. They obviously satisfy an identical recursion relation, and upon recalling the definition of M we observe that the recursion relation in question can be expressed

$$\frac{1}{\tau} \bigg\{ \frac{\mathcal{D}_n(N) - \mathcal{D}_{n-1}(N)}{\tau} - \frac{\mathcal{D}_{n-1}(N) - \mathcal{D}_{n-2}(N)}{\tau} \bigg\} = -\omega^2 \mathcal{D}_{n-1}(N)$$

This in the limit becomes a differential equation

$$\frac{d^2 \mathcal{D}(t)}{dt^2} = -\omega^2 \mathcal{D}(t) \tag{62.1}$$

descriptive of a function D(t) for which we seek the value at $t = N\tau = t_2 - t_1$. To start the recursive construction off we need initial data; we have

$$\mathcal{D}_1 = \omega \tau [2 - (\omega \tau)^2] \quad \text{giving} \quad \mathcal{D}(0) = 0 \tag{62.2}$$

and

$$\frac{\mathcal{D}_2 - \mathcal{D}_1}{\tau} = \frac{\omega\tau}{\tau} \left\{ [2 - (\omega\tau)^2]^2 - 1 - [2 - (\omega\tau)^2] \right\}$$
$$= \omega \left\{ 1 - 3(\omega\tau)^2 + (\omega\tau)^4 \right\} \quad \text{giving} \quad \mathcal{D}'(0) = \omega \tag{62.3}$$

It follows from (62) that $\mathcal{D}(t) = \sin \omega t$. Returning with this information to (61) we obtain

$$\begin{split} I_N &= \left(\frac{2\pi i \hbar \tau}{m}\right)^{\frac{N}{2}} \sqrt{\frac{\omega \tau}{\sin \omega (t_2 - t_1)}} \\ &= R^{N+1} \cdot \sqrt{\frac{m \omega}{2\pi i \hbar \sin \omega (t_2 - t_1)}} \quad \text{with} \quad R(\tau) \equiv \sqrt{\frac{2\pi i \hbar \tau}{m}} \end{split}$$

To obtain a non-trivial result in the limit $\tau \downarrow 0$ we must a bandon the prefactor. To that end we make the replacement

$$ds_1 d_2 \cdots d_N \longrightarrow R \cdot ds_1 \cdot R \cdot ds_2 \cdot R \cdots R \cdot ds_N \cdot R$$

which is, in effect, to assign a "measure" to path space. Thus—following a cleaned-up version of the path blazed by Feynman—do we assign direct meaning to the statement

$$A(t_2 - t_1) = \int_{\text{all generators}} e^{\frac{i}{\hbar} \frac{m}{2} \int_{t_1}^{t_2} \{\dot{s}^2 - \omega^2 s^2\} dt} \mathcal{D}s(t) = \sqrt{\frac{m\omega}{2\pi i \hbar \sin \omega (t_2 - t_1)}}$$
(63)

Our success, it will be noted, was entirely Gaussian in origin. And hard won!

There is, however, a "softer" way to proceed. We might consider that the functional integral concept had already told us what it had to say when at (60.1) it ascribed a certain non-obvious *structure* to the propagator, and that it is to conditions (51) that we should look for more particular information about the left side $A(t_2 - t_1)$. To illustrate with minimal clutter the kind of analysis I have in mind, consider the case of a free particle. For such a system it is a familiar fact that the classical action can be described

$$S_0(x_2,t_2;x_1,t_1) = \frac{m}{2} \frac{(x_2-x_1)^2}{t_2-t_1}$$

What condition on $A(t_2 - t_1)$ is forced by the requirement that, consistently with (51.2),

$$K(x_2, t_2; x_1, t_1) = A(t_2 - t_1) \cdot e^{\frac{i}{\hbar} \frac{m}{2} (x_2 - x_1)^2 / (t_2 - t_1)} \quad \longrightarrow \quad \delta(x_2 - x_1)$$

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as $(t_2 - t_1) \downarrow 0$? Familiarly

$$\delta(x-a) = \lim_{\sigma \to 0} \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\left[\frac{x-a}{\sigma}\right]^2\right\}$$

so we write

$$e^{\frac{i}{\hbar}\frac{m}{2}(x_2-x_1)^2/(t_2-t_1)} = \exp\left\{-\frac{1}{2}\left[\frac{x_2-x_1}{\sqrt{i\hbar(t_2-t_1)/m}}\right]^2\right\}$$

and conclude that $A(t_2 - t_1)$ has necessarily the form

$$A(t_2 - t_1) = \sqrt{\frac{m}{2\pi\hbar(t_2 - t_1)}} \cdot \{1 + \text{arbitrary power series in } (t_2 - t_1)\}$$

This result is consistent with the result obtained from (63) in the free particle limit $\omega \downarrow 0$. Much sharper conclusions can be drawn from (51.3); one wants

$$\begin{split} A(t_2 - t_1) \cdot e^{\frac{i}{\hbar} \frac{m}{2} (x_2 - x_1)^2 / (t_2 - t_1)} \\ &= A(t_2 - t) A(t - t_1) \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar} \frac{m}{2} (x_2 - x)^2 / (t_2 - t)} e^{\frac{i}{\hbar} \frac{m}{2} (x - x_1)^2 / (t - t_1)} \, dx \end{split}$$

which after performance of the Gaussian integral is found to entail

$$A(t_2 - t_1) = A(t_2 - t)A(t - t_1)\sqrt{\frac{2\pi i\hbar}{m}\frac{(t_2 - t)(t - t_1)}{(t_2 - t_1)}}$$

It implication is that $A(\bullet)$ satisfies a functional equation of the form

$$A(x+y) = A(x)A(y)\sqrt{\frac{\alpha x \cdot \alpha y}{\alpha(x+y)}}$$
 with $\alpha \equiv \sqrt{\frac{2\pi i\hbar}{m}}$

This can be written G(x + y) = G(x)G(y) with $G(x) \equiv A(x)\sqrt{\alpha x}$, and if $\Gamma(x) \equiv \log G(x)$ we have $\Gamma(x + y) = \Gamma(x) + \Gamma(y)$. Therefore

$$\frac{\Gamma(x+y) - \Gamma(x)}{y} = \frac{\Gamma(y)}{y} \quad \text{for all } x$$

from which (taking Y to the limit $y \downarrow 0$) we obtain

$$\frac{d\Gamma(x)}{dx} = k$$
 whence $\Gamma(x) = kx + c$

But the functional condition satisfied by $\Gamma(x)$ enforces c = 0, so we have $G(x) = e^{kx}$ giving $A(x) = \sqrt{\frac{1}{\alpha x}}e^{kx}$. Thus do we obtain

$$K_{\text{free particle}} = \sqrt{\frac{m}{2\pi i\hbar(t_2 - t_1)}} \cdot e^{k(t_2 - t_1)} \exp\left\{\frac{i}{\hbar}S_{\text{free particle}}\right\}$$

The central exponential can be gauged away by adjustment of the energy scale, since $V(x) \longrightarrow V(x) + k$ induces $S \longrightarrow S - k(t_2 - t_1)$. This result is not only consistent with, but actually reproduces, the result implicit in (63). What information could, alternatively, have been gleaned from the requirement (51.1)that $K(x,t;\bullet,\bullet) = A(t) \exp\{\frac{i}{\hbar}S(x,t;\bullet,\bullet)\}$ satisfy the Schrödinger equation? The first of the equations (68) reduces (by $A_{xx} = 0$) to precisely the Hamilton-Jacobi equation, which S by construction satisfies exactly. The second of equations (68) in Chapter I reads

$$(A^2)_t + (\frac{x - x_1}{t - t_1}A^2)_x = 0$$

giving

$$A(t-t_1) = A(t_0) \cdot \sqrt{\frac{t_0}{t-t_1}}$$

which is again consistent with but much weaker than the result implicit in (63). The evidence of this discussion suggests that after-the-fact constructions of $A(t_2 - t_1)$ proceed most effectively from the composition rule (51.3).

And there is, in fact, a still "softer" line of argument which is sufficient to the needs of some applications. Looking back again to (60.1), we note that *ratios* of propagators are described by a formula

$$\frac{K(x_2, t_2; x_1, t_1)}{K(\tilde{x}_2, t_2; \tilde{x}_1, t_1)} = e^{\frac{i}{\hbar} \{S(x_2, t_2; x_1, t_1) - S(\tilde{x}_2, t_2; \tilde{x}_1, t_1)\}}$$

from which all reference to $A(t_2 - t_1)$ has dropped away. This result becomes most vivid when \tilde{x}_1 is a "vacuum point"—a point at which the particle can be *at rest with zero energy*; we have

$$S(\tilde{x}, t_2; \tilde{x}, t_1) = \begin{cases} -E_0(t_2 - t_1) & \text{when } \tilde{x} \text{ is an equilibrium point} \\ 0 & \text{when } \tilde{x} \text{ is a "vacuum point"} \end{cases}$$

and in the latter case

$$K(x_2, t_2; x_1, t_1) = K(\tilde{x}, t_2; \tilde{x}, t_1) \cdot e^{\frac{i}{\hbar}S(x_2, t_2; x_1, t_1)}$$
(64)

For a free particle

$$S_{\text{free particle}}(x_2, t_2; x_1, t_1) = \frac{m}{2} \frac{(x_2 - x_1)^2}{t_2 - t_1}$$

shows that *every* point is a "vacuum point":

$$S_{\text{free particle}}(x, t_2; x, t_1) = 0 \text{ for all } x$$

For an oscillator

$$S_{\text{oscillator}}(x, t_2; x, t_1) = \frac{m\omega}{2\sin\omega(t_2 - t_1)} \bigg[(x_2^2 + x_1^2)\cos\omega(t_2 - t_1) - 2x_2x_1 \bigg]$$

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there is a single vacuum point, situated at the origin. For the system

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

a solitary equilibrium point resides at $\tilde{x} = -g/\omega^2$, where the rest energy is $E_0 = -mg^2/\omega^2$; to make \tilde{x} into a vacuum point one must adjust the zero of the energy scale. For a particle in free fall V(x) = mgx there is *no* equilibrium point, no vacuum point, and it becomes therefore impossible to make use of (64).

The Feynman formalism—clearly and explicitly—takes classical mechanics as its point of departure, and achieves quantum mechanics by a functional integration process, a process that (see the figure) "gives Hamilton's comparison

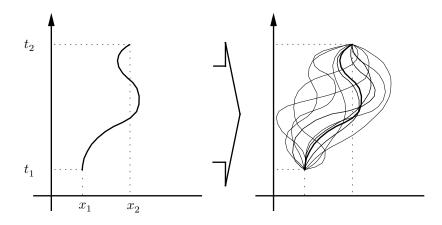


FIGURE 4: Representation of the Feynman quantization procedure.

paths a physical job to do." It is, in effect, a *quantization procedure*, and is today widely considered to be "the quantization procedure of choice." Run in reverse, it provides fresh insight into the placement of classical mechanics within a quantum world, and it is that aspect of the Feynman formalism that I want now to explore. Let