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PATH INTEGRALS AND ASSOCIATED VARIATIONS

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Path integrals and associated variations

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Abstract: Several procedures associated with the variation of the action in Feynman path integrals are described, as follows: construction of the semiclassical approximation, integration by parts, and differentiation with respect to a parameter. Moreover, integrands containing Gaussian factors are discussed, and the occurrence of the Morse index is noted. Some (rigorous) results are extended to the case where Gaussian factors are present.

1. Introduction.

Path integrals were suggested by Feynman as a way of representing solutions to the Schrödinger equation [1] [2]. In particular, we consider the Green's function for a quantum particle on R^n under the influence of a potential V,

$$-i^{-1}\hbar\partial_t G(t;y,x) - [-(\hbar^2/2m)\nabla_y^2 + V(y)]G(t;y,x) = 0 \quad \text{for} \quad t>0, \tag{1.1a}$$

$$\lim_{t\searrow 0} G(t;y,x) = \delta(y-x), \tag{1.1b}$$

and Feynman's ansatz is:

$$G(t;y,x) = N\int_{\substack{\gamma(0)=x\\ \gamma(t)=y}} \mathcal{D}(\gamma)\exp\left\{\frac{i}{\hbar}\int_0^t d\tau\left[\frac{1}{2}m\sum_{j=1}^{n}\left(\frac{d\gamma^j}{d\tau}\right)^2 - V(\gamma(\tau))\right]\right\}. \tag{1.2a}$$

We integrate here (in a way which will be made precise) over paths $\gamma: [0,t] \to R^n$, subject to the two endpoint conditions as indicated. The symbol $\mathcal{D}(\gamma)$ is a kind of generalized measure, and N, a normalizing constant, which depends on the definition of the integral that is adopted. Note that $\int d\tau\ldots$ is the classical action $S(\gamma)$ along the path γ. We will often take $\hbar = 1$ (for Planck's constant divided by 2π), and the above integral can then be written as

$$G(t;y,x) = N\int_{\gamma(0)=x,\ \gamma(t)=y} \mathcal{D}(\gamma)\, e^{iS(\gamma)}. \tag{1.2b}$$

The path integral suggests a way of quantizing a given classical system. One can say that it constitutes an alternative to the quantization methods based on the Schrödinger equation or on the Heisenberg quantization rules. The path integral, however, differs from these two other methods in several respects. In particular, it is based on the Lagrangian, and on the action, rather than on the Hamiltonian. The action in turn leads to a number of variational relations in the classical domain, and these should find their quantum analogues in the path integral formalism [3] [4].

In the present article we discuss three variational procedures which are associated with integrals such as in (1.2). The first applies to the semiclassical limit of quantum mechanics ($\hbar \to 0$). In this case the quantum particle

should move (nearly) along the classical path γ_0. We then make a (functional) power series expansion of $S(\gamma)$ around $S(\gamma_0)$. The quadratic term is of particular interest here.

The second procedure depends on integration by parts. It yields a form of quantum-mechanical equations of motion, and also functional differential equations for generating functionals. The rule $[p_j, q^k] = i^{-1}\delta_j^k$ can also be investigated in this way. The third procedure depends on differentiating path integrals with respect to parameters, and illustrates in particular a connection between the classical equation $p_j = \partial S/\partial q^j$ and the quantum rule $p_j = i^{-1} \times \partial/\partial q^j$. Moreover, the differentiability properties of path integrals is a subject of independent interest.

We should also comment about mathematical rigor in this article. Many discussions of the path integral are at the level of heuristic manipulations, and in fact, the mathematical theory is still in its beginnings. We should therefore like to point out, that the material which we present does have a mathematical basis. In particular, we state in various places some sufficient conditions on the potential for the validity of a given relation, even though we do not give proofs (except in the appendix). Most likely, a relation in question would remain valid also for some other potentials.

The article is organized as follows. In sec. 2 we review one definition of the path integral. In sec. 3 we discuss some integrability properties and evaluations, and in particular, we discuss Gaussian functions. The three variational procedures are then discussed in turn in secs. 4 - 6. Finally, in the appendix we take up again integrals involving Gaussian factors, and we present some extensions of results proved previously.

We may note that some of the above topics were much discussed on earlier occasions, and could be considered as folklore. We make no attempt here to provide extensive references.

2. A definition of Feynman-type integrals.

A number of definitions of path integrals have been proposed. The more recent ones exploit the Hilbert space structure of the integral, as suggested by the kinetic part of the action in (1.2). Explicitly, we may write

$$S(\gamma) = S_T(\gamma) + S_V(\gamma), \tag{2.1}$$

$$S_T(\gamma) = \frac{1}{2}m\int_0^t d\tau \sum_{j=1}^{n} (d\gamma^j/d\tau)^2 = \frac{1}{2}m\langle\dot\gamma,\dot\gamma\rangle. \tag{2.2a}$$

Moreover, by redefining $V(y)$ if necessary, we may suppose that $x = (0) = 0$. Then the conditions

$$\langle\dot\gamma,\dot\gamma\rangle < \infty, \qquad \gamma(0) = 0 \tag{2.2b}$$

define a real Hilbert space $\mathcal{H}_0$ of paths.

We think therefore of $e^{iS_T(\eta)}$ as characterizing the integral, whose integrands will be some functions $f(\eta)$. Such an integrand may contain the factor $e^{iS_V(\eta)}$, the factor $\delta(\eta(t)-y)$ for the second endpoint condition, and/or other contributions. It becomes then natural to consider an oscillatory Gaussian integral over an (abstract) real Hilbert space $\mathcal{H}$, and path integrals would then be obtained by specialization. Since we do not regard as a space of paths, we refer to such an integral as a Feynman-type integral rather than as a path integral.

We now follow [5], and turn to constructing a definition for an integral of the general form

$$\int_{\mathcal{H}} \mathcal{D}(\xi)\, e^{\frac{1}{2}i\kappa\langle\xi,\xi\rangle} F(\xi). \tag{2.3}$$

Here κ is a mass parameter, which is restricted by: $\operatorname{Im}\kappa \geq 0$, $\kappa \neq 0$.

We consider first the case $\dim \mathcal{H} = k < \infty$. We set

$$I^{b,\alpha}(f) = [(b-i\kappa)/2\pi]^{\frac{1}{2}k} \int d^k u\, e^{-\frac{1}{2}b\langle u-\alpha,\, u-\alpha\rangle} e^{\frac{1}{2}i\kappa\langle u,u\rangle} f(u), \tag{2.4a}$$

where $\alpha \in \mathcal{H}$, and where

$$\operatorname{Re} b > 0 \quad \text{and} \quad -\tfrac{1}{4}\pi < \arg(b-i\kappa)^{\frac{1}{2}} < \tfrac{1}{4}\pi. \tag{2.4b}$$

Note that the factor $[(b\ldots]^{\frac{1}{2}k}$ is adjusted so that $I^{b,0}(1)=1$. Next, we are interested in the limit as $b\to 0$. (For definiteness, we specify a unique nontangential limit.) If this limit exists and is independent of α, we call this limit the Feynman integral of f, and we denote it by $I(f)$, or as in (2.3).

The arbitrary vector α has been included in order to guarantee translational invariance of the integral, or of the generalized measure $\mathcal{D}(\xi)$.

In the finite-dimensional case we will sometimes write this integral using $d^k u$, as follows:

$$(-i\kappa/2\pi)^{\frac{1}{2}k} \int d^k u\, e^{\frac{1}{2}i\kappa\langle u,u\rangle} f(u). \tag{2.5a}$$

If $\kappa > 0$, it may be convenient to write the normalizing factor as

$$(-i\kappa/2\pi)^{\frac{1}{2}k} = (\kappa/2\pi)^{\frac{1}{2}k} \exp(-\tfrac{1}{4}i\pi k). \tag{2.5b}$$

If $\dim\mathcal{H} = \infty$, then we start by introducing the set $\mathcal{P}$ of finite-dimensional, orthogonal projections, and $\hat{\mathcal{Q}}$, the family of increasing sequences of such projections, defined explicitly by:

$$\hat{\mathcal{Q}} = \{\{P_j\} : P_k \in \mathcal{P},\ P_{k+1} \geq P_k \ \text{ for } \forall k,\ \lim_{j\to\infty} P_j = 1\}. \tag{2.6}$$

Choose $\Pi = \{P_j\} \in \hat{\mathcal{Q}}$, and let

$$I_\Pi^{b,\alpha}(F) = \lim_{j\to\infty} I^{b,P_j\alpha}(F(P_j\,\cdot)). \tag{2.7}$$

If the (nontangential) limit $I_\Pi^{b,\alpha}(F)$ as $b\to 0$ exists and is independent of α, we denote it by $I_\Pi(F)$. However, we should have independence of Π. It is not always convenient to require that the $I_\Pi(F)$'s should be equal for $\forall \Pi \in \hat{\mathcal{Q}}$, so we introduce some smaller families of projections. Let $P \in \mathcal{P}$, and let

$$\mathcal{Q}(P) = \{\{P_j\} \in \hat{\mathcal{Q}} : P_k \geq P \ \text{ for } \forall k\}. \tag{2.8}$$

We now specify that the $I_\Pi(F)$'s should be equal whenever $\Pi \in \mathcal{Q}(P)$, for some $P \in \mathcal{P}$. (More general families of sequences of projections were envisaged in [5].) Under this condition, $I_\Pi(F)$ is the Feynman integral of F, and (as before) is denoted by $I(F)$, or as in (2.3).

In dealing with path integrals as in (1.2), we set $x=0$ and include the factor $\delta(\eta(t)-y)$ in the integrand, as was suggested above. We observe that

$$\eta(\tau) = \int_0^t d\tau'\, \dot\eta(\tau')\dot\theta_\tau(\tau') = \langle\dot\eta, \dot\theta_\tau\rangle \quad \text{where} \quad \theta_\tau(\tau') = \min(\tau,\tau'), \tag{2.9}$$

and in particular, $\eta(t) = \langle\dot\eta, \dot\theta_t\rangle$. It is therefore convenient to use the family $\mathcal{Q}(\bar{P})$ where $\bar{P}$ projects onto the subspace $\{v\theta_t : v\in\mathbb{R}^n\}$. The δ-function can then be eliminated directly in each approximating integral.

We remark that if we write G as a path integral with a δ-function, then no additional normalising factors are needed. However, eliminating the δ-function then leaves a factor, which can be identified with N of (1.2). Then

$$N = (-im/2\pi t)^{\frac{1}{2}n}. \tag{2.10}$$

When we speak of integrability of F in the text, we refer to the Feynman integral $I(F)$. The reference family of sequences will be $\hat{\mathcal{Q}}$ in case of an integral over an abstract space, and will be $\mathcal{Q}(\bar{P})$ in case of a path integral for a Schrödinger particle.

An alternative definition of Feynman-type integrals, depending on infinite-dimensional Gaussian measures and on analytic continuation, is given in the appendix. For the examples in the text, the two definitions are equivalent.

3. Integrability, Gaussian functions, and the Morse index.

Feynman-type integrals, such as defined in sec. 2, involve conditional convergence or analyticity, and are therefore more difficult to investigate than positive-definite integrals. Integrable functions can be described at present by listing special cases, rather than by giving general criteria.

In a finite number of dimensions, various sufficient conditions for

Feynman-integrability of a function can be given. Typically, these conditions restrict the growth at infinity and smoothness in such a way, that if a more rapid growth is desired, then a greater smoothness must be imposed. E.g., functions in L_1 are (Feynman-) integrable, and entire functions of order less than two are integrable.

For infinitely many dimensions, we first note the following integrands which can be integrated in closed form (provided certain restrictions are met): linear exponentials, Gaussians, and polynomials. This rather special class can be greatly enlarged by taking suitable superpositions. In particular, let us integrate $e^{i\langle\beta,\xi\rangle}$ with respect to a bounded measure μ:

$$F_\mu(\xi) := \int_{\mathcal{H}} d\mu(\beta)\, e^{i\langle\beta,\xi\rangle} \quad \text{where} \quad \int d|\mu|(\beta) < \infty. \tag{3.1a}$$

Such F_μ are integrable, and

$$I(F_\mu) = \int d\mu(\beta)\, \exp\left[\tfrac{1}{2}(i\kappa)^{-1}\langle\beta,\beta\rangle\right]. \tag{3.1b}$$

(Cf. [5]. A number of other authors also investigated such F.) Moreover, if $\zeta_1,\dots,\zeta_\ell \in \mathcal{H}$ and

$$\int d|\mu|(\beta)\,(1+|\langle\zeta_1,\beta\rangle|)\cdots(1+|\langle\zeta_\ell,\beta\rangle|) < \infty, \tag{3.2a}$$

then

$$F(\xi) = \langle\zeta_1,\xi\rangle \quad \langle\zeta_\ell,\xi\rangle \int d\mu(\beta)\, e^{i\langle\beta,\xi\rangle} \tag{3.2b}$$

is Feynman-integrable [6]. This function can be described as the Fourier transform of a distribution, F_μ being the Fourier transform of the measure μ.

It can be shown [6] that if the potential V is the Fourier transform of a measure on R^n with finite moments,

$$V(y) = \int_{R^n} d\nu(w)\, e^{iwy} \quad \text{with} \quad \int d|\nu|(w)(1+|w|)^\ell < \infty \tag{3.3}$$

for some integer $\ell \geq 0$, then the path integral (1.2) can be put into the form $\int \mathcal{D}(\xi)\, e^{\frac{1}{2}im\langle\xi,\xi\rangle} F(\xi)$ with F such that

$$F(\xi) = \int d\mu(\beta)\, e^{i\langle\beta,\xi\rangle} \quad \text{and} \quad \int d|\mu|(\beta)(1+\|\beta\|)^\ell < \infty. \tag{3.4}$$

The latter condition implies (3.2a). Moreover, the resulting path integral indeed satisfies the equations (1.1) for the Green's function. (We emphasize that a condition as in (3.3) is sufficient but not necessary for the validity of (1.1) or of other relations that will follow.)

Let us turn to Gaussian functions. We start with the finite-dimensional case, and consider a function g which is the restriction to R^n of an entire function of order less than two, and also

$$f(u) = e^{\frac{1}{2}i\kappa\langle u,Lu\rangle} g(u), \tag{3.5a}$$

$$I(f) = e^{-\frac{1}{4}i\pi k}(\kappa/2\pi)^{\frac{1}{2}k} \int d^k u\, e^{\frac{1}{2}i\kappa\langle u,u\rangle} e^{\frac{1}{2}i\kappa\langle u,Lu\rangle} g(u), \tag{3.5b}$$

where $\kappa > 0$ and L is a real (linear) operator. The two exponents in the integrand of (3.5b) combine into $\frac{1}{2}i\kappa\langle u,(1+L)u\rangle$, and if we proceed heuristically and make the change of variable $v = (1+L)^{\frac{1}{2}}u$, then we obtain

$$[\det(1+L)]^{-\frac{1}{2}} e^{-\frac{1}{4}i\pi k}(\kappa/2\pi)^{\frac{1}{2}k} \int d^k v\, e^{\frac{1}{2}i\kappa\langle v,v\rangle} g((1+L)^{-\frac{1}{2}}v). \tag{3.6}$$

Let us examine the various possibilities. First we note that L can be assumed symmetric, and so it can be diagonalized by an orthogonal transformation. Next, if $1+L>0$, then there is no ambiguity, and $I(f)$ is clearly equal to the expression in (3.6).

The case where $1+L$ has zero as an eigenvalue has to be excluded. The transformation then becomes singular, and moreover, the integral in (3.5) will not in general converge.

The case of particular interest to us is when $1+L$ has negative eigenvalues. In this case $g((1+L)^{-\frac{1}{2}}v)$ and $[\det(1+L)]^{-\frac{1}{2}}$ have to be specified more precisely. Since g is analytic, it is determined once the square root is chosen, but the choice is of no consequence, since an odd power in any variable will make the term integrate to zero. With regard to $[\det(1+L)]^{-\frac{1}{2}}$, it can be shown that this factor acquires the phase factor $e^{-\frac{1}{2}i\pi} = -i$ for each negative eigenvalue. The number of these eigenvalues is by definition the Morse index, denoted by $\mathrm{ind}(1+L)$ (cf. [7][8]). Therefore

$$I(f) = |\det(1+L)|^{-\frac{1}{2}} \exp[(-\tfrac{1}{2}i\pi)\,\mathrm{ind}(1+L)]\, I(g((1+L)^{-\frac{1}{2}}\cdot)). \tag{3.7}$$

Further details regarding the proof of this equation as well as references can be found in the appendix.

To appreciate the role of the phase factor, consider the case of one dimension, $g=1$, and $1+L=-1$. We observe that

$$I(1) = e^{-\frac{1}{4}i\pi}(\kappa/2\pi)^{\frac{1}{2}} \int du\, e^{\frac{1}{2}i\kappa u^2} = 1, \tag{3.8a}$$

and in an analogous way it follows that

$$I_-(1) := e^{\frac{1}{4}i\pi}(\kappa/2\pi)^{\frac{1}{2}} \int du\, e^{-\frac{1}{2}i\kappa u^2} = 1. \tag{3.8b}$$

We now see that

$$I(f) = e^{-\frac{1}{4}i\pi}(\kappa/2\pi)^{\frac{1}{2}} \int du\, e^{-\frac{1}{2}i\kappa u^2} = I_-(1)\left(e^{-\frac{1}{4}i\pi}/e^{\frac{1}{4}i\pi}\right) = \exp(-\tfrac{1}{2}i\pi). \tag{3.8c}$$

In other words, $e^{-\frac{1}{2}i\pi}$ is just the quotient of two normalizing phase factors, i.e. for the integrals $I(1)$ and $I_-(1)$.

A formula analogous to (3.7), but for functions as in (3.2b), defined on $\mathcal{H}$ of arbitrary dimension, is given in the appendix.

The Morse index was discussed in conjunction with (rigorous) path integrals in [8] - [10]. It occurs in the formulas of the semiclassical approximation (cf. the next section), and in this context it is also known as the Maslov index.

We conclude this section with the example of the harmonic oscillator in one dimension. In this case the potential part of the action, $\frac{1}{2}m\omega^2\int d\tau\, \eta^2(\tau)$, yields a Gaussian integrand. However, the variable of integration is $\dot\eta$ rather than η, and $\eta(\tau)$ is a scalar product, $\langle \dot\eta, \dot\theta_\tau\rangle$, cf. (2.9). We observe that

$$\int_0^t d\tau\, \dot\theta_\tau(\tau')\,\dot\theta_\tau(\tau'') = \min(\tau',\tau'') , \tag{3.9a}$$

from which follows

$$\int_0^t d\tau\, \eta^2(\tau) = \int_0^t d\tau'\,\dot\eta(\tau') \int_0^t d\tau''\,\dot\eta(\tau'') \min(\tau',\tau'') . \tag{3.9b}$$

We see that $\min(\tau',\tau'')$ is the kernel of an integral operator M. The corresponding Morse index can be easily computed, since the operator in question is the inverse to $-d^2/d\sigma^2$. A calculation for a mixed momentum-coordinate representation yields [10]

$$\operatorname{ind}(-\omega^2 M) = [(\omega t/\pi) + \tfrac{1}{2}] , \tag{3.10}$$

where $[..]$ denotes the entire part.

4. The semiclassical approximation.

From the point of view of path integrals, the semiclassical approximation is an example of the stationary phase approximation. We recall that this approximation has the following form (for a one-dimensional integral):

$$\int_{-\infty}^{\infty} du\, e^{ixg(u)} f(u) \approx \int_{-\infty}^{\infty} du\, \exp\{ix[g(u_0) + \tfrac{1}{2}(u-u_0)^2 g''(u_0)]\} f(u_0) = \\ = f(u_0)\, e^{ixg(u_0)} |g''(u_0)|^{-\frac{1}{2}} e^{\pm\frac{1}{4}i\pi} (2\pi/x)^{\frac{1}{2}} \quad \text{as} \quad x\to\infty . \tag{4.1}$$

Here we assume that u_0 is the only critical point of g on the support of f and that u_0 is nondegenerate. We take $\pm\frac{1}{4}i\pi$ if $g''(u_0) \gtrless 0$. (Additional smoothness and integrability conditions are needed as well.)

The situation with path integrals is analogous, even though these integrals are infinite-dimensional. We have here the oscillatory factor $e^{(i/\hbar)S}$, and we are interested in the behavior as $\hbar\to 0$, i.e. as $\hbar^{-1}\to\infty$. A critical path defined by $\delta S/\delta\eta = 0$ is just a classical path. Let us assume for simplicity that there is a unique such path for the conditions assumed in the path integral, and that we have a particle on R^1. We then make a functional power-series expansion for S:

$$S(\eta) = S(\eta_0) + \tfrac{1}{2}\iint_0^t d\tau\, d\tau' (\eta-\eta_0)(\tau)(\eta-\eta_0)(\tau')[\delta^2 S/\delta\eta(\tau)\delta\eta(\tau')]_{\eta=\eta_0} + \dots . \tag{4.2}$$

We neglect higher-order terms.

The second-order term for the potential part of S can be evaluated as follows:

$$[\delta^2/\delta\eta(\tau)\delta\eta(\tau')] \int_0^t d\tau''\, V(\eta(\tau''))\Big|_{\eta=\eta_0} = [\delta/\delta\eta(\tau)] \int_0^t d\tau\, V'(\eta(\tau))\,\delta\eta(\tau'')/\delta\eta(\tau')\Big|_{\eta=\eta_0} \tag{4.3a}$$

But $\delta\eta(\tau'')/\delta\eta(\tau') = \delta(\tau'-\tau'')$, so

$$[\delta/\delta\eta(\tau)]\, V'(\eta(\tau'))\Big|_{\eta=\eta_0} = V''(\eta_0(\tau'))\,\delta(\tau-\tau') , \tag{4.3b}$$

and, with the notation $\eta-\eta_0 = \chi\hbar^{\frac{1}{2}}$, we obtain the term $\int d\tau\, V''\chi^2$. One sees in the same way as in eqs. (3.9) that this term has the form

$$\tfrac{1}{2}\hbar \int_0^t d\tau\, \chi^2(\tau)\, V''(\eta_0(\tau)) = \tfrac{1}{2} m\hbar \langle \dot\chi, L\dot\chi\rangle , \tag{4.5a}$$

where L is the integral operator with the kernel

$$m^{-1}\int_0^t d\tau\, V''(\eta_0(\tau))\,\dot\theta_\tau(\tau')\,\dot\theta_\tau(\tau'') . \tag{4.5b}$$

Let us return to the (approximated) action $S(\eta)$. For the kinetic part S_T, the expansion through the second order will just reproduce the original function. Therefore

$$\hbar^{-1}S(\eta) \approx \hbar^{-1}S(\eta_0) + \tfrac{1}{2}m\langle\dot\chi,\dot\chi\rangle + \tfrac{1}{2}m\langle\dot\chi, L\dot\chi\rangle , \tag{4.6}$$

and the path integral for the Green's function, with S approximated as above, becomes

$$e^{(i/\hbar)S(\eta_0)} N \int_{\chi(0)=\chi(t)=0} \mathcal{D}(\chi)\, e^{\frac{1}{2}im\langle\dot\chi,\dot\chi\rangle} e^{\frac{1}{2}im\langle\dot\chi, L\dot\chi\rangle} = \\ = e^{(i/\hbar)S(\eta_0)} N |\det(1+L)|^{-\frac{1}{2}} \exp[(-\tfrac{1}{2}i\pi)\operatorname{ind}(1+L)] . \tag{4.7}$$

Let us suppose that V'' is bounded, $|V''| \le B$. Since $|\dot\theta_\tau| \le 1$ and also

$$\int_0^t d\tau\, |\dot\chi| \le \|\dot\chi\|\cdot\|1\| = \|\dot\chi\|\, t^{\frac{1}{2}} \tag{4.8}$$

we easily obtain

$$|\langle\dot\chi, L\dot\chi\rangle| \le (B/m)\, t^2 \|\dot\chi\|^2 , \qquad \|L\| \le (B/m)\, t^2 . \tag{4.9}$$

Therefore for t sufficiently small, $1+L>0$, and $\operatorname{ind}(1+L) = 0$. However, as t increases, $1+L$ may acquire the eigenvalue zero, and negative eigenvalues.

In one dimension, an eigenvalue zero can be interpreted as the occurrence of a turning point in the corresponding classical system. Indeed, let us look again at the case of the harmonic oscillator, where the semiclassical approximation is exact. The first two zeros of $-\omega^2 M$ [cf. eq. (3.10)] occur for

$$\omega t/\pi + \tfrac{1}{2} = 1, 2, \quad \text{so that} \quad \omega t = \tfrac{1}{2}\pi, \ \tfrac{3}{2}\pi , \tag{4.10}$$

respectively, i.e., are one swing apart.

An extensive analysis of such turning points and of the accompanying changes of phase can be found in the treatise of Maslov [11]. A detailed mathematical investigation of the semiclassical limit is described in [9], where the following hypothesis is made on the potential:

$$V(y) = \int d\nu(\omega)\, e^{i\omega y} \quad \text{with} \quad \int d|\nu|(\omega)\, e^{\varepsilon|\omega|} < \infty , \tag{4.11}$$

for some $\varepsilon > 0$.

5. Integration by parts.

The definition of Feynman-type integrals as given in sec. 2 ensured translational invariance of the generalized measure $\mathcal{D}(\xi)$. In a one-dimensional set-up this invariance and a heuristic interchange of operations lead to the following equations:

$$\begin{aligned} 0 &= (d/db)_{b=0} (-i\kappa/2\pi)^{\frac12} \int du\, e^{\frac12 i\kappa(u+b)^2} f(u+b) \\ &= (-i\kappa/2\pi)^{\frac12} \int du\, (d/du)\, e^{\frac12 i\kappa(u+b)^2} f(u+b)\big|_{b=0} \\ &= (-i\kappa/2\pi)^{\frac12} \int du\, e^{\frac12 i\kappa u^2} [i\kappa u f(u) + f'(u)] . \end{aligned} \tag{5.1}$$

These equations could be called integration-by-parts formulae.

Let us put these equations into a more general setting. Let $S \in \mathcal{H}$, and let F be such that $D_S F(\xi)$ and $\langle S,\xi\rangle F(\xi)$ are integrable. Then

$$\int \mathcal{D}(\xi)\, e^{\frac12 i\kappa\langle\xi,\xi\rangle} [i\kappa\langle S,\xi\rangle F(\xi) + D_S F(\xi)] = 0 . \tag{5.2}$$

As a special case, we obtain the following quantum-mechanical equation of motion:

$$\begin{aligned} &\int_{\eta(0)=0} \mathcal{D}(\eta)\, e^{\frac12 im\langle\dot\eta,\dot\eta\rangle} \exp[-i\textstyle\int_0^t d\tau\, V(\eta(\tau))]\, \delta(\eta(t)-y) \\ &\quad \times \int_0^t d\sigma\, f(\sigma)\, [m\ddot\eta^j(\sigma) + (\partial^j V)(\eta(\sigma))] = 0 . \end{aligned} \tag{5.3}$$

To derive (5.3), one can use the following relation, which is easily verifiable for polynomials in η:

$$-(d^2/d\sigma^2)\langle \dot\theta_\sigma, \delta/\delta\dot\eta\rangle = \delta/\delta\eta(\sigma) . \tag{5.4}$$

The scalar product $\langle\dot\theta_\sigma, \delta/\delta\dot\eta\rangle$ is just the Gâteaux derivative $D_{\dot\theta_\sigma}$.

Equation (5.3) is valid for potentials V such that ([6]; cf. also [12])

$$V(y) = \int d\nu(\omega)\, e^{i\omega y} \quad \text{with} \quad \int d|\nu|(\omega)(1+|\omega|) < \infty. \tag{5.5}$$

The quantity $\ddot\eta$ in (5.3) should be interpreted as a distribution: $\langle f,\ddot\eta^j\rangle = -\langle\dot f,\dot\eta^j\rangle$, and f should vanish in neighborhoods of 0 and t, and have a continuous derivative.

The foregoing ideas could also be expressed as follows. We introduce the notation

$$\langle f\rangle = N \int_{\eta(0)=x,\ \eta(t)=y} \mathcal{D}(\eta)\, e^{iS(\eta)} f(\eta) , \tag{5.6a}$$

and apply a Gâteaux derivative inside the integral, as before. Then (heuristically),

$$i\langle (D_S S) f\rangle + \langle D_S f\rangle = 0 . \tag{5.6b}$$

This is a form of the Schwinger action principle.

We remark also that the rule $[p_j, q^k] = i^{-1}\delta_j^k$ can be derived (heuristically) from (5.6b) in the form

$$\langle m\dot\eta^j(\sigma+\varepsilon)\eta^k(\sigma) - \eta^k(\sigma) m\dot\eta^j(\sigma-\varepsilon) - i^{-1}\delta^{jk}\rangle \to 0 \tag{5.7}$$

as $\varepsilon \searrow 0$ [1][2]. A weaker relation of this kind is proved in [6]. (We might note here, that in path integrals, quantities can be ordered only according to time. This is the reason for the particular form of (5.7).)

An alternative way of exploiting integration by parts depends on introducing external sources and generating functions. Let $J \in \mathcal{H}_0$, and set

$$T(J) = \int_{\eta(0)=0} \mathcal{D}(\eta)\, e^{\frac12 im\langle\dot\eta,\dot\eta\rangle} \exp[-i\textstyle\int_0^t d\tau\, V(\eta(\tau))]\, e^{i\langle\eta,J\rangle}\, \delta(\eta(t)-y) . \tag{5.8}$$

Then, in place of (5.3), we obtain

$$\begin{aligned} &\int_{\eta(0)=0} \mathcal{D}(\eta)\, e^{\frac12 im\langle\dot\eta,\dot\eta\rangle} \exp[-i\textstyle\int_0^t d\tau\, V(\eta(\tau))]\, e^{i\langle\eta,J\rangle} \delta(\eta(t)-J) \\ &\quad \times \int_0^t d\sigma\, f(\sigma)\, [m\ddot\eta^l(\sigma) + (\partial^l V)(\eta^1(\sigma),\dots,\eta^n(\sigma)) - J^l(\sigma)] = 0 . \end{aligned} \tag{5.9a}$$

We now observe that applying $i^{-1}\delta/\delta J^l(\sigma)$ to $T(J)$ results in a factor $\eta^l(\sigma)$ in the integrand. Therefore (5.9a) can be transformed to

$$m\frac{d^2}{d\sigma^2}\Big[\frac1i \frac{\delta}{\delta J^l(\sigma)}\Big] T(J) + (\partial^l V)\Big(\frac1i\frac{\delta}{\delta J^1(\sigma)},\dots,\frac1i\frac{\delta}{\delta J^n(\sigma)}\Big) T(J) = J^l(\sigma) T(J). \tag{5.9b}$$

The last equation is meaningful a priori only for a polynomial potential V. This equation can be verified explicitly for the harmonic oscillator. (See the appendix.)

Equations such as (5.7b) are sometimes called Schwinger's equations. They were suggested primarily for quantum field theory, where typically one considers polynomial interactions. Such equations provide a way of describing quantum systems without noncommuting operators (except for anticommuting objects in case of fermionic fields).

6. Differentiation with respect to parameters.

This section is devoted to two kinds of questions. One of these complements the preceding discussion in the following way. In secs. 4 and 5 we considered variations of η for which the endpoints were held fixed. In the present section we vary just the endpoints of η, in particular y.

The second kind of questions concerns differentiability or analyticity in κ (or m), in $\hbar$, and in other parameters.

We make a digression, and introduce a phase-space form of path integrals, as follows (we now use q in place of y):

$$G(t;q,x) = N\int_{\eta(0)=x,\ \eta(t)=q} \mathcal{D}(\eta)\mathcal{D}(p)\, e^{iS(p,\eta)}\ , \tag{6.1}$$

$$S(p,\eta) = \int_0^t d\tau\,(p\dot\eta - H) = \int_0^t d\tau\left[\textstyle\sum_{j=1}^n p_j\dot\eta^j - \sum(2m)^{-1}p_j{}^2 - V\right] \tag{6.2a}$$

$$= \langle p,\dot\eta\rangle - (2m)^{-1}\langle p,p\rangle - \int_0^t d\tau\, V. \tag{6.2b}$$

We think of $\langle p,\dot\eta\rangle - (2m)^{-1}\langle p,p\rangle$ as characterizing the integral, while $\int d\tau\, V$ and the endpoint condition at t could contribute to the integrand, as before. When the integrand does not depend on p, then the p-integration can be done explicitly (at least at the heuristic level), and one is led back to the path integral over η, as e.g. in (1.2).

Mathematical definitions of the integral over phase space can be constructed by adapting that of sec. 2 and that of the appendix, (cf. [13]), or otherwise.

We now assume a particle on R^1, and we recall the familiar relations of classical mechanics,

$$p = \partial S/\partial q\ , \qquad H = -\partial S/\partial t\ , \tag{6.3a}$$

which imply

$$i^{-1}\partial_q e^{iS} = p e^{iS}\ , \quad -i^{-1}\partial_t e^{iS} = H e^{iS}. \tag{6.3b}$$

We apply these derivatives to (6.1), and (heuristically) interchange differentiation and integration (the same endpoint conditions are to be understood):

$$i^{-1}\partial_q G(t;q,x) = N\int \mathcal{D}(\eta)\mathcal{D}(p)\, p(t)\, e^{iS}, \tag{6.4a}$$

$$-i^{-1}\partial_t G(t;q,x) = N\int \mathcal{D}(\eta)\mathcal{D}(p)\, H(t)\, e^{iS}. \tag{6.4b}$$

We observe that eq. (6.4a) would have to be modified in the Hilbert space approach, since there $q=\eta(t)$ and $p(t)$ are objects of different kinds: q is a scalar product, $q=\langle\dot\eta,\dot\theta_t\rangle$, while $p(t)$ can only have a distribution-theoretic meaning. This difference is of course implied by the form of the scalar products, $\langle p,\dot\eta\rangle$, $\langle\dot\eta,\dot\eta\rangle$, and $\langle p,p\rangle$. In [13] the following variant of (6.4a) is proved,

$$i^{-1}\partial_q G(t;q,x) = N\int\mathcal{D}(\eta)\mathcal{D}(p)\, e^{iS}\, t^{-1}\int_0^t d\tau\, p(\tau) + \mathcal{O}(t^2)\ , \tag{6.5}$$

where V is assumed to be such as in (5.5).

The factor $t^{-1}\int d\tau\, p$ comes from one term when $\langle p,\dot\eta\rangle$ is developed with the help of a suitable orthonormal basis:

$$\langle p,\dot\eta\rangle = \langle p,\dot\theta_t\rangle\langle\dot\theta_t,\dot\eta\rangle/\langle\dot\theta_t,\dot\theta_t\rangle + \ldots = q\,t^{-1}\int_0^t d\tau\, p(\tau) + \ldots\ . \tag{6.6}$$

On the other hand, eq. (6.4b) cannot be valid in the given form, since $p^2(t)$ is not an integrable factor, and neither is $\int d\tau\, p^2(\tau)$.

We turn to derivatives with respect to other parameters. First of all, let us observe that a heuristic interchange of operations can be very misleading here. Indeed, if we were to calculate $\partial_\kappa[I^{(\kappa)}(F)]$ by such an interchange, we would get $i\langle\zeta,\zeta\rangle$ in the integrand, which is a nonintegrable factor. However, in all known examples $I(F)$ is analytic in κ for $\mathrm{Im}\,\kappa>0$. However, information on differentiability and analyticity has been obtained by other methods, and we list two in particular.

(i) Assume that V is continuous except on a set of capacity zero. Then an analysis based on holomorphic semigroups yields analyticity in κ for $\mathrm{Im}\,\kappa>0$ [14].

(ii) If the integrand F is the Fourier transform of a measure of bounded variation, then $I(F)$ can be reduced to a measure-theoretic integral, whose differentiability can perhaps be reduced from the properties of the measure.

The latter method was used extensively in [9], and our appendix also includes a result which illustrates this point.

Appendix. Gaussian factors and the mathematical theory.

We first summarize another definition of Feynman-type integrals. This definition depends on analytic continuation in the variance (here, $i\kappa^{-1}$) from the real positive values. However, in order to ensure translational invariance, we have to employ a more complicated procedure. We consider

$$J(b,\alpha,b_1;F) := \int\mathcal{D}(\zeta)\, e^{-\frac{1}{2}\langle\zeta-\alpha,\zeta-\alpha\rangle} e^{-\frac{1}{2}b_1\langle\zeta,\zeta\rangle} F(\zeta)\ . \tag{A.1}$$

The integral here is the Gaussian measure-theoretic integral with variance $(b+b_1)^{-1}$. We suppose that J as a function of b, b_1 is analytic in a region which includes the set $\{\mathrm{Re}\, b>0,\ \mathrm{Re}\, b_1\geq 0\}$. If $\lim_{b\to 0} J(b,\alpha,-i\kappa;F)$ exists as a nontangential limit and is independent of α, we call this the Feynman-type integral of F in the sense of analytic continuation (s.a.c.) and denote it by $J(F)$.

In this appendix our assertions about integrability will refer to both integrals I and J, and we will indicate this in the propositions that follow.

Proposition 1.—(a) Take $\mathcal{H}=R^k$ and κ real. Let g be the restriction to R^k of an entire function of order less than two, and let $L:R^k\to R^k$ be symmetric and such that $1+L$ is nonsingular. Then the following function is integrable,

$$f(u) := \exp\left(\tfrac{1}{2} i\kappa \langle u, Lu\rangle\right) g(u)\,, \tag{A.2a}$$

and

$$I(f) = J(f) = |\det(1+L)|^{-\frac{1}{2}} \exp\left[(-\tfrac{1}{2} i\pi)\,\mathrm{ind}(1+L)\right] I\left(g((1+L)^{-\frac{1}{2}}\cdot)\right). \tag{A.2b}$$

(b) Let κ be real, as before. Let $S_1, \dots, S_\ell \in \mathcal{H}$ (of arbitrary dimension), and let μ be a measure on $\mathcal{H}$ satisfying

$$\int d|\mu|(\beta)(1+|\langle S_1,\beta\rangle|)\dots(1+|\langle S_\ell,\beta\rangle|) < \infty. \tag{A.3}$$

Let L be symmetric, of trace class, and such that $1+L$ is nonsingular. Then the following function is integrable,

$$F(\xi) := e^{\frac{1}{2} i\kappa\langle \xi, L\xi\rangle}(-i)^\ell \langle S_1,\xi\rangle \dots \langle S_\ell, \xi\rangle \int d\mu(\beta)\, e^{i\langle\beta,\xi\rangle}\,, \tag{A.4a}$$

and

$$I(F) = J(F) = |\det(1+L)|^{-\frac{1}{2}} \exp\left[(-\tfrac{1}{2} i\pi)\,\mathrm{ind}(1+L)\right](-1)^\ell \int d\mu(\beta) \times D_{S_1}\dots D_{S_\ell} \exp\left[\tfrac{1}{2}(i\kappa)^{-1}\langle\beta,(1+L)^{-1}\beta\rangle\right]. \tag{A.4b}$$

<u>Proof</u>: (a): We exploit the fact that integrability was proved in [15] by taking the convergence factor $e^{-\frac{1}{2}\langle u, Bu\rangle}$ with B an operator (which $\to 0$), rather than $e^{-\frac{1}{2}b\langle u,u\rangle}$. A linear change of variables like $w = (1+|L|)^{-\frac{1}{2}} u$ in the Feynman integral is therefore admitted (cf. [12]). Here $|L| = (L^2)^{\frac{1}{2}}$. If L is diagonalized, then $|L|$ is the result of replacing each eigenvalue λ of L, necessarily real, by $|\lambda|$. Next, for each negative eigenvalue of $1+L$, we can effect the transformation $v^j = \pm i w^j$ by contour integration. Moreover, for each such eigenvalue one obtains the factor $e^{-\frac{1}{2}i\pi}$, as the argument of sec. 3 shows (eqs. (3.8)). The result is as in (A.2b).

(b): We consider first the integral J(F). We complexify $\mathcal{H}$, but we retain a bilinear scalar product, rather than introduce a Hermitian one. The measure-theoretic Gaussian integral of $F_{L,\beta}(\xi) = e^{\frac{1}{2}i\kappa\langle\xi,L\xi\rangle} e^{i\langle\beta,\xi\rangle}$ can be factorized with respect to the eigenvectors of L, with eigenvalues λ_j, and this integral can be expressed as

$$J(b,\alpha,b_1;F_{L,\beta}) = e^{-\frac{1}{2}b\langle\alpha,\alpha\rangle}\left\{\prod_{j=1}^{\infty}\left[1 - i\kappa\lambda_j(b+b_1)^{-1}\right]\right\} \times \exp\left\{-\tfrac{1}{2}(b+b_1)^{-1}\langle\beta - ib\alpha, \left[1-i\kappa L(b+b_1)^{-1}\right](\beta - ib\alpha)\rangle\right\}, \tag{A.5a}$$

$$-\tfrac{1}{4}\pi < \arg(1-i\kappa\lambda_j)^{\frac{1}{2}} < \tfrac{1}{4}\pi. \tag{A.5b}$$

Since $\sum|\lambda_j| < \infty$, the infinite product converges. As a convergent limit of finite products, which constitute a uniformly bounded family of analytic functions, this infinite product is analytic in b, b_1 when $\mathrm{Re}(b+b_1) > 0$ (or in a larger region). The same holds for the exponential. We may therefore continue analytically to $b_1 = -i\kappa$, and then to the boundary value $b = 0$.

We return to F. For $b, b_1 > 0$ one can interchange integrations and differentiations so as to obtain

$$J(b,\alpha,b_1;F) = (-1)^\ell \int d\mu(\beta)\, D_{S_1}\dots D_{S_\ell}\, J(b,\alpha,b_1;F_{L,\beta})\,, \tag{A.6}$$

the D_{S_j} acting on β. The factor $\exp\left[-\frac{1}{2}(b+b_1)^{-1}\langle\beta,\beta\rangle\right]$ in (A.5a) implies that the last expression is analytic in b, b_1 when $\mathrm{Re}(b+b_1) > 0$, and we can let $b_1 = -i\kappa$. The handling of the approach to the boundary value $b = 0$ is analogous to that in case $L = 0$, and is as described in [6].

For I(F), we can argue as follows: Replace $e^{\frac{1}{2}i\kappa\langle\xi,\xi\rangle}$ by $e^{-\frac{1}{2}b_1\langle\xi,\xi\rangle}$. Then the $I^{b,\alpha}(F(P_j\cdot))$ constitute a sequence of functions analytic in b, b_1 when $\mathrm{Re}(b+b_1) > 0$, the sequence having (locally) uniform bounds. Moreover, $I^{b,\alpha}(F(P_j\cdot)) \to I^{b,\alpha}(F)$ for $b, b_1 > 0$ by dominated convergence. Therefore this limit holds also for $b_1 = -i\kappa$. The limit to $b = 0$ of $I^{b,\alpha}(F)$ then goes as before. □

The assertion of (b) with $\ell = 0$ (but in a different framework) was stated in [8], and a different proof was outlined there.

We were concerned in this article with asymptotic limits, and we state therefore the following:

<u>Corollary 2</u>.—With reference to proposition 1,

$$\lim_{\kappa\to\infty} I(\varphi) = \varphi(0)\,|\det(1+L)|^{-\frac{1}{2}} \exp\left[(-\tfrac{1}{2}i\pi)\,\mathrm{ind}(1+L)\right]. \tag{A.7}$$

where $\varphi = f$ and the hypotheses of (a) are assumed, or else, $\varphi = F$ and the hypotheses of (b) are assumed.

Part (a) follows from proposition 7 of [12], which applies to g. Part (b) follows by dominated convergence. □

We next consider the harmonic oscillator, with or without perturbations. To avoid complications with the Morse index, we restrict the time interval.

<u>Proposition 3</u>.—Let $V_0(y) = \frac{1}{2}Ky^2$ (for a particle on $\mathbb{R}^n$). Assume that $t < \pi(m/K)^{\frac{1}{2}}$. Let $V = V_0 + V_1$ where

$$V_1(y) = \int d\nu(w)\, e^{iwy}\,. \tag{A.8}$$

(a) If $\int d|\nu|(w) < \infty$, then the path integral (1.2) converges (as I or J) and satisfies eqs. (1.1) for the Green's function.
(b) If $\int d|\nu|(w)(1+|w|) < \infty$, then the equations of motion (5.3) are fulfilled.
(c) If $V_1 = 0$, then the functional differential equations (5.9b) are fulfilled.

<u>Outline of proof</u>: (a): The path integral in question is discussed in detail in [16], but our criteria for integrability differ from those of <u>loc. cit</u>. Now, integrability as I or as J follows from proposition 1, and for verification of eqs. (1.1) we refer to [16].
(b): Equations (5.3) follow if the path integral converges for each of the two terms [12]. However, the convergence follows from proposition 1, in the same

way as for the case $V_0 = 0$ treated in [6].
(c): If $V_1 = 0$, then all integrations and differentiations reduce to algebraic operations involving exponentials and polynomials. In particular, there is no problem with interchanges of operations. (□)

We turn to the questions of differentiability and analyticity. These questions relate e.g. to the problem of the asymptotic expansion as $\hbar \to 0$, and various assertions along these lines were made in [9]. We state here a simple "folk lemma", as an application of proposition 1 and of related techniques.

We consider the following integral:

$$\varphi(\kappa, g) = \int \mathcal{D}(\xi) e^{\frac{1}{2} i\kappa \langle \xi, \xi \rangle} e^{\frac{1}{2} i\kappa \langle \xi, L\xi \rangle} e^{-ig W(\xi)} F(\xi) , \qquad (A.9)$$

where L is symmetric (and real), of trace class, and such that $1 + L$ is nonsingular. Assume that

$$F(\xi) = \int d\mu(\beta) e^{i\langle \beta, \xi \rangle} , \qquad W(\xi) = \int d\rho(\beta) e^{i\langle \beta, \xi \rangle} , \qquad (A.10a)$$

where

$$\int d|\mu|(\beta) < \infty , \qquad \int d|\rho|(\beta) < \infty . \qquad (A.10b)$$

<u>Lemma</u> <u>4</u>.—(a) If $1 + L > 0$, then φ is analytic in κ in $\{\mathrm{Im}\, \kappa > 0\}$.
(b) If μ and ρ have finite moments of orders 2n, then φ is of class $\mathcal{C}^n$ in κ for κ real, $\kappa \neq 0$.
(c) The function φ is entire in g for κ real. If $1 + L > 0$, then φ is entire in g also when $\mathrm{Im}\, \kappa > 0$.

<u>Outline of proof</u>: Following [17] (cf. also [6][16]), e^{-igW_F} is the Fourier transform of a bounded measure ν, so that we can write

$$I(F) = [\det(1+L)]^{-\frac{1}{2}} \int d\nu(\beta) \exp\left[\tfrac{1}{2}(i\kappa)^{-1} \langle \beta, (1+L)^{-1} \beta \rangle\right] . \qquad (A.11)$$

and (a) follows. Moreover, as shown in [6], lemma 2, if two measures have finite moments of a given order, then so does their convolution. We can therefore differentiate in (A.11) with respect to κ for κ real, and (b) follows. Part (c) is in effect shown in [17] for the case $L = 0$, $F = 1$, and κ real, but the indicated techniques allow one easily to relax these restrictions. (□)

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