

TRUE MEASURES FOR REAL TIME PATH INTEGRALS

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ABSTRACT

Coherent state matrix elements of (real time) quantum mechanical propagators can be written as limits of well-defined phase-space path integrals involving a Brownian diffusion process on phase space. These limits are taken for diverging diffusion constant.

1. INTRODUCTION

Real time path integrals in quantum mechanics give the integral kernel of the unitary evolution operator $\exp(-i\hbar H)$.

$$[\exp(-i\hbar H)](q'', q') = \lim_{N \rightarrow \infty} \int \dots \int \exp \left\{ -\sum_{l=0}^N [(q_{l+1} - q_l)^2 / 2i\epsilon + i\epsilon V(q_l)] \right\} \prod_{l=1}^N \frac{dq_l}{\sqrt{2\pi i\epsilon}} \quad (1.1)$$

$$\text{with } \epsilon = \hbar/N, \quad q_{N+1} = q'', \quad q_0 = q'$$

$$= N^{-1} \int \exp \left[-\frac{1}{2i} \int_0^T \dot{q}^2 dt - i \int_0^T V(q) dt \right] \prod_t dq(t) \quad (1.2)$$

$$\text{with } q(T) = q'', \quad q(0) = q'$$

One derives (1.1) by using the Trotter product formula for unitary operators; (1.1) is exact for quite a large class of potentials V (see Nelson, [1]). In (1.2) the limit for $N \rightarrow \infty$ has been taken implicitly. The resulting Feynman path integral is however only an "integral" in name. The infinite product of Lebesgue measures $\prod_t dq(t)$

does not make mathematical sense, and the normalization constant N is undefined.

Analogous expressions can be written for the operator $\exp(-tH)$.

$$\begin{aligned} & [\exp(-tH)](q'', q') \\ &= \lim_{N \rightarrow \infty} \int \dots \int \exp \left\{ - \sum_{l=0}^N [(q_{l+1} - q_l)^2 / 2\epsilon - \epsilon V(q_l)] \right\} \prod_{l=1}^N \frac{dq_l}{\sqrt{2\pi\epsilon}} \\ &= N^{-1} \int \exp \left[- \frac{1}{2} \int \dot{q}^2 dt - \int V(q) dt \right] \prod_{t_1} dq(t) \end{aligned} \quad (1.3)$$

In this case however the formal expression (1.3) can be rewritten as

$$[\exp(-tH)](q'', q') = \int \exp \left[- \int_0^T V(q) dt \right] d\mu_W(q) \quad (1.4)$$

where μ_W is the (Wiener) measure for the Brownian process pinned at both initial and final points ($q(0) = q'$, $q(T) = q''$) and with connected covariance ($t_2 > t_1$)

$$\begin{aligned} \langle q(t_2) q(t_1) \rangle^c &= \langle q(t_2) q(t_1) \rangle - \langle q(t_2) \rangle \langle q(t_1) \rangle \\ &= t_1 \left(1 - \frac{t_2}{T} \right). \end{aligned}$$

Formally, different factors in (1.3) have combined to give rise to the Wiener measure in (1.4) (see e.g. the discussion in Reed & Simon, [2]). As a result (1.4) is a true integral on path space, with a genuine underlying measure. One can therefore use the full artillery of measure and integration theory when using (1.4); this has made the Feynman-Kac formula (1.4) a powerful tool in mathematical physics.

This is in marked contrast to the Feynman path integral (1.2). No formal recombination of factors, leading up to a genuine measure on path space, is possible here. Several attempts have been made in the past at defining the Feynman path integral in a mathematically sound way without having recourse to the discrete time slicing of (1.1). In [3] Gel'fand and Yaglom introduce an extra term $-\frac{1}{2\nu} \int \dot{q}^2 dt$ in the exponent, in order to produce a Wiener measure in combination with $N^{-1} \prod dq(t)$. The limit for $\nu \rightarrow \infty$ should then have given the integral kernel for $\exp(-tH)$. As was pointed out by Cameron [4], this procedure fails because $\exp \left[\frac{1}{2} \int \dot{q}^2 dt \right]$ is not measurable with respect to Wiener measure. In [5] Itô proposed to introduce the two extra terms $-\frac{1}{2\nu} \int (\dot{q}^+ + \dot{q}^-) dt$ into the exponent in the integrand of (1.2); again the limit $\nu \rightarrow \infty$ should be taken in the end. This approach works for a limited class of potentials V . Note that, because of the presence of second order derivatives, two boundary values are needed at both $t=0$, $t=T$ (not only $q(0) = q'$, $q(T) = q''$; extra boundary conditions for $\dot{q}(0)$, $\dot{q}(T)$ have to be introduced). This means that the new object is no longer a true configuration space path integral. In [6] Albeverio and Hoegh-Krohn circumvent the absence of a measure by considering the Feynman path integral as a kind of Fourier integral. Their approach works for all potentials V which can be written as the Fourier transform of a bounded measure. In [7] Combe, Hoegh-Krohn,

Rodriguez, Sirugue and Sirugue-Collin define Feynman path integrals in momentum space (as opposed to configuration space). The measure in their path integrals corresponds to a Poisson process; the paths in its support are typically only piecewise continuous. Their approach works for any potential V which is the sum of a quadratic part and the Fourier transform of a bounded measure.

We here present a different approach, using also true measures on path space. Our approach is closer again, in spirit, to the older Gel'fand-Yaglom and Itô ideas, in the sense that we introduce a stochastic process (a Wiener process in our case) with a diffusion constant ν tending to ∞ in the end. Our approach differs from all the above in that we consider phase space path integrals rather than configuration space (or momentum space) integrals. The class of potentials we can treat is quite different too; it contains e.g. all polynomial potentials which are bounded below.

2. PHASE SPACE PATH INTEGRALS

The standard (formal) procedure for obtaining a path integral is to write the Trotter product formula

$$\exp(-iTH) = \lim_{N \rightarrow \infty} \left[\exp\left(-i \frac{T}{N} (-\Delta)\right) \exp\left(-i \frac{T}{N} V\right) \right]^N, \quad (2.1)$$

and to insert the formal resolution of the identity $\int dx |x\rangle \langle x| = 1$ between every two factors. This leads to (1.1), and thus (formally) to (1.2). A different procedure is to insert alternatively (formal) resolutions of the identity in configuration space ($\int dq |q\rangle \langle q| = 1$) and in momentum space ($\int dp |p\rangle \langle p| = 1$). The result is

$$\begin{aligned} & \langle q'' | \exp(-iTH) | q' \rangle \\ &= \lim_{N \rightarrow \infty} \int \dots \int \exp \left\{ \sum_{l=0}^N [i p_{l+\frac{1}{2}} (q_{l+1} - q_l) - i \hat{H}(p_{l+\frac{1}{2}}, q_l)] \right\} \\ & \quad \prod_{l=0}^N \frac{dp_{l+\frac{1}{2}}}{2\pi} \prod_{l=1}^N dq_l \end{aligned}$$

$$\text{with } q_{N+1} = q'', \quad q_0 = q'$$

$$\hat{H}(p, q) = \langle p | H | q \rangle / \langle p | q \rangle$$

$$= M \int \exp \left(i \int [p \dot{q} - H(p, q)] dt \right) \prod_t [dp(t) dq(t)] \quad (2.2)$$

$$\text{with } q(T) = q'', \quad q(0) = q'$$

(no boundary conditions on p)

This is the phase space path integral for $[\exp(-iTH)](q'', q')$. There exists however another procedure for the construction of the phase space path integral for $\exp(-iTH)$: the coherent state path integral.

The (canonical) coherent states $|p, q\rangle$ are normalized vectors, labeled by phase space points, and defined by

$$|p, q\rangle = \exp[i(pQ - qP)] |0\rangle$$

where $|0\rangle$ is the harmonic oscillator ground state :

$$(P^2 + Q^2 - 1) |0\rangle = 0$$

It is well-known (see e.g. Klauder & Sudarshan [8]) that the coherent states give rise to a resolution of the identity

$$\int \frac{dpdq}{2\pi} |p,q\rangle \langle p,q| = \mathbb{1} \quad (2.3)$$

Unlike the resolutions of the identity introduced above, (2.3) is not just a formal expression : the vectors involved are true, normalized vectors, and the integral is weakly convergent.

If we insert (2.3) between every two factors in (2.1) we obtain (see Klauder [9]) the following expression for the coherent state matrix elements of $\exp(-iTH)$.

$$\begin{aligned} & \langle p'', q'' | \exp(-iTH) | p', q' \rangle \\ &= \lim_{N \rightarrow \infty} \int \dots \int \prod_{l=1}^N \frac{dp_l dq_l}{2\pi} \exp \left\{ \sum_{l=0}^N \left[\frac{i}{2} (p_l q_{l+1} - p_{l+1} q_l) \right. \right. \\ & \quad \left. \left. - iH(p_{l+1}, q_{l+1}; p_l, q_l) \right] \right\} \end{aligned}$$

$$\text{with } p_{N+1} = p'', q_{N+1} = q'', p_0 = p', q_0 = q'$$

$$H(p_2, q_2; p_1, q_1) = \frac{\langle p_2, q_2 | H | p_1, q_1 \rangle}{\langle p_2, q_2 | p_1, q_1 \rangle}$$

$$= \mathcal{M} \int \exp \left[\frac{i}{2} \int (pdq - qdp) - i \int H(p, q) dt \right] \prod_t [dp(t) dq(t)] \quad (2.4)$$

$$\text{with } p(0) = p', q(0) = q', p(T) = p'', q(T) = q''$$

$$H(p, q) = \langle p, q | H | p, q \rangle$$

The path integral (2.4) is very similar to (2.2) ; the Hamiltonian function $H(p, q)$ entering the exponent in the integrand is different however. Integrating (2.4) over p', p'' leads to the integral kernel $[\exp(-iTH)](q'', q')$.

Note that in (2.4) as well as in (2.2) the only terms involving \dot{p} or \dot{q} in the exponent have the form $\int p \dot{q} dt = \int p dq$ or $\int q \dot{p} dt = \int q dp$. Since these expressions are perfectly well-defined stochastic integrals with respect to Wiener measure, it is now legitimate to introduce two extra terms $-\frac{1}{2\nu} \int (\dot{p}^2 + \dot{q}^2) dt$ in the exponent, and to recombine these with $\mathcal{M} \prod_t [dp(t) dq(t)]$ in order to lead to a Wiener measure. The resulting expression is a mathematically well-defined object. Our claim is that in the limit for $\nu \rightarrow \infty$ it also leads to the right answer.

3. PHASE SPACE PATH INTEGRALS WITH WIENER MEASURE

3.1 The Theorem

Let us start by stating our result. In [10] we have proved that

$$\lim_{v \rightarrow \infty} 2\pi e^{vT/2} \int \exp \left[\frac{i}{2} \int (pdq - qdp) - i \int h(p,q) dt \right] d\mu_W^v(p) d\mu_W^v(q) \\ = \langle p'', q'' | \exp(-iTH) | p', q' \rangle \quad (3.1)$$

Here the μ_W^v are the Wiener measures associated to two independent Brownian processes (one in p , one in q), with diffusion constants v , as is apparent from the connected covariance (x is either p or q)

$$\langle x(t_2)x(t_1) \rangle^c = \langle x(t_2)x(t_1) \rangle - \langle x(t_2) \rangle \langle x(t_1) \rangle \\ = vt_1 \left(1 - \frac{t_2}{T}\right) \quad (t_2 > t_1)$$

The processes are pinned at both initial and final points

$$p(0) = p', \quad q(0) = q', \quad p(T) = p'', \quad q(T) = q''$$

The connection between the operator H and the function $h(p,q)$ is given by

$$H = \int \frac{dp dq}{2\pi} |p,q\rangle h(p,q) \langle p,q| \quad (3.2)$$

The function $h(p,q)$ can be calculated from the diagonal matrix elements $H(p,q) = \langle p,q | H | p,q \rangle$ by the prescription

$$h(p,q) = \{ \exp [-(\partial_p^2 + \partial_q^2)/2] H \} (p,q) \quad (3.3)$$

Of course we have to impose some conditions on the operator H in order for (3.1) to hold. As was proved in [10], (3.1) is true for all Hamiltonians H satisfying the following three conditions

$$1) \text{ For all } \alpha > 0 : \int dp dq |h(p,q)|^2 \exp [-\alpha(p^2 + q^2)] < \infty \quad (3.4)$$

$$2) \text{ For some } \beta < \frac{1}{2} : \int dp dq |h(p,q)|^4 \exp [-\beta(p^2 + q^2)] < \infty \quad (3.5)$$

3) The set of finite linear combinations of coherent states,

$$\left\{ \sum_{j=1}^J \alpha_j |p_j, q_j\rangle ; J < \infty \right\}, \text{ is a core for } H. \quad (3.6)$$

Remark.

Note that the function $h(p,q)$ is different from both $H(p,q)$ in (2.4) and $\hat{H}(p,q)$ in (2.2). One sees from (3.2) that $h(p,q)$ is the anti-normal ordered symbol of H (while $H(p,q)$ is the normal ordered symbol). The relationship (3.3) can be inverted, leading to

$$H(p,q) = \int \frac{dp' dq'}{2\pi} \exp [-(p-p')^2/2 - (q-q')^2/2] h(p',q')$$

3.2 Examples

1. For any Hamiltonian H polynomial in P and Q , the corresponding function $h(p,q)$ is a polynomial too; (3.4) and (3.5) are then trivially satisfied. The third condition is satisfied if e.g. H is bounded below. This means we can handle, for instance,

$$P^2 + Q^2 + \lambda Q^4 \quad (\lambda > 0)$$

$$P^2 - \mu Q^4 + \lambda Q^6 \quad (\lambda > 0)$$

$$P Q^2 P$$

As the last example shows, we don't have to restrict ourselves to Hamiltonians which can be split into kinetic and potential parts. This is of course one of the advantages of working with phase space path integrals.

2. Any function $h(p,q)$ which is bounded below, and which satisfies both (3.4) and (3.5) defines a Hamiltonian H (through (3.2)) for which (3.1) will hold.

Note that if $h(p,q)$ has the form $h(p,q) = p^2 + v(q)$, then H has the form $H = P^2 + V(Q)$, where V is an entire function:

$$V(q) = \frac{1}{2} + \int \frac{dq'}{\sqrt{2\pi}} \exp[-(q-q')^2/2] v(q')$$

3. We need not restrict ourselves to selfadjoint operators. (3.1) is still true for maximal symmetric operators such as

$$\frac{1}{2} (PQ^3 + Q^3P) \quad (\text{deficiency indices } (0,1)).$$

We do however still require condition (3.6).

3.3 Sketch Of The Proof

We shall only outline the main ideas of the proof. For all the technical details (and there are many), the reader is referred to [10].

Let us first look at what happens if $h = 0$. In that case, one finds that the expression in the left hand side of (3.1), for finite v , gives the integral kernel of a contraction semigroup on $L^2(\mathbb{R}^2; dp dq/2\pi)$. More precisely,

$$\begin{aligned} 2\pi e^{vT/2} \int \exp\left[\frac{i}{2} \int (pdq - qdp)\right] d\mu_W^v(p) d\mu_W^v(q) \\ = [\exp(-vAT)](p'', q''; p', q') \end{aligned} \quad (3.7)$$

$$\text{with } A = \frac{1}{2} \left[(-i\partial_q + \frac{p}{2})^2 - (-i\partial_p + \frac{q}{2})^2 - 1 \right].$$

This operator A has a purely discrete spectrum. Its eigenvalues are the nonnegative entire numbers $0, 1, 2, \dots$; each eigenvalue is infinitely degenerate. (Note that A can be seen as the Hamiltonian of a 2-dimensional charged particle in a constant magnetic field, restricted to the plane orthogonal to the field. The eigenvalues of A are then the

familiar Landau levels). Let P_0 be the orthogonal projection operator, in $L^2(\mathbb{R}^2; dp dq/2\pi)$, onto the space spanned by the eigenvectors of A with eigenvalue 0. It turns out that P_0 is an integral operator. Explicit computation shows that its integral kernel is equal to the coherent state "overlap function",

$$P_0(p'', q''; p', q') = \langle p'', q'' | p', q' \rangle \quad (3.8)$$

This means that the range $P_0 L^2(\mathbb{R}^2; dp dq/2\pi)$ of P_0 is exactly given by the functions $F(p, q) = \langle p, q | f \rangle$, with $f \in \mathcal{H} = L^2(\mathbb{R})$. As v tends to ∞ , obviously $\lim_{v \rightarrow \infty} \exp(-vAT) = P_0$, hence

$$\lim_{v \rightarrow \infty} 2\pi e^{vT/2} \int \exp\left[\frac{i}{2} \int (pdq - qdp)\right] d\mu_W^v(p) d\mu_W^v(q) = \langle p'', q'' | p', q' \rangle \quad (3.9)$$

(3.9) is exactly statement (3.1), restricted to the case $h = 0$. For the general case, $h \neq 0$, one finds again that the path integral in the left hand side of (3.1), for finite v , is the integral kernel of a contraction semigroup on $L^2(\mathbb{R}^2; dp dq/2\pi)$.

$$2\pi e^{vT/2} \int \exp\left[\frac{i}{2} \int (pdq - qdp) - i \int h(p, q) dt\right] d\mu_W^v(p) d\mu_W^v(q) = \{\exp[-(vA + ih)T]\} (p'', q''; p', q') \quad (3.10)$$

The generator of the semigroup is now $vA + ih$, where A is as defined above, and h is the multiplication operator by the function $h(p, q)$. As v tends to ∞ , the presence of the vA -term will force the contraction semigroup to "live" on $P_0 L^2(\mathbb{R}^2; dp dq/2\pi)$ only. On the other hand only the first term of the decomposition $h = P_0 h P_0 + (1 - P_0) h P_0 + h(1 - P_0)$ contributes in this limit. Hence

$$\lim_{v \rightarrow \infty} \exp[-(vA + ih)T] = P_0 \exp(-i P_0 h P_0 T) P_0 \quad (3.11)$$

Note that $P_0 h P_0$ is no longer a multiplication operator. Due to the connection (3.8) between P_0 and the coherent states, one finds

$$\begin{aligned} & \{P_0 \exp(-i P_0 h P_0 T) P_0\} (p'', q''; p', q') \\ & = \langle p'', q'' | \exp(-iTH) | p', q' \rangle, \end{aligned}$$

$$\text{with } H = \int \frac{dpdq}{2\pi} |p, q\rangle h(p, q) \langle p, q|.$$

Together with (3.10) and (3.11), this implies (3.1).

3.4 Extensions And Open Problems.

The same approach works for other kinematical variables. In [10] spin path integrals were treated. In [11] an outline is given of the procedure for generalized coherent states, associated with general Lie groups. In [12] a detailed treatment of affine coherent state path

integrals will be given.

Open problems we intend to study in the future are for instance path integrals of systems with constraints, an extension of our present work to more singular potentials, and the implementation of our ideas in field theory.

4. REFERENCES

1. Nelson, E., J. Math. Phys. 5, 332 (1964).
2. Reed, M. and Simon, B., "Methods of Modern Mathematical Physics", Vol. II. (Academic Press, New York, 1975).
3. Gel'fand, I.M. and Yaglom, A.M., J. Math. Phys. 1 (1960), 48.
4. Cameron, R.H., J. Anal. Math. 10, 287 (1962/1963).
5. Itô, K., Proc. of 5th Berkeley Symposium on Mathematical Statistics and Probability, Vol. 2, Part 1, p.145 (Univ. of California Press, Berkeley, 1967).
6. Albeverio, S.A. and Hoegh-Krohn, R.J., "Mathematical Theory of Feynman Path Integrals" (Springer-Verlag, Berlin, 1976).
7. Combe, P., Hoegh-Krohn, R., Rodriguez, R., Sirugue, M. and Sirugue-Collin, M., Comm. Math. Phys. 77, 269 (1980).
8. Klauder, J.R. and Sudarshan, E.C.G., "Fundamentals of Quantum Optics" (Benjamin, New York, 1968).
9. Klauder, J.R., in "Path Integrals", George J. Papadopoulos and J.T. Devreese (eds.), P.5 (Plenum, New York, 1978).
10. Daubechies, I. and Klauder, J.R., "Quantum Mechanical Path Integrals with Wiener Measures for All Polynomial Hamiltonians. II", J. Math. Phys. 26, 2239 (1985)
11. Klauder, J.R., "Coherent-State Path Integrals for Group Representations", at the 14th International Colloquium on Group Theoretical Methods in Physics, Seoul (S-Korea), August 26-30, 1985.
12. Daubechies, I., Klauder, J.R. and Paul, T., in preparation.

REMARKS ON THE TIME TRANSFORMATION TECHNIQUE
FOR PATH INTEGRATION

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Abstract

The time transformation technique has proven very useful and has indeed added a new dimension to path integral calculation. However, it is not all well understood why the nonintegrable position-dependent time transformation works in path integration. To provide a basis for the time transformation technique, we consider a modified Feynman's path integral, called the "promotor," $P(\vec{x}, \vec{x}'; \tau) = \int \exp[(i/\hbar) \int (L + E) dt] D\vec{x}$, by integration of which the energy-dependent Green's function can be evaluated. In order to implement the time transformation in actual path integration, we propose a scaling rule for local time intervals. Since the standard isometric time slicing cannot be applied equipollently before and after the position-dependent time transformation, an anisometric time slicing is proposed, which leads to a unique consistent scaling rule for a finite time interval. We find that the time transformation, even if nonintegrable, can work inside a path integral because the dominant contribution comes from the path along which the transformation is integrable.