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Quantum Mechanical Path Integrals with Wiener Measures for all Polynomial Hamiltonians

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We construct arbitrary matrix elements of the quantum evolution operator for a wide class of self-adjoint canonical Hamiltonians, including those which are polynomial in the Heisenberg operators, as the limit of well defined path integrals involving Wiener measure on phase space, as the diffusion constant diverges. A related construction achieves a similar result for an arbitrary spin Hamiltonian.

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Path integrals for evolution operators of quantum mechanical systems are almost always defined as the limits of expressions involving finitely many integrals.[1] Efforts to define them as integrals involving genuine measures on path spaces of continuous paths, or as limits of such integrals, have been largely unrewarding.[2] In our earlier work on this subject we have succeeded in establishing quantum mechanical path integrals with genuine measures for the limited class of quadratic Hamiltonians.[3]

In this paper, taking an alternative but closely related approach, we succeed in constructing arbitrary matrix elements of the quantum evolution operator as limits of well defined path integrals involving Wiener measure on phase space as the diffusion constant diverges. Our construction works for any self-adjoint Hamiltonian of a wide but special class (defined below) which includes all Hamiltonians polynomial in the canonical (Heisenberg) operators. A similar construction leads to an analogous description of arbitrary matrix elements of the quantum evolution operator for an arbitrary Hamiltonian composed of spin operators for any fixed spin $s > 0$, extending earlier work.[4] As above, these matrix elements are defined as limits of well defined path integrals involving Wiener measure defined here on the unit sphere, again as the diffusion constant diverges. Finally we comment on how the spin path-integral expression passes to the canonical one as $s \to \infty$. We content ourselves here with a statement of our principal results, reserving a precise formulation and detailed proofs to a separate article.[5] For clarity we confine our discussion to a single degree of freedom. The notation is that of our earlier papers.

Canonical case.—For all $(p,q) \in R^2$ let

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

denote the canonical coherent states, where $|0\rangle$ is a normalized vector that satisfies $(Q + iP)|0\rangle = 0$. It follows[6] that a general operator H can be expressed as

$$H = \int h(p,q)|p,q\rangle\langle p,q|\, dp\, dq/2\pi,$$

where

$$h(p,q) = \exp[-(\partial^2/\partial p^2 + \partial^2/\partial q^2)/2]\langle p,q|H|p,q\rangle.$$

For H the unit operator I, this expression yields $h = 1$; for H a polynomial in P and Q, it follows that h is a polynomial in p and q. The special class of Hamiltonians we are able to discuss includes all those for which $h(p,q)$ is polynomially bounded. We suppose hereafter that H denotes the self-adjoint Hamiltonian of interest, and thus that h is real.

Now we introduce additional canonical coherent states

$$|p,q,n\rangle \equiv \exp[i(pQ-qP)]|n\rangle, \quad n=0,1,2,\ldots,$$

where $|n\rangle$ denotes the normalized nth excited state of a harmonic oscillator of unit frequency; clearly $|p,q,0\rangle \equiv |p,q\rangle$. For any β with $|\beta|<1$ it follows that[7]

$$|p,q\rangle\rangle \equiv \sum_{n=0}^{\infty} \oplus\, \beta^{n/2}|p,q,n\rangle$$

defines a vector in an associated direct-sum Hilbert space $\mathscr{H}$. We define four operators in $\mathscr{H}$ as follows:

$$E_\beta \equiv \int |p,q\rangle\rangle\langle\langle p,q|dp\,dq/2\pi = \sum_{n=0}^{\infty}\oplus\,|\beta|^n I_n, \quad A \equiv \sum_{n=0}^{\infty}\oplus\, nI_n, \quad B_\beta \equiv \int h(p,q)|p,q\rangle\rangle\langle\langle p,q|\,dp\,dq/2\pi,$$

$$C_\beta \equiv \int \exp[-i\epsilon h(p,q)]|p,q\rangle\rangle\langle\langle p,q|\,dp\,dq/2\pi.$$

In arriving at the second form for E_β we have used the basic fact that

$$\int |p,q,n\rangle\langle p,q,m|\,dp\,dq/2\pi = \langle m|n\rangle I_n = \delta_{mn}I_n,$$

where I_n denotes the unit operator in the nth direct-sum subspace. Observe that E_1 is the identity operator in $\mathscr{H}$, while $P \equiv E_0$ is the projection onto the 0th subspace $\mathscr{H}$. A real h implies that B_β is a symmetric operator in $\mathscr{H}$.

Now choose the following parameters: N is a variable positive integer, T a fixed positive time interval, $\epsilon \equiv T/(N+1)$, and $\beta \equiv (1-\epsilon\nu/2)/(1+\epsilon\nu/2)$, ν fixed and positive (ν is the diffusion constant, as will become apparent). With these identifications, and for polynomially bounded h, we are able to prove[5,8] ("s" means strong) *Lemma 1:*

$$\underset{N\to\infty}{\text{s-lim}}\, C_\beta^N = \exp(-\nu TA - iTB_1). \tag{1}$$

Furthermore, under the same conditions, we can prove *Lemma 2:*

$$\underset{\nu\to\infty}{\text{s-lim}}\, \exp(-\nu TA - iTB_1) = P\exp(-iTPB_1P)P. \tag{2}$$

Observe that PB_1P restricted to the 0th subspace is just the self-adjoint Hamiltonian H. Consequently, for any $|\phi\rangle$, $|\psi\rangle \in \mathscr{H}$, the matrix element of the evolution operator is given by

$$\langle\phi|e^{-iTH}|\psi\rangle = \lim_{\nu\to\infty}\lim_{N\to\infty}\langle\langle\phi|C_\beta^N|\psi\rangle\rangle, \tag{3}$$

where $|\phi\rangle\rangle$, $|\psi\rangle\rangle \in \mathscr{H}$ are vectors with 0th entry $|\phi\rangle$, $|\psi\rangle$, respectively, and zero in all remaining entries, $n>0$.

We now proceed to give a path-integral expression for (3). With the parameters chosen as above it follows that

$$\langle\langle p'',q''|C_\beta^N|p',q'\rangle\rangle = \int\cdots\int \prod_{l=0}^{N}\langle\langle p_{l+1},q_{l+1}|p_l,q_l\rangle\rangle \prod_{l=1}^{N}\{\exp[-i\epsilon h(p_l,q_l)]dp_l\,dq_l/2\pi\},$$

where $(p',q')\equiv(p_0,q_0)$ and $(p'',q'')\equiv(p_{N+1},q_{N+1})$. We observe that[3b]

$$\langle\langle p_2,q_2|p_1,q_1\rangle\rangle = \frac{1+\epsilon\nu/2}{\epsilon\nu}\exp\left\{\frac{i}{2}(p_1q_2-q_1p_2) - \frac{1}{2\epsilon\nu}[(p_2-p_1)^2+(q_2-q_1)^2]\right\}.$$

The form of this expression makes evident the result of the limit $N\to\infty$ ($\epsilon\to 0$) as

$$\lim_{N\to\infty}\langle\langle p'',q''|C_\beta^N|p',q'\rangle\rangle = 2\pi e^{\nu T/2}\int \exp\{i\int_0^T[\tfrac{1}{2}(p\dot{q}-q\dot{p})-h(p,q)]dt\}d\mu_W^\nu(p,q),$$

where μ_W^ν is a product of two pinned Wiener measures concentrated on continuous paths with a normalized connected covariance given for $t_1 \leq t_2$ by $\langle x(t_1)x(t_2)\rangle^c = \nu t_1(1-t_2/T)$ for $x \equiv p$ or q; here the role of ν as diffusion constant is apparent. Note that $\int(p\dot{q}-q\dot{p})dt$ interpreted as $\int(p\,dq - q\,dp)$ involves well-defined stochastic integrals in any[9] (Itô or Stratonovich) sense. Finally, we obtain the following *Theorem:*

$$\langle\phi|e^{-iTH}|\psi\rangle = \lim_{\nu\to\infty}\int\langle\phi|p'',q''\rangle[2\pi e^{\nu T/2}\int\exp(iS)d\mu_W^\nu]\langle p',q'|\psi\rangle\left(\frac{dp''\,dq''}{2\pi}\right)\left(\frac{dp'\,dq'}{2\pi}\right),$$

where S denotes the "classical action,"

$$S \equiv \int_0^T [\tfrac{1}{2}(p\dot{q} - q\dot{p}) - h(p,q)]dt.$$

This result achieves our stated goal of a path-integral representation.

It is important to compare our results here with those obtained earlier. In Ref. 3 we were able to find an expression for quadratic Hamiltonians which involves the function $H(p,q) = \langle p,q|H|p,q\rangle$ as the Hamiltonian function in S (rather than h), at the expense of introducing Wiener measures with nonvanishing drift terms determined by the usual Hamilton equations of motion.[3b] Thus, at least for the limited set of Hamiltonians in common, we gain a clearer understanding of the true underlying distinction between two formal but otherwise identical path-integral expressions given by[10]

$$\mathcal{N}\int \exp(iS)\prod_t dp(t)\,dq(t),$$

where $S = \int[\tfrac{1}{2}(p\dot{q} - q\dot{p}) - h(p,q)]dt$ or $S = \int[\tfrac{1}{2}(p\dot{q} - q\dot{p}) - H(p,q)]dt$. If $\hbar \to 0$ recall that $h(p,q) \to H_c(p,q)$, $H(p,q) \to H_c(p,q)$, where $H_c(p,q)$ denotes the usual classical Hamiltonian. This fact explains how yet another expression, involving Wiener measures without drift and the function $H(p,q)$ representing the Hamiltonian, can be valid insofar as the leading term of the stationary-phase approximation is concerned, since in that approximation both H and h are equivalent to H_c [neglecting terms $O(\hbar)$].[11]

The rigorous path-integral definition described in this paper enables variable transformations (e.g., canonical transformations) to be examined much more critically than in the usual formal formulation. Such a possibility provides just one motivation for our seeking to define quantum mechanical path integrals in terms of genuine measures on continuous paths.

Spin case.—With regard to a path integral for spin s we can proceed analogously. Fix $s > 0$, and for $(\theta,\phi) \in S^2$ let

$$|\theta,\phi\rangle \equiv \exp(-i\phi S_3)\exp(-i\theta S_2)|s_s\rangle \in \mathcal{H}_s$$

denote normalized spin-coherent states, where $S_3|s_s\rangle = s|s_s\rangle$, and $\vec{S}^2 = s(s+1)I_s$. It follows that

$$H = N_s\int h(\theta,\phi)|\theta,\phi\rangle\langle\theta,\phi|d\Omega,$$

where $N_s = (2s+1)/4\pi$, $d\Omega = \sin\theta\, d\theta\, d\phi$, represents any operator in $\mathcal{H}_s$. Here the relation between h and H is expressed[12] in terms of the usual spherical harmonics Y_{lm} by

$$h(\theta,\phi) = \sum_{l=0}^{2s}\sum_{m=-l}^{l}\frac{(2s+l+1)!}{(2s+1)!}\frac{(2s-l)!}{(2s)!}Y_{lm}(\theta,\phi)\int Y_{lm}^*(\theta',\phi')\langle\theta',\phi'|H|\theta',\phi'\rangle d\Omega'.$$

Evidently for H the identity operator I_s, $h=1$; while for any operator H, h is well defined. Hereafter we assume that H is the self-adjoint spin-operator Hamiltonian of interest, and thus h is real. Next we introduce additional normalized spin-coherent states

$$|\theta,\phi,j_m\rangle \equiv \exp(i-\phi S_3)\exp(-i\theta S_2)|j_m\rangle$$

appropriate to spin j and magnetic quantum number m, where $S_3|j_m\rangle = m|j_m\rangle$; clearly $|\theta,\phi,s_s\rangle \equiv |\theta,\phi\rangle$. For any β with $|\beta| < 1$ it follows that

$$|\theta,\phi\rangle\rangle \equiv \sum_{l=0}^{\infty}\oplus\;(2l+2s+1)^{1/2}\beta^{l(l+2s+1)/4}|\theta,\phi,l+s_s\rangle$$

defines a vector in an associated direct-sum Hilbert space $\mathcal{H}_s$. Four operators are defined on $\mathcal{H}_s$ as follows:

$$E_\beta \equiv \int|\theta,\phi\rangle\rangle\langle\langle\theta,\phi|(d\Omega/4\pi) = \sum_{l=0}^{\infty}\oplus\;|\beta|^{l(l+2s+1)/2}I_{l+s}, \quad A \equiv \sum_{l=0}^{\infty}\oplus\;\tfrac{1}{2}l(l+2s+1)I_{l+s},$$

$$B_\beta \equiv \int h(\theta,\phi)|\theta,\phi\rangle\rangle\langle\langle\theta,\phi|(d\Omega/4\pi), \quad C_\beta \equiv \int\exp[-i\epsilon h(\theta,\phi)]|\theta,\phi\rangle\rangle\langle\langle\theta,\phi|(d\Omega/4\pi).$$

Here we have used the fact that

$$(2j+1)\int|\theta,\phi,j_m\rangle\langle\theta,\phi,j'_m|(d\Omega/4\pi) = \delta_{jj'}I_j$$

for all $j, j' \geqslant m$. We choose N a variable positive integer, T a fixed positive time integral, $\epsilon \equiv T/(N+1)$, and $\beta = 1 - \epsilon\nu$, ν fixed and positive. Then again we are able to prove, *mutatis mutandis,* (1) and (2), with (3) as a consequence. As for the path-integral expression it follows that

$$\langle\langle \theta'', \phi'' | C_\beta^N | \theta', \phi' \rangle\rangle = \int \cdots \int \prod_{p=0}^{N} \langle\langle \theta_{p+1}, \phi_{p+1} | \theta_p, \phi_p \rangle\rangle \prod_{p=1}^{N} \exp[-i\epsilon h(\theta_p, \phi_p)](d\Omega_p/4\pi),$$

where, for $0 < \epsilon << 1$, and up to $O(\epsilon^2)$ terms,

$$\langle\langle \theta_2, \phi_2 | \theta_1, \phi_1 \rangle\rangle = \sum_{l=0}^{\infty} (2l+2s+1)[1 - \tfrac{1}{2}\epsilon\nu l(l+2s+1)] \langle \theta_2, \phi_2, l+s_s | \theta_1, \phi_1, l+s_s \rangle$$

$$= (1+s\epsilon\nu)\langle \theta_2, \phi_2 | \theta_1, \phi_1 \rangle \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (4\pi)[1 - \tfrac{1}{2}\epsilon\nu l(l+1)] Y_{lm}(\theta_2, \phi_2) Y_{lm}^*(\theta_1, \phi_1).$$

Note here that

$$\langle \theta_2, \phi_2 | \theta_1, \phi_1 \rangle \equiv \left[\cos\frac{\theta_2 - \theta_1}{2} \cos\frac{\phi_2 - \phi_1}{2} + i \cos\frac{\theta_2 + \theta_1}{2} \sin\frac{\phi_2 - \phi_1}{2} \right]^{2s} \quad (4)$$

while

$$(e^{t\nu\Delta/2})(\theta_2, \phi_2; \theta_1, \phi_1) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \exp[-\tfrac{1}{2}t\nu l(l+1)] Y_{lm}(\theta_2, \phi_2) Y_{lm}^*(\theta_1, \phi_1), \quad (5)$$

with Δ the Laplacian on the unit sphere, is the Markov transition element for Brownian motion on the sphere with diffusion constant ν. Consequently,

$$\lim_{N \to \infty} \langle\langle \theta'', \phi'' | C_\beta^N | \theta', \phi' \rangle\rangle = 4\pi e^{s\nu T/2} \int \exp\{i \int_0^T [s \cos\theta\dot{\phi} - h(\theta, \phi)] dt\} d\mu_W^\nu \theta, \phi). \quad (6)$$

Here μ_W^ν denotes a pinned Wiener measure on the unit sphere with diffusion constant ν and weight given by (5) for $t = T$. To obtain (6) it is necessary to expand (4) to second-order differentials and use an appropriate form of the Itô calculus.[4] Here $\int \cos\theta\dot{\phi}\, dt = \int \cos\theta\, d\phi$ represents a well defined stochastic integral (in any sense). Finally we observe that

$$\langle \phi | e^{-iTH} | \psi \rangle = \lim_{\nu \to \infty} \int \langle \phi | \theta'', \phi'' \rangle (N_s e^{s\nu T/2} \int e^{iS} d\mu_W^\nu) \langle \theta', \phi' | \psi \rangle d\Omega'' d\Omega',$$

with $S = \int_0^T [s \cos\theta\dot{\phi} - h(\theta, \phi)] dt$, represents the desired path-integral expression.

In the spin case remarks entirely similar to those of the canonical case apply to an alternative path-integral definition in which Brownian motion on the sphere in the presence of drift and alternative expressions for the classical Hamiltonians arise. See Ref. 4.[10]

Lastly we remark that if we rescale ν in the spin case to ν/s, set $p = s^{1/2}\cos\theta$, $q = s^{1/2}\phi$ $(-\pi < \phi \leq \pi)$, and formally take the limit $s \to \infty$, then it follows that the spin path integral becomes the canonical path integral (modulo a trivial phase change).

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[6]J. R. Klauder and E. C. G. Sudarshan *Fundamentals of Quantum Optics* (Benjamin, New York, 1968), Chaps. 7 and 8.

[7]The normalization of the vectors $|p,q\rangle\rangle$ differs by a factor $(1-|\beta|)^{1/2}$ from that in Ref. 3b.

[8]One can prove that $\nu A + iB_1$, where $B_1 = \lim_{\beta \to 1} B_\beta$, generates a strongly continuous contraction semigroup which we denote by $\exp[-\nu TA - iTB_1]$.

[9]See, e.g., K. Itô, in *Mathematical Problems in Theoretical Physics,* edited by H. Araki (Springer-Verlag, New York, 1975), p. 218.

[10]Compare, in this regard, R. Shankar, Phys. Rev. Lett. **45**, 1088 (1980).

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[12]See, e.g., F. T. Arecchi, E. Courtens, R. Gilmore, and H. Thomas, Phys. Rev. A **6**, 2211 (1972).