Sums over paths adapted to quantum theory in phase space

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I. In the WWM formalism [1], it is well known that information about a quantum system is stored in the "evolution function" or "twisted exponential", this is to say, the solution of the (twisted product) Schrödinger equation:

$$2i\,\frac{\partial \chi_H}{\partial t} = H \times \chi_H; \qquad \chi_H(0) = 1. \tag{1}$$

Here H denotes the classical hamiltonian of the system under consideration, χ_H is the corresponding evolution function (then, χ_H is a function of time and phase-space coordinates) and $\times$ denotes the twisted product. We take units with $\hbar = 2$.

A Fourier transformation with respect to t gives us the spectral projectors ("Wigner functions") for each value of the energy E:

$$\Pi_H(E) = \frac{1}{4\pi}\int \chi_H(t)\, \exp(itE/2)\, dt. \tag{2}$$

The spectrum of H is simply the support of $\Pi_H(E)$ on the E-axis. We prove the following: the evolution function may be expressed as a Feynman-type integral:

$$\chi_H(u;t) = \iint \mathcal{D}[x(\tau)]\, \mathcal{D}[y(\tau)]\, \exp\biggl[-\frac{i}{2}\int (H(x) - 2yJ\dot{y} + 2xJ\dot{y})\, d\tau\biggr] \tag{3}$$

where the phase-space trajectories have to fulfil $x(0) = y(0)$, $y(t) = u$; aJb denotes the symplectic product of the vectors a, b.

Proof.

$$\chi_H(u;t) = \lim_{N\to\infty} \exp\Bigl(-\frac{it}{2N}\Bigr) \times \cdots \times \exp\Bigl(-\frac{it}{2N}\Bigr) =: \chi_H^{(N)}(u;t),$$

where

$$\begin{aligned}\chi_H^{(N)}(u;t) &= \exp\Big(-\frac{it}{2N}\Big) \times \chi_H^{(N-1)}(u;t) \\ &= \iint \underline{dx_N}\,\underline{dy_N}\ \exp\Big[-\frac{i}{2}\Big(\frac{t}{N}\,H(x_N) - 2uJx_N - 2x_NJy_N - 2y_NJu\Big)\Big]\chi_H^{(N-1)}(y_N) \qquad (4)\\ &= \cdots = \int \cdots \int \prod_{j=2}^{N} \underline{dx_j}\,\underline{dy_j}\ \exp\Big\{-\frac{i}{2}\Big[\sum_{j=1}^{N}\frac{t}{N}\,H(x_j) + \sum_{j=2}^{N} 2(x_j - y_j)J(y_{j+1} - y_j)\Big]\Big\}\end{aligned}$$

with $x_1 = y_2, u = y_{N+1}$; the limit of which expression we represent by (3). Here $\underline{dx} = (2\pi)^{-n}\,dx$. □

II. (A classical interlude). In much the same way as the classical action is selected by the Euler–Lagrange equations for the ordinary Lagrangian, we may regard the integrand in (3) as a "Lagrangian" dependent on the variables x, y. The Euler–Lagrange equations give then:

$$\dot{x}_c = J\,\frac{\partial H}{\partial x_c}; \qquad \dot{y}_c = \tfrac{1}{2}x_c\,. \tag{5}$$

We remark that the first equations are nothing but Hamilton's equations; then $x_c(\tau)$ is a classical trajectory governed by H and $y_c(\tau) = \frac{1}{2}(x(\tau) + x(0))$; the trajectory is chosen in such a way that $y_c(\tau) = u$. A simple calculation gives for the phase in (3):

$$g_c(u;t) = \int_0^t \big(H(x_c) + \tfrac{1}{2}x_cJ\dot{x}_c)\big)\,d\tau - x_c(0)Ju. \tag{6}$$

Contrary to appearances, this function does not depend on $x_c(0)$. In classical mechanics g_c makes a lot of sense [2, 3]. It may be directly related to the action associated to the trajectory $x_c(\tau)$. Let us introduce $(q(\tau), p(\tau)) = x_c(\tau)$; $(q_i, p_i) = x_c(0)$; $(q_f, p_f) = x_c(t)$; $\rho = q_f - q_i$, $u = (r, k)$. Then we have:

$$g_c(u;t) = g_c(r,k;t) = k\rho - S(r + \tfrac{1}{2}\rho, r - \tfrac{1}{2}\rho; t), \tag{7}$$

where $S(q_f, q_i; t)$ is the action and k turns out to be $\frac{1}{2}\big(\frac{\partial S}{\partial q_f} - \frac{\partial S}{\partial q_i}\big)$ (Legendre transformation). Weinstein [2] calls g_c the *Poincaré generating function* and proves its invariance under linear canonical changes of coordinates. Using (7) one gets the following modified Hamilton–Jacobi equation for g_c:

$$\frac{\partial g_c}{\partial t} = H\Big(u + \frac{1}{2}\,J\,\frac{\partial g_c}{\partial u}\Big). \tag{8}$$

III. Let us consider quadratic hamiltonians, of the form $H = \frac{1}{2}{}^tuBu + {}^tcu + d$ where B is a symmetric $2n \times 2n$ matrix, c is a vector in $\mathbb{R}^{2n}$ and d is a scalar constant. Now, clearly the usual "trick" for quadratic hamiltonians allowing to calculate propagators by factoring out the classical paths, works also in the present context. This will permit us to calculate with ease the evolution function for any quadratic hamiltonian. We write it in the form:

$$\chi_H(u;t) = F(t)\,\exp\big(-\tfrac{i}{2}g_c(u;t)\big), \tag{9}$$

and calculate in turn $g_c(u;t)$, $F(t)$. We make the following Ansatz:

$$g_c(u;t) = {}^t u\, G(t) u + {}^t u\, k(t) + v(t). \tag{10}$$

Let us define $L := JB$, $R := JG$. Replacing expression (10) in (9) gives:

$$\dot R = \tfrac{1}{2}(L - RL + RL - RLR); \quad \dot k = \tfrac{1}{2}(1 - GJ)BJk + (1 - GJ)c; \quad \dot v = d - \tfrac{1}{8}{}^t kJBJk + \tfrac{1}{2}{}^t cJk. \tag{11}$$

The first of these equations is a variant of the "matrix Riccati equation" interesting in its own right [4]. The solution is:

$$R(t) = -(\Sigma(t) + 1)^{-1}(\Sigma(t) - 1), \tag{12}$$

where $\Sigma(t)$ solves $\dot\Sigma = -L\Sigma = -\Sigma L$, with $\Sigma(0) = 1$. From the group property $\chi(t)\times\chi(t') = \chi(t+t')$ one gets:

$$F(t)\, F(t')\ \det{}^{1/2} G(t + t') = F(t + t')\ \det{}^{1/2}(G(t) + G(t')), \tag{13}$$

from which we infer: $F(t) = \det^{-1/2}(\frac{1}{2}(\Sigma(t) + 1))$.

IV. Let us put in what follows $c = 0$, $d = 0$ for simplicity (as long as $\det B \neq 0$, the general ease may be brought to that form except for a trivial summand).

In order to calculate the Poincaré generating functions and spectra what remains to be done is, in essence, the calculation of matrix exponentials. This can be greatly simplified using Williamson's classification theorem [5] for normal canonical forms. The solutions for $n = 1$ are well known: see Table 1.

Table 1:

Hamiltonian type	Eigenvalues of L	Generating function	Spectrum
1	real	$2H\,\mathrm{th}\,\frac{t}{2}$	TAC
3, 4	null	Ht	TAC
5	pure imaginary	$2H\,\mathrm{tg}\,\frac{t}{2}$	DPP

The solutions for $\mathbb{R}^4$ may be separated into two classes, in an obvious way, according to whether the Hamiltonian decomposes in direct sum of two $\mathbb{R}^2$-hamiltonians or not. The indecomposable cases are given in Table 2.

In the tables TAC means *transient absolutely continuous spectrum* and DPP *discrete pure point spectrum* [6]. Whenever H_1, H_2 appear it is to be reckoned that $H = H_1 + H_2$ and the Poisson bracket of H_1 and H_2 is zero.

We offer two comments:

(i) Calculation of g is relatively simpler than calculation of the action S. This is due to its canonical invariance. The simplicity of the evolution function relative to the usual propagator may be traced back to that. Also the pre-exponential factor is computed much more easily.

(ii) We know very little about the singular case ($\det B = 0$, $c \neq 0$) when $n > 1$.

Table 2:

Hamiltonian type	Eigenvalues of L	Generating function	Spectrum
1	real	$2H_1 \operatorname{th} \frac{t}{2} + H_2 t \operatorname{sech}^2 \frac{t}{2}$	TAC
2	complex	$\dfrac{2H_1 \sinh at + 2H_2 \sin bt}{\cosh at + \cos bt}$	TAC
4	null	Ht	TAC
5	pure imaginary	$2H_1 \operatorname{tg} \frac{t}{2} + H_2 t \sec^2 \frac{t}{2}$	DPP

References

[1] J. M. Gracia-Bondía, "The Hydrogen atom in the phase-space formulation of quantum mechanics", Phys. Rev. A **30** (1984), 691–697.

[2] A. Weinstein, "The invariance of Poincaré's generating function for canonical transformations", Invent. Math. **16** (1972), 202–213.

[3] M. A. Marinov, "An alternative to the Hamiltonian–Jacobi approach in classical mechanics", J. Phys. A **12** (1979), 31–47.

[4] P. Winternitz, "Lie groups and symmetries of nonlinear differential equations", Preprint, Université de Montréal, 1976.

[5] P. Broadbridge, "Normal forms for classical and boson systems", Physica A **99** (1979), 494–512.

[6] J. E. Avron and B. Simon, "Transient and recurrent spectrum", J. Funct. Anal. **43** (1981), 1–31.