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Phase-Space Propagators for Quantum Quadratic Hamiltonians in One and Two Dimensions

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After a summary of the fundamental concepts of quantum mechanics in phase space we apply the Moshinsky-Winternitz classification of the time-independent quadratic Hamiltonians in one and two dimensions to give the explicit form of the phase-space propagators, and make some comments on their spectra.

1. PHASE-SPACE QUANTUM MECHANICS

The idea of building a quantum formalism in phase space starts at the beginning of the 1930s (Weyl, 1931; Wigner, 1932). At this time it was thought to associate quantum operators with every classical observable through certain correspondence rule (Groenewold, 1946; Moyal, 1949; Agarwal and Wolf, 1970; Krüger and Poffin, 1977). Wigner introduced the function which takes his name; this function describes a quantum state and is defined on the classical phase space associated with the problem under study. Since then many attempts have been made to accomplish a systematic study of this alternative to the usual quantum theory.

A simple approach to the Weyl correspondence and the Wigner function is given in de Groot (1974). A deeper approach can be found in Várilly and Gracia-Bondía (1988), Gracia-Bondía (1986), and Amiet and Hugenin (1981). The key idea lies in associating to every quantum operator a function in the variables q and p. This new formalism has certain advantages in relation to the traditional approach. For example, some calculations are simpler when we use phase-space functions than with the use of the operators; we circumvent the problems that arise with domains of non-bounded operators; and in this formalism the classical limit of the quantum

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expressions can easily be obtained by performing the limit when $\hbar$ goes to zero.

We restrict ourselves to spinless particles without constraints and we stipulate that we are working in Cartesian coordinates (the integrals will always be taken from $-\infty$ to $+\infty$).

Let us consider an observable A related to a certain physical system with n degrees of freedom. The Weyl-Wigner correspondence gives us a one-to-one mapping between quantum observables and real-valued functions or distributions defined on the $2n$-dimensional phase space and vice versa:

$$\underset{\sim}{W}: \quad A \to a(\mathbf{q}, \mathbf{p})$$
$$\tilde{W}: \quad a(\mathbf{q}, \mathbf{p}) \to A$$

by means of the following expressions (de Groot, 1974):

$$\begin{aligned} a(\mathbf{q}, \mathbf{p}) &= \int d\mathbf{u} \left[\exp\left(\frac{i}{\hbar} \mathbf{qu}\right)\right] \langle \mathbf{p} + \tfrac{1}{2}\mathbf{u} | A | \mathbf{p} - \tfrac{1}{2}\mathbf{u}\rangle \\ &= \int d\mathbf{v} \left[\exp\left(\frac{i}{\hbar} \mathbf{pv}\right) \langle \mathbf{q} - \tfrac{1}{2}\mathbf{v} | A | \mathbf{q} + \tfrac{1}{2}\mathbf{v}\rangle \right. \end{aligned} \tag{1}$$

$$\begin{aligned} A &= \left(\frac{1}{2\pi\hbar}\right)^n \int d\mathbf{q}\, d\mathbf{p}\, a(\mathbf{q}, \mathbf{p}) \int d\mathbf{v} \left[\exp\left(\frac{i}{\hbar}\mathbf{pv}\right)\right] \left|\mathbf{q} + \frac{\mathbf{v}}{2}\right\rangle \left\langle \mathbf{q} - \frac{\mathbf{v}}{2}\right| \\ &= \left(\frac{1}{2\pi\hbar}\right)^n \int d\mathbf{q}\, d\mathbf{p}\, a(\mathbf{q}, \mathbf{p}) \int d\mathbf{u} \left[\exp\left(\frac{i}{\hbar}\mathbf{qu}\right)\right] \left|\mathbf{p} - \frac{\mathbf{u}}{2}\right\rangle \left\langle \mathbf{p} + \frac{\mathbf{u}}{2}\right| \end{aligned} \tag{2}$$

The magnitudes $a(\mathbf{q}, \mathbf{p})$ obtained in this way are not classical. The theory elaborated starting from these functions is a reformulation of quantum mechanics. It is well known that we cannot reduce quantum mechanics to classical statistical mechanics as Weyl had originally guessed.

Let us consider a quantum state represented by the density operator

$$\rho(t) = \sum_j \alpha_j |\psi_j(t)\rangle\langle\psi_j(t)|$$

with $0 \leq \alpha_j \leq 1$, $\sum_j \alpha_j = 1$, and $\{|\psi_j(t)\rangle\}$ an orthonormal system.

The Wigner function associated with this state is defined as

$$W_\rho(\mathbf{q}, \mathbf{p}, t) = \left(\frac{1}{2\pi\hbar}\right)^n \underset{\sim}{W}[\rho(t)]$$

The mean value of the observable A in the state ρ turns out to be

$$\bar{A} = \int d\mathbf{q}\, d\mathbf{p}\, W_\rho(\mathbf{q}, \mathbf{p}, t) a(\mathbf{q}, \mathbf{p})$$

This and other properties seem to suggest treating $W_\rho(\mathbf{q}, \mathbf{p}, t)$ as a probability density function in phase space. However, this happens to be false: the Wigner function is not necessarily a positive-definite function (Hudson, 1974; Soto and Claverie, 1983a,b).

Let $f(\mathbf{q}, \mathbf{p})$ and $g(\mathbf{q}, \mathbf{p})$ be functions defined on the phase space. Let F and G be operators such that

$$\tilde{W}[f(\mathbf{q}, \mathbf{p})] = F, \qquad \tilde{W}[g(\mathbf{q}, \mathbf{p})] = G$$

We want to know the function associated with the operator FG:

$$\underset{\sim}{W}[FG] = \underset{\sim}{W}[(\tilde{W}f)(\tilde{W}g)]$$

This function is called the twisted product of the functions $f(\mathbf{q}, \mathbf{p})$ and $g(\mathbf{q}, \mathbf{p})$, and we denote it as $(f \times g)(\mathbf{q}, \mathbf{p})$.

By using (1) and (2), it turns out that

$$(f \times g)(u) = \left(\frac{1}{\pi\hbar}\right)^{2n} \int dv\, dw\, f(v) g(w) \exp\left[\frac{2i}{\hbar}(u^{\mathrm{T}}Jv + v^{\mathrm{T}}Jw + w^{\mathrm{T}}Ju)\right] \quad (3)$$

where

$$J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$$

I_n is the n-dimensional identity matrix and $u^{\mathrm{T}} = (\mathbf{q}, \mathbf{p})$, $v^{\mathrm{T}} = (\mathbf{q}', \mathbf{p}')$, and $w^{\mathrm{T}} = (\mathbf{q}'', \mathbf{p}'')$ are variables on the phase space.

It has been rigorously proved that (3) is meaningful for functions belonging to the Schwartz space (Várilly and Gracia-Bondía (1988)). The proof is also generalizable to elements belonging to a subset of generalized functions that turns out to be a *-algebra of distributions that contains all the polynomials, all the functions defined on the Schwartz space, and all the distributions having compact support. In particular we can calculate twisted products in which quadratic Hamiltonians in coordinates and momenta take part (this fact is essential in order to calculate their propagators).

In general $(f \times g)(u) \neq (g \times f)(u)$, which is the phase-space counterpart of the fact that in general two quantum observables do not commute.

Let us consider a conservative system $[H \neq H(t)]$. Its quantum mechanical evolution operator is

$$U(t) = e^{-(it/\hbar)\mathscr{H}}$$

where $\mathscr{H}$ is the operator representing the Hamiltonian in conventional quantum mechanics.

The propagator in our formalism is defined as the transformed function by the Weyl–Wigner correspondence of the evolution operator:

$$\chi(u;\,t)=\underset{\sim}{W}\left[\exp\left(-\frac{it}{\hbar}\mathscr{H}\right)\right]=\underset{\sim}{W}\left\{\exp\left(-\frac{it}{\hbar}\,\tilde{W}[H]\right)\right\} \tag{4}$$

$H(u)$ is the classical Hamiltonian of the system. The propagator is the main object in this formalism.

If we define

$$\Pi_H(u;\,E)=\frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}\chi_H(u;\,t)\,e^{iEt/\hbar}\,dt$$

we can obtain the quantum values of the energy as the support on E of the function $\Pi_H(u;\,E)$.

Let us consider classical Hamiltonians of the following type:

$$H=\tfrac{1}{2}u^{\mathrm{T}}Bu+c^{\mathrm{T}}u+d$$

We call them quadratic Hamiltonians. Here B is a real, symmetric, constant $2n\times 2n$ matrix, c is a real, constant column vector, and d is a real number. We have

$$u^{\mathrm{T}}(t)=(q_1(t),\ldots,q_n(t),p_1(t),\ldots,p_n(t))$$

We define the $\Sigma(t)$ matrix and the $a(t)$ vector as follows:

$$u(t)=\Sigma(t)u(0)+a(t) \tag{5}$$

Using this expression in the Hamiltonian equations, we find

$$\dot{\Sigma}=JB\Sigma,\qquad \dot{a}=JBa+Jc$$

By hypothesis, $B\neq B(t)$, $J\neq J(t)$, and obviously $\Sigma(0)=I$. The solution of the differential systems turns out to be

$$\begin{aligned}\Sigma t&=e^{JBt}\\ a(t)&=(JB)^{-1}(e^{JBt}-I)Jc\\ &=t\left[I+\frac{1}{2!}(JBt)+\frac{1}{3!}(JBt)(JBt)+\cdots\right]Jc\end{aligned} \tag{6}$$

Note that the first expression for $a(t)$ is meaningful as a series expansion in spite of the fact that the matrix $(JB)^{-1}$ could not exist.

It is easy to check that $\Sigma(t)$ is a symplectic matrix for every time, that is,

$$\Sigma^{\mathrm{T}}J\Sigma=J \tag{7}$$

Through rather cumbersome calculations, it can be shown (Gracia-Bondía, 1986; Amiet and Hugenin, 1981) that

$$\chi(u;\, t) = \frac{\exp[i\beta(t)/\hbar]}{\{\det[(\Sigma+I)/2]\}^{1/2}} \exp\left[\frac{i}{\hbar}(u^{\mathrm{T}}Gu + u^{\mathrm{T}}K)\right] \tag{8}$$

where

$$G \equiv G(t) = J(\Sigma+I)^{-1}(\Sigma-I) \tag{9}$$

$$K \equiv K(t) = 2J(\Sigma+I)^{-1}a \tag{10}$$

$\beta(t)$ is a time-dependent phase, which does not depend on the phase-space coordinates. In order to be evaluated, equation (8) has to be substituted into the Schrödinger equation, which in our formalism is

$$i\hbar\, \partial\chi/\partial t = H \times \chi$$

It turns out that

$$\beta(t) = \int_0^t (\tfrac{1}{2}c^{\mathrm{T}}JK + \tfrac{1}{8}K^{\mathrm{T}}JBJK - d)\, d\tau$$

Note that K is here a time-dependent vector.

It is important here to remark that the determinant of $(\Sigma+I)$ is different from zero in the situations that we consider in this paper.

Notice that if we have a homogeneous Hamiltonian, that is,

$$H = \tfrac{1}{2}u^{\mathrm{T}}Bu$$

then

$$a(t) = 0, \qquad K(t) = 0, \qquad \beta(t) = 0$$

2. CLASSIFICATION OF QUADRATIC HAMILTONIANS

2.1. Homogeneous Quadratic Hamiltonians

Let us consider two homogeneous quadratic Hamiltonians

$$H = \tfrac{1}{2}u^{\mathrm{T}}Bu, \qquad \tilde{H} = \tfrac{1}{2}u^{\mathrm{T}}\tilde{B}u$$

where B and $\tilde{B}$ are different real matrices such that there exists a symplectic matrix S that relates them

$$\tilde{B} = S^{\mathrm{T}}BS$$

$$\tilde{H}(u) = \tfrac{1}{2}u^{\mathrm{T}}\tilde{B}u = \tfrac{1}{2}u^{\mathrm{T}}S^{\mathrm{T}}BSu$$

If we consider the symplectic change of coordinates $\tilde{u} = Su$,

$$\tilde{H}(u) = \tfrac{1}{2}\tilde{u}^{\mathrm{T}}B\tilde{u} = H(\tilde{u})$$

we see that the Hamiltonian associated with $\tilde{B}$ in the u variables is equivalent to that associated with B in the $\tilde{u}$ variables.

It is easy to obtain

$$\tilde{\Sigma} = e^{J\tilde{B}t} = S^{-1}e^{JBt}S = S^{-1}\Sigma S$$

$$\tilde{G} = J(\tilde{\Sigma}+I)^{-1}(\tilde{\Sigma}-I) = S^{\mathrm{T}}GS$$

It is clear that the matrix G is transformed by S as B is. With this result in mind, it is easy to show that the propagators associated with $H(u)=\frac{1}{2}u^{\mathrm{T}}Bu$ and $\tilde{H}(u)=\frac{1}{2}u^{\mathrm{T}}\tilde{B}u$ are related by

$$\chi_{\tilde{B}}(S^{-1}u;\, t)=\chi_B(u;\, t)$$

We see that if we know χ_B, it suffices to make the corresponding coordinate transformation to obtain $\chi_{\tilde{B}}$. This result lead us to classify the homogeneous quadratic Hamiltonians into equivalence classes under symplectic transformations and calculate the propagators for the representative Hamiltonians of each class only. For this classification we have followed Moshinsky and Winternitz (1980). The authors classify the matrices of the form JB that belong to the Lie algebra $sp(2n,\mathbb{R})$ of the symplectic group $Sp(2n,\mathbb{R})$ into orbits under $Sp(2n,\mathbb{R})$.

The canonical forms in the cases $n=1$ and $n=2$ are:

(i) $n=1$:

$$B_1=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}; \qquad H_1=\tfrac{1}{2}(p^2+q^2) \qquad \text{(harmonic oscillator)}$$

$$B_2=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}; \qquad H_2=\tfrac{1}{2}(p^2-q^2) \qquad \text{(harmonic barrier)}$$

$$B_3=\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}; \qquad H_3=\tfrac{1}{2}p^2 \qquad \text{(free particle)}$$

(ii) $n=2$:

$$B_1=\begin{pmatrix}-1 & 0 & 0 & 0\\ 0 & -\lambda & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & \lambda\end{pmatrix}, \qquad B_2=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -\lambda & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & \lambda\end{pmatrix}$$

$$B_3=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \lambda & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & \lambda\end{pmatrix}, \qquad B_4=\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}$$

$$B_5 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix}_{\varepsilon=\pm 1}, \qquad B_6 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix}_{\varepsilon=\pm 1}$$

Here the units are chosen in order to eliminate some arbitrary constants.

Each of the Hamiltonians associated with the preceding matrices may be written in the form $H = H_1 + H_2$, where H_i is the Hamiltonian describing a harmonic oscillator, a harmonic barrier, or a free particle moving in the i direction. These cases are called orthogonally decomposable. We have to be careful with realization of $sp(4, \mathbb{R})$ used by Moshinsky and Winternitz.

There are five more cases, called orthogonally indecomposable:

$$B_7 = \begin{pmatrix} 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \end{pmatrix} \qquad B_8 = \begin{pmatrix} 0 & 0 & 0 & -\varepsilon/2 \\ 0 & 0 & \varepsilon/2 & 0 \\ 0 & \varepsilon/2 & 1 & 0 \\ -\varepsilon/2 & 0 & 0 & 1 \end{pmatrix}_{\varepsilon=\pm 1}$$

$$B_9 = \begin{pmatrix} -1 & 0 & 0 & -\lambda/2 \\ 0 & -1 & \lambda/2 & 0 \\ 0 & \lambda/2 & 1 & 0 \\ -\lambda/2 & 0 & 0 & 1 \end{pmatrix} \qquad B_{10} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$B_{11} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

To evaluate the Hamiltonians

$$H = \tfrac{1}{2} u^{\mathrm{T}} B u, \qquad u^{\mathrm{T}} = (q_1, q_2, p_1, p_2)$$

2.2. Nonhomogeneous Quadratic Hamiltonians

We have

$$H = \tfrac{1}{2} u^{\mathrm{T}} B u + c^{\mathrm{T}} u + d$$

Two situations occur:

(i) det $B \neq 0$. Using the change $\tilde{u} = d - \frac{1}{2} c^{\mathrm{T}} B^{-1} c$, we have

$$H = \tfrac{1}{2} \tilde{u}^{\mathrm{T}} B \tilde{u} + d', \qquad d' = d - \tfrac{1}{2} c^{\mathrm{T}} B^{-1} c$$

It is easy to prove that the constant d' adds a factor $\exp[(-i/\hbar) t d']$ to the propagator corresponding to the homogeneous part.

(ii) det $B=0$. This situation is complicated; we do not know a general method to attack it yet.

In the case $n=1$, we found 40 nonhomogeneous different Hamiltonians with det $B=0$. We classified them under symplectic changes of coordinates and we found that, if we eliminate the nonquadratic ones (i.e., linear in q, p), they can be grouped into two orbits whose representatives are

$$H_p=\tfrac{1}{2}(p^2+p), \qquad H_q=\tfrac{1}{2}(p^2+q) \tag{11}$$

H_q represents essentially a gravitational field, and H_p corresponds to a free particle, $H_p=\frac{1}{2}(p+\frac{1}{2})^2-\frac{1}{8}$.

3. EXPLICIT FORM OF THE PROPAGATORS

The calculation for one-dimensional homogeneous Hamiltonians has already been given (Garcia-Bondía, 1986). Formulas (6), (8), and (9) are used:

$$\chi_1=\exp\left(\frac{-2i}{\hbar}H_1\tan\frac{t}{2}\right)\sec\frac{t}{2}$$

$$\chi_2=\exp\left(\frac{-2i}{\hbar}H_2\tanh\frac{t}{2}\right)\operatorname{sech}\frac{t}{2}$$

$$\chi_3=\exp\left(\frac{-it}{\hbar}H_3\right)$$

As we see, χ depends on q and p through the Hamiltonian. We carried out the computations for H_q, H_q

$$\chi_p=\exp[(-it/\hbar)H_p], \qquad \chi_q=\exp\left[-\frac{it}{\hbar}H_q-\frac{it^3}{96\hbar}\right]$$

For $n=2$ the computations are more cumbersome. The results are:

1. $$H_1=\tfrac{1}{2}(p_1^2-q_1^2)+\tfrac{1}{2}\lambda(p_2^2-q_2^2)=H_{1,1}+\lambda H_{1,2}$$

$$\chi_1=\frac{\exp[(-2i/\hbar)H_{1,1}\tanh(t/2)]}{\cosh(t/2)}\times\frac{\exp[(-2i/\hbar)H_{1,2}\tanh(\lambda t/2)]}{\cosh(\lambda t/2)}$$

2. $$H_2=\tfrac{1}{2}(p_1^2+q_1^2)+\tfrac{1}{2}\lambda(p_2^2-q_2^2)=H_{2,1}+\lambda H_{2,2}$$

$$\chi_2=\frac{\exp[(-2i/\hbar)H_{2,1}\tan(t/2)]}{\cos(t/2)}\times\frac{\exp[(-2i/\hbar)H_{2,2}\tanh(\lambda t/2)]}{\cosh(\lambda t/2)}$$

3. $$H_3 = \tfrac{1}{2}(p_1^2 + q_1^2) + \tfrac{1}{2}\lambda(p_2^2 + q_2^2) = H_{3,1} + \lambda H_{3,2}$$

$$\chi_3 = \frac{\exp[(-2i/\hbar)H_{3,1}\tan(t/2)]}{\cos(t/2)} \times \frac{\exp[(-2i/\hbar)H_{3,2}\tan(\lambda t/2)]}{\cos(\lambda t/2)}$$

4. $$H_4 = \tfrac{1}{2}p_1^2 + \tfrac{1}{2}(p_2^2 - q_2^2) = H_{4,1} + H_{4,2}$$

$$\chi_4 = \exp\left(\frac{-it}{\hbar} H_{4,1}\right) \frac{\exp[(-2i/\hbar)H_{4,2}\tanh(t/2)]}{\cosh(t/2)}$$

5. $$H_5 = \tfrac{1}{2}(p_1^2 + q_1^2) + \tfrac{1}{2}\varepsilon p_2^2 = H_{5,1} + H_{5,2}$$

$$\chi_5 = \frac{\exp[(-2i/\hbar)H_{5,1}\tan(t/2)]}{\cos(t/2)} \exp\left(\frac{-it}{\hbar} H_{5,2}\right)$$

6. $$H_6 = \tfrac{1}{2}p_1^2 + \tfrac{1}{2}\varepsilon p_2^2$$

$$\chi_6 = \exp[(-it/\hbar)H_6]$$

In the orthogonally decomposable cases we can split the Hamiltonian into two parts, each depending on the variables (q_1, p_2), (q_2, p_2), respectively. The propagator is obtained as a function of the variables (q, p) through these two parts.

7. $$H_7 = \tfrac{1}{4}(2p_1 q_2 - 2p_2 q_1)$$

$$\chi_7 = \frac{\exp[(-4i/\hbar)H_7 \tan(t/4)]}{\cos^2(t/4)}$$

8. $$H_8 = \tfrac{1}{2}(p_1^2 + p_2^2) + \tfrac{1}{4}\varepsilon(2p_1 q_2 - 2p_2 q_1) = H_{8,1} + H_{8,2}$$

$$\chi_8 = \frac{1}{\cos^2(\varepsilon t/4)} \exp\left(\frac{-4i}{\hbar} H_{8,1} \tan\frac{t}{4}\right) \exp\left(\frac{-4i}{\hbar} H_{8,2} \frac{t/4}{\cos^2(t/4)}\right)$$

(the variables no longer appear separated in H_8);

9. $$H_9 = \tfrac{1}{2}(p_1^2 - q_1^2 + p_2^2 - q_2^2) + \tfrac{1}{4}\lambda(2p_1 q_2 - 2p_2 q_1) = H_{9,1} + H_{9,2}$$

$$\chi_9 = \frac{2}{\cosh t + \cos(\lambda t/2)} \times \exp\left[\frac{-i/\hbar}{\cosh t + \cos(\lambda t/2)}\left(2H_{9,1}\sinh t + \frac{4}{\lambda} H_{9,2} \sin\frac{\lambda t}{2}\right)\right]$$

10. $$H_{10} = \tfrac{1}{2}(2q_1 p_1 + 2q_2 p_2) + \tfrac{1}{2}(2q_2 p_1) = H_{10,1} + H_{10,2}$$

$$\chi_{10} = \frac{1}{\cosh^2(t/2)} \exp\left(\frac{-2i}{\hbar} H_{10,1} \tanh\frac{t}{2}\right) \exp\left(\frac{-2i}{\hbar} H_{10,2} \frac{t/2}{\cosh^2(t/2)}\right)$$

11. $H_{11} = \frac{1}{2}(q_2^2 + 2p_1 p_2)$

$$\chi_{11} = \exp\left(\frac{-it}{\hbar} H_{11}\right) \exp\left[\frac{-i}{3\hbar}\left(\frac{t}{2}\right)^3 p_1^2\right]$$

The computation of the propagators for quadratic Hamiltonians in higher dimensions requires subtler techniques than the mere direct computation. It will be the object of a later study.

4. SPECTRAL ANALYSIS

The Fourier transform of χ_B with respect to the time gives us the spectral projectors parameterized by the energy E:

$$\Pi_B(u; E) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} \chi_B(u; t) \exp\frac{itE}{\hbar}\, dt \tag{12}$$

The support of Π_B gives the quantum spectrum of the observable H in this formalism. If we are only interested in the spectrum, it is enough to calculate

$$F(E) = \frac{1}{(2\pi\hbar)^n} \int \Pi_B(u; E)\, d^{2n}u = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} \psi(t) \exp\frac{itE}{\hbar}\, dt \tag{13}$$

where the spectral function $\psi(t)$ is given by

$$\psi(t) = \frac{1}{(2\pi\hbar)^n} \int \chi_B(u; t)\, d^{2n}u \tag{14}$$

The computations have been done already in the case $n = 1$ (Gracia-Bondía, 1986).

(i) Free particle:

$$\Pi(u; E) = \delta(p^2/2 - E)$$

Then $E \in \mathbb{R}^+$.

(ii) Harmonic oscillator:

$$\Pi(u; E) = \sum_{k=0}^{\infty} 2(-1)^k L_k(2H)\, \delta(2n + 1 - E)$$

where L_k denotes the ordinary Laguerre polynomial of order n. The spectrum is

$$E \in \{2(n + 1/2),\ n = 0, 1, \ldots\}$$

note that here $\hbar = 2$.

(iii) Harmonic barrier:

$$\Pi(u;\, E) = e^{iH} \operatorname{sech}\left(\frac{\pi E}{2}\right) {}_1F_1\left(\frac{1+iE}{2}, 1; -2iH\right)$$

${}_1F_1$ is the Kummer function of the first kind. The spectrum is $E = \mathbb{R}$.

(iv) Gravitational field:

$$\Pi(u, E) = 2 \operatorname{Ai}(p^2 + q - 2E)$$

where $Ai(x)$ is the Airy function. The spectrum is $E = \mathbb{R}$.

In the case $n = 2$ we have two kinds of propagators, those associated with the decomposable as well as the indecomposable cases. The decomposable ones are of the form

$$\chi(q_1, q_2, p_1, p_2;\, t) = \chi_1(q_1, p_1;\, t)\chi_2(q_2, p_2;\, t)$$

and Π is expressed in terms of the convolution of Π_1 and Π_2, which are of the form previously seen.

Let us consider the indecomposable cases.

Using formula (12) and χ_{11}, we have for the spectral projector

$$\Pi_{11}(u;\, E) = \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} e^{iEt/\hbar}\, e^{-itH_{11}/\hbar}\, e^{-it^3 p_1^2/24\hbar}\, dt$$

which turns out to be an Airy integral (Watson, 1966, p. 188):

$$\Pi_{11}(q_1, q_2, p_1, p_2;\, E)$$
$$= \begin{cases} \dfrac{2\pi}{3(2\pi\hbar)^{1/2}} \left(\dfrac{24\hbar}{p_1^2}\right)^{1/3} \left(\dfrac{\gamma}{3}\right)^{1/2} \left\{ J_{-1/3}\left(2\left(\dfrac{\gamma}{3}\right)^{3/2}\right) + J_{1/3}\left(2\left(\dfrac{\gamma}{3}\right)^{3/2}\right) \right\}, & \gamma > 0 \\ \dfrac{2}{3(2\pi\hbar)^{1/2}} \left(\dfrac{24\hbar}{p_1^2}\right)^{1/3} (-\gamma)^{1/2} K_{1/3}\left(2\left(\dfrac{-\gamma}{3}\right)^{3/2}\right), & \gamma < 0 \end{cases}$$

where J_ν are Bessel functions of the first kind, K_ν the modified Bessel functions (or Kelvin functions), and

$$\gamma = \frac{E - H_{11}}{\hbar} \left(\frac{24\hbar}{p_1^2}\right)^{1/3}$$

The spectrum is then $E = \mathbb{R}$.

When $\det B \neq 0$, it is possible to use $\psi(t)$ instead $\Pi(u, E)$. In that case

$$\psi(t) = \frac{i^n}{[\det(\Sigma - I)]^{1/2}} \tag{15}$$

This is a general result in n dimensions and we prove it in the Appendix.

We apply this formula to B_7, B_8, B_9, and B_{10}. We omit the intermediate computations and present the matrices Σ_k associated with the matrices B_k of (6) only and the ψ_k:

$$\Sigma_7 = \begin{pmatrix} \cos\frac{1}{2}t & \sin\frac{1}{2}t & 0 & 0 \\ -\sin\frac{1}{2}t & \cos\frac{1}{2}t & 0 & 0 \\ 0 & 0 & \cos\frac{1}{2}t & \sin\frac{1}{2}t \\ 0 & 0 & -\sin\frac{1}{2}t & \cos\frac{1}{2}t \end{pmatrix}$$

$$\psi_7(t) = \frac{-1}{4\sin^2(t/4)}$$

$$\Sigma_8 = \begin{pmatrix} \cos\frac{1}{2}\varepsilon t & \sin\frac{1}{2}\varepsilon t & t\cos\frac{1}{2}\varepsilon t & t\sin\frac{1}{2}\varepsilon t \\ -\sin\frac{1}{2}\varepsilon t & \cos\frac{1}{2}\varepsilon t & -t\sin\frac{1}{2}\varepsilon t & t\cos\frac{1}{2}\varepsilon t \\ 0 & 0 & \cos\frac{1}{2}\varepsilon t & \sin\frac{1}{2}\varepsilon t \\ 0 & 0 & -\sin\frac{1}{2}\varepsilon t & \cos\frac{1}{2}\varepsilon t \end{pmatrix}$$

$$\psi_8(t) = \frac{-1}{4\sin^2(t/4)}$$

$$\Sigma_9 = \begin{pmatrix} (\cosh t\cos\frac{1}{2}\lambda t) & (\cosh t\sin\frac{1}{2}\lambda t) & (\sinh t\cos\frac{1}{2}\lambda t) & (\sinh t\sin\frac{1}{2}\lambda t) \\ (-\cosh t\sin\frac{1}{2}\lambda t) & (\cosh t\cos\frac{1}{2}\lambda t) & (-\sinh t\sin\frac{1}{2}\lambda t) & (\sinh t\cos\frac{1}{2}\lambda t) \\ (\sinh t\cos\frac{1}{2}\lambda t) & (\sinh t\sin\frac{1}{2}\lambda t) & (\cosh t\cos\frac{1}{2}\lambda t) & (\cosh t\sin\frac{1}{2}\lambda t) \\ (-\sinh t\sin\frac{1}{2}\lambda t) & (\sinh t\cos\frac{1}{2}\lambda t) & (-\cosh t\sin\frac{1}{2}\lambda t) & (\cosh t\cos\frac{1}{2}\lambda t) \end{pmatrix}$$

$$\psi_9(t) = \frac{-1}{4[\sinh^2(t/2)+\sin^2(\lambda t/4)]}$$

$$\Sigma_{10} = \begin{pmatrix} e^t & te^t & 0 & 0 \\ 0 & e^t & 0 & 0 \\ 0 & 0 & e^{-t} & 0 \\ 0 & 0 & -te^{-t} & e^{-t} \end{pmatrix}$$

$$\psi_{10}(t) = \frac{-1}{4\sinh^2(t/2)}$$

Using formula (13), we obtain

$$F_7(E)=F_8(E)=\frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}\frac{-e^{itE/\hbar}}{4\sin^2(t/4)}\,dt$$
$$=\frac{4}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}e^{i\alpha x}(e^{ix}-e^{-ix})^{-2}\,dx$$

where $t=4x$ and $\alpha=4E/\hbar$.

Operating formally, we have

$$F_7(E)=F_8(E)=\frac{4}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}e^{i\alpha x}\,e^{-2ix}(1-e^{-2ix})^{-2}\,dx$$
$$=\frac{4}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}e^{i(\alpha-2)x}$$
$$\times\left[1+\sum_{k=1}^{\infty}\frac{2\cdot 3\cdots(2+k-1)}{k!}\,e^{-2ikx}\right]dx$$
$$=\frac{4}{(2\pi\hbar)^{1/2}}\sum_{k=0}^{\infty}(k+1)\int_{-\infty}^{\infty}e^{ix(\alpha-2-2k)}\,dx$$
$$=\frac{4}{(2\pi\hbar)^{1/2}}\sum_{k=0}^{\infty}(k+1)2\pi\delta(\alpha-2-2k) \tag{16}$$

We recall that the energy spectrum is the support of $F(E)$, which in this case is

$$E=\tfrac{1}{4}\hbar(2+2k)=\tfrac{1}{2}\hbar(k+1),\qquad k=0,1,\ldots$$

which corresponds to the energy levels of the two-dimensional quantum oscillator.

Proceeding formally as in the previous cases, we obtain

$$F_{10}(E)=\frac{-1}{4(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}\frac{e^{itE/\hbar}}{\sinh^2(t/2)}\,dt$$
$$=\frac{-2}{(2\pi\hbar)^{1/2}}\sum_{k=0}^{\infty}(k+1)\int_{-\infty}^{\infty}e^{iy(2E/\hbar+i(2+2k))}\,dy$$
$$=\frac{-4\pi}{(2\pi\hbar)^{1/2}}\sum_{k=0}^{\infty}(k+1)\delta\left(\frac{2E}{\hbar}+i(2+2k)\right) \tag{17}$$

$$F_9(E)=\frac{-1}{4(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}\frac{e^{itE/\hbar}}{\sinh^2(t/2)+\sin^2(\lambda t/2)}\,dt$$
$$=\frac{-1}{(2\pi\hbar)^{1/2}}\sum_{k,l=0}^{\infty}\int_{-\infty}^{\infty}\exp\left\{t\left[-(k+l+1)+i\left(\lambda(k-l)+\frac{E}{\hbar}\right)\right]\right\}dt$$
$$=-\left(\frac{2\pi}{\hbar}\right)^{1/2}\sum_{k,l=0}^{\infty}\delta\left(\frac{E}{\hbar}+\lambda(k-l)+i(k+l+1)\right) \tag{18}$$

The Dirac deltas $\delta(z_0)$, where z_0 is a complex number, are well-defined distributions on the test space of the entire functions exponentially bounded at infinity (Gelfand and Shilov, 1964; Vo-Khac Khoan, 1972). This kind of distribution is often called an ultradistribution and the space of the ultradistributions denoted by $\mathbb{Z}'$ (Gelfand and Shilov, 1964; Vo-Khac Khoan, 1972). However, $F_9(E)$ and $F_{10}(E)$ are not well defined ultradistributions, since the series in (17) and (18) do not converge in the weak topology on $\mathbb{Z}'$. A further study is necessary in order to make precise what kind of generalized functions $F_9(E)$ and $F_{10}(E)$ are and to determine their respective supports.

5. APPENDIX

The aim of this Appendix is to prove that if $\det B \neq 0$, then

$$\psi(t) = \frac{i^n}{[\det(\Sigma - I)]^{1/2}}$$

We make the proof in three steps.

Lemma 1. G is a real, symmetric matrix. Equation (7) implies that $\Sigma^{\mathrm{T}} = -J\Sigma^{-1}J$.

Transposing (9), we have

$$\begin{aligned} G^{\mathrm{T}} &= (\Sigma^{\mathrm{T}} - I)(\Sigma^{\mathrm{T}} + I)^{-1} J^{\mathrm{T}} \\ &= -(-J\Sigma^{-1}J - I)(-J\Sigma^{-1}J + I)^{-1}J \\ &= -J(-\Sigma^{-1} + I)J[-J(\Sigma^{-1} + I)J]^{-1}J \\ &= J(I - \Sigma^{-1})(\Sigma^{-1} + I)^{-1} \\ &= J(\Sigma - I)\Sigma^{-1}[(I + \Sigma)\Sigma^{-1}]^{-1} \\ &= J(\Sigma - I)(\Sigma + I)^{-1} \\ &= G \end{aligned}$$

G is a real matrix, which comes straighforwardly from its definition.

As a consequence of this lemma, there exists an orthogonal real matrix R such that $G = R^T DR$, where D is a real, diagonal matrix. We have by (14)

$$\begin{aligned} \psi(t) &= \frac{1}{(2\pi\hbar)^n} \int \chi(u;\, t)\, d^{2n}u \\ &= \frac{F(t)}{(2\pi\hbar)^n} \int \exp\left(\frac{i}{\hbar} u^{\mathrm{T}} G u\right) d^{2n}u \\ &= \frac{F(t)}{(2\pi\hbar)^n} \int \exp\left(\frac{i}{\hbar} u^{\mathrm{T}} R^{\mathrm{T}} D R u\right) d^{2n}u \end{aligned}$$

$$=\frac{F(t)}{(2\pi\hbar)^n}\int \exp\left(\frac{i}{\hbar}v^{\mathrm{T}}Dv\right)|\det(R^{-1})|\,d^{2n}v$$

where $v=Ru$. We have $|\det(R^{-1})|=1$ because of the orthogonality of R.

If we denote by $\{\lambda_i, i=1,\ldots,2n\}$ the common eigenvalues of G and D, we have

$$\psi(t)=\frac{F(t)}{(2\pi\hbar)^n}\int \exp\left(\frac{i}{\hbar}\sum_{j=1}^{2n}\lambda_j v_j^2\right)dv_1\cdots dv_{2n} \tag{A1}$$

Lemma 2. $\det B\neq 0 \Rightarrow \det G(t)\neq 0$ a.e.

Let

$$\det G=(\det J)\det(\Sigma+1)^{-1}\det(\Sigma-I)=\frac{\det(\Sigma-I)}{\det(\Sigma+I)}$$

which shows that $\det G=0$ if and only if $\det(\Sigma-I)=0$.

Let W be the Jordan canonical form of JB. Then there exists a nonsingular matrix S such that

$$(\Sigma-I)=(e^{JBt}-I)=S^{-1}(e^{Wt}-I)S$$

Therefore

$$\det(\Sigma-I)=\det(e^{Wt}-I)=\prod_{j=1}^{2n}(e^{\gamma_j t}-1)$$

where $\{\gamma_j\}$ are the eigenvalues of W repeated as many times as shown by their multiplicity. Hence, if $\det(\Sigma-I)=0$, at least for one of these eigenvalues $e^{\gamma_j t}-1=0$, and consequently $t=0$ or $t_k=2k\pi i/\gamma_j$.

The second alternative is only possible when γ_j is purely imaginary. Note that the eigenvalues γ_j of JB can never be zero because $\det B\neq 0$ by hypothesis.

We have proved that $\det G(t)$ can at most be zero for a numerable set of instants of time.

Let us go back to (A1). Here, $\lambda_j\neq 0$ a.e. because of Lemma 2, and therefore the integral giving $\psi(t)$ is well defined,

$$\psi(t)=\frac{F(t)}{(2\pi\hbar)^n}\prod_{j=1}^{2n}\left[\int_{-\infty}^{\infty}\exp\left(\frac{i}{\hbar}\lambda_j v_j^2\right)dv_j\right]$$

We have a product of Fresnel integrals, which are well known (see, e.g., Marsden, 1973, p. 262), and give

$$\int_{-\infty}^{\infty}\exp\left(\frac{i}{\hbar}\lambda_j v_j^2\right)dv_j=\left(\frac{\pi\hbar}{\lambda_j}\right)^{1/2}e^{i\pi/4}$$

Therefore,

$$\begin{aligned}
\psi(t) &= \frac{F(t)}{(2\pi\hbar)^n} \prod_{j=1}^{2n} \left(\frac{\pi\hbar}{\lambda_j}\right)^{1/2} e^{i\pi/4} \\
&= \frac{F(t)}{(2\pi\hbar)^n} \frac{(\pi\hbar)^n e^{in\pi/2}}{(\prod_{j=1}^{2n} \lambda_j)^{1/2}} \\
&= \frac{F(t)\, e^{in\pi/2}}{2^n (\det G)^{1/2}} \\
&= \frac{e^{in\pi/2}}{2^n} \frac{1}{\{\det[(\Sigma+I)/2]\}^{1/2}} \frac{1}{\{\det[J(\Sigma+I)^{-1}(\Sigma-I)]\}^{1/2}} \\
&= \frac{e^{in\pi/2}}{[\det(\Sigma+I)\det(\Sigma+I)^{-1}\det(\Sigma-I)]^{1/2}} \\
&= \frac{i^n}{[\det(\Sigma-I)]^{1/2}}
\end{aligned}$$

proving our claim.

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