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Quadratic Hamiltonians in phase-space quantum mechanics

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Abstract. The dynamical evolution is described within the phase-space formalism by means of the Moyal propagator, which is the symbol of the evolution operator. Quadratic Hamiltonians on the phase space are distinguished in that their Moyal bracket with any function equals their Poisson bracket. It is shown that, for general time-independent quadratic Hamiltonians, the Moyal propagators transform covariantly under linear canonical transformations; they are then derived and classified in a fully explicit manner using the theory of Hamiltonian normal forms. We present several tables of propagators. It is proved that these propagators belong to the Moyal algebra of distributions, and that the spectrum of the Hamiltonian may be obtained directly as the support of the Fourier transform of the Moyal propagator with respect to time. From that, the quantum-mechanical problem for these Hamiltonians is, in principle, completely solved. The appropriate path-integral formalism for phase-space quantum mechanics, leading back to the same results, is outlined in an appendix.

1. Introduction

The phase-space approach to non-relativistic quantum mechanics of spinless particles, also called the Weyl-Wigner-Moyal (WWM) formalism, has of late received renewed attention [1]. In this formalism, observables are directly given by symbols (functions or distributions) in the phase space $\boldsymbol{R}^{2n}$. These are univocally related to the operators in the ordinary formulations of quantum mechanics by the Weyl correspondence rule. Information about the dynamics of a quantum-mechanical system in the WWM description is stored in the *evolution function*, or *Moyal propagator*, i.e. the symbol associated to the unitary evolution operator of the given system.

Here we present a completely explicit calculation of the evolution function for time-independent quadratic Hamiltonians, from which one may derive the Green functions. In a sense, this paper is a continuation of the programme set out by Moshinky and Winternitz [2] to solve Schrödinger equations for Hamiltonians that are second-order polynomials in position and momentum coordinates; these authors went no further than $n = 2$. There is much advantage in using quantum theory in phase space, as we shall see, because it allows full exploitation of the underlying canonical symmetry.

The structure of the paper is as follows. In § 2 we review briefly the WWM formalism. We introduce the Moyal propagators as the evolution functions in phase space and the spectral projectors, and derive a formula to compute the Green functions in this formalism. Section 3 is devoted to the study of the Moyal propagators of general quadratic Hamiltonians; general results are given which are valid in the time-independent case. In § 4 we proceed to the effective calculation of the Moyal propagators for

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non-singular homogeneous quadratic Hamiltonians. We give a table of these Moyal propagators up to $n=5$. Section 5 is devoted to the study of the singular and inhomogeneous cases; we finish this section with a couple of tables also. In § 6 we deal with the calculation of spectra.

We include two appendices. Appendix 1 is concerned with technical results which make the present approach rigorous. In particular, we prove that the Moyal propagators are well behaved generalised functions belonging to an algebra under the twisted product, called the Moyal algebra, and that the support of the Fourier transform of the Moyal propagator coincides with the spectrum of the Hamiltonian. Appendix 2 outlines a Feynman path-integral approach to define the Moyal propagator for an arbitrary Hamiltonian.

2. The WWM formalism

The Weyl map transforms a function or distribution f on the phase space $\boldsymbol{R}^{2n}$ with coordinates $\boldsymbol{q}$, $\boldsymbol{p}$ into an operator $W(f)$ by

$$W(f)=\frac{1}{(2\pi)^n}\int_{\boldsymbol{R}^{2n}} \mathscr{F}f(\boldsymbol{\sigma},\boldsymbol{\tau})\Omega(\boldsymbol{\sigma},\boldsymbol{\tau})\,\mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}\boldsymbol{\tau} \tag{2.1}$$

where $\mathscr{F}f$ is the ordinary Fourier transform of f. Throughout the paper, we use the convention that $\hbar=2$. The operator kernel $\Omega(\boldsymbol{\sigma},\boldsymbol{\tau})$ is given by

$$\Omega(\boldsymbol{\sigma},\boldsymbol{\tau})=\exp[\mathrm{i}(\boldsymbol{\sigma}\cdot\boldsymbol{Q}+\boldsymbol{\tau}\cdot\boldsymbol{P})]=\exp[\mathrm{i}(\sigma_1Q_1+\ldots+\sigma_nQ_n+\tau_1P_1+\ldots+\tau_nP_n)] \tag{2.2}$$

where $Q_1,\ldots,Q_n$, $P_1,\ldots,P_n$ are respectively the position and momentum operators in n dimensions. The operators (2.2) satisfy the canonical commutation relations in Weyl's form:

$$\Omega(\boldsymbol{\sigma}_1,\boldsymbol{\tau}_1)\Omega(\boldsymbol{\sigma}_2,\boldsymbol{\tau}_2)=\Omega(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2,\boldsymbol{\tau}_1+\boldsymbol{\tau}_2)\exp[-\mathrm{i}(\boldsymbol{\sigma}_1\boldsymbol{\tau}_2-\boldsymbol{\sigma}_2\boldsymbol{\tau}_1)]. \tag{2.3}$$

The map $f\mapsto W(f)$ gives a one-to-one correspondence between functions (or distributions) and operators. Since the product of operators is non-commutative, we must use a non-commutative product of functions on phase space, corresponding to the product of operators, and usually called the *twisted product* [3, 4]. The twisted product of f and g will be written $f\times g$; we demand that $W(f\times g)=W(f)W(g)$, or equivalently $f\times g=W^{-1}[W(f)W(g)]$. From (2.1) and (2.3) we find

$$\begin{aligned}(f\times g)(\boldsymbol{q},\boldsymbol{p})=\frac{1}{(2\pi)^{2n}}\int_{\boldsymbol{R}^{4n}} & f(\boldsymbol{q}_1,\boldsymbol{p}_1)g(\boldsymbol{q}_2,\boldsymbol{p}_2)\\ &\times\exp[\mathrm{i}(\boldsymbol{q}\cdot\boldsymbol{p}_1-\boldsymbol{p}\cdot\boldsymbol{q}_1+\boldsymbol{q}_1\cdot\boldsymbol{p}_2-\boldsymbol{p}_1\cdot\boldsymbol{q}_2\\ &+\boldsymbol{q}_2\cdot\boldsymbol{p}-\boldsymbol{p}_2\cdot\boldsymbol{q})]\,\mathrm{d}\boldsymbol{q}_1\,\mathrm{d}\boldsymbol{p}_1\,\mathrm{d}\boldsymbol{q}_2\,\mathrm{d}\boldsymbol{p}_2.\end{aligned} \tag{2.4a}$$

We simplify the notation by introducing ${}^t\boldsymbol{u}=(\boldsymbol{q},\boldsymbol{p})=(q_1,\ldots,q_n,p_1,\ldots,p_n)$ where ${}^t\boldsymbol{u}$ is the transpose of $\boldsymbol{u}$, and the matrix

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

where I_n is the $n\times n$ identity matrix. Now, (2.4a) can be written as

$$(f\times g)(\boldsymbol{u})=\frac{1}{(2\pi)^{2n}}\int_{\boldsymbol{R}^{4n}} f(\boldsymbol{v})g(\boldsymbol{w})\exp[\mathrm{i}({}^t\boldsymbol{u}J\boldsymbol{v}+{}^t\boldsymbol{v}J\boldsymbol{w}+{}^t\boldsymbol{w}J\boldsymbol{u})]\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{w} \tag{2.4b}$$

where ${}^t\boldsymbol{u}J\boldsymbol{v}$ is the 'symplectic scalar product' of $\boldsymbol{u}$ and $\boldsymbol{v}$.

Quantum theory in phase space may be developed entirely in terms of the twisted product without reference to the conventional formulation.

The Grossmann–Royer operators $\Pi(\boldsymbol{u})$ may be defined [5] by

$$\Pi(\boldsymbol{q}, \boldsymbol{p}) = \frac{1}{\pi^n} \int_{\boldsymbol{R}^{2n}} \exp[-\mathrm{i}(\boldsymbol{q} \cdot \boldsymbol{\sigma} + \boldsymbol{p} \cdot \boldsymbol{\tau})] \Omega(\boldsymbol{\sigma}, \boldsymbol{\tau}) \, \mathrm{d}\boldsymbol{\sigma} \, \mathrm{d}\boldsymbol{\tau}. \tag{2.5}$$

It can be proved that

$$\Pi(\boldsymbol{q}, \boldsymbol{p}) \Psi(\boldsymbol{\zeta}) = 2^n \exp[\mathrm{i}\boldsymbol{p}(\boldsymbol{\zeta} - \boldsymbol{q})] \Psi(2\boldsymbol{q} - \boldsymbol{\zeta})$$

for wavefunctions Ψ defined on the position space. From (2.1) and (2.5) it follows that

$$W(f) = \frac{1}{(4\pi)^n} \int_{\boldsymbol{R}^{2n}} f(\boldsymbol{u}) \Pi(\boldsymbol{u}) \, \mathrm{d}\boldsymbol{u}. \tag{2.6}$$

The utility of the Grossmann–Royer operators is shown by the identity

$$\operatorname{Tr} \Pi(\boldsymbol{u}) \Pi(\boldsymbol{v}) = (4\pi)^n \delta(\boldsymbol{u} - \boldsymbol{v})$$

which implies the inversion formula:

$$f(\boldsymbol{u}) = \operatorname{Tr}[W(f) \Pi(\boldsymbol{u})]. \tag{2.7}$$

In particular we find that

$$W^{-1}(|\Psi_1\rangle\langle\Psi_2|)(\boldsymbol{u}) = \langle\Psi_2|\Pi(\boldsymbol{u})|\Psi_1\rangle = 2^n \int_{\boldsymbol{R}^n} \overline{\Psi_2(\boldsymbol{q} + \boldsymbol{\zeta})} \, \Psi_1(\boldsymbol{q} - \boldsymbol{\zeta}) \exp(\mathrm{i}\boldsymbol{p} \cdot \boldsymbol{\zeta}) \, \mathrm{d}\boldsymbol{\zeta} \tag{2.8}$$

and for $\Psi_1 = \Psi_2$ we recover, but for a constant factor, the time-honoured formula for 'Wigner functions' [6]. In general

$$\begin{aligned} W^{-1}(A) = \operatorname{Tr}[\Pi(\boldsymbol{q}, \boldsymbol{p}) A] &= \int_{\boldsymbol{R}^n} \langle\boldsymbol{\zeta}|\Pi(\boldsymbol{q}, \boldsymbol{p}) A|\boldsymbol{\zeta}\rangle \, \mathrm{d}\boldsymbol{\zeta} \\ &= 2^n \int_{\boldsymbol{R}^n} \exp[\mathrm{i}\boldsymbol{p}(\boldsymbol{\zeta} - \boldsymbol{q})] \langle 2\boldsymbol{q} - \boldsymbol{\zeta}|A|\boldsymbol{\zeta}\rangle \, \mathrm{d}\boldsymbol{\zeta} \\ &= \int_{\boldsymbol{R}^n} \exp(\tfrac{1}{2}\mathrm{i}\boldsymbol{p} \cdot \boldsymbol{\xi}) \langle \boldsymbol{q} - \tfrac{1}{2}\boldsymbol{\xi}|A|\boldsymbol{q} + \tfrac{1}{2}\boldsymbol{\xi}\rangle \, \mathrm{d}\boldsymbol{\xi}. \end{aligned} \tag{2.9}$$

Let H be a time-independent classical Hamiltonian and let $W(H)$ be the operator determined by H via the Weyl correspondence. We shall always assume that $W(H)$ is self-adjoint. The *evolution function* or *Moyal propagator* associated with H is given by

$$\Xi_H(\boldsymbol{u}, t) = W^{-1}[\exp(-\tfrac{1}{2}\mathrm{i} W(H) t)] = 1 - \frac{\mathrm{i}Ht}{2} - \frac{H \times H}{2^2 \cdot 2!} t^2 + \mathrm{i} \frac{H \times H \times H}{2^3 \cdot 3!} t^3 + \ldots.$$

The Fourier transform of Ξ_H with respect to t gives us the spectral projectors parametrised by the energy E:

$$\Gamma_H(\boldsymbol{u}, E) = \frac{1}{4\pi} \int_{\boldsymbol{R}} \Xi_H(\boldsymbol{u}, t) \, \mathrm{e}^{\mathrm{i}tE/2} \, \mathrm{d}t. \tag{2.10}$$

These are, but for a constant factor, the Wigner functions corresponding to wavefunctions which are generalised eigenfunctions of $W(H)$ with eigenvalue E. We prove this assertion for the simplest case in which $W(H)$ has a pure non-degenerate discrete spectrum. The twisted product of H and Γ_H is

$$(H\times\Gamma_H(E))(\boldsymbol{u})=\frac{1}{4\pi}\int_{\boldsymbol{R}}(H\times\Xi_H(t))(\boldsymbol{u})\,\mathrm{e}^{\mathrm{i}tE/2}\,\mathrm{d}t.$$

Making use of the phase space version of the Schrödinger equation:

$$(H\times\Xi_H(t))(\boldsymbol{u})=2\mathrm{i}\frac{\partial}{\partial t}\Xi_H(\boldsymbol{u},t) \tag{2.11}$$

(recall that $\hbar=2$), we have

$$\begin{aligned}(H\times\Gamma_H(E))(\boldsymbol{u})&=\frac{1}{4\pi}\int_{\boldsymbol{R}}\left(2\mathrm{i}\frac{\partial}{\partial t}\Xi_H(\boldsymbol{u},t)\right)\mathrm{e}^{\mathrm{i}t/E/2}\,\mathrm{d}t\\&=\frac{E}{4\pi}\int_{\boldsymbol{R}}\Xi_H(\boldsymbol{u},t)\,\mathrm{e}^{\mathrm{i}tE/2}\,\mathrm{d}t\\&=E\Gamma_H(\boldsymbol{u},E).\end{aligned}$$

The second equality comes from integrating by parts. We have finally obtained that

$$(H\times\Gamma_H(E))(\boldsymbol{u})=E\Gamma_H(\boldsymbol{u},E).$$

The Weyl transform of this equation is written

$$W(H)\,W(\Gamma_H(E))=EW(\Gamma_H(E)).$$

Therefore, $W(\Gamma_H(E))$ is the orthogonal projector onto the proper subspace of $W(H)$ with eigenvalue E. If ϕ_E is the normalised eigenvector of $W(H)$ with eigenvalue E, then $\Gamma_H(\boldsymbol{u},E)$ is, save for a constant factor, the Wigner function corresponding to ϕ_E.

The foregoing suggests that the spectrum Sp H of $W(H)$ is the support on the variable E of the function (more correctly, the distribution-valued measure)$\Gamma_H(\boldsymbol{u},E)$. We prove this in appendix 1.

Green functions, defined as transition amplitudes from the state $|\boldsymbol{q}_i\rangle$ at time $t_0=0$ to the state $|\boldsymbol{q}_f\rangle$ at time t, can be evaluated using the phase-space Moyal propagator [7]. Writing $U(t)=\mathrm{e}^{-\mathrm{i}tW(H)/2}$, a formal calculation gives

$$G(\boldsymbol{q}_f,\boldsymbol{q}_i,t)=\left(\frac{1}{4\pi}\right)^n\int_{\boldsymbol{R}^n}\Xi_H\left(\frac{\boldsymbol{q}_f+\boldsymbol{q}_i}{2},\boldsymbol{p};t\right)\exp[\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{q}_f-\boldsymbol{q}_i)/2]\,\mathrm{d}\boldsymbol{p}.$$

To see this, we observe that, by (2.9):

$$\begin{aligned}&\left(\frac{1}{4\pi}\right)^n\int_{\boldsymbol{R}^n}[W^{-1}(U(t))]\left(\frac{\boldsymbol{q}_f+\boldsymbol{q}_i}{2},\boldsymbol{p};t\right)\exp[\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{q}_f-\boldsymbol{q}_i)/2]\,\mathrm{d}\boldsymbol{p}\\&\quad=\left(\frac{1}{4\pi}\right)^n\int_{\boldsymbol{R}^n}\int_{\boldsymbol{R}^n}\exp[\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{q}_f-\boldsymbol{q}_i)/2]\\&\quad\quad\times\exp(\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{v}/2)\left\langle\frac{\boldsymbol{q}_f+\boldsymbol{q}_i-\boldsymbol{v}}{2}\right|U(t)\left|\frac{\boldsymbol{q}_f+\boldsymbol{q}_i+\boldsymbol{v}}{2}\right\rangle\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{p}\\&\quad=\int_{\boldsymbol{R}^n}\int_{\boldsymbol{R}^n}\left\langle\frac{\boldsymbol{q}_f+\boldsymbol{q}_i-\boldsymbol{v}}{2}\right|U(t)\left|\frac{\boldsymbol{q}_f+\boldsymbol{q}_i+\boldsymbol{v}}{2}\right\rangle\left(\frac{1}{4\pi}\right)^n\\&\quad\quad\times\exp[\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{q}_f-\boldsymbol{q}_i+\boldsymbol{v})/2]\,\mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{v}\\&\quad=\int_{\boldsymbol{R}^n}\mathrm{d}\boldsymbol{v}\left\langle\frac{\boldsymbol{q}_f+\boldsymbol{q}_i-\boldsymbol{v}}{2}\right|U(t)\left|\frac{\boldsymbol{q}_f+\boldsymbol{q}_i+\boldsymbol{v}}{2}\right]\delta(\boldsymbol{q}_f-\boldsymbol{q}_i+\boldsymbol{v})\\&\quad=\langle\boldsymbol{q}_f|U(t)|\boldsymbol{q}_i\rangle=G(\boldsymbol{q}_f,\boldsymbol{q}_i,t).\end{aligned}$$

We can now build a *twisted functional calculus* with the symbols, with an important difference: its elements are *concrete functions* (or distributions) in phase space. The general formula for this is

$$f^{\times}(H) := \int_{\mathrm{Sp}\,H} f(E)\Gamma_H(\boldsymbol{u}, E)\,\mathrm{d}E.$$

Some important elements of a functional calculus are

(*a*) The aforesaid *evolution function* or *Moyal propagator*:

$$\Xi_H(\boldsymbol{u};\, t) = \int_{\mathrm{sp}\,H} \Gamma_H(\boldsymbol{u};\, E)\,\mathrm{e}^{-\mathrm{i}tE/2}\,\mathrm{d}E$$

(*b*) the *resolvent function*:

$$R_H(\boldsymbol{u};\, \lambda) = \int_{\mathrm{Sp}\,H} \frac{\Gamma_H(\boldsymbol{u};\, E)}{E-\lambda}\,\mathrm{d}E$$

defined for $\lambda \in \boldsymbol{C}$, $\lambda \notin \mathrm{Sp}\,H$, which verifies $R_H(\boldsymbol{u};\, \lambda) \times (H-\lambda) = 1$;

(*c*) the *twisted powers*:

$$H^{\times n}(\boldsymbol{u}) := H \times \ldots \times H(\boldsymbol{u}) = \int_{\mathrm{Sp}\,H} E^n\Gamma_H(\boldsymbol{u};\, E)\,\mathrm{d}E = 2^n\mathrm{i}^n \frac{\partial^n \Xi_H}{\partial t^n}\bigg|_{t=0}.$$

We finish this section by giving the law of evolution of the observables. In conventional quantum mechanics, observables evolve in the Heisenberg picture according to

$$F(t) = e^{\mathrm{i}Ht/2}F(0)\,\mathrm{e}^{-\mathrm{i}Ht/2}.$$

If $f(t) = W^{-1}[F(t)]$, we have

$$f(t) = W^{-1}[\mathrm{e}^{\mathrm{i}Ht/2}F(0)\,\mathrm{e}^{-\mathrm{i}Ht/2}] = \Xi_H^*(t) \times f(0) \times \Xi_H(t) \tag{2.12}$$

which is the corresponding law of motion for observables in phase-space quantum theory.

3. Quadratic Hamiltonians

The general expression for the n-dimensional quadratic Hamiltonian is given by

$$H(t) = \tfrac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}B(t)\boldsymbol{u} + {}^{\mathrm{t}}\boldsymbol{u}\boldsymbol{c}(t) + d(t)$$

where $B(t)$ is a $2n \times 2n$ symmetric matrix, $\boldsymbol{c}(t)$ is a $2n$-vector and $d(t)$ is a real function of t.

Since the Hamiltonian is quadratic, the corresponding system of Hamilton equations is linear. Therefore, the solution to the classical equations of motion has the form:

$$\boldsymbol{u}(t, t_0) = \Sigma(t, t_0)\boldsymbol{u}_0 + \boldsymbol{a}(t, t_0) \tag{3.1}$$

where $\Sigma(t, t_0)$ is a $2n \times 2n$ matrix and $\boldsymbol{u}_0$ is given by the initial condition $\boldsymbol{u}(t_0, t_0) = \boldsymbol{u}_0$. Therefore, $\Sigma(t_0, t_0) = I$ and $\boldsymbol{a}(t_0, t_0) = 0$. The functions Σ and $\boldsymbol{a}$ obey the following pair of differential equations:

$$\dot{\Sigma}(t, t_0) = JB(t)\Sigma(t, t_0) \tag{3.2a}$$

$$\dot{\boldsymbol{a}}(t, t_0) = JB(t)\boldsymbol{a}(t, t_0) + J\boldsymbol{c}(t) \tag{3.2b}$$

subject to the given initial conditions (the dot means $\partial/\partial t$). They can be written as

$$\Sigma(t, t_0) = \exp\left(\int_{t_0}^{t} JB(\tau)\,\mathrm{d}\tau\right)$$

$$\boldsymbol{a}(t, t_0) = \int_{t_0}^{t} \Sigma(t, \tau)Jc(\tau)\,\mathrm{d}\tau.$$

A symplectic matrix is a $2n \times 2n$ matrix S for which ${}^{\mathrm{t}}SJS = J$. One can easily check that $\Sigma(t, t_0)$ is symplectic for all t. If we transpose (3.2a), omitting the dependence on time for simplicity, we have

$${}^{\mathrm{t}}\dot{\Sigma} = {}^{\mathrm{t}}\Sigma\,{}^{\mathrm{t}}B\,{}^{\mathrm{t}}J = -{}^{\mathrm{t}}\Sigma BJ.$$

We then obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}({}^{\mathrm{t}}\Sigma J\Sigma) = 0$$

that is, ${}^{\mathrm{t}}\Sigma J\Sigma = K$, where K is a constant $2n \times 2n$ matrix. Since $\Sigma(t_0, t_0) = I$, we have $K = J$ and hence $\Sigma(t, t_0)$ is symplectic.

We define the 'Moyal bracket' $\{\cdot, \cdot\}_M$ as

$$\{f, g\}_M := -\tfrac{1}{2}\mathrm{i}(f \times g - g \times f).$$

The quantum evolution law (2.12) may be written in differential form as a Heisenberg-Liouville equation:

$$\partial\boldsymbol{u}(t, t_0)/\partial t = \{\boldsymbol{u}(t, t_0), H\}_M.$$

On the other hand, classical Hamiltonian mechanics gives

$$\partial\boldsymbol{u}(t, t_0)/\partial t = \{\boldsymbol{u}(t, t_0), H\}_P$$

where $\{\cdot, \cdot\}_P$ denotes the Poisson bracket.

Let $\hat{\partial}f/\partial q_j := \partial f/\partial p_j$, $\hat{\partial}f/\partial p_j := -\partial f/\partial q_j$. Then, if f or g is a polynomial, we have

$$f \times g = \sum_{r \in N^{2n}} \frac{\mathrm{i}^{r_1+\ldots+r_{2n}}}{r_1!\ldots r_{2n}!} \frac{\partial^{r_1+\ldots+r_{2n}}f}{\partial^{r_1}u_1\ldots\partial^{r_{2n}}u_{2n}} \frac{\hat{\partial}^{r_1+\ldots+r_{2n}}g}{\partial^{r_1}u_1\ldots\partial^{r_{2n}}u_{2n}}$$

by integration by parts; moreover, this formula holds as an asymptotic series in more general cases [8]. In particular, for H quadratic, we get

$$\begin{aligned} H \times f &= Hf + \mathrm{i}\{H, f\}_P - \frac{1}{2}\sum_{i,j=1}^{2n} B_{ij}\frac{\hat{\partial}^2 f}{\partial u_i \partial u_j} \\ f \times H &= Hf - \mathrm{i}\{H, f\}_P - \frac{1}{2}\sum_{i,j=1}^{2n} B_{ij}\frac{\hat{\partial}^2 f}{\partial u_i \partial u_j}. \end{aligned} \tag{3.3}$$

It is clear that $\{H, f\}_P = \{H, f\}_M$ for any f if and only if H is a polynomial at most quadratic in the phase-space coordinates; this was first pointed out by Uhlhorn [9], and forms the starting point for the deformation theory of Bayen *et al* [10]. Note that this corresponds to linear classical dynamics. That property sets apart this particular class of Hamiltonians, as it makes feasible a fully explicit solution of the corresponding quantum problem in phase space. In fact, it can be argued that Moyal's is the proper setting for quantum mechanics of quadratic Hamiltonians, as it allows one to bring in the full power of canonical symmetry. The latter is hidden in the conventional formalism, making the solution of the Schrödinger equation for quadratic Hamiltonians a painful business in general.

There is another property that singles out quadratic Hamiltonians in $\boldsymbol{R}^{2n}$: if we call 'canonoid' any coordinate transformation in phase space that preserves the form of Hamilton's equations corresponding to a given fixed Hamiltonian, then the following holds: a transformation of $\boldsymbol{R}^{2n}$ is canonical if and only if it is canonoid for all quadratic Hamiltonians [11]. This result has been recently extended to Banach symplectic spaces [12].

It is an open problem to see whether the link between the canonoid–canonical relationship and the equality of Moyal and Poisson brackets generalises to other phase spaces (homogeneous symplectic manifolds) quantised *à la* Moyal (see, for instance [13]).

The components of $\boldsymbol{u}$ in (3.1) must change with time according to the law of evolution of the observables:

$$\boldsymbol{u}(t, t_0) = \Xi_H^*(t, t_0) \times \boldsymbol{u}_0 \times \Xi_H(t, t_0)$$

or

$$\Xi_H(t, t_0) \times \boldsymbol{u}(t, t_0) = \boldsymbol{u}_0 \times \Xi_H(t, t_0).$$

Here the propagators $\Xi_H(t, t_0)$ still obey equation (2.11), with $\Xi_H(t_0, t_0) = 1$.

From (3.1) we obtain

$$\begin{aligned}(\Xi_H \times \boldsymbol{u})(t, t_0) &= \left(\boldsymbol{u} - \mathrm{i}J\frac{\partial}{\partial \boldsymbol{u}}\right)\Xi_H(t, t_0) \\ &= \left(\Sigma^{-1}(t, t_0)\boldsymbol{u} + \mathrm{i}\Sigma^{-1}(t, t_0)J\frac{\partial}{\partial \boldsymbol{u}} - \Sigma^{-1}(t, t_0)\boldsymbol{a}(t, t_0)\right)\Xi_H(t, t_0) \qquad (3.4)\end{aligned}$$

where $\partial/\partial\boldsymbol{u}$ denotes the gradient with respect to $\boldsymbol{u}$.

Formula (3.4) can be written as

$$(\Sigma^{-1} + I)J\frac{\partial \Xi_H}{\partial \boldsymbol{u}} = -\mathrm{i}[(I - \Sigma^{-1})\boldsymbol{u} + \Sigma^{-1}\boldsymbol{a}]\Xi_H.$$

If we multiply by Σ, this yields

$$(I + \Sigma)J\partial\Xi_H/\partial\boldsymbol{u} = -\mathrm{i}[(\Sigma - I)\boldsymbol{u} + \boldsymbol{a}]\Xi_H.$$

Now, assuming that $(\Sigma + I)$ is non-singular (non-exceptional case), we have

$$\partial\Xi_H/\partial\boldsymbol{u} = \mathrm{i}[J(\Sigma + I)^{-1}(\Sigma - I)\boldsymbol{u} + J(\Sigma + I)^{-1}\boldsymbol{a}]\Xi_H.$$

This is a system of partial differential equations having the solution

$$\Xi_H = F(t, t_0)\exp[\tfrac{1}{2}\mathrm{i}({}^{\mathrm{t}}\boldsymbol{u}G\boldsymbol{u} + {}^{\mathrm{t}}\boldsymbol{u}k)] \qquad (3.5)$$

with

$$G = J(\Sigma + I)^{-1}(\Sigma - I) = J - 2J(\Sigma + I)^{-1} \qquad (3.6a)$$

$$\boldsymbol{k} = 2J(\Sigma + I)^{-1}\boldsymbol{a} = (J - G)\boldsymbol{a}. \qquad (3.6b)$$

The matrix G is symmetric. To prove it, we introduce $\Sigma^{\#} := (\Sigma - I)(\Sigma + I)^{-1}$ which is the 'Cayley transform' of Σ and note that $G = J\Sigma^{\#}$. Then

$$\begin{aligned}{}^{\mathrm{t}}G &= -{}^{\mathrm{t}}\Sigma^{\#}J = (I + {}^{\mathrm{t}}\Sigma)^{-1}(I - {}^{\mathrm{t}}\Sigma)J = (I + J\Sigma^{-1}J^{-1})^{-1}(I - J\Sigma^{-1}J^{-1})J \\ &= J(I + \Sigma^{-1})^{-1}(I - \Sigma^{-1}) = J(\Sigma + I)^{-1}(\Sigma - I) = J\Sigma^{\#} = G.\end{aligned}$$

In order to obtain $F(t, t_0)$ in (3.5), we need to use the Schrödinger equation (2.11). After some calculation, one obtains

$$F(t, t_0) = \left[\det\left(\frac{I+\Sigma(t, t_0)}{2}\right)\right]^{-1/2} \exp[\mathrm{i}\beta(t, t_0)/2] \tag{3.7}$$

provided that the determinant does not vanish. The exponential term is given by

$$\beta(t, t_0) = \int_{t_0}^{t} [\tfrac{1}{2}{}^{t}\boldsymbol{c}(\tau)J\boldsymbol{k}(\tau, t_0) + \tfrac{1}{8}{}^{t}\boldsymbol{k}(\tau, t_0)JB(\tau)J\boldsymbol{k}(\tau, t_0) - d(\tau)]\, \mathrm{d}\tau. \tag{3.8}$$

Note that β vanishes when H is homogeneous of degree 2. Formulae equivalent to (3.5)–(3.8) appeared already in [14]. We have rederived them for the benefit of the reader.

From now on, we shall suppose that B, $\boldsymbol{c}$ and d do not depend on time, so as to obtain fully explicit results. Under this assumption, equations (3.2) are easily solved and their solutions are

$$\Sigma(t) := \Sigma(t, 0) = \Sigma(t+t_0, t_0) = \mathrm{e}^{JBt} \tag{3.9a}$$

$$\boldsymbol{a}(t) := \boldsymbol{a}(t, 0) = \boldsymbol{a}(t+t_0, t_0) = (JB)^{-1}[\exp(JBt) - I]J\boldsymbol{c} = (\Sigma(t) - I)B^{-1}\boldsymbol{c}. \tag{3.9b}$$

Equation (3.9b) makes sense only if $\det B \neq 0$. On the other hand, if $\det B = 0$, we have

$$\boldsymbol{a}(t) = \left[t + JB\frac{t^2}{2} + \ldots + (JB)^{n-1}\frac{t^n}{n!} + \ldots\right]J\boldsymbol{c}$$

that we shall take as the meaning of (3.9b) by convention.

We next study the exceptional case. Let T be the Jordan canonical form of JB. Then, there exists a non-singular matrix S such that $T = S^{-1}JBS$. Hence

$$\mathrm{e}^{JBt} + I = S\,\mathrm{e}^{Tt}S^{-1} + SS^{-1} = S(\mathrm{e}^{Tt} + I)S^{-1}.$$

Thus $\det(\Sigma + I) = \det(\mathrm{e}^{Tt} + I)$. Therefore, if T has the eigenvalues $\lambda_1, \ldots, \lambda_{2n}$ we have

$$\det(\Sigma + I) = (\mathrm{e}^{\lambda_1 t} + 1)\ldots(\mathrm{e}^{\lambda_{2n} t} + 1). \tag{3.10}$$

Thus, $\det(\Sigma + I) = 0$ iff some factor $(\mathrm{e}^{\lambda_k t} + 1)$ vanishes. In that case, $\lambda_k t = (2n+1)\pi\mathrm{i}$ or

$$t = \frac{(2n+1)\pi\mathrm{i}}{\lambda_k}.$$

Since t must be real, λ_k is thus purely imaginary. In such a case, the singularities of the Moyal propagator will be equally spaced in time. This situation really occurs, as we shall see.

We present now a crucial result for the study of quadratic Hamiltonians: covariance of the Moyal propagators under linear canonical transformations.

Theorem 1. Let $H = \frac{1}{2}{}^{t}\boldsymbol{u} + {}^{t}\boldsymbol{u}\boldsymbol{c} + d$ be a time-independent quadratic Hamiltonian and let S be a real $2n \times 2n$ symplectic matrix. If we define a new Hamiltonian by $H' = \frac{1}{2}{}^{t}\boldsymbol{u}B'\boldsymbol{u} + {}^{t}\boldsymbol{u}\boldsymbol{c}' + d$ with $B' = {}^{t}SBS$, $\boldsymbol{c}' = {}^{t}S\boldsymbol{c}$, then

$$\Xi_{H'}(\boldsymbol{u}, t) = \Xi_H(S\boldsymbol{u}, t). \tag{3.11}$$

Proof. According to (3.5) and (3.7)

$$\Xi_{H'}(\boldsymbol{u}, t) = \left[\det\left(\frac{I+\Sigma'(t)}{2}\right)\right]^{-1/2} \exp[\mathrm{i}\beta'(t)/2] \exp[\tfrac{1}{2}\mathrm{i}({}^{\mathrm{t}}\boldsymbol{u}G'\boldsymbol{u} + {}^{\mathrm{t}}\boldsymbol{u}\boldsymbol{k}')] \tag{3.12}$$

where

$$\Sigma' = \mathrm{e}^{JB't} = \mathrm{e}^{J{}^{\mathrm{t}}SBSt} = \mathrm{e}^{S^{-1}JBtS} = S^{-1}\,\mathrm{e}^{JBt}S = S^{-1}\Sigma S. \tag{3.13}$$

Therefore

$$\det\left(\frac{I+\Sigma'}{2}\right) = \det\left[S^{-1}\left(\frac{I+\Sigma}{2}\right)S\right] = \det\left(\frac{I+\Sigma}{2}\right)$$

and

$$G' = J(\Sigma'+I)^{-1}(\Sigma'-I) = J(S^{-1}\Sigma S+I)^{-1}(S^{-1}\Sigma S-I)$$
$$= JS^{-1}(\Sigma+I)^{-1}(\Sigma-I)S = {}^{\mathrm{t}}SGS.$$

Thus

$${}^{\mathrm{t}}\boldsymbol{u}G'\boldsymbol{u} = {}^{\mathrm{t}}\boldsymbol{u}{}^{\mathrm{t}}SGS\boldsymbol{u} = {}^{\mathrm{t}}(S\boldsymbol{u})G(S\boldsymbol{u}) \tag{3.14}$$

$$\boldsymbol{k}' = (J-G')\boldsymbol{a}'$$
$$\boldsymbol{a}' = (JB')^{-1}[\exp(JB't)-I]\boldsymbol{c}' = (J{}^{\mathrm{t}}SBS)^{-1}[S^{-1}\Sigma S - I]J{}^{\mathrm{t}}S\boldsymbol{c}$$
$$= S^{-1}(JB)^{-1}(\Sigma - I)J\boldsymbol{c} = S^{-1}\boldsymbol{a}$$

and so

$$\boldsymbol{k}' = (J - {}^{\mathrm{t}}SGS)S^{-1}\boldsymbol{a} = ({}^{\mathrm{t}}SJS - {}^{\mathrm{t}}SGS)S^{-1}\boldsymbol{a} = {}^{\mathrm{t}}S\boldsymbol{k}.$$

Hence

$${}^{\mathrm{t}}\boldsymbol{u}\boldsymbol{k}' = {}^{\mathrm{t}}\boldsymbol{u}{}^{\mathrm{t}}S\boldsymbol{k} = {}^{\mathrm{t}}(S\boldsymbol{u})\boldsymbol{k}. \tag{3.15}$$

To complete the proof, it remains to check that $\beta'(t) = \beta(t)$. This follows from

$${}^{\mathrm{t}}\boldsymbol{c}'J\boldsymbol{k}' = {}^{\mathrm{t}}\boldsymbol{c}SJ{}^{\mathrm{t}}S\boldsymbol{k} = {}^{\mathrm{t}}\boldsymbol{c}J\boldsymbol{k}$$
$${}^{\mathrm{t}}\boldsymbol{k}'JB'J\boldsymbol{k}' = {}^{\mathrm{t}}\boldsymbol{k}SJ{}^{\mathrm{t}}SBSJ{}^{\mathrm{t}}S\boldsymbol{k} = {}^{\mathrm{t}}\boldsymbol{k}JBJ\boldsymbol{k}.$$

Together with (3.13)-(3.15), this proves (3.11).

Corollary. H and H' have the same spectrum.

Proof. Note that equation (2.10) implies that

$$\Gamma_{H'}(\boldsymbol{u}, E) = \Gamma_H(S\boldsymbol{u}, E)$$

and that the support on E of this function represents the spectrum of the corresponding Hamiltonian. Note also that the transformation $H \mapsto H'$ is equivalent to the coordinate change $\boldsymbol{u}' = S\boldsymbol{u}$.

Theorem 2. Let $H=\frac{1}{2}{}^{t}\boldsymbol{u}B\boldsymbol{u}+{}^{t}\boldsymbol{u}\boldsymbol{c}+d$ be a time-independent quadratic Hamiltonian and $\boldsymbol{u}_0=(\boldsymbol{q}_0,\boldsymbol{p}_0)$ a $2n$-vector. If we define a new Hamiltonian by $H':=\frac{1}{2}{}^{t}\boldsymbol{u}B\boldsymbol{u}+{}^{t}\boldsymbol{u}\boldsymbol{c}'+d'$ with $\boldsymbol{c}'=B\boldsymbol{u}_0+\boldsymbol{c}$ and $d'=\frac{1}{2}{}^{t}\boldsymbol{u}_0B\boldsymbol{u}_0+{}^{t}\boldsymbol{u}_0\boldsymbol{c}+d$, then

$$\Xi_{H'}(\boldsymbol{u},t)=\Xi_H(\boldsymbol{u}+\boldsymbol{u}_0,t).$$

Proof. $\Xi_{H'}(\boldsymbol{u},t)$ is again given by (3.12), but in the present case $B'=B$, so $\Sigma'=\Sigma$ and hence $G'=J(\Sigma')^{\#}=J\Sigma^{\#}=G$. Moreover, from (3.2*b*) and (3.6*b*) we get $\boldsymbol{a}'=\boldsymbol{a}+(\Sigma-I)\boldsymbol{u}_0$ and thus $\boldsymbol{k}'=\boldsymbol{k}+2G\boldsymbol{u}_0$. A tedious calculation now gives

$$\begin{aligned}\beta'(t)&=\int_0^t[\tfrac{1}{2}{}^{t}\boldsymbol{c}'(\tau)J\boldsymbol{k}'(\tau)+\tfrac{1}{8}{}^{t}\boldsymbol{k}'(\tau)JB(\tau)J\boldsymbol{k}'(\tau)-d']\,\mathrm{d}\tau\\&=\beta(t)+\int_0^t[{}^{t}\boldsymbol{u}_0\dot{G}(\tau)\boldsymbol{u}_0+{}^{t}\boldsymbol{u}_0\dot{\boldsymbol{k}}(\tau)]\,\mathrm{d}\tau=\beta(t)+{}^{t}\boldsymbol{u}_0G(t)\boldsymbol{u}_0+{}^{t}\boldsymbol{u}_0\boldsymbol{k}(t).\end{aligned}$$

From this $\Xi_{H'}(\boldsymbol{u},t)=\Xi_H(\boldsymbol{u}+\boldsymbol{u}_0,t)$ follows at once. As before, the spectra of H and H' coincide.

As an obvious corollary of theorems 1 and 2, if S is a real symplectic matrix and $\boldsymbol{u}_0$ a real $2n$-vector, we have

$$\Xi_{H'}(\boldsymbol{u},t)=\Xi_H(S\boldsymbol{u}+\boldsymbol{u}_0,t)\tag{3.16}$$

where H' is the quadratic Hamiltonian obtained by replacing $\boldsymbol{u}$ in $H=\frac{1}{2}{}^{t}\boldsymbol{u}B\boldsymbol{u}+{}^{t}\boldsymbol{u}\boldsymbol{c}+d$ by $S\boldsymbol{u}+\boldsymbol{u}_0$. Also, we have $\mathrm{Sp}\,H=\mathrm{Sp}\,H'$. In other words, for quadratic Hamiltonians, *the Moyal propagator is covariant and the spectrum is invariant under the group* $\mathrm{ISp}(2n,\boldsymbol{R})$ *of inhomogeneous canonical transformations.*

Equation (3.16) gives us a method to obtain the Moyal propagators for all the time-independent quadratic Hamiltonians. We may group these Hamiltonians in equivalence classes. H and H' belong to the same class if and only if we can find an inhomogeneous symplectic transformation connecting them. If we find the Moyal propagator for one representative of a class, we can find the Moyal propagators of all Hamiltonians of the class from (3.16). Once we have found simple representatives (called, in the homogeneous case, normal forms [15]) two main difficulties still arise: one is to determine which class contains a given Hamiltonian; the other is to obtain the matrix S relating this Hamiltonian with its corresponding normal form; however, we will not go into these questions here. On the other hand, we reassert, the spectra of two Hamiltonians belonging to the same class are identical.

A transformation from H into $H'=H+d$, d being a constant, shifts the spectrum $\mathrm{Sp}\,H$ into $\mathrm{Sp}\,H'=\mathrm{Sp}\,H+d=\{x\in\boldsymbol{R}\colon x=y+d,\ y\in\mathrm{Sp}\,H\}$, as one can easily deduce from (3.8) and (2.10). Here $\Xi_{H'}(\boldsymbol{u},t)=\Xi_H(\boldsymbol{u},t)\,\mathrm{e}^{-\mathrm{i}dt/2}$.

At this point, we wish to remark that, given an homogeneous Hamiltonian $H=\frac{1}{2}{}^{t}\boldsymbol{u}B\boldsymbol{u}$, there exists a class of *complex* symplectic transformations $B\mapsto B'={}^{t}SBS$, where B' is again a real symmetric matrix, so that $H'=\frac{1}{2}{}^{t}\boldsymbol{u}B'\boldsymbol{u}$ is also a Hamiltonian. Moreover, the conclusion (3.11) of theorem 1 holds under this more general class of transformations. (However, if we are looking for the class of complex symplectic transformations for which ${}^{t}SBS$ is real and symmetric for every real symmetric B, we find that either S is real or else $S=\mathrm{i}M$, where M is real. Such an M is not symplectic, since ${}^{t}MJM=-J$; but if we write

$$M=\begin{pmatrix}M_{11}&M_{12}\\M_{21}&M_{22}\end{pmatrix}\qquad\tilde{M}=\begin{pmatrix}-M_{11}&-M_{12}\\M_{21}&M_{22}\end{pmatrix}$$

where $M_{ij}\in\boldsymbol{R}^{n\times n}$ for $i,j=1,2$, then $\tilde{M}$ is symplectic.)

4. Classification of the Moyal propagators in the non-singular case

In the present section, we consider those Hamiltonians H for which $\det B \neq 0$. In that case, we can write

$$H = \tfrac{1}{2}{}^{t}(u + B^{-1}c)B(u + B^{-1}c) + d' \qquad \text{with } d' = d - \tfrac{1}{2}{}^{t}cB^{-1}c$$

so that H is equivalent to $H' = \frac{1}{2}{}^{t}uBu + d'$, and therefore the study of the quadratic Hamiltonians whose quadratic form B is non-singular can be reduced to the study of the non-singular homogeneous quadratic Hamiltonians.

Here, we intend to find the Moyal propagators of these Hamiltonians. After (3.11), we need only obtain the Moyal propagators for the normal forms, which are simple representatives of the equivalence by conjugacy classes. The normal forms have been classified and one can find an extensive study of them in the literature. The classification begins with the following result.

Proposition. (i) If B is symmetric and λ is an eigenvalue of JB, then so are $-\lambda$, $\bar{\lambda}$, $-\bar{\lambda}$ and they all have the same multiplicity. The eigenvalue 0 always appears with even multiplicity.

(ii) Let λ_i, $1 \leqslant k$, denote the eigenvalues of JB and let V_i be the corresponding generalised eigenspaces of JB, i.e.

$$(\lambda_i I - JB)^{m_i} v = 0 \qquad \text{iff } v \in V_i \qquad \text{for } m_i \text{ integer} \geqslant 1.$$

Then each V_i is invariant under JB, $\boldsymbol{R}^{2n} = \oplus_{i=1}^{k} V_i$ and

$$\det(\lambda I - JB) = \prod_{i=1}^{k} (\lambda - \lambda_i)^{d_i} \qquad \text{with } d_i = \dim V_i \geqslant m_i.$$

(iii) The invariant subspaces V_i are symplectically orthogonal:

$${}^{t}vJv' = 0 \qquad \text{if } v \in V_i,\ v' \in V_j;\ \lambda_i \neq \pm\lambda_j, \pm\bar{\lambda}_j.$$

Proof. Straightforward linear algebra. For instance, (i) follows from observing that the characteristic polynomial of JB is even.

According to (ii) and (iii), JB and therefore $\frac{1}{2}JBt$, can be reduced by blocks. This decomposition carries over to the quantum context: the propagator associated to a decomposable matrix JB is given by the ordinary product of propagators corresponding to each indecomposable block. The equality of ordinary and twisted products in this case follows immediately from the definition of twisted product.

The classification theory of normal forms for linear canonical systems was initiated by Williamson [16] and developed by many others. Here we use the classification scheme due to Koçak [17].

The possibilities for the indecomposable blocks are:

(*a*) JB has two real eigenvalues α, $-\alpha (\alpha > 0)$;

(*b*) JB has two purely imaginary eigenvalues $i\beta$, $-i\beta (\beta > 0)$;

(*c*) JB has four distinct complex eigenvalues $\pm\alpha \pm i\beta (\alpha, \beta > 0)$.

We here present a list of the indecomposable normal forms.

(a) The eigenvalues are α, $-\alpha(\alpha>0)$:

$$JB=\begin{pmatrix} M & 0 \\ 0 & -{}^{\mathrm{t}}M \end{pmatrix} \qquad \text{with} \qquad M=\begin{pmatrix} \alpha & & & \\ 1 & \alpha & & \\ & \ddots & \ddots & \\ & & 1 & \alpha \end{pmatrix} \in \boldsymbol{R}^{k\times k}. \tag{4.1}$$

(b) The eigenvalues are $\mathrm{i}\beta, -\mathrm{i}\beta$ ($\beta>0$). We have four inequivalent types:
(i)

$$\begin{gathered} JB=\begin{pmatrix} Q & 0 \\ R & -{}^{\mathrm{t}}Q \end{pmatrix} \qquad \text{with} \qquad Q=\begin{pmatrix} A & & & \\ I & A & & \\ & \ddots & \ddots & \\ & & I & A \end{pmatrix} \\ R=\begin{pmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & \\ & & & \varepsilon I \end{pmatrix} \end{gathered} \tag{4.2}$$

where Q, $R\in \boldsymbol{R}^{k\times k}$ with k even, $I=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $A=\begin{pmatrix} 0 & -\beta \\ \beta & 0 \end{pmatrix}$, and $\varepsilon=\pm 1$.

(ii)

$$\begin{gathered} JB=\begin{pmatrix} U & V \\ -V & -{}^{\mathrm{t}}U \end{pmatrix} \qquad U=\begin{pmatrix} 0 & & & \\ 1 & 0 & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{pmatrix} \\ V=\begin{pmatrix} & & & -\varepsilon\beta \\ & & \cdot^{\cdot^{\cdot}} & \\ & \varepsilon\beta & & \\ -\varepsilon\beta & & & \end{pmatrix} \end{gathered} \tag{4.3}$$

where U, $V\in \boldsymbol{R}^{k\times k}$ with k odd, $\varepsilon=\pm 1$.

(c) The eigenvalues are $\pm\alpha\pm\mathrm{i}\beta(\alpha,\beta>0)$:

$$JB=\begin{pmatrix} K & 0 \\ 0 & -{}^{\mathrm{t}}K \end{pmatrix} \qquad \text{with} \qquad K=\begin{pmatrix} C & & & \\ I & C & & \\ & \ddots & \ddots & \\ & & I & C \end{pmatrix} \in \boldsymbol{R}^{2k\times 2k} \tag{4.4}$$

where $I=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $C=\begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix}$.

A decomposable form is constructed simply as a direct sum of indecomposable forms, here called 'canonical blocks'. For instance, if Y and Z are two normal forms of dimensions $2m$ and $2n$ respectively, their composition could be

$$X=\begin{pmatrix} Y & 0 \\ 0 & Z \end{pmatrix}. \tag{4.5}$$

However, if we construct the Hamiltonian as $H=-\frac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}JX\boldsymbol{u}$, the coordinates are ordered as ${}^{\mathrm{t}}\boldsymbol{u}=(q_1,\ldots,q_m,p_1,\ldots,p_m,q_{m+1},\ldots,q_{m+n},p_{m+1},\ldots,p_{m+n})$.

We will maintain the convention that ${}^{t}\boldsymbol{u}=(q_1,\ldots,q_{m+n},p_1,\ldots,p_{m+n})$, so that the direct sum (4.5) must be rewritten

$$X=\begin{pmatrix} Y_1 & 0 & Y_2 & 0\\ 0 & Z_1 & 0 & Z_2\\ Y_3 & 0 & Y_4 & 0\\ 0 & Z_3 & 0 & Z_4\end{pmatrix}$$

where $Y_j\in \boldsymbol{R}^{m\times m}$, $Z_j\in\boldsymbol{R}^{n\times n}$ $(j=1,2,3,4)$.

In general, if we call X the composition of s canonical blocks of the form $Y_k=\begin{pmatrix} Y_{k1} & Y_{k2}\\ Y_{k3} & Y_{k4}\end{pmatrix}$, $k=1,\ldots,s$, then $X=\begin{pmatrix} X_1 & X_2\\ X_3 & X_4\end{pmatrix}$, where each X_j is a block diagonal direct sum of the Y_{kj}. Note, in particular, that this convention preserves the form of $J=\begin{pmatrix} 0 & I_n\\ -I_n & 0\end{pmatrix}$ under direct sums.

Now we proceed to the effective calculation of the Moyal propagators. Since the Hamiltonians considered in this section are homogeneous, we have to obtain G and $\det((\Sigma+I)/2)$ only. Formula (3.6a) yields

$$G=J\frac{\Sigma-I}{\Sigma+I}=J\frac{\mathrm{e}^{JBt}-I}{\mathrm{e}^{JBt}+I}=J\frac{\mathrm{e}^{JBt/2}-\mathrm{e}^{-JBt/2}}{\mathrm{e}^{JBt/2}+\mathrm{e}^{-JBt/2}}=J\tanh\frac{JBt}{2}.$$

If JB is a canonical form, we can write $JB=L+N$ where N is nilpotent and L can be one of the following forms:

(i) diagonal as in (4.1);

(ii) block diagonal as in (4.2) and (4.4); here the blocks are equal to A and C respectively;

(iii) antidiagonal as in (4.3).

The function $\tanh z$ is analytic except when $\operatorname{Im} z=(2n+1)\frac{1}{2}\pi$. Because $N^k=0$, we have the matrix-valued series expansion:

$$\tanh\frac{JBt}{2}=\tanh\frac{Lt}{2}+\sum_{n=1}^{k-1}\frac{1}{n!}\left(\frac{Nt}{2}\right)^n\frac{\mathrm{d}^n}{\mathrm{d}z^n}\bigg|_{z=Lt/2}(\tanh z). \tag{4.6}$$

To elucidate the right-hand side of (4.6), we examine the following three possibilities.

Case 1. L is diagonal as in (4.1). Then

$$\tanh\frac{Lt}{2}=L\left(\frac{1}{\alpha}\tanh\frac{\alpha t}{2}\right). \tag{4.7}$$

Note that $[(1/\alpha)L]^2=I$. The nth derivative is

$$\frac{\mathrm{d}^n}{\mathrm{d}z^n}\bigg|_{z=Lt/2}(\tanh z)=\begin{cases}\dfrac{1}{\alpha}L\dfrac{\mathrm{d}^n}{\mathrm{d}z^n}\bigg|_{z=\alpha t/2}(\tanh z) & \text{if } n \text{ is even}\\[2ex] I\dfrac{\mathrm{d}^n}{\mathrm{d}z^n}\bigg|_{z=\alpha t/2}(\tanh z) & \text{if } n \text{ is odd.}\end{cases}$$

If we define $g_H(\boldsymbol{u},t)$ as

$$g_H(\boldsymbol{u},t):=-{}^{t}\boldsymbol{u}G\boldsymbol{u}=-{}^{t}\boldsymbol{u}J\left(\tanh\frac{L+N}{2}\right)\boldsymbol{u}$$

we have

$$g_H(\boldsymbol{u},t)=\frac{2}{\alpha}H_1\tanh\frac{\alpha t}{2}+H_2 t\,\mathrm{sech}^2\frac{\alpha t}{2}+\ldots+\frac{H_k t^{k-1}}{2^{k-2}(k-1)!}\frac{\mathrm{d}^{k-1}}{\mathrm{d}z^{k-1}}\bigg|_{z=\alpha t/2}(\tanh z).$$

Here

$$H_1:=-\tfrac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}JL\boldsymbol{u}\qquad H_2:=-\tfrac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}JN\boldsymbol{u}\qquad \text{and if } n=2,\ldots,k-1$$
$$H_{n+1}:=-\tfrac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}JN^nP^{n+1}\boldsymbol{u}\qquad \text{where } P^n=\begin{cases}(1/\alpha)\,L & \text{if } n \text{ is odd}\\ I & \text{if } n \text{ is even.}\end{cases}\tag{4.8}$$

Obviously, $H=H_1+H_2$.

Case 2. L is block diagonal as in (4.2) and (4.4). If JB is given by (4.2), then

$$\tanh\frac{JBt}{2}=L\frac{1}{\beta}\tan(\tfrac{1}{2}\beta t)+\sum_{n=1}^{k-1}\frac{1}{n!}\left(\frac{t}{2}\right)^n N^nP^{n+1}\frac{\mathrm{d}^n}{\mathrm{d}z^n}\bigg|_{z=\beta t/2}(\tan z)\tag{4.9}$$

where $P^n=(-1)^{(n-1)/2}(1/\beta)L$ if n is odd, and $P^n=(-1)^{(n+2)/2}I$ if n is even.

To derive this formula, we recall that $A=\begin{pmatrix}0 & -\beta\\ \beta & 0\end{pmatrix}$ and note that

$$\tanh\begin{pmatrix}0 & -\frac{1}{2}\beta t\\ \frac{1}{2}\beta t & 0\end{pmatrix}=\tfrac{1}{2}\begin{pmatrix}-1 & -\mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}\tanh\begin{pmatrix}\frac{1}{2}\mathrm{i}\beta t & 0\\ 0 & -\frac{1}{2}\mathrm{i}\beta t\end{pmatrix}\begin{pmatrix}-1 & -\mathrm{i}\\ \mathrm{i} & 1\end{pmatrix}$$
$$=A\frac{1}{\beta}\tanh(\tfrac{1}{2}\beta t)$$

and so

$$\tanh\frac{Lt}{2}=L\frac{1}{\beta}\tan(\tfrac{1}{2}\beta t).\tag{4.10a}$$

If, for simplicity, we write $T=(1/\beta)L$, we easily obtain that $T^2=-I$; $T^3=-T$; $T^4=I$. It is also clear that (4.10a) can be written as

$$\tanh(\tfrac{1}{2}\beta tT)=T\tan(\tfrac{1}{2}\beta t)\tag{4.11}$$

and (4.11) implies that

$$\frac{\mathrm{d}^n}{\mathrm{d}z^n}\bigg|_{z=(\beta t/2)T}(\tanh z)=T^{-n+1}\frac{\mathrm{d}^n}{\mathrm{d}z^n}\bigg|_{z=\beta t/2}(\tan z)\tag{4.12}$$

Hence (4.9) follows. Also

$$g_H(\boldsymbol{u},t)=\frac{2}{\beta}H_1\tan\frac{\beta t}{2}+\sum_{n=1}^{k-1}\frac{1}{n!}\frac{t^n}{2^{n-1}}H_{n+1}\frac{\mathrm{d}^n}{dz^n}\bigg|_{z=\beta t/2}(\tan z)\tag{4.13}$$

where $H_1,\ldots,H_k$ are defined here as in (4.8). Note that $H=H_1+H_2$ again.

If JB is given by (4.4), then

$$L=\alpha\begin{pmatrix}I & 0\\ 0 & -I\end{pmatrix}+\beta\begin{pmatrix}T & 0\\ 0 & T\end{pmatrix}$$

where T is a direct sum of $2k$ blocks of the form $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. After some calculation, we obtain that

$$\left.\frac{\mathrm{d}^n}{\mathrm{d}z^n}\right|_{z=Lt/2} (\tanh z) = \begin{pmatrix} f_{1,n}I + g_{1,n}T & 0 \\ 0 & f_{2,n}I + g_{2,n}T \end{pmatrix}$$

where

$$f_{1,n} = \frac{\partial^n}{\partial y \partial^{n-1} x}\left(\frac{\sin 2y}{\cosh 2x + \cos 2y}\right)\Bigg|_{\substack{x=\alpha t/2 \\ y=\beta t/2}}$$

$$g_{1,n} = \frac{\partial^n}{\partial x^n}\left(\frac{\sin 2y}{\cosh 2x + \cos 2y}\right)\Bigg|_{\substack{x=\alpha t/2 \\ y=\beta t/2}}$$

$$f_{2,n} = \frac{\partial^n}{\partial y \partial^{n-1} x}\left(\frac{\sin 2y}{\cosh 2x + \cos 2y}\right)\Bigg|_{\substack{x=-\alpha t/2 \\ y=\beta t/2}}$$

$$g_{2,n} = \frac{\partial^n}{\partial x^n}\left(\frac{\sin 2y}{\cosh 2x + \cos 2y}\right)\Bigg|_{\substack{x=-\alpha t/2 \\ y=\beta t/2}}.$$

If W now denotes

$$W = \begin{pmatrix} 0 & & & \\ I & 0 & & \\ & \ddots & \ddots & \\ & & I & 0 \end{pmatrix} \qquad \text{where } I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

we have

$$\tanh\frac{JBt}{2} = \sum_{n=0}^{k-1} \frac{1}{n!}\left(\frac{t}{2}\right)^n \begin{pmatrix} f_{1,n}W^n + g_{1,n}W^nT & 0 \\ 0 & (-1)^n f_{2,n}{}^{\mathrm{t}}W^n + (-1)^n g_{2,n}{}^{\mathrm{t}}W^nT \end{pmatrix}. \tag{4.14}$$

From this, $g_H(\boldsymbol{u}, t)$ may be computed explicitly, but we shall omit the (rather complicated) general formula. The lower-multiplicity cases are exhibited in table 1.

Case 3. L is of antidiagonal form as in (4.3).

In this case, formulae (4.9) and (4.13) are reproduced. The proof is as follows: $\tanh z$ is an odd function and consequently only the odd powers of z will appear in its Taylor expansion on a neighbourhood of zero. If we define K as $(1/\varepsilon\beta)L$, then

$$K = \begin{pmatrix} 0 & \cdots & 0 & J \\ 0 & \cdots & J & 0 \\ \vdots & \ddots & \vdots & \vdots \\ J & \cdots & 0 & 0 \end{pmatrix} \qquad \text{with } J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

and we have $K^2 = -I$, $K^3 = -K$, $K^4 = I$, and

$$\tanh\frac{Lt}{2} = \tanh\frac{\varepsilon\beta t}{2}K = \varepsilon K \tan\frac{\beta t}{2} = \frac{L}{\beta}\tan\frac{\beta t}{2}. \tag{3.10b}$$

From (4.10b) a straightforward calculation gives (4.12), with T replaced by K, and hence we have proved the validity of (4.9) and (4.13) in the present case.

From the preceding formulae, one can now write down the desired Moyal propagators.

Expression (4.13) becomes singular at $t=(2m+1)\pi/\beta$, m an integer, as expected. However, $\Xi_H(\boldsymbol{u}, (2m+1)\pi/\beta)$ is a well defined distribution, a multiple of Dirac's δ in fact, and the map $t \mapsto \Xi_H(\boldsymbol{u}, t)$ is everywhere continuous in the appropriate topologies (see appendix 1).

For the decomposable Hamiltonians, the matrix $\tanh(JBt/2)$ is obtained as a direct sum of the expressions for the corresponding indecomposable summands of JB. To obtain $\det((\Sigma+I)/2)$, we have to find the eigenvalues of JB and then apply (3.10). The set of eigenvalues of JB is the union of all the eigenvalues of each canonical block Y_k, since JB may be written as a direct sum of these blocks by permuting the q and p coordinates. The details are straightforward.

As remarked before, if H can be written as a sum of Hamiltonians $H=H_1(\boldsymbol{u}_1)+\ldots+H_s(\boldsymbol{u}_s)$, where $\boldsymbol{u}=(\boldsymbol{u}_1,\ldots,\boldsymbol{u}_s)$ and the several $\boldsymbol{u}_i$ lie in symplectically orthogonal subspaces, then

$$\Xi_H(\boldsymbol{u}, t)=\prod_{1\leqslant i\leqslant s}\Xi_{H_i}(\boldsymbol{u}_i, t)=\prod_{1\leqslant i\leqslant s}^{\times}\Xi_{H_i}(\boldsymbol{u}_i, t). \tag{4.15}$$

This fact extends to the singular case ($\det B=0$).

We end this section with a pair of useful results.

Lemma 1. Let $H_1=\frac{1}{2}{}^t\boldsymbol{u}A\boldsymbol{u}$ and $H_2=\frac{1}{2}{}^t\boldsymbol{u}B\boldsymbol{u}$ be two homogeneous quadratic Hamiltonians of dimension $2n$, where A and B are symmetric matrices. Then $JB \mapsto H_B$ is a Lie algebra isomorphism. In particular, the classical Poisson bracket $\{H_A, H_B\}_P$ is identically zero if and only if the commutator $[JA, JB]$ vanishes.

Proof. We may write

$$\{H_A, H_B\}_P=\sum_{i=1}^{n}\left(\frac{\partial H_A}{\partial u_i}\frac{\partial H_B}{\partial u_{i+n}}-\frac{\partial H_A}{\partial u_{i+n}}\frac{\partial H_B}{\partial u_i}\right)={}^t\left(\frac{\partial H_A}{\partial \boldsymbol{u}}\right)J\left(\frac{\partial H_B}{\partial \boldsymbol{u}}\right)$$

where $\partial/\partial\boldsymbol{u}$ denotes the gradient, as before. Since $\partial H_A/\partial\boldsymbol{u}=A\boldsymbol{u}$ and $\partial H_B/\partial\boldsymbol{u}=B\boldsymbol{u}$, we have that

$$\{H_A, H_B\}_P={}^t\boldsymbol{u}AJB\boldsymbol{u}=-{}^t\boldsymbol{u}BJA\boldsymbol{u}=\tfrac{1}{2}{}^t\boldsymbol{u}(AJB-BJA)\boldsymbol{u}.$$

Assume now that the Poisson bracket is identically zero. We have equivalently that $JAJB-JBJA=0$.

Theorem 3. Let $H=\frac{1}{2}{}^t\boldsymbol{u}B\boldsymbol{u}$ be any homogeneous time-independent quadratic Hamiltonian. Then the classical Poisson brackets $\{H, g_H(\boldsymbol{u}, t)\}_P$ and $\{H, \Xi_H(\boldsymbol{u}, t)\}_P$ are always zero.

Proof. In the expansion (4.6), all the terms commute since $[L, N]=0$. It follows that $\{H_m, H_n\}_P=0$ in all cases, and hence $\{H, g_H(\boldsymbol{u}, t)\}_P=0$. (We leave the details to the reader.)

We remark that theorem 3 is formally a corollary of the result [18]: $\{H, H^{\times n}\}_P=0$.

We summarise the results up to now in table 1, which includes all non-singular homogeneous indecomposable types up to dimension $n=5$. In table 1, $\alpha>0$, $\beta>0$ and $\varepsilon=\pm 1$.

Table 1. Non-singular homogeneous Hamiltonians.

Indecomposable Hamiltonians with $\det B \neq 0$.

$n=1$ (case a): $H=\alpha q p$; $\Xi_H(\boldsymbol{u},t)=\operatorname{sech}\left(\frac{\alpha t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\alpha}H\tanh\frac{\alpha t}{2}\right)$.

$n=1$ (case b): $H=\frac{1}{2}\varepsilon\beta(q^2+p^2)$; $\Xi_H(\boldsymbol{u},t)=\sec\left(\frac{\beta t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\beta}H\tan\frac{\beta t}{2}\right)$.

$n=2$ (case a): $H=H_1+H_2$; $H_1=\alpha(q_1p_1+q_2p_2)$, $H_2=q_1p_2$;

$$\Xi_H(\boldsymbol{u},t)=\operatorname{sech}^2\left(\frac{\alpha t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\alpha}H_1\tanh\frac{\alpha t}{2}-\frac{\mathrm{i}t}{2}H_2\operatorname{sech}^2\frac{\alpha t}{2}\right).$$

$n=2$ (case b): $H=H_1+H_2$; $H_1=\beta(q_1p_2-q_2p_1)$, $H_2=\frac{1}{2}\varepsilon(q_1^2+q_2^2)$;

$$\Xi_H(\boldsymbol{u},t)=\sec^2\left(\frac{\beta t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\beta}H_1\tan\frac{\alpha t}{2}-\frac{\mathrm{i}t}{2}H_2\sec^2\frac{\beta t}{2}\right).$$

$n=2$ (case c): $H=H_1+H_2$; $H_1=\alpha(q_1p_1+q_2p_2)$, $H_2=\beta(q_1p_2-q_2p_1)$;

$$\Xi_H(\boldsymbol{u},t)=\frac{2}{\cosh\alpha t+\cos\beta t}\exp\left(-\frac{\mathrm{i}}{\alpha}H_1\frac{\sinh\alpha t}{\cosh\alpha t+\cos\beta t}-\frac{i}{\beta}H_2\frac{\sin\beta t}{\cosh\alpha t+\cos\beta t}\right).$$

$n=3$ (case a): $H=H_1+H_2$; $H_1=\alpha(q_1p_1+q_2p_2+q_3p_3)$, $H_2=q_1p_2+q_2p_3$;

$H_3=q_1p_3$;

$$\Xi_H(\boldsymbol{u},t)=\operatorname{sech}^3\left(\frac{\alpha t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\alpha}H_1\tanh\frac{\alpha t}{2}-\frac{\mathrm{i}t}{2}H_2\operatorname{sech}^2\frac{\alpha t}{2}+\frac{\mathrm{i}t^2}{4}H_3\tanh\frac{\alpha t}{2}\operatorname{sech}^2\frac{\alpha t}{2}\right).$$

$n=3$ (case b): $H=H_1+H_2$; $H_1=\varepsilon\beta(\frac{1}{2}q_2^2-q_1q_3+\frac{1}{2}p_2^2-p_1p_3)$, $H_2=q_1p_2+q_2p_3$;

$H_3=-\frac{1}{2}\varepsilon(q_1^2+p_3^2)$;

$$\Xi_H(\boldsymbol{u},t)=\sec^3\left(\frac{\beta t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\beta}H_1\tan\frac{\beta t}{2}-\frac{\mathrm{i}t}{2}H_2\sec^2\frac{\beta t}{2}+\frac{\mathrm{i}t^2}{4}H_3\tan\frac{\beta t}{2}\sec^2\frac{\beta t}{2}\right).$$

$n=4$ (case a): $H=H_1+H_2$; $H_1=\alpha(q_1p_1+q_2p_2+q_3p_3+q_4p_4)$,

$H_2=q_1p_2+q_2p_3+q_3p_4$, $H_3=q_1p_3+q_2p_4$, $H_4=q_1p_4$;

$$\Xi_H(\boldsymbol{u},t)=\operatorname{sech}^4\left(\frac{\alpha t}{2}\right)\exp\left[-\frac{\mathrm{i}}{\alpha}H_1\tanh\frac{\alpha t}{2}-\frac{\mathrm{i}t}{2}H_2\operatorname{sech}^2\frac{\alpha t}{2}\right.$$
$$\left.+\frac{\mathrm{i}t^2}{4}H_3\tanh\frac{\alpha t}{2}\operatorname{sech}^2\frac{\alpha t}{2}+\frac{\mathrm{i}t^3}{24}H_4\left(1-4\tanh^2\frac{\alpha t}{2}+3\tanh^4\frac{\alpha t}{2}\right)\right].$$

$n=4$ (case b): $H=H_1+H_2$; $H_1=\beta(q_1p_2-q_2p_1+q_3p_4-q_4p_3)$,

$H_2=q_1p_3+q_2p_4-\frac{1}{2}\varepsilon(q_3^2+q_4^2)$, $H_3=-\varepsilon(q_1q_4-q_2q_3)$, $H_4=\frac{1}{2}\varepsilon(q_1^2+q_2^2)$;

$$\Xi_H(\boldsymbol{u},t)=\sec^4\left(\frac{\beta t}{2}\right)\exp\left[-\frac{\mathrm{i}}{\beta}H_1\tan\frac{\beta t}{2}-\frac{\mathrm{i}t}{2}H_2\sec^2\frac{\beta t}{2}\right.$$
$$\left.+\frac{\mathrm{i}t^2}{4}H_3\tan\frac{\beta t}{2}\sec^2\frac{\beta t}{2}+\frac{\mathrm{i}t^3}{24}H_4\left(1+4\tan^2\frac{\beta t}{2}+3\tan^4\frac{\beta t}{2}\right)\right].$$

Table 1. (continued)

$n=4$ (case c): $H = H_1+H_2+H_3$; $H_1=\alpha(q_1p_1+q_2p_2+q_3p_3+q_4p_4)$,

$H_2=\beta(q_1p_2-q_2p_1+q_3p_4-q_4p_3)$, $H_3=q_1p_3+q_2p_4$, $H_4=q_2p_3-q_1p_4$;

$$\Xi_H(u,t)=\frac{4}{(\cosh\alpha t+\cos\beta t)^2}\exp\left[-\frac{\mathrm{i}}{\alpha}H_1\frac{\sinh\alpha t}{\cosh\alpha t+\cos\beta t}-\frac{\mathrm{i}}{\beta}H_2\frac{\sin\beta t}{\cosh\alpha t+\cos\beta t}\right.$$
$$\left.-\mathrm{i}tH_3\frac{1+\cosh\alpha t\cos\beta t}{(\cosh\alpha t+\cos\beta t)^2}-\mathrm{i}tH_4\frac{\sinh\alpha t\sin\beta t}{(\cosh\alpha t+\cos\beta t)^2}\right].$$

$n=5$ (case a): $H=H_1+H_2$; $H_1=\alpha(q_1p_1+q_2p_2+q_3p_3+q_4p_4+q_5p_5)$,

$H_2=q_1p_2+q_2p_3+q_3p_4+q_4p_5$, $H_3=q_1p_3+q_2p_4+q_3p_5$,

$H_4=q_1p_4+q_2p_5$, $H_5=q_1p_5$;

$$\Xi_H(u,t)=\operatorname{sech}^5\left(\frac{\alpha t}{2}\right)\exp\left[-\frac{\mathrm{i}}{\alpha}H_1\tanh\frac{\alpha t}{2}-\frac{\mathrm{i}t}{2}H_2\operatorname{sech}^2\frac{\alpha t}{2}\right.$$
$$+\frac{\mathrm{i}t^2}{4}H_3\tanh\frac{\alpha t}{2}\operatorname{sech}^2\left(\frac{\alpha t}{2}\right)+\frac{\mathrm{i}t^3}{24}H_4\left(1-4\tanh^2\frac{\alpha t}{2}+3\tanh^4\frac{\alpha t}{2}\right)$$
$$\left.-\frac{\mathrm{i}t^4}{48}H_5\left(2\tanh\frac{\alpha t}{2}-5\tanh^3\frac{\alpha t}{2}+3\tanh^5\frac{\alpha t}{2}\right)\right].$$

$n=5$ (case b): $H=H_1+H_2$; $H_1=-\varepsilon\beta(q_1q_5-q_2q_4+\frac{1}{2}q_3^2+p_1p_5-p_2p_4+\frac{1}{2}p_3^2)$,

$H_2=q_1p_2+q_2p_3+q_3p_4+q_4p_5$, $H_3=-\varepsilon(q_1q_3-\frac{1}{2}q_2^2+p_3p_5-\frac{1}{2}p_4^2)$,

$H_4=q_1p_4+q_2p_5$, $H_5=-\frac{1}{2}\varepsilon(q_1^2+p_5^2)$;

$$\Xi_H(u,t)=\sec^5\left(\frac{\beta t}{2}\right)\exp\left[-\frac{\mathrm{i}}{\beta}H_1\tan\frac{\beta t}{2}-\frac{\mathrm{i}t}{2}H_2\sec^2\frac{\beta t}{2}\right.$$
$$+\frac{\mathrm{i}t^2}{4}H_3\tan\frac{\beta t}{2}\sec^2\frac{\beta t}{2}+\frac{\mathrm{i}t^3}{24}H_4\left(1+4\tan^2\frac{\beta t}{2}+3\tan^4\frac{\beta t}{2}\right)$$
$$\left.-\frac{\mathrm{i}t^4}{48}H_5\left(2\tan\frac{\beta t}{2}+5\tan^3\frac{\beta t}{2}+3\tan^5\frac{\beta t}{2}\right)\right].$$

5. Classification of the Moyal propagators in the singular case

We study the homogeneous Hamiltonians first. In the homogeneous case, there are two indecomposable normal forms:

(a)

$$JB=\begin{pmatrix}U & 0\\ R & -{}^tU\end{pmatrix}\qquad U=\begin{pmatrix}0 & & & \\ 1 & 0 & & \\ & \ddots & \ddots & \\ & & 1 & 0\end{pmatrix}\qquad R=\begin{pmatrix}0 & & & \\ & \ddots & & \\ & & 0 & \\ & & & \pm1\end{pmatrix}$$

(b)

$$JB=\begin{pmatrix}U & 0\\ 0 & -{}^tU\end{pmatrix}$$

In case (a), U and R have $\frac{1}{2}(k+1)$ rows, where k is odd; in case (b), U has $k+1$ rows, where k is even.

In both cases JB is nilpotent: $(JB)^k \neq 0$, $(JB)^{k+1} = 0$. The Taylor expansion of $\tanh z$ at $z = 0$ is

$$\tanh z = \sum_{m=1}^{\infty} \frac{2^{2m}(2^{2m}-1)}{(2m)!} B_{2m} z^{2m-1}$$

where B_{2m} are the Bernoulli numbers. Therefore

$$\tanh \frac{JBt}{2} = \sum_{m=1}^{[(k+1)/2]} \frac{2^{2m}(2^{2m}-1)}{(2m)!} B_{2m} \left(\frac{JBt}{2}\right)^{2m-1}$$

where

$$\left[\frac{k+1}{2}\right] = \begin{cases} (k+1)/2 & \text{if } k \text{ odd: case } (a) \\ k/2 & \text{if } k \text{ even: case } (b). \end{cases}$$

Also

$$g_H(\boldsymbol{u};\, t) = H_1 t + \sum_{m=2}^{[(k+1)/2]} \frac{4(2^{2m}-1)t^{2m-1}}{(2m)!} B_{2m} H_{2m-1}$$

where

$$H_1 = \tfrac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}B\boldsymbol{u} \qquad H_{2m-1} = \tfrac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}\underbrace{(BJBJ\ldots JB)}_{4m-3 \text{ factors}}\boldsymbol{u}.$$

By applying formula (3.10), we obtain $\det[(\Sigma + I)/2] = 1$.

The analysis for the homogeneous decomposable case is exactly the same as when $\det B \neq 0$; in particular, (4.15) remains valid.

The study of the inhomogeneous singular Hamiltonians is more complicated. We cannot reduce the study of the Moyal propagators to the homogeneous case. We know no general method to classify these Hamiltonians into equivalence classes under coordinate changes of the type $\boldsymbol{u}' = S\boldsymbol{u} + \boldsymbol{u}_0$, S being a real symplectic matrix. Thus, we classify the Hamiltonians for each dimension and study them case by case.

In table 2, we list the singular homogeneous indecomposable types up to dimension $n = 5$. In table 3, we list representatives of the inhomogeneous singular Hamiltonians for $n = 1$ and $n = 2$. In all cases, $\alpha > 0$, $\beta > 0$ and $\varepsilon = \pm 1$.

Table 2. Singular homogeneous Hamiltonians.

Indecomposable Hamiltonians with $\det B = 0$.

$n = 1$: $H = -\frac{1}{2}\varepsilon q^2$; $\Xi_H(\boldsymbol{u}, t) = \exp(-\frac{1}{2}\mathrm{i}Ht)$.

$n = 2$: $H = q_1 p_2 - \frac{1}{2}\varepsilon q_2^2$; $\Xi_H(\boldsymbol{u}, t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht - \frac{\varepsilon}{3}\left(\frac{t}{2}\right)^3 q_1^2\right)\right]$.

$n = 3$: $H = q_1 p_2 + q_2 p_3 - \frac{1}{2}\varepsilon q_3^2$;

$\Xi_H(\boldsymbol{u}, t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht + \frac{\varepsilon}{3}\left(\frac{t}{2}\right)^3 (2q_3 q_1 - q_2^2) - \frac{2\varepsilon}{15}\left(\frac{t}{2}\right)^5 q_1^2\right)\right]$.

$n = 3$: $H = q_1 p_2 + q_2 p_3$; $\Xi_H(\boldsymbol{u}, t) = \exp(-\frac{1}{2}\mathrm{i}Ht)$.

Table 2. (continued)

$n=4$: $H = q_1p_2 + q_2p_3 + q_3p_4 - \frac{1}{2}\varepsilon q_4^2$;

$$\Xi_H(\boldsymbol{u},t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht + \frac{1}{3}\left(\frac{t}{2}\right)^3(-2q_1p_4 + 2\varepsilon q_4p_2 - \varepsilon q_3^2) + \frac{2\varepsilon}{15}\left(\frac{t}{2}\right)^5(2q_1q_3 - q_2^2) - \frac{17\varepsilon}{315}\left(\frac{t}{2}\right)^7 q_1^2\right)\right].$$

$n=5$: $H = q_1p_2 + q_2p_3 + q_3p_4 + q_4p_5 - \frac{1}{2}\varepsilon q_5^2$;

$$\Xi_H(\boldsymbol{u},t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht - \frac{1}{3}\left(\frac{t}{2}\right)^3(2q_1p_4 + 2q_2p_5 - 2\varepsilon q_3q_5 + \varepsilon q_4^2)\right.\right.$$
$$\left.\left. + \frac{2\varepsilon}{15}\left(\frac{t}{2}\right)^5(2q_2q_4 - 2q_1q_5 - q_3^2) + \frac{17\varepsilon}{315}\left(\frac{t}{2}\right)^7(2q_1q_3 - q_2^2) - \frac{62\varepsilon}{2835}\left(\frac{t}{2}\right)^9 q_1^2\right)\right].$$

$n=5$: $H = q_1p_2 + q_2p_3 + q_3p_4 + q_4p_5$;

$$\Xi_H(\boldsymbol{u},t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht - \frac{1}{3}\left(\frac{t}{2}\right)^3(2q_1p_4 + 2q_2p_5)\right)\right].$$

Table 3. Singular inhomogeneous Hamiltonians.

Inhomogeneous case: $H = \frac{1}{2}{}^t\boldsymbol{u}B\boldsymbol{u} + {}^t\boldsymbol{c}\boldsymbol{u}$; $\det B = 0$, $\boldsymbol{c} \neq 0$.

$n=1$: $H = aq + bp$; $\Xi_H(\boldsymbol{u},t) = \exp(-\frac{1}{2}\mathrm{i}Ht)$.

$n=1$: $H = -\frac{1}{2}\varepsilon q^2 + ap$; $\Xi_H(\boldsymbol{u},t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht - \frac{\varepsilon a^2}{24}t^3\right)\right]$.

$n=2$: $H = aq_1 + bq_2 + ep_1 + fp_2$; $\Xi_H(\boldsymbol{u},t) = \exp(-\frac{1}{2}\mathrm{i}Ht)$.

$n=2$: $H = q_1p_2 - \frac{1}{2}\varepsilon q_2^2 + ap_1$;

$$\Xi_H(\boldsymbol{u},t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht - \frac{\varepsilon}{24}(q_1^2 - 2aq_2)t^3 - \frac{\varepsilon a^2}{240}t^5\right)\right].$$

$n=2$: $H = -\frac{1}{2}\varepsilon q_2^2 + aq_1 + bp_1 + ep_2$; $\Xi_H(\boldsymbol{u},t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht - \frac{\varepsilon e^2}{24}t^3\right)\right]$.

$n=2$: $H = -\frac{1}{2}\varepsilon q_1^2 - \frac{1}{2}\varepsilon' q_2^2 + ap_1 + bp_2$; $\Xi_H(\boldsymbol{u},t) = \exp\left[-\frac{\mathrm{i}}{2}\left(Ht - \frac{\varepsilon a^2 + \varepsilon' b^2}{24}t^3\right)\right]$.

$n=2$: $H = H_1 + H_2$; $H_1 = \alpha q_2p_2$, $H_2 = aq_1 + bp_1$;

$$\Xi_H(\boldsymbol{u},t) = \operatorname{sech}\left(\frac{\alpha t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\alpha}H_1\tanh\frac{\alpha t}{2} - \frac{\mathrm{i}t}{2}H_2\right).$$

$n=2$: $H = H_1 + H_2$; $H_1 = -\frac{1}{2}\varepsilon\beta(q_2^2 + p_2^2)$, $H_2 = aq_1 + bp_1$;

$$\Xi_H(\boldsymbol{u},t) = \sec\left(\frac{\beta t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\beta}H_1\tan\frac{\beta t}{2} - \frac{\mathrm{i}t}{2}H_2\right).$$

$n=2$: $H = H_1 + H_2$; $H_1 = \alpha q_2p_2$, $H_2 = -\frac{1}{2}\varepsilon q_1^2 + ap_1$;

$$\Xi_H(\boldsymbol{u},t) = \operatorname{sech}\left(\frac{\alpha t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\alpha}H_1\tanh\frac{\alpha t}{2} - \frac{\mathrm{i}t}{2}H_2 + \frac{\mathrm{i}\varepsilon a^2}{48}t^3\right).$$

$n=2$: $H = H_1 + H_2$; $H_1 = -\frac{1}{2}\varepsilon\beta(q_2^2 + p_2^2)$, $H_2 = -\frac{1}{2}\varepsilon' q_1^2 + ap_1$;

$$\Xi_H(\boldsymbol{u},t) = \sec\left(\frac{\beta t}{2}\right)\exp\left(-\frac{\mathrm{i}}{\beta}H_1\tan\frac{\beta t}{2} - \frac{\mathrm{i}t}{2}H_2 + \frac{\mathrm{i}\varepsilon a^2}{48}t^3\right).$$

6. Spectral analysis

As we prove in appendix 1, the spectrum of a Hamiltonian H can be identified with the support on E of the spectral projector $\Gamma_H(\boldsymbol{u}, E)$. A possible way to obtain properties of the spectra of the quadratic Hamiltonians is then to do Fourier analysis on the Moyal propagators studied here. We show how this comes about for $n=1$. From the previous tables we extract six representative Hamiltonians, which cover all possible cases.

(i) Trivial.

$$H=0 \qquad \Xi_H(\boldsymbol{u};\, t)=1.$$

We have $\Gamma_H(\boldsymbol{u};\, E)=\delta(E)$; Sp $H=\{0\}$.

(ii) Free particle.

$$H=\tfrac{1}{2}p^2 \qquad \Xi_H(\boldsymbol{u};\, t)=\exp(-\tfrac{1}{2}\mathrm{i}p^2 t).$$

We have $\Gamma_H(\boldsymbol{u};\, E)=\delta(\tfrac{1}{2}p^2-E)$; Sp $H=\boldsymbol{R}^+$.

(iii) Free-fall Hamiltonian.

$$H=\tfrac{1}{2}p^2+q \qquad \Xi_H(\boldsymbol{u};\, t)=\exp[-\tfrac{1}{2}\mathrm{i}(Ht+t^3/24)].$$

From

$$\mathrm{Ai}(x)=\frac{1}{2\pi}\int_{\boldsymbol{R}}\exp(\mathrm{i}\nu x+\tfrac{1}{3}\mathrm{i}\nu^3)\,\mathrm{d}\nu$$

we have

$$\Gamma_H(\boldsymbol{u};\, E)=2^{1/3}\,\mathrm{Ai}(2^{1/3}(H-E)) \qquad \mathrm{Sp}\, H=\boldsymbol{R}.$$

(iv) Harmonic barrier.

$$H=\tfrac{1}{2}(p^2-q^2) \qquad \Xi_H(\boldsymbol{u};\, t)=\mathrm{sech}\left(\frac{t}{2}\right)\exp\left(-\mathrm{i}H\tanh\frac{t}{2}\right).$$

Using Kummer's formula:

$${}_1F_1(a,1,z)=\frac{1}{\Gamma(a)\Gamma(1-a)}\int_0^1 \mathrm{e}^{zt}t^{a-1}(1-t)^{-a}\,\mathrm{d}t$$

one can show

$$\Gamma_H(\boldsymbol{u};\, E)=\frac{1}{2}\,\mathrm{sech}\left(\frac{\pi E}{2}\right)\mathrm{e}^{-\mathrm{i}H}\;{}_1F_1(\tfrac{1}{2}(1-\mathrm{i}E),1,2\mathrm{i}H)$$

and consequently Sp $H=\boldsymbol{R}$.

(v) Harmonic oscillator.

$$H=\tfrac{1}{2}(p^2+q^2)$$

$$\Xi_H(\boldsymbol{u};\, t)=\begin{cases}\sec\left(\dfrac{t}{2}\right)\exp\left(-\mathrm{i}H\tan\dfrac{t}{2}\right) & \text{if } t\neq(2k+1)\pi,\ k\in\mathbb{Z}\\ (-1)^{k+1}2\pi\mathrm{i}\delta & \text{if } t=(2k+1)\pi,\ k\in\mathbb{Z}.\end{cases}$$

Using the formula for the generating function of the Laguerre polynomials:

$$\sum_{k=0}^{\infty} L_k(x)y^k = (1-y)^{-1}\exp[xy/(y-1)]$$

one gets

$$\Gamma_H(\boldsymbol{u}; E) = \sum_{k=0}^{\infty} 2\delta(E-(2k+1))(-1)^k L_k(2H)\mathrm{e}^{-H}$$

and Sp $H = \{1, 3, 5, 7, \ldots\}$, as expected (recall that $\hbar = 2$).

(vi) Harmonic 'antioscillator'.

$$H = -\tfrac{1}{2}(p^2+q^2)$$

$$\Xi_H(\boldsymbol{u}; t) = \begin{cases} \sec\left(\frac{t}{2}\right)\exp\left(-\mathrm{i}H\tan\frac{t}{2}\right) & \text{if } t \neq (2k+1)\pi,\ k\in\mathbb{Z} \\ (-1)^k 2\pi\mathrm{i}\delta & \text{if } t = (2k+1)\pi,\ k\in\mathbb{Z}. \end{cases}$$

Although we have lumped together the two cases (v) and (vi) in table 1, they must be carefully distinguished now. We have the following proposition.

Proposition. Let S be a complex symplectic $2n\times 2n$ matrix such that $S = \mathrm{i}M$ with M real. Let $H' = \frac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}B'\boldsymbol{u}$ and $H = \frac{1}{2}{}^{\mathrm{t}}\boldsymbol{u}B\boldsymbol{u}$ be two homogeneous Hamiltonians, subject to $B' = {}^{\mathrm{t}}SBS$. Then Sp $H' = -$Sp H.

Proof. Since (3.11) remains valid for complex S, and according to (3.5) and (3.7),

$$\Xi_{H'}(\boldsymbol{u}, t) = \Xi_H(S\boldsymbol{u}, t) = \left[\det\left(\frac{I+\Sigma}{2}\right)\right]^{-1/2} \exp[\tfrac{1}{2}\mathrm{i}\,{}^{\mathrm{t}}(S\boldsymbol{u})G(S\boldsymbol{u})]$$

$$= \left[\det\left(\frac{I+\Sigma}{2}\right)\right]^{-1/2} \exp[-\tfrac{1}{2}\mathrm{i}\,{}^{\mathrm{t}}(M\boldsymbol{u})G(M\boldsymbol{u})] = \overline{\Xi_H(M\boldsymbol{u}, t)}$$

(where we have omitted the term with $\beta(t)$ which vanishes if the Hamiltonian is homogeneous). Then

$$\Gamma_{H'}(\boldsymbol{u}, E) = \frac{1}{4\pi}\int \Xi_{H'}(\boldsymbol{u}, t)\mathrm{e}^{\mathrm{i}tE/2}\,\mathrm{d}t$$

$$= \frac{1}{4\pi}\int \overline{\Xi_H(M\boldsymbol{u}, t)}\,\mathrm{e}^{\mathrm{i}tE/2}\,\mathrm{d}t = \Gamma_H(M\boldsymbol{u}, -E).$$

If we denote the support on E of $\Gamma_H(\boldsymbol{u}, E)$ by $\mathrm{supp}_E\Gamma_H(\boldsymbol{u}, E)$, we finally have

$$\mathrm{Sp}\ H' = \mathrm{supp}_E\ \Gamma_{H'}(\boldsymbol{u}, E) = \mathrm{supp}_E\ \Gamma_H(M\boldsymbol{u}, -E) = -\mathrm{Sp}\ H.$$

For the harmonic 'antioscillator', we now obtain

$$\Gamma_H(\boldsymbol{u}; E) = \sum_{k=0}^{\infty} 2\delta(E+(2k+1))(-1)^k L_k(-2H)\mathrm{e}^{H}$$

and Sp $H = \{-1, -3, -5, -7, \ldots\}$.

For $n > 1$, the calculation of Fourier transforms in the indecomposable cases becomes computationally very difficult. In principle, we could obtain the spectra in the decomposable cases by convolution of the spectral projectors for the indecomposable Hamiltonians. A very simple case is the isotropic harmonic oscillator in $\boldsymbol{R}^{2n}$, where we get

$$\Gamma_H(\boldsymbol{u}; E) = 2^n \sum_{k=0}^{\infty} (-1)^k \binom{n+k-1}{k} e^{-H} L_k^{n-1}(2H)\delta(E-(2k+n)).$$

Here L_k^{n-1} denotes the associated Laguerre polynomial of order $n-1$ and degree k. Note that the correct degeneration of levels is obtained.

7. Conclusion

The programme set out by Moshinsky and Winternitz [2] may be implemented completely in the Moyal formulation. This is better adapted to dealing with quadratic Hamiltonians because of its underlying canonical symmetry. By use of formulae such as those developed in § 2 and appendix 1, all physical questions related to the corresponding dynamical problems can be treated directly from our explicit formulae. If one is reluctant to abandon the conventional formalism, one can always derive the Green functions from our Moyal propagators.

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Appendix 1. Quadratic Hamiltonians and the Moyal algebra

In this appendix, we examine the mathematical basis of the Moyal formalism more closely and establish the following results: the Moyal propagator for any non-singular (time-independent) quadratic Hamiltonian lies in the Moyal algebra of tempered distributions [4]; the operator corresponding to such a Hamiltonian is self-adjoint, and its spectrum is given by the support (on E) of the Fourier transform of the Moyal propagator.

The twisted product (2.4) of functions on $\boldsymbol{R}^{2n}$ can be extended in a natural manner to a certain class of distributions on $\boldsymbol{R}^{2n}$. Let $\mathscr{S}(\boldsymbol{R}^{2n})$ denote the Schwartz space of smooth rapidly decreasing functions on $\boldsymbol{R}^{2n}$ and let $\mathscr{S}'(\boldsymbol{R}^{2n})$ be its dual space of tempered distributions. Then if $f, g \in \mathscr{S}(\boldsymbol{R}^{2n})$, we also have $f \times g \in \mathscr{S}(\boldsymbol{R}^{2n})$; by duality, one can extend the twisted product to the case where either f or g lies in $\mathscr{S}'(\boldsymbol{R}^{2n})$, in which case $f \times g$ is also a tempered distribution; and by a further extension, both f

and g can be tempered distributions provided at least one of them lies in

$$\mathcal{M}(\boldsymbol{R}^{2n}) = \{f \in \mathcal{S}'(\boldsymbol{R}^{2n}) : f \times h,\ h \times f \in \mathcal{S}(\boldsymbol{R}^{2n}) \text{ whenever } h \in \mathcal{S}(\boldsymbol{R}^{2n})\}$$

which turns out to be an involutive algebra of distributions under the twisted product, called the Moyal algebra (with complex conjugation as the involution). For details of this extension, we refer to [4].

If $\mathcal{M}(\boldsymbol{R}^{2n})$ is to be considered as a natural 'algebra of observables' for phase-space quantum mechanics, one must show that it contains the Moyal propagators $\Xi_H(\boldsymbol{u}; t)$ for a large class of Hamiltonians H. We now show that this class includes all non-singular quadratic Hamiltonians. This is also a step in the proof of self-adjointness for $W(H)$.

It is known that a tempered distribution T lies in $\mathcal{M}(\boldsymbol{R}^{2n})$ if and only if the corresponding operator $W(T)$ on $L^2(\boldsymbol{R}^n)$ and its adjoint $W(T)^* = W(\overline{T})$ are defined on the dense subspace $\mathcal{S}(\boldsymbol{R}^n)$ and leave $\mathcal{S}(\boldsymbol{R}^n)$ invariant [4]. As in the calculation of the formula for the Green function, we find, for $\Psi \in \mathcal{S}(\boldsymbol{R}^n)$, that

$$\begin{aligned}[W(\Xi_H(t))\Psi](\boldsymbol{x}) &\\ &= \frac{1}{(4\pi)^n} \int_{\boldsymbol{R}^n} \int_{\boldsymbol{R}^n} \Xi_H(\tfrac{1}{2}(\boldsymbol{x}+\boldsymbol{y}), \boldsymbol{z}; t) \exp[\tfrac{1}{2}\mathrm{i}\,{}^t\boldsymbol{z}(\boldsymbol{x}-\boldsymbol{y})]\Psi(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}\, \mathrm{d}\boldsymbol{z}. \qquad \text{(A1.1)}\end{aligned}$$

It thus remains to establish that $W(\Xi_H(t))\Psi$ and $W(\overline{\Xi_H(t)})\Psi$ lie in $\mathcal{S}(\boldsymbol{R}^n)$ whenever $\Psi \in \mathcal{S}(\boldsymbol{R}^n)$ for suitable Hamiltonians H.

Theorem 4. If H is a non-singular time-independent quadratic Hamiltonian, then $\Xi_H(t)$ lies in $\mathcal{M}(\boldsymbol{R}^{2n})$ for all $t \in \boldsymbol{R}$.

Proof. If S is a real symplectic $2n \times 2n$ matrix and $\boldsymbol{u}_0 \in \boldsymbol{R}^{2n}$, it is clear that the change of variables $\tilde{f}(\boldsymbol{u}) = f(S\boldsymbol{u} + \boldsymbol{u}_0)$ leaves $\mathcal{S}(\boldsymbol{R}^{2n})$ invariant, and from (2.4) we see that $\tilde{f} \times \tilde{g} = (f \times g)^{\sim}$; thus $\mathcal{M}(\boldsymbol{R}^{2n})$ is also invariant under $f \mapsto \tilde{f}$. By (3.16) it thus suffices to establish the theorem for $H = \frac{1}{2}{}^t\boldsymbol{u}B\boldsymbol{u}$, where JB is a simple representative of its symplectic conjugacy class. Moreover, by (4.15), we may suppose that JB is indecomposable.

If JB is given by (4.1) or (4.4), we find that $\Xi_H(\boldsymbol{q}, \boldsymbol{p}; t) = \exp(\mathrm{i}\,{}^t\boldsymbol{p}K\boldsymbol{q})$, where K denotes the upper left $n \times n$ block of $\tanh(JBt/2)$. In these cases, (A1.1) reduces to

$$\begin{aligned}[W(\Xi_H(t))\Psi](\boldsymbol{x}) &\\ &= \frac{1}{(4\pi)^n} \int_{\boldsymbol{R}^n} \exp[\tfrac{1}{2}\mathrm{i}\,{}^t\boldsymbol{z}(I+K)\boldsymbol{x}] \int_{\boldsymbol{R}^n} \exp[-\tfrac{1}{2}\mathrm{i}\,{}^t\boldsymbol{y}\,{}^t(I-K)\boldsymbol{z}]\Psi(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y}\, \mathrm{d}\boldsymbol{z} \qquad \text{(A1.2)}\end{aligned}$$

and $W(\overline{\Xi_H(t)})\Psi$ equals the right-hand side of (A1.2) with K replaced by $-K$, so the desired follows from the invariance of $\mathcal{S}(\boldsymbol{R}^n)$ under the Fourier transform, provided that the matrices $I \pm K$ are non-singular.

If JB is given by (4.2) or (4.3), then (A1.1) reduces to a less simple form, since quadratic exponential terms appear in the analogue of (A1.2). However, since $\mathcal{S}(\boldsymbol{R}^n)$ is stable under translations and multiplication by $\exp[\frac{1}{2}\mathrm{i}\,{}^t\boldsymbol{x}F\boldsymbol{x}]$, for any real symmetric matrix F, one verifies that the same result holds as in the previous cases: $W(\Xi_H(t))$ and its adjoint preserve $\mathcal{S}(\boldsymbol{R}^n)$ provided that $I - K$ and $I + K$ are non-singular.

From (4.6), one verifies that in all cases $\det(I+K)\det(I-K)=\det(I+\tanh(Lt/2))$, where L is the semisimple part of JB. From (4.7), (4.10) and (4.14), the value of $D=\det(I+\tanh(Lt/2))$ can be computed for each of the indecomposable cases (a), (b) and (c) of § 4. The results are:

$$\text{case }(a):\qquad D=\operatorname{sech}^{2k}\left(\frac{\alpha t}{2}\right)$$

$$\text{case }(b):\qquad D=\sec^{2k}\left(\frac{\beta t}{2}\right)$$

$$\text{case }(c):\qquad D=\frac{[(2+2\cosh\alpha t\cos\beta t)^2+(2\sinh\alpha t\sin\beta t)^2]^k}{(\cosh\alpha t+\cos\beta t)^{4k}}.$$

Thus D *does not vanish* for any t, as required. (In case (b), the values $t=(2m+1)\pi/\beta$, m integer, deserve a comment: at such values, $\Xi_H(t)$ is proportional to a δ distribution concentrated at a point, which in any case lies in $\mathcal{M}(\boldsymbol{R}^{2n})$.)

Now let H be a non-singular quadratic Hamiltonian. From (3.3), it is clear that $H\in\mathcal{M}(\boldsymbol{R}^{2n})$. Let $W_0(H)$ denote the operator defined by (2.1) or (2.6) with f replaced by H, whose domain is $\mathcal{S}(\boldsymbol{R}^n)$. Moreover, $W_0(\Xi_H(t))$, similarly defined as an operator with domain $\mathcal{S}(\boldsymbol{R}^n)$ from the functional form (3.5) by means of (A1.1), forms a continuous group of operators on $\mathcal{S}(\boldsymbol{R}^n)$ which extends to a group $\mathrm{U}(t)$ of unitary operators on $L^2(\boldsymbol{R}^n)$. Let $\frac{1}{2}\mathrm{i}\,W(H)t$ denote the generator of this unitary group. Then clearly $\mathcal{S}(\boldsymbol{R}^n)\subset\mathcal{D}(W(H))$ and $W(H)\Psi=W_0(H)\Psi$ for all $\Psi\in\mathcal{S}(\boldsymbol{R}^n)$. By theorem 4, the domain $\mathcal{S}(\boldsymbol{R}^n)$ of $W_0(H)$ is invariant under the unitary group $\mathrm{U}(t)$.

From a theorem of Taylor [19, prop. B.3], we conclude that $W_0(H)$ is essentially self-adjoint and $W(H)$ is its unique self-adjoint extension. Thus the functional calculus properties dealt with in § 2 are rigorously valid for non-singular quadratic Hamiltonians.

The foregoing is also true for singular quadratic Hamiltonians; in fact, a theorem by Wang [20] guarantees that, if f is any real smooth function such that all its derivatives of order at least two are bounded, then $\Xi_f(\boldsymbol{u},t)$ exists as an element of $\mathcal{M}$. The proof, however, is involved and demands familiarity with the methods of pseudodifferential operator theory; this is why we chose to present here an elementary proof within our sphere of interest.

Finally, we consider the spectrum of $W(H)$, which we have denoted $\mathrm{Sp}\,H$. We show that this coincides with $\mathrm{supp}_E\,\Gamma_H$. If $\Psi\in\mathcal{S}(\boldsymbol{R}^n)$, let $f_\Psi(\boldsymbol{u})=W^{-1}(|\Psi\rangle\langle\Psi|)(\boldsymbol{u})$. From the formulae of § 2 we see that

$$\langle\Psi|\exp(-\mathrm{i}\,W(H)t/2)|\Psi\rangle=\frac{1}{(4\pi)^n}\int_{\boldsymbol{R}^{2n}}f_\Psi(\boldsymbol{u})\Xi_H(\boldsymbol{u},t)\,\mathrm{d}\boldsymbol{u}. \tag{A1.3}$$

By the spectral theorem, we may write

$$\langle\Psi|\exp(-\mathrm{i}\,W(H)t/2)|\Psi\rangle=\int_{\mathrm{Sp}\,H}\mathrm{e}^{-\mathrm{i}tE/2}\,\mathrm{d}\mu_\Psi(E) \tag{A1.4}$$

where μ_Ψ is the spectral measure associated with Ψ [21].

Equation (2.10) defines a function $\Gamma_H(E)$ with values in $\mathcal{S}'(\boldsymbol{R}^{2n})$ or, more precisely, a $\mathcal{S}'(\boldsymbol{R}^{2n})$-valued measure $\Gamma_H(\mathrm{d}E)$ for which

$$\Xi_H(\boldsymbol{u}, t) = \int_{\boldsymbol{R}} \mathrm{e}^{-\mathrm{i}tE/2}\Gamma_H(\boldsymbol{u}, \mathrm{d}E) \tag{A1.5}$$

where the integral in (A1.5) extends, in fact, over $\mathrm{supp}_E\,\Gamma_H$. Define the complex measure ν_Ψ by

$$\mathrm{d}\nu_\Psi(E) = \int_{\boldsymbol{R}^{2n}} f_\Psi(\boldsymbol{u})\Gamma_H(\boldsymbol{u}, \mathrm{d}E).$$

Clearly $\mathrm{supp}\,\nu_\Psi \subset \mathrm{supp}_E\,\Gamma_H$. Then

$$\int_{\boldsymbol{R}^{2n}} f_\Psi(\boldsymbol{u})\Xi_H(\boldsymbol{u}, t)\,\mathrm{d}u = \int_{\boldsymbol{R}}\int_{\boldsymbol{R}^{2n}} \mathrm{d}\boldsymbol{u}\,\mathrm{e}^{-\mathrm{i}tE/2} f_\Psi(\boldsymbol{u})\Gamma_H(\boldsymbol{u}, \mathrm{d}E) = \int_{\boldsymbol{R}} \mathrm{e}^{-\mathrm{i}tE/2}\,\mathrm{d}\nu_\Psi(E).$$

Together with (A1.3) and (A1.4), this implies that the complex measures μ_Ψ, ν_Ψ have the same Fourier transforms and hence coincide.

Since $\mathrm{Sp}\,H = \bigcup_\Psi \mathrm{supp}\,\mu_\Psi$ [21], we thus obtain that $\mathrm{Sp}\,H \subset \mathrm{supp}_E\,\Gamma_H$.

On the other hand, if $E \in \mathrm{supp}_E\,\Gamma_H$, $\Gamma_H(\mathrm{d}E)$ and therefore $W_0(\Gamma_H(\mathrm{d}E))$ are not identically zero on any neighbourhood V of E. Thus we can find $\Phi \in \mathcal{S}(\boldsymbol{R}^n)$ so that $\langle\Phi|\,W_0(\Gamma_H(\mathrm{d}E))|\Phi\rangle \not\equiv 0$ on V. Since

$$\langle\Phi|\,W_0(\Gamma_H(\mathrm{d}E))|\Phi\rangle = \int_{\boldsymbol{R}^{2n}} f_\Phi(\boldsymbol{u})\Gamma_H(\boldsymbol{u}, \mathrm{d}E) = \mathrm{d}\nu_\Phi(E)$$

we find that $V \cap \mathrm{supp}\,\mu_\Phi = V \cap \mathrm{supp}\,\mu_\Phi \neq \emptyset$ and hence $V \cap \mathrm{Sp}\,H \neq \emptyset$. Thus $E \in \mathrm{Sp}\,H$. We conclude that $\mathrm{supp}_E\,\Gamma_H \subset \mathrm{Sp}\,H$.

We have proven that $\mathrm{supp}_E\Gamma_H = \mathrm{Sp}\,H$ whenever $W(H)$ is self-adjoint and $\Xi_H(t) \in \mathcal{M}(\boldsymbol{R}^{2n})$ for all t. In particular, the methods sketched in § 6 do indeed lead to the calculation of spectra in our case.

We remark that the measure $\Gamma_H(\mathrm{d}E)$ is always discrete or absolutely continuous in the present context. Thus the notation $\Gamma_H(\boldsymbol{u}, E)\,\mathrm{d}E$ employed throughout the paper, instead of $\Gamma_H(\boldsymbol{u}, \mathrm{d}E)$, is justified. In the discrete case, the $\Gamma_H(\boldsymbol{u}, E)$ belong to $\mathcal{S}(\boldsymbol{R}^{2n})$; otherwise, they are tempered distributions that do *not* belong to the Moyal algebra.

Appendix 2. The path-integral form for the Moyal propagator

The ordinary exponential function can be defined as

$$\mathrm{e}^x = \lim_{N\to\infty} (1 + x/N)^N.$$

This gives a heuristic suggestion for the calculation of Moyal propagators. Let us write $\Xi_H(\boldsymbol{u}; t) = \prod_{1\leqslant k\leqslant N}^{\times} \Xi_H(\boldsymbol{u}; t/N)$. Considering, for simplicity, a time-independent Hamiltonian, one has

$$\Xi_H\left(\boldsymbol{u}; \frac{t}{N}\right) = 1 - \frac{\mathrm{i}t}{2N} H + \mathrm{O}\left(\frac{t^2}{N^2}\right) = \exp\left(-\frac{\mathrm{i}tH}{2N}\right) + \mathrm{O}\left(\frac{t^2}{N^2}\right).$$

We conjecture then

$$\Xi_H(\boldsymbol{u};\,t)=\lim_{N\to\infty}\underbrace{\mathrm{e}^{-\mathrm{i}tH/2N}\times\ldots\times\mathrm{e}^{-\mathrm{i}tH/2N}}_{(N\text{ times})}=:\lim_{N\to\infty}\Xi_H^{(N)}(\boldsymbol{u};\,t).$$

The explicit form of $\Xi_H^{(N)}$ is calculated now, following [22] (the subscripts under the integral signs will be omitted):

$$\begin{aligned}\Xi_H^{(N)}(\boldsymbol{u};\,t)&=\left[\exp\left(-\frac{\mathrm{i}tH}{2N}\right)\Xi_H^{(N-1)}\right](\boldsymbol{u};\,t)\\&=(2\pi)^{-2n}\iint \mathrm{d}\boldsymbol{y}_N\,\mathrm{d}\boldsymbol{x}_N\\&\quad\times\exp\{-\tfrac{1}{2}\mathrm{i}[(t/N)H(\boldsymbol{y}_N)-2\,{}^{\mathrm{t}}\boldsymbol{u}J\boldsymbol{y}_N-2\,{}^{\mathrm{t}}\boldsymbol{y}_NJ\boldsymbol{x}_N-2\,{}^{\mathrm{t}}\boldsymbol{x}_NJ\boldsymbol{u}]\}\Xi_H^{(N-1)}(\boldsymbol{x}_N;\,t)\\&=(2\pi)^{-4n}\iiiint \mathrm{d}\boldsymbol{y}_N\,\mathrm{d}\boldsymbol{x}_N\,\mathrm{d}\boldsymbol{y}_{N-1}\,\mathrm{d}\boldsymbol{x}_{N-1}\\&\quad\times\exp\{-\tfrac{1}{2}\mathrm{i}[(t/N)H(\boldsymbol{y}_N)+(t/N)H(\boldsymbol{y}_{N-1})2\,{}^{\mathrm{t}}\boldsymbol{u}J\boldsymbol{y}_N-2\,{}^{\mathrm{t}}\boldsymbol{y}_NJ\boldsymbol{x}_N-2\,{}^{\mathrm{t}}\boldsymbol{x}_NJ\boldsymbol{u}\\&\quad-2\,{}^{\mathrm{t}}\boldsymbol{x}_NJ\boldsymbol{y}_{N-1}-2\,{}^{\mathrm{t}}\boldsymbol{y}_{N-1}J\boldsymbol{x}_{N-1}-2\,{}^{\mathrm{t}}\boldsymbol{x}_{N-1}J\boldsymbol{x}_N]\}\Xi_H^{(N-2)}(\boldsymbol{x}_{N-1};\,t)\\&=\ldots=(2\pi)^{-2Nn}\int\ldots\int\prod_{j=1}^{N}\mathrm{d}\boldsymbol{y}_j\,\mathrm{d}\boldsymbol{x}_j\\&\quad\times\exp\left[-\frac{\mathrm{i}}{2}\left(\sum_{i=1}^{N}\frac{t}{N}H(\boldsymbol{y}_i)-2\sum_{i=1}^{N}({}^{\mathrm{t}}\boldsymbol{x}_{i+1}J\boldsymbol{y}_i+{}^{\mathrm{t}}\boldsymbol{y}_iJ\boldsymbol{x}_i+{}^{\mathrm{t}}\boldsymbol{x}_iJ\boldsymbol{x}_{i+1})\right)\right]\end{aligned}\tag{A2.1}$$

where we made the little trick of twisted-multiplying the last factor by 1 in order to get a more rounded expression; also, we put $\boldsymbol{x}_{N+1}=\boldsymbol{u}$.

Assume now that N is even. We rewrite the second part in the exponent in (A2.1):

$$\begin{aligned}G_N:={}&{}^{\mathrm{t}}\boldsymbol{y}_1J\boldsymbol{x}_1+{}^{\mathrm{t}}(\boldsymbol{y}_2-\boldsymbol{y}_1)J\boldsymbol{x}_2+{}^{\mathrm{t}}(\boldsymbol{y}_3-\boldsymbol{y}_2)J\boldsymbol{x}_3+\ldots+{}^{\mathrm{t}}(\boldsymbol{y}_N-\boldsymbol{y}_{N-1})J\boldsymbol{x}_N\\&+{}^{\mathrm{t}}\boldsymbol{x}_{N+1}J\boldsymbol{y}_N+{}^{\mathrm{t}}(\boldsymbol{x}_1-\boldsymbol{x}_3)J\boldsymbol{x}_2+{}^{\mathrm{t}}(\boldsymbol{x}_3-\boldsymbol{x}_5)J\boldsymbol{x}_4+\ldots+{}^{\mathrm{t}}(\boldsymbol{x}_{N-1}-\boldsymbol{x}_{N+1})J\boldsymbol{x}_N\end{aligned}$$

and apply the method of stationary phase to perform the integral over the $\boldsymbol{x}$. That is, we equate to zero the derivatives of the previous expression with respect to the $\boldsymbol{x}$, which yields

$$\begin{aligned}\boldsymbol{x}_{2k}&=\boldsymbol{y}_1+\sum_{i=1}^{k-1}(\boldsymbol{y}_{2i+1}-\boldsymbol{y}_{2i})\\\boldsymbol{x}_{2k-1}&=\boldsymbol{u}+\sum_{i=k}^{N/2}(\boldsymbol{y}_{2i-1}-\boldsymbol{y}_{2i})\qquad 1\leqslant k\leqslant N/2.\end{aligned}\tag{A2.2}$$

Instead of writing the resulting expression as an iterated integral over the $\boldsymbol{y}$, we go over directly to the continuous limit. Let us introduce the time parameter τ, such that $0\leqslant\tau\leqslant t$, and assume $\boldsymbol{x}_{2k}=\boldsymbol{x}(\tau_{2k})$; $\boldsymbol{x}_{2k+1}=\tilde{\boldsymbol{x}}(\tau_{2k+1})$; $\boldsymbol{y}_k=\boldsymbol{y}(\tau_k)$. The limit $N\to\infty$ in the expression (A2.2) gives the following relations among the continuous trajectories $\boldsymbol{x}(\tau)$,

$\tilde{x}(\tau)$, $y(\tau)$:

$$x(\tau)=y(t)-\frac{1}{2}\int_{\tau}^{t}\dot{y}(s)\,\mathrm{d}s=\frac{y(\tau)+y(t)}{2}$$

$$\tilde{x}(\tau)=u+\frac{1}{2}\int_{0}^{\tau}\dot{y}(s)\,\mathrm{d}s=\frac{y(\tau)-y(0)}{2}+u.$$

We find also

$$\text{`}\lim_{N\to\infty}\text{'}\, G_N={}^{\mathrm{t}}y(t)J\tilde{x}(t)+{}^{\mathrm{t}}uJy(0)+\frac{1}{2}\int_0^t {}^{\mathrm{t}}\tilde{x}(\tau)J\dot{y}(\tau)\,\mathrm{d}\tau$$
$$+\frac{1}{2}\int_0^t {}^{\mathrm{t}}x(\tau)J\dot{y}(\tau)\,\mathrm{d}\tau-\int_0^t {}^{\mathrm{t}}x(\tau)J\dot{\tilde{x}}(\tau)\,\mathrm{d}\tau$$
$$=\frac{1}{4}\int_0^t {}^{\mathrm{t}}y(\tau)J\dot{y}(\tau)\,\mathrm{d}\tau+\tfrac{1}{2}{}^{\mathrm{t}}uJy(0)$$

after some work (where $\frac{1}{2}(y(0)+y(t))=u$ must be used).

We have, then, the following expressions for the Moyal propagator as a normalised integral over paths:

$$\Xi_H(u;\,t)=\int\!\!\int \mathscr{D}[x(\tau)]\mathscr{D}[y(\tau)]$$
$$\times\exp\left(-\frac{\mathrm{i}}{2}\int_0^t [H(y(\tau))-2\,{}^{\mathrm{t}}x(\tau)J\dot{x}(\tau)+2\,{}^{\mathrm{t}}y(\tau)J\dot{x}(\tau)]\,\mathrm{d}\tau\right)$$
$$\text{with } x(0)=u \qquad \text{(A2.3)}$$

or

$$\Xi_H(u;\,t)=\int \mathscr{D}[y(\tau)]$$
$$\times\exp\left[-\frac{\mathrm{i}}{2}\left(\int_0^t [H(y(\tau))+\tfrac{1}{2}{}^{\mathrm{t}}y(\tau)J\dot{y}(\tau)]\,\mathrm{d}\tau\right)+{}^{\mathrm{t}}y(0)Ju\right]. \qquad \text{(A2.4)}$$

The former is from (A2.1); the latter comes from our stationary phase calculation. In (A2.4) one has the condition $\frac{1}{2}(y(0)+y(t))=u$. (Taking N odd in the argument leading to (A2.4) is messier, but the final result is the same.)

Formula (A2.1) can be applied in principle to direct calculations of evolution functions, at least in simple cases. The one example known to the authors of such a calculation, which gives the evolution function for the harmonic oscillator again, may be found in [23]. On the other hand, it is fruitful, as in conventional quantum mechanics, to examine the expansion of (A2.4) around classical paths. We can consider the expressions under the integral sign in the 'integrands' of (A2.3) and (A2.4) as Lagrangians of sorts. In the second case, for instance, the Euler–Lagrange equations $(\mathrm{d}/\mathrm{d}t)\partial L/\partial\dot{y}=\partial L/\partial y$ give

$$\partial H/\partial y=-J\dot{y}$$

i.e. Hamilton's equations! We will denote by $y_{\mathrm{cl}}(\tau)$ a path obeying the classical dynamics with $\frac{1}{2}(y_{\mathrm{cl}}(0)+y_{\mathrm{cl}}(t))=u$. The exponent of (A2.4) for these paths:

$$g_{\mathrm{cl}}(u;\,t)=\int_0^t [H(y_{\mathrm{cl}}(\tau))+\tfrac{1}{2}{}^{\mathrm{t}}y_{\mathrm{cl}}(\tau)J\dot{y}_{\mathrm{cl}}(\tau)]\,\mathrm{d}\tau+{}^{\mathrm{t}}y(0)Ju$$

is obviously a symmetrical form of the classical action. One arrives as well at the last formula from (A2.3). Note that the 'Lagrangian' under the integral sign in (A2.3) or (A2.4) is a singular one, so it would seem that we are not entitled to use the Euler–Lagrange equations. The proper theory [24], however, gives also in the present case Hamilton's equations as a kind of necessary constraint†.

If the Hamiltonian is quadratic, the Moyal propagator can be calculated solely from the classical paths, in much the same way as the path integral calculation proceeds for the propagator in the standard theory, for quadratic Lagrangians. In effect, application of the method of stationary phase in (A2.4) gives at once

$$\Xi_H(\boldsymbol{u};\, t) = F(t)\exp[-\tfrac{1}{2}\mathrm{i}g_{\mathrm{cl}}(\boldsymbol{u};\, t)].$$

We leave it to the reader to check that in this case g_{cl} is the same quantity that we have denoted by g_H throughout the paper.

One can now calculate $F(t)$ from the path integral, but it is easier to get it from the group property of Ξ_H (as noted in [25]). We obtain anew the basic formulae employed in the paper; the details are omitted. Note that this derivation of the general form of the evolution function for quadratic Hamiltonians gives immediately the pre-exponential factor, in contradistinction to our method in § 3.

It is clear that we could employ the method of stationary phase in (A2.3) or (A2.4) to obtain the *point de départ* of a semiclassical expansion of the Moyal propagator for arbitrary Hamiltonians [26].

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