

Quantization of Gaussians

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Dedicated to the memory of Boris Pavlov.

Abstract. Our paper is devoted to the oscillator semigroup, which can be defined as the set of operators whose kernels are centered Gaussian. Equivalently, they can be defined as the Weyl quantization of centered Gaussians. We use the Weyl symbol as the main parametrization of this semigroup. We derive formulas for the tracial and operator norm of the Weyl quantization of Gaussians. We identify the subset of Gaussians, which we call *quantum degenerate*, where these norms have a singularity.

1. Introduction

Throughout our paper we will use the Weyl quantization, which is the most natural correspondence between quantum and classical states. For a function k = k(x, p), with $x, p \in \mathbb{R}^d$, we will denote by Op(k) its Weyl quantization. Then function k is called the Weyl symbol (or the Wigner function) of the operator Op(k).

The Heisenberg uncertainty relation says that one cannot compress a state both in position and momentum without any limits. This is different than in classical mechanics, where in principle a state can have no dispersion both in position and momentum.

One can ask what happens to a quantum state when we compress its Weyl symbol. To be more precise, consider the Gaussian function $e^{-\lambda(x^2+p^2)}$, where $\lambda > 0$ is an arbitrary parameter that controls the "compression". It is easy to compute the Weyl quantization of $e^{-\lambda(x^2+p^2)}$ and express it in terms of the quantum harmonic oscillator

$$H = \hat{x}^2 + \hat{p}^2 = \sum_{j=1}^d (\hat{x}_j^2 + \hat{p}_j^2).$$
(1.1)

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There are 3 distinct regimes of the parameter λ :

$$Op\left(e^{-\lambda(x^{2}+p^{2})}\right) = \begin{cases} (1-\lambda^{2})^{-d/2} \exp\left[-\frac{1}{2}\log\frac{(1+\lambda)}{(1-\lambda)}H\right], & 0 < \lambda < 1, \\ 2^{-d}\mathbb{1}_{\{d\}}(H), & \lambda = 1, \\ (\lambda^{2}-1)^{-d/2}(-1)^{(H-d)/2} \exp\left[-\frac{1}{2}\log\frac{(1+\lambda)}{(\lambda-1)}H\right], & 1 < \lambda. \end{cases}$$
(1.2)

Thus, for $0 < \lambda < 1$, the quantization of the Gaussian is proportional to a thermal state of H. As λ increases to 1, it becomes "less mixed"–its "temperature" decreases. At $\lambda = 1$ it becomes pure—its "temperature" becomes zero and it is the ground state of H. For $1 < \lambda < \infty$, when we compress the Gaussian, it is no longer positive—due to the factor $(-1)^{(H-d)/2}$ it has eigenvalues with alternating signs. Besides, it becomes "more and more mixed", contrary to the naive classical picture.

Thus, at $\lambda = 1$ we observe a kind of a "phase transition": For $0 \leq \lambda < 1$ the quantization of a Gaussian behaves more or less according to the classical intuition. For $1 < \lambda$ the classical intuition stops to work—compressing the classical symbol makes its quantization more "diffuse".

It is easy to compute the trace of (1.2):

$$\operatorname{Tr}\operatorname{Op}\left(\mathrm{e}^{-\lambda(x^{2}+p^{2})}\right) = \frac{1}{2^{d}\lambda^{d}}.$$
(1.3)

Evidently, (1.3) does not see the "phase transition" at $\lambda = 1$. However, if we consider the trace norm, this phase transition appears—the trace norm of (1.2) is differentiable except at $\lambda = 1$:

$$\operatorname{Tr} \left| \operatorname{Op} \left(e^{-\lambda (x^2 + p^2)} \right) \right| = \begin{cases} \frac{1}{2^d \lambda^d} & \lambda \leq 1, \\ \frac{1}{2^d}, & 1 \leq \lambda. \end{cases}$$
(1.4)

Note that (1.4) can be viewed as a kind of quantitative "uncertainty principle".

Our paper is devoted to operators that can be written as the Weyl quantization of a (centered) Gaussian, more precisely, operators of the form $aOp(e^{-A})$, where A is a quadratic form with a strictly positive real part and $a \in \mathbb{C}$. Such operators form a semigroup called the *oscillator semigroup*. We denote it by $Osc_{++}(\mathbb{C}^{2d})$. We also considered its subsemigroup, called the *normalized oscillator semigroup* and denoted $Osc_{++}^{nor}(\mathbb{C}^{2d})$, which consists of operators

$$\pm \sqrt{\det(\mathbb{1} + A\theta)} \operatorname{Op}(e^{-A}),$$

where θ is -i times the symplectic form ω .

The oscillator semigroup is closely related to the complex symplectic group $Sp(\mathbb{C}^{2d})$. In particular, there exists a natural 2–1 epimorphism from $Osc^{nor}_{++}(\mathbb{C}^{2d})$ onto $Sp_{++}(\mathbb{C}^{2d})$, which is a certain natural subsemigroup of $Sp(\mathbb{C}^{2d})$.

The oscillator semigroup is also closely related to the better known *meta*plectic group, denoted $Mp(\mathbb{R}^{2d})$. The metaplectic group is generated by operators of the form $\pm \sqrt{\det(\mathbb{1} + B\omega)} \operatorname{Op}(e^{iB})$, where *B* is a real symmetric matrix. There exists a natural 2–1 epimorphism from $Mp(\mathbb{R}^{2d})$ to the real symplectic group $Sp(\mathbb{R}^{2d})$. Not all elements of the metaplectic group can be written as Weyl quantizations of a Gaussian.

The situation with the oscillator semigroup is somewhat different than with the metaplectic group. All elements of the oscillator semigroup are quantizations of a Gaussian, however, not all of them correspond to a (complex) symplectic transformation. Those that do not correspond to quadratic forms A satisfying $det(1 + A\theta) = 0$. We call such quadratic forms "quantum degenerate". Classically, they are of course nondegenerate. Only their quantization is degenerate. In particular, for a quantum degenerate A, the operator $Op(e^{-A})$ is not proportional to an element of $Osc_{++}^{nor}(\mathbb{C}^{2d})$. The set of quantum degenerate matrices can be viewed as a place where some kind of a phase transition takes place in the oscillator semigroup. For instance, as we show in our paper, the trace norm of $Op(e^{-A})$ depends smoothly on quantum nondegenerate A's, however, its smoothness typically breaks down at quantum degenerate A's.

It is also natural to mention another type of an oscillator semigroup, which we denote $\operatorname{Osc}_+(\mathbb{C}^{2d})$. It is the semigroup generated by the operators of the form $a\operatorname{Op}(e^{-A})$, where $A \ge 0$. $\operatorname{Osc}_+(\mathbb{C}^{2d})$ contains both $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$ and $Mp(\mathbb{R}^{2d})$. It is in some sense the closure of $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$. We mention this semigroup only in passing, concentrating on $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$, which is easier, because, as we mentioned above, all elements of $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$ have Gaussian symbols. Note that the convenient notation ++ for > 0 and + for ≥ 0 , which we use, is borrowed from Howe [16].

Most of the time our discussion of the oscillator semigroup is representation independent (without invoking a concrete Hilbert space on which $Op(e^{-A})$ acts). Perhaps the most obvious representation is the so-called Schrödinger representation, where the Hilbert space is $L^2(\mathbb{R}^d)$, \hat{x} is identified with the operator of multiplication by x and \hat{p} is $\frac{1}{i}\partial_x$. Another possible representation is the Fock representation (or, which is essentially equivalent, the Bargmann–Fock representation, see, e.g., [11]). In both Schrödinger and Bargmann–Fock representations the oscillator semigroup consists of operators with centered Gaussian kernels.

Let us now discuss the literature on operators with Gaussian kernels, or equivalently, on quantizations of Gaussians. Probably, the best known reference on this subject is a paper [16] by Howe. In fact, we follow to some extent the terminology from [16]. His paper contains, for instance, a formula of composition of operators with Gaussian kernels, a criterion for positivity of such operators and the proof that there exists a 2–1 epimorphism from the normalized oscillator semigroup to a subsemigroup of $Sp(\mathbb{C}^{2d})$. Howe works mostly in the Schrödinger representation. Instead of the Weyl symbol, he occasionally considers the so-called *Weyl transform*, which is essentially the Fourier transform of the Weyl symbol.

Another important work on the subject is a paper [15] by Hilgert, who realized that the oscillator semigroup is isomorphic to a semigroup described by Bargmann,

Brunet and Kramer (see [2], [6], and [7]). Hilgert uses mostly the *Fock–Bargmann* representation.

The book of Folland [14] contains a chapter on the oscillator semigroup, which sums up the main points of [15] and [16].

The existence of the "phase transition" at quantum degenerate positive Gaussians has been known for quite a long time, where the earliest reference we could find is the paper [20] by Unterberger.

Our paper differs from [14, 15, 16] by using the Weyl quantization as the basic tool for the description of the oscillator semigroup. It is in some sense parallel to the presentation of the metaplectic group contained in [11, Sect. 10.3]. The Weyl quantization is in our opinion a natural tool in this context. First of all, it is symplectically invariant (unlike the Fock–Bargmann transform or the Schrödinger representation). Because of that, the analysis based on the Weyl quantization is particularly convenient and yields simple formulas. Secondly, the Weyl quantization allows us to make a direct contact with the quantum–classical correspondence principle. This semiclassical aspect is hidden when one uses the Weyl transform, which is also symplectically invariant.

An operation, that we introduce, which we find interesting is the product # in the set of symmetric matrices. More precisely, it is defined so that $Op(e^{-A})Op(e^{-B})$ is proportional to $Op(-e^{A\#B})$. Whenever defined, # is associative, however it is not always well defined. # can be viewed as a semiclassical noncommutative distortion of the usual sum of square matrices. As we show, quantum nondegenerate matrices with a positive part form a semigroup, which is essentially isomorphic to the oscillator semigroup.

Among new results obtained in our paper, there is a formula for the absolute value of an operator $Op(e^{-A})$, its trace norm and its operator norm.

There exists a close relationship between the set of complex matrices equipped with # and the complex symplectic group. This relationship is quite intricate–it is almost a bijection, after removing some exceptional elements in both sets. One of new results of our paper is a detailed description of this relationship, see in particular Theorem 18.

An interesting recent paper of Viola [21] gives a formula for the norm of an element of the oscillator semigroup. Our formula for $\|\operatorname{Op}(e^{-A})\|$ is in our opinion simpler than Viola's.

As an application of the formula for the trace norm of $Op(e^{-A})$ we give a proof of the boundedness of the Weyl quantization with an explicit estimate of the of the operator norm. This result, which is a version of the so-called Calderon– Vaillancourt Theorem for the Weyl quantization, follows the ideas of Cordes [10] and Kato [18], however, the estimate of the norm seems to be new.

Elements of the oscillator semigroup can be viewed as exponentials of quantum quadratic Hamiltonians, that is $e^{-Op(H)}$, where *H* is a classical quadratic Hamiltonian with a positive real part. One example of such a Hamiltonian is $\hat{H}_{\psi} := e^{i\psi}\hat{p}^2 + e^{-i\psi}\hat{x}^2$ for $|\psi| < \frac{\pi}{2}$, which is often called the *Davies harmonic oscillator*. It has been noted by a number of authors that this operator has interesting, often counterintuitive properties. In particular, [1] and [21] point out that $e^{-z\hat{H}_{\psi}}$ can be defined as a bounded operator only for z that belong to a subset of the complex plane of a rather curious shape. We reproduce this result using methods developed in this article.

The oscillator semigroup provides a natural framework for a discussion of holomorphic semigroups $z \mapsto e^{-zOp(H)}$ associated with accretive quadratic Hamiltonians Op(H). We briefly discuss this issue at the end of our paper.

Finally, let us mention that one can explicitly compute the Weyl symbol of various functions of the harmonic oscillator, not only of its exponential. In particular, formulas in terms of special functions for the Weyl symbol of the resolvent of the harmonic oscillator can be found in [12]; see also [8], where the inverse of the harmonic oscillator is considered.

2. Notation

Let $L(\mathbb{C}^n)$ denote the set of $n \times n$ matrices. For $R \in L(\mathbb{C}^n)$ we will write \overline{R} , $R^{\#}$, resp. R^* for its complex conjugate, transpose, resp. Hermitian adjoint. Elements of \mathbb{C}^n are represented by column matrices, so that for $v, w \in \mathbb{C}^n$ the (sesquilinear) scalar product of v and w can be denoted by v^*w .

By $\sigma(R)$ we will denote the spectrum of R.

We set

$$L^{\operatorname{reg}}(\mathbb{C}^n) := \{ R \in L(\mathbb{C}^n) \mid R + 1 \text{ is invertible} \}.$$

$$(2.1)$$

For $R \in L^{\operatorname{reg}}(\mathbb{C}^n)$, its *Cayley transform* is defined by

$$c(R) := (\mathbb{1} - R)(\mathbb{1} + R)^{-1}.$$

The Cayley transform is a bijection on $L^{\operatorname{reg}}(\mathbb{C}^n)$ and it is involutive, i.e.,

$$c(c(R)) = R. (2.2)$$

For $A \in L(\mathbb{C}^n)$, we write A > 0, resp. $A \ge 0$ if

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$$v^*Av > 0, \quad v \in \mathbb{C}^n, \quad v \neq 0,$$

esp. $v^*Av \ge 0, \quad v \in \mathbb{C}^n.$ (2.3)

 ${\rm Sym}(\mathbb{R}^n),$ resp. ${\rm Sym}(\mathbb{C}^n)$ denotes the set of symmetric real, resp. complex $n\times n$ matrices. We also set

$$\operatorname{Sym}_{+}(\mathbb{R}^{n}) := \{ A \in \operatorname{Sym}(\mathbb{R}^{n}) \mid A \ge 0 \},$$
(2.4)

$$\operatorname{Sym}_{++}(\mathbb{R}^n) := \{ A \in \operatorname{Sym}(\mathbb{R}^n) \mid A > 0 \},$$
(2.5)

$$\operatorname{Sym}_{+}(\mathbb{C}^{n}) := \{ A \in \operatorname{Sym}(\mathbb{C}^{n}) \mid \operatorname{Re} A \ge 0 \},$$
(2.6)

$$\operatorname{Sym}_{++}(\mathbb{C}^n) := \{ A \in \operatorname{Sym}(\mathbb{C}^n) \mid \operatorname{Re} A > 0 \}.$$
(2.7)

Note that $\operatorname{Sym}_{++}(\mathbb{C}^n)$ is sometimes called the (generalized) Siegel upper half-plane. It is sometimes denoted S_n or \mathfrak{S}_n [16]. The following proposition can be found in [16]:

Proposition 1. If $A \in \text{Sym}_{++}(\mathbb{C}^n)$, then A^{-1} exists and belongs to $\text{Sym}_{++}(\mathbb{C}^n)$.

 $\begin{array}{l} \textit{Proof. Let } A = A_{\rm r} + {\rm i}A_{\rm i} \text{ with } A_{\rm r} \in {\rm Sym}_{++}(\mathbb{R}^n), \, A_{\rm i} \in {\rm Sym}(\mathbb{R}^n). \text{ Let } B := \sqrt{A_{\rm r}}, \\ C := B^{-1}A_{\rm i}B^{-1}. \text{ Then } A = B(\mathbbm{1} + {\rm i}C)B \text{ and } A^{-1} = B^{-1}(\mathbbm{1} + {\rm i}C)^{-1}B^{-1}. \text{ Clearly}, \\ (\mathbbm{1} + {\rm i}C)^{-1} \in {\rm Sym}_{++}(\mathbb{C}^n). \text{ Hence } A^{-1} \in {\rm Sym}_{++}(\mathbb{C}^n). \end{array}$

Every $n \times n$ symmetric matrix A defines a quadratic form on \mathbb{R}^n by

$$\mathbb{R}^n \ni y \mapsto y^\# A y \in \mathbb{C}. \tag{2.8}$$

We will often write A for the function (2.8). Thus, in particular,

$$\mathrm{e}^{-A}(y) = \mathrm{e}^{-y^{\#}Ay}.$$

We will often need to use the square root of a complex number a. If it is clear from the context that a is positive and real, then \sqrt{a} will always denote the positive square root. If a is a priori arbitrary, then $\pm\sqrt{a}$ will denote both values of the square root. If a given formula involves only one of possible values of the square root, then we will write $\epsilon\sqrt{a}$ where $\epsilon = 1$ or $\epsilon = -1$.

3. The Weyl quantization

Recall that for any $k \in \mathscr{S}'(\mathbb{R}^d \times \mathbb{R}^d)$

$$Op(k)(x, y) = (2\pi)^{-d} \int k \left(\frac{x+y}{2}, p\right) e^{ip(x-y)} dp$$
(3.1)

is called the Weyl–Wigner quantization of the symbol k, see, e.g., [17, Sect. 18.5] or [11]. We can recover the symbol of a quantization from its distributional kernel by

$$k(x, p) = \int \operatorname{Op}(k) \left(x + \frac{z}{2}, x - \frac{z}{2} \right) e^{-izp} dz.$$
 (3.2)

For sufficiently nice functions k, m we can define the *star product* * (sometimes called the *Moyal star*) such that Op(k)Op(m) = Op(k * m) holds. On the level of symbols we have

$$(k*m)(x, p) := e^{\frac{i}{2}(\partial_{x_1}\partial_{p_2} - \partial_{p_1}\partial_{x_2})} k(x_1, p_1)m(x_2, p_2)\Big|_{\substack{x:=x_1=x_2\\p:=p_1=p_2}}.$$
(3.3)

Write $y = \begin{bmatrix} x \\ p \end{bmatrix}$, $\omega := \begin{bmatrix} 0 & \mathbb{1}_d \\ -\mathbb{1}_d & 0 \end{bmatrix}$, and $\theta := \begin{bmatrix} 0 & -i\mathbb{1}_d \\ i\mathbb{1}_d & 0 \end{bmatrix} = -i\omega$. One can rewrite (3.3) in a more compact form:

$$(k*m)(y) = e^{-\frac{1}{2}\partial_{y_1}\theta\partial_{y_2}}k(y_1)m(y_2)\Big|_{y:=y_1=y_2}.$$
(3.4)

Here is an integral form of (3.4):

$$(k*m)(y) = \pi^{-2d} \int dy_1 \int dy_2 e^{2(y-y_1)\theta(y-y_2)} k(y_1) m(y_2), \qquad (3.5)$$

(see, e.g., [11, Theorem 8.70(4)]). For the product of three symbols, we have (k*m*n)(y)

$$= e^{-\frac{1}{2}\partial_{y_1}\theta\partial_{y_2} - \frac{1}{2}\partial_{y_1}\theta\partial_{y_3} - \frac{1}{2}\partial_{y_2}\theta\partial_{y_3}}k(y_1)m(y_2)n(y_3)\Big|_{y:=y_1=y_2=y_3}$$

$$= \pi^{-3d} \int dy_1 \int dy_2 \int dy_3 e^{(y-y_1)\theta(y-y_2) + (y-y_2)\theta(y-y_3) + (y-y_1)\theta(y-y_3)} \qquad (3.6)$$

$$\times e^{-\frac{1}{2}(y-y_1)\theta(y-y_1) - \frac{1}{2}(y-y_2)\theta(y-y_2) - \frac{1}{2}(y-y_3)\theta(y-y_3)}k(y_1)m(y_2)n(y_3)\Big|_{y=y_1=y_2=y_3}.$$

4. Product

Let $A, B \in \text{Sym}(\mathbb{C}^{2d})$. Suppose that

the matrix
$$\begin{bmatrix} \theta A \theta & -\theta \\ \theta & \theta B \theta \end{bmatrix}$$
 is invertible. (4.1)

We then define $A \# B \in \text{Sym}(\mathbb{C}^{2d})$ by

$$A \# B := \begin{bmatrix} -\mathbb{1} \\ \mathbb{1} \end{bmatrix}^{\#} \begin{bmatrix} \theta A \theta & -\theta \\ \theta & \theta B \theta \end{bmatrix}^{-1} \begin{bmatrix} -\mathbb{1} \\ \mathbb{1} \end{bmatrix}.$$
(4.2)

For the time being, the definition of the product # may seem strange. As we will soon see in Sect. 6, it is motivated by the product of operators with Gaussian symbols.

The following proposition gives a condition which guarantees that A#B is well defined.

Proposition 2. Condition (4.1) holds iff the inverse of $(1 + A\theta B\theta)$ exists. We then have

$$\begin{bmatrix} \theta A \theta & -\theta \\ \theta & \theta B \theta \end{bmatrix}^{-1} = \begin{bmatrix} (\theta A \theta + B^{-1})^{-1} & (\theta + \theta B \theta A \theta)^{-1} \\ -(\theta + \theta A \theta B \theta)^{-1} & (\theta B \theta + A^{-1})^{-1} \end{bmatrix}$$

$$= \begin{bmatrix} B \theta (\mathbb{1} + A \theta B \theta)^{-1} \theta & (\mathbb{1} + B \theta A \theta)^{-1} \theta \\ -(\mathbb{1} + A \theta B \theta)^{-1} \theta & A \theta (\mathbb{1} + B \theta A \theta)^{-1} \theta \end{bmatrix}, \quad (4.3)$$

$$A \# B = (\theta A \theta + B^{-1})^{-1} + (\theta B \theta + A^{-1})^{-1} \\ + (\theta + \theta A \theta B \theta)^{-1} - (\theta + \theta B \theta A \theta)^{-1}. \quad (4.4)$$

Proof. It is well known how to compute an inverse of a 2×2 block matrix. This yields (4.3), which implies (4.4).

Clearly,

$$\theta(1 + A\theta B\theta)^{\#}\theta = (1 + B\theta A\theta). \tag{4.5}$$

Therefore, the inverse of $(1 + A\theta B\theta)$ exists iff the inverse of $(1 + B\theta A\theta)$ exists. If this is the case, then all terms in (4.3) and (4.4) are well defined.

Proposition 3. The product # is associative, i.e., if $A, B, C \in \text{Sym}(\mathbb{C}^{2d})$ and A#B, B#C, (A#B)#C and A#(B#C) are well defined, then

$$(A\#B)\#C = A\#(B\#C). \tag{4.6}$$

Besides,

$$A\#0 = 0\#A = A, \qquad A\#(-A) = 0,$$

$$\overline{A\#B} = \overline{B}\#\overline{A}, \qquad (-A)\#(-B) = -B\#A$$

Proof. We check that

$$(A\#B)\#C = A\#(B\#C) = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}^{\#} \begin{bmatrix} \theta A\theta + \frac{1}{2}\theta & -\frac{1}{2}\theta & -\frac{1}{2}\theta \\ \frac{1}{2}\theta & \theta B\theta + \frac{1}{2}\theta & -\frac{1}{2}\theta \\ \frac{1}{2}\theta & \frac{1}{2}\theta & \theta C\theta + \frac{1}{2}\theta \end{bmatrix}^{-1} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}.$$
(4.7)

(Compare with (3.6)). This yields (4.6). The remaining statements are straightforward. $\hfill \Box$

Note that it is useful to think of # as a noncommutative deformation of the addition. In fact, we have

$$A \# B = A + B + O(A^2 + B^2).$$
(4.8)

5. Quantum non-degenerate matrices

Define

$$\operatorname{Sym}^{\operatorname{qnd}}(\mathbb{C}^{2d}) := \{ A \in \operatorname{Sym}(\mathbb{C}^{2d}) : \det(\mathbb{1} + A\theta) \neq 0 \},$$
(5.1)

$$\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d}) := \left\{ A \in \operatorname{Sym}_{++}(\mathbb{C}^{2d}) : \operatorname{det}(\mathbb{1} + A\theta) \neq 0 \right\},$$
(5.2)
$$\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{R}^{2d}) := \left\{ A \in \operatorname{Sym}(\mathbb{R}^{2d}) : \operatorname{det}(\mathbb{1} + A\theta) \neq 0 \right\},$$
(5.3)

$$\operatorname{Sym}^{\operatorname{qua}}(\mathbb{R}^{2a}) := \{ A \in \operatorname{Sym}(\mathbb{R}^{2a}) : \operatorname{det}(\mathbb{1} + A\theta) \neq 0 \},$$
(5.3)

$$\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{R}^{2d}) := \left\{ A \in \operatorname{Sym}_{++}(\mathbb{R}^{2d}) : \operatorname{det}(\mathbb{1} + A\theta) \neq 0 \right\}.$$
(5.4)

("qnd" stands for quantum non-degenerate).

There are several equivalent formulas for the product (4.2). It is actually not so obvious to pass from one of them to another. In the following proposition we give a few of them.

Proposition 4. Let $A, B \in \text{Sym}^{\text{qnd}}(\mathbb{C}^{2d})$ such that $(\mathbb{1} + A\theta B\theta)^{-1}$ exists. Then

$$A \# B = c (c(A\theta)c(B\theta))\theta \tag{5.5}$$

$$= (\mathbb{1} + A\theta)^{-1} (A\theta + B\theta) (\mathbb{1} + A\theta B\theta)^{-1} (\mathbb{1} + A\theta)\theta$$
(5.6)

$$= (\mathbb{1} + B\theta)(\mathbb{1} + A\theta B\theta)^{-1}(A\theta + B\theta)(\mathbb{1} + B\theta)^{-1}\theta$$
(5.7)

$$= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(A\theta + B\theta)(\mathbb{1} - A\theta)^{-1}\theta$$
(5.8)

$$= (\mathbb{1} - B\theta)^{-1} (A\theta + B\theta) (\mathbb{1} + B\theta A\theta)^{-1} (\mathbb{1} - B\theta)\theta.$$
(5.9)

We have

$$\mathbb{1} + A\theta B\theta = (\mathbb{1} + A\theta)(\mathbb{1} + A\#B\theta)^{-1}(\mathbb{1} + B\theta),$$
(5.10)
and $A\#B \in \operatorname{Sym}^{\operatorname{qnd}}(\mathbb{C}^{2d}).$

Proof. To see (5.5), it is enough to show that

$$c(A\#B\theta) = c(A\theta)c(B\theta).$$
(5.11)

Equation (4.4) can be rewritten as

$$\begin{split} A \# B &= B \theta (\mathbbm{1} + A \theta B \theta)^{-1} \theta + A \theta (\mathbbm{1} + B \theta A \theta)^{-1} \theta \\ &+ (\mathbbm{1} + A \theta B \theta)^{-1} \theta - (\mathbbm{1} + B \theta A \theta)^{-1} \theta \\ &= (\mathbbm{1} + B \theta) (\mathbbm{1} + A \theta B \theta)^{-1} \theta - (\mathbbm{1} - A \theta) (\mathbbm{1} + B \theta A \theta)^{-1} \theta. \end{split}$$

Therefore,

$$1 - A \# B \theta = (A \theta - 1) B \theta (1 + A \theta B \theta)^{-1} + (1 - A \theta) (1 + B \theta A \theta)^{-1}
 = (1 - A \theta) (1 + B \theta A \theta)^{-1} (1 - B \theta);
 (5.12)

 1 + A \# B \theta = (1 + B \theta) A \theta (1 + B \theta A \theta)^{-1} + (1 + B \theta) (1 + A \theta B \theta)^{-1}
 = (1 + B \theta) (1 + A \theta B \theta)^{-1} (1 + A \theta).
 (5.13)$$

Hence,

$$\begin{aligned} c(A\#B\theta) \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(\mathbb{1} - B\theta)(\mathbb{1} + A\theta)^{-1}(A\theta B\theta + \mathbb{1})(\mathbb{1} + B\theta)^{-1} \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(\mathbb{1} - B\theta)(B\theta + (\mathbb{1} + A\theta)^{-1}(\mathbb{1} - B\theta))(\mathbb{1} + B\theta)^{-1} \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(B\theta + (\mathbb{1} - B\theta)(\mathbb{1} + A\theta)^{-1})(\mathbb{1} - B\theta)(\mathbb{1} + B\theta)^{-1} \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(\mathbb{1} + B\theta A\theta)(\mathbb{1} + A\theta)^{-1}(\mathbb{1} - B\theta)(\mathbb{1} + B\theta)^{-1} \\ &= c(A\theta)c(B\theta). \end{aligned}$$

Thus (5.5) is proven.

Next note that

$$c(A\theta)c(B\theta) = (1 + A\theta)^{-1}(1 - A\theta)(1 - B\theta)(1 + B\theta)^{-1} = (1 + A\theta)^{-1}(1 - A\theta - B\theta + A\theta B\theta)(1 + B\theta)^{-1}.$$
(5.14)

Therefore,

$$1 - c(A\theta)c(B\theta) = 2(1 + A\theta)^{-1}(A\theta + B\theta)(1 + B\theta)^{-1}$$
(5.15)

$$1 + c(A\theta)c(B\theta) = 2(1 + A\theta)^{-1}(1 + A\theta B\theta)(1 + B\theta)^{-1}.$$
(5.16)

Next we insert (5.15) and (5.16) into

$$A\#B = c(c(A\theta)c(B\theta))\theta$$
(5.17)

$$= \left(\mathbb{1} - c(A\theta)c(B\theta)\right) \left(\mathbb{1} + c(A\theta)c(B\theta)\right)^{-1}\theta$$
(5.18)

$$= \left(\mathbb{1} + c(A\theta)c(B\theta)\right)^{-1} \left(\mathbb{1} - c(A\theta)c(B\theta)\right)\theta, \tag{5.19}$$

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obtaining (5.6), resp. (5.7).

We know that A#B is symmetric. Applying the transposition to (5.6), resp. (5.7), we obtain (5.8), resp. (5.9), where we use $\theta^{\#} = -\theta$, $A^{\#} = A$, $B^{\#} = B$.

Equation (5.10) is proven in (5.13). This implies that $1 + A \# B\theta$ is invertible. Hence $A \# B \in \text{Sym}^{\text{qnd}}(\mathbb{C}^{2d})$.

The set $\operatorname{Sym}^{\operatorname{qnd}}(\mathbb{C}^{2d})$ equipped with (4.2) is not a semigroup. It is enough to see that for $A = B = \begin{bmatrix} i & 0 \\ 0 & i \end{bmatrix}$ we have $\mathbb{1} + A\theta B\theta = 0$, so A#B is not defined.

Proposition 5. Sym₊₊ (\mathbb{C}^{2d}) is a semigroup.

Proof. Let A and B belong to $\operatorname{Sym}_{++}(\mathbb{C}^{2d})$. The matrix $\begin{bmatrix} \theta A \theta & -\theta \\ \theta & \theta B \theta \end{bmatrix}$ belongs to $\operatorname{Sym}_{++}(\mathbb{C}^{2d})$. Hence, so does its inverse. Thus, (4.2) also belongs to $\operatorname{Sym}_{++}(\mathbb{C}^{2d})$. This shows that A # B is well defined and belongs to $\operatorname{Sym}_{++}(\mathbb{C}^{2d})$.

Proposition 6. Sym^{qnd}₊₊(\mathbb{C}^{2d}) is also a semigroup.

Proof. Let A and B belong to $\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$. We already know that A#B is well defined, and hence $1 + A\theta B\theta$ is invertible (see Proposition 2). Using (5.10) and the invertibility of $1 + A\theta$, $1 + B\theta$, we can conclude that $1 + A\#B\theta$ is invertible. Hence $A\#B \in \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$.

6. Oscillator semigroup

Following [16, 14], the oscillator semigroup $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$ is defined as the set of operators on $L^2(\mathbb{R}^d)$ whose Weyl symbols are centered Gaussian, that is operators of the form $a\operatorname{Op}(e^{-A})$, where $a \in \mathbb{C}, A \in \operatorname{Sym}_{++}(\mathbb{C}^{2d})$ and $A(x,p) = \begin{bmatrix} x \\ p \end{bmatrix}^{\#} A \begin{bmatrix} x \\ p \end{bmatrix}$. (In [16], this semigroup is denoted by Ω).

There are several equivalent characterizations of $\text{Osc}_{++}(\mathbb{C}^{2d})$. Here is one of them:

Proposition 7. $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$ equals the set of operators on $L^2(\mathbb{R}^d)$ with centered Gaussian kernels. More precisely, the integral kernel of $\operatorname{aOp}(e^{-A})$ for $A = \begin{bmatrix} B & D \\ D^{\#} & F \end{bmatrix}$ is $\operatorname{ce}^{-C(x,y)}$, where

$$c = \frac{2^{-d}a}{\sqrt{\det(F)}},\tag{6.1}$$

$$C(x,y) = -\frac{1}{4} \begin{bmatrix} x \\ y \end{bmatrix}^{\#} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} B - DF^{-1}D^{\#} & -iDF^{-1} \\ -iF^{-1}D^{\#} & F^{-1} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$
$$= -\frac{1}{4} \begin{bmatrix} x \\ y \end{bmatrix}^{\#} \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix},$$

and

$$c_{11} = B - DF^{-1}D^{\#} - iDF^{-1} - iF^{-1}D^{\#} + F^{-1},$$

$$c_{12} = B - DF^{-1}D^{\#} + iDF^{-1} - iF^{-1}D^{\#} - F^{-1},$$

$$c_{21} = B - DF^{-1}D^{\#} - iDF^{-1} + iF^{-1}D^{\#} - F^{-1},$$

$$c_{22} = B - DF^{-1}D^{\#} + iDF^{-1} + iF^{-1}D^{\#} + F^{-1}.$$

Proof. The formula follows by elementary Gaussian integration. The detailed computations can be found in [14]. \Box

Proposition 8. Let A and B belong to $\text{Sym}_{++}(\mathbb{C}^{2d})$. Then the following product formula holds:

$$Op(e^{-A})Op(e^{-B}) = \frac{\epsilon}{\sqrt{\det(A\theta B\theta + 1)}}Op(e^{-A\#B}),$$
(6.2)

where $\epsilon = 1$ or $\epsilon = -1$. Consequently, $Osc_{++}(\mathbb{C}^{2d})$ is a semigroup and

$$\operatorname{Osc}_{++}(\mathbb{C}^{2d}) \ni c\operatorname{Op}(e^{-A}) \mapsto A \in \operatorname{Sym}_{++}(\mathbb{C}^{2d})$$
 (6.3)

is an epimorphism.

Proof. Formula (3.5) assures us that

$$(e^{-y^{\#}Ay} * e^{-y^{\#}By})(y) = \pi^{-2d} \int dy_1 \int dy_2 \exp\left(-2(y-y_2)\theta(y-y_1) - y_1^{\#}Ay_1 - y_2^{\#}By_2\right)$$
$$= \pi^{-2d} \int dy_1 \int dy_2 \exp\left(-\begin{bmatrix}y_1\\y_2\end{bmatrix}^{\#}\begin{bmatrix}A & -\theta\\\theta & B\end{bmatrix}\begin{bmatrix}y_1\\y_2\end{bmatrix} - 2\begin{bmatrix}y_1\\y_2\end{bmatrix}^{\#}\begin{bmatrix}-\theta y\\\theta y\end{bmatrix}\right)$$
(6.4)
$$= \det\begin{bmatrix}A & -\theta\\\theta & B\end{bmatrix}^{-1/2} \exp\left(\begin{bmatrix}-\theta y\\\theta y\end{bmatrix}^{\#}\begin{bmatrix}A & -\theta\\\theta & B\end{bmatrix}^{-1}\begin{bmatrix}-\theta y\\\theta y\end{bmatrix}\right).$$

Then we check that

$$\det \begin{bmatrix} A & -\theta \\ \theta & B \end{bmatrix} = \det(\mathbb{1} + A\theta B\theta), \tag{6.5}$$

$$\begin{bmatrix} -\theta y \\ \theta y \end{bmatrix}^{\#} \begin{bmatrix} A & -\theta \\ \theta & B \end{bmatrix}^{-1} \begin{bmatrix} -\theta y \\ \theta y \end{bmatrix} = -\begin{bmatrix} -y \\ y \end{bmatrix}^{\#} \begin{bmatrix} \theta A \theta & -\theta \\ \theta & \theta B \theta \end{bmatrix}^{-1} \begin{bmatrix} -y \\ y \end{bmatrix}.$$
(6.6)

Again, following [16, 14], we introduce the normalized oscillator semigroup, denoted $\operatorname{Osc}_{++}^{\operatorname{nor}}(\mathbb{C}^{2d})$, as

$$\left\{\pm\sqrt{\det(\mathbb{1}+A\theta)}\operatorname{Op}\left(\mathrm{e}^{-A}\right) | A \in \operatorname{Sym}_{++}^{\operatorname{qnd}}\left(\mathbb{C}^{2d}\right)\right\}.$$

(In [16], this semigroup is denoted by Ω^0).

Proposition 9. $\operatorname{Osc}_{++}^{\operatorname{nor}}(\mathbb{C}^{2d})$ is a subsemigroup of $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$ and

$$\operatorname{Osc}_{++}^{\operatorname{nor}}(\mathbb{C}^{2d}) \ni \pm \sqrt{\operatorname{det}(\mathbb{1} + A\theta)} \operatorname{Op}(\mathrm{e}^{-A}) \mapsto A \in \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$$
(6.7)

is a 2–1 epimorphism of semigroups.

Proof. It is enough to check that

$$\sqrt{\det(\mathbb{1} + A\theta)} \operatorname{Op}(e^{-A}) \sqrt{\det(\mathbb{1} + B\theta)} \operatorname{Op}(e^{-B})
= \epsilon \sqrt{\det(\mathbb{1} + A \# B\theta)} \operatorname{Op}(e^{-A \# B}),$$
(6.8)

where $\epsilon = 1$ or $\epsilon = -1$. Indeed, (5.10) implies

$$\det(\mathbb{1} + A\theta B\theta) = \det(\mathbb{1} + A\theta)\det(\mathbb{1} + A\#B\theta)^{-1}\det(\mathbb{1} + B\theta).$$
(6.9)

Now we need to use (6.2).

7. Positive elements of the oscillator semigroup

We define

$$\operatorname{Sym}_{p}(\mathbb{R}^{2d}) := \left\{ A \in \operatorname{Sym}_{++}(\mathbb{R}^{2d}) \mid \sigma(A\theta) \subset [-1,1] \right\},\tag{7.1}$$

$$\operatorname{Sym}_{p}^{\operatorname{qnd}}(\mathbb{R}^{2d}) := \left\{ A \in \operatorname{Sym}_{p}(\mathbb{R}^{2d}) \mid \det(A\theta + 1) \neq 0 \right\}.$$
(7.2)

Proposition 10. Let $a \in \mathbb{C}$ and $A \in \text{Sym}_{++}(\mathbb{C}^{2d})$. Then

- (1) $(a \operatorname{Op}(e^{-A}))^* = \overline{a} \operatorname{Op}(e^{-\overline{A}}).$
- (2) $a \operatorname{Op}(e^{-A})$ is Hermitian iff $a \in \mathbb{R}$ and $A \in \operatorname{Sym}_{++}(\mathbb{R}^{2d})$.
- (3) $a \operatorname{Op}(e^{-A})$ is positive iff $a > 0, A \in \operatorname{Sym}_p(\mathbb{R}^{2d})$.

Proof. Claims (1) and (2) follow from the obvious identity $Op(a)^* = Op(\overline{a})$.

Let us prove (3). A is a positive definite real matrix and ω is a symplectic matrix. It is well known, that they can be simultaneously diagonalized, that is, one can find a basis of \mathbb{R}^{2d} such that if we write $\mathbb{R}^{2d} = \bigoplus_{i=1}^{d} \mathbb{R}^2$, then ω is the direct sum of $\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$ and A is the direct sum of $\begin{bmatrix} \lambda_i & 0 \\ 0 & \lambda_i \end{bmatrix}$ with $\lambda_i > 0$. After an appropriate metaplectic transformation, we can represent the Hilbert space $L^2(\mathbb{R}^d)$ as $\bigotimes_{i=1}^{d} L^2(\mathbb{R})$ and $\operatorname{Op}(e^{-A})$ can be represented as $\bigotimes_{i=1}^{d} \operatorname{Op}(e^{-\lambda_i(x_i^2 + p_i^2)})$. Next we use (1.2) to see that the positivity of $\operatorname{Op}(e^{-A})$ is equivalent to $\lambda_i \leq 1$, $i = 1, \ldots, d$, which in turn is equivalent to $\sigma(A\theta) \subset [-1, 1]$ (the eigenvalues of $A\theta$ are of the form $\pm \lambda_i$).

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Proposition 11. Sym_p^{qnd}(\mathbb{R}^{2d}) = { $A \in Sym_{++}(\mathbb{R}^{2d}) \mid \sigma(A\theta) \subset] - 1, 1[$ }.

Proof. We use the basis mentioned at the end of the proof of Proposition 10. \Box

Proposition 12. det $(\mathbb{1} + A\theta) = det(\mathbb{1} + \overline{A}\theta)$. Consequently, Sym^{qnd}(\mathbb{C}^{2d}) and Sym^{qnd}(\mathbb{C}^{2d})

are invariant with respect to complex conjugation.

Proof. We use

$$\theta(1 + A\theta)\theta = 1 + \theta A, \tag{7.3}$$

$$(1 + \theta A)^{\#} = 1 - A\theta,$$
 (7.4)

$$1 - A\theta = 1 + A\theta. \tag{7.5}$$

Theorem 13. (1) If $A \in \text{Sym}_{++}(\mathbb{C}^{2d})$, then $\overline{A} \# A \in \text{Sym}_p(\mathbb{R}^{2d})$. (2) If $A \in \text{Sym}_{++}^{\text{qnd}}(\mathbb{C}^{2d})$, then $\overline{A} \# A \in \text{Sym}_p^{\text{qnd}}(\mathbb{R}^{2d})$.

Proof. (1) Let $A \in \text{Sym}_{++}(\mathbb{C}^{2d})$. Then

$$Op(e^{-A})^*Op(e^{-A}) = \frac{1}{\sqrt{\det(\mathbb{1} + \overline{A}\theta A\theta)}} e^{-\overline{A}\#A}$$
(7.6)

is a positive operator. Therefore, by Proposition 10(3), $\overline{A} # A \in \operatorname{Sym}_{p}(\mathbb{R}^{2d})$.

(2) $\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$ is a semigroup, invariant with respect to the conjugation, and hence $\overline{A} \# A \in \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$. By (1), $\overline{A} \# A \in \operatorname{Sym}_{p}(\mathbb{R}^{2d})$. But by definition $\operatorname{Sym}_{p}^{\operatorname{qnd}}(\mathbb{R}^{2d}) = \operatorname{Sym}_{p}(\mathbb{R}^{2d}) \cap \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$.

8. Complex symplectic group

A linear operator R on \mathbb{R}^{2d} is called *symplectic* if

$$R^{\#}\omega R = \omega. \tag{8.1}$$

The set of symplectic operators on \mathbb{R}^{2d} will be denoted $Sp(\mathbb{R}^{2d})$. It is the well known symplectic group in dimension 2d.

In our paper a more important role is played by the complex version of the symplectic group. More precisely, we will say that a complex linear operator R on \mathbb{C}^{2d} is symplectic if (8.1) holds. (Of course, we can replace ω in (8.1) with θ). The set of complex symplectic operators on \mathbb{C}^{2d} will be denoted $Sp(\mathbb{C}^{2d})$. It is also a group, called the *complex symplectic group* in dimension 2d.

We define

$$Sp_{+}(\mathbb{C}^{2d}) := \{ R \in Sp(\mathbb{C}^{2d}) \mid R^{*}\theta R \le \theta \},$$
(8.2)

$$Sp_{++}(\mathbb{C}^{2d}) := \{ R \in Sp(\mathbb{C}^{2d}) \mid R^* \theta R < \theta \}.$$

$$(8.3)$$

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Both $Sp_+(\mathbb{C}^{2d})$ and $Sp_{++}(\mathbb{C}^{2d})$ are semigroups satisfying

$$Sp(\mathbb{R}^{2d}) \cap Sp_{++}(\mathbb{C}^{2d}) = \emptyset,$$
 (8.4)

$$Sp_{++}(\mathbb{C}^{2d}) \subset Sp_{+}(\mathbb{C}^{2d}),$$

$$(8.5)$$

$$Sp(\mathbb{R}^{2d}) \subset Sp_+(\mathbb{C}^{2d}).$$
 (8.6)

We also set

$$Sp_{\rm h}(\mathbb{C}^{2d}) := \left\{ R \in Sp(\mathbb{C}^{2d}) : \overline{R} = R^{-1} \right\}$$

$$(8.7)$$

$$= \{ R \in Sp(\mathbb{C}^{2d}) : R^*\theta = \theta R \},$$
(8.8)

$$Sp_{\mathbf{p}}(\mathbb{C}^{2d}) := \left\{ R \in Sp_{\mathbf{h}}(\mathbb{C}^{2d}) : \ \sigma(R) \subset]0, \infty[\right\}.$$

$$(8.9)$$

Below we state a few properties of $Sp_{++}(\mathbb{C}^{2d})$ and $Sp_p(\mathbb{C}^{2d})$. It will be convenient to defer their proofs to the next section.

Proposition 14. $Sp_{\mathbf{p}}(\mathbb{C}^{2d}) \subset Sp_{++}(\mathbb{C}^{2d}).$

Let t > 0. Note that $\mathbb{C} \setminus [-\infty, 0] \ni z \mapsto z^t \in \mathbb{C}$ is a well defined holomorphic function. In the proposition below $\sigma(R) \subset [0, \infty[$, therefore R^t is well defined.

Proposition 15. Let $R \in Sp_p(\mathbb{C}^{2d})$. Then $R^t \in Sp_p(\mathbb{C}^{2d})$.

Proposition 16. Let $R \in Sp_{++}(\mathbb{C}^{2d})$. Then $\overline{R}^{-1}R \in Sp_p(\mathbb{C}^{2d})$.

The next result, which is an analog of the polar decomposition, was noted by Howe (see [16, Proposition (23.7.2)]):

Proposition 17. Every $R \in Sp_{++}(\mathbb{C}^{2d})$ may be decomposed in the following way: R = TS.(8.10)where $T := \overline{R}\sqrt{\overline{R}^{-1}R} \in Sp(\mathbb{R}^{2d})$ and $S := \sqrt{\overline{R}^{-1}R} \in Sp_{p}(\mathbb{C}^{2d})$.

9. Relationship between Sym and symplectic group

Let us define

$$Sp^{\operatorname{reg}}(\mathbb{C}^{2d}) = \left\{ R \in Sp(\mathbb{C}^{2d}) \mid R + 1 \text{ is invertible} \right\},$$
 (9.1)

$$Sp_{\rm h}^{\rm reg}(\mathbb{C}^{2d}) = \left\{ R \in Sp_{\rm h}(\mathbb{C}^{2d}) \mid R + 1 \text{ is invertible} \right\}.$$

$$(9.2)$$

Theorem 18. (1) Sym^{qnd} $(\mathbb{C}^{2d}) \ni A \mapsto c(A\theta) \in Sp^{reg}(\mathbb{C}^{2d})$ is a bijection. Its inverse is

$$Sp^{\operatorname{reg}}(\mathbb{C}^{2d}) \ni R \mapsto c(R)\theta \in \operatorname{Sym}^{\operatorname{qnd}}(\mathbb{C}^{2d}).$$
 (9.3)

Besides, if $A, B \in \text{Sym}^{\text{qnd}}(\mathbb{C}^{2d})$ and $A \# B \in \text{Sym}^{\text{qnd}}(\mathbb{C}^{2d})$ is well defined, then

$$c(A\#B\theta) = c(A\theta)c(B\theta).$$
(9.4)

- (2) $\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d}) \ni A \mapsto c(A\theta) \in Sp_{++}(\mathbb{C}^{2d})$ is an isomorphism of semigroups. (3) $\operatorname{Sym}^{\operatorname{qnd}}(\mathbb{R}^{2d}) \ni A \mapsto c(A\theta) \in Sp_{\mathrm{h}}^{\operatorname{reg}}(\mathbb{C}^{2d})$ is a bijection.

(4)
$$\operatorname{Sym}_{p}^{\operatorname{qnd}}(\mathbb{R}^{2d}) \ni A \mapsto c(A\theta) \in Sp_{p}(\mathbb{C}^{2d})$$
 is a bijection.

Proof. (1) Let $A \in \text{Sym}^{\text{qnd}}(\mathbb{C}^{2d})$. Then,

$$c(A\theta)^{\#}\theta c(A\theta) = (\mathbb{1} - \theta A)^{-1} (\mathbb{1} + \theta A)\theta(\mathbb{1} - A\theta)(\mathbb{1} + A\theta)^{-1}$$
$$= (\mathbb{1} - \theta A)^{-1} (\mathbb{1} - \theta A\theta A\theta)(\mathbb{1} + A\theta)^{-1}$$
$$= (\mathbb{1} - \theta A)^{-1} (\mathbb{1} - \theta A)\theta(\mathbb{1} + A\theta)(\mathbb{1} + A\theta)^{-1} = \theta$$

Hence, $c(A\theta) \in Sp(\mathbb{C}^{2d})$.

Conversely, let $R \in Sp^{\operatorname{reg}}(\mathbb{C}^{2d})$. Then

$$\begin{split} \left((\mathbbm{1} - R)(\mathbbm{1} + R)^{-1}\theta \right)^{\#} &= -\theta(\mathbbm{1} + R^{\#})^{-1}(\mathbbm{1} - R^{\#}) \\ &= -(\theta + R^{\#}\theta)^{-1}(\mathbbm{1} - R^{\#}) = -(\theta(\mathbbm{1} + R^{-1}))^{-1}(\mathbbm{1} - R^{\#}) \\ &= -(\mathbbm{1} + R^{-1})^{-1}(\theta - \theta R^{\#}) = -(\mathbbm{1} + R^{-1})^{-1}(\mathbbm{1} - R^{-1})\theta \\ &= (\mathbbm{1} + R)^{-1}(\mathbbm{1} - R)\theta. \end{split}$$

Hence, $c(R)\theta \in \text{Sym}(\mathbb{C}^{2d})$.

Clearly, $A\theta + 1$ is invertible iff $c(A\theta) \in L^{\operatorname{reg}}(\mathbb{C}^{2d})$. Thus

$$\operatorname{Sym}^{\operatorname{qnd}}(\mathbb{C}^{2d}) \ni A \mapsto c(A\theta) \in Sp^{\operatorname{reg}}(\mathbb{C}^{2d})$$

is a bijection.

To see (9.4) it is enough to use (5.5).

(2) We have

$$c(A\theta)^*\theta c(A\theta) = (\mathbb{1} + \theta \overline{A})^{-1} (\mathbb{1} - \theta \overline{A})\theta (\mathbb{1} - A\theta)(\mathbb{1} + A\theta)^{-1}$$

= $(\mathbb{1} + \theta \overline{A})^{-1} (\mathbb{1} - \theta \overline{A}\theta - \theta A\theta + \theta \overline{A}\theta A\theta)(\mathbb{1} + A\theta)^{-1}$
= $\theta - 2(\mathbb{1} + \theta \overline{A})^{-1}\theta (\overline{A} + A)\theta (\mathbb{1} + A\theta)^{-1}.$

Thus,

$$c(A\theta)^*\theta c(A\theta) < \theta \tag{9.5}$$

iff $\overline{A} + A > 0$. Hence $\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d}) \ni A \mapsto c(A\theta) \in Sp_{++}(\mathbb{C}^{2d})$ is a bijection. It is a homomorphism because of (9.4).

(3) Let $A \in \text{Sym}^{\text{qnd}}(\mathbb{R}^{2d})$. Then

$$\overline{c(A\theta)} = \frac{\mathbb{1} + A\theta}{\mathbb{1} - A\theta} = c(A\theta)^{-1}.$$
(9.6)

Hence, $c(A\theta) \in Sp_h(\mathbb{C}^{2d})$.

Conversely, let $R \in Sp_{\rm h}^{\rm reg}(\mathbb{C}^{2d})$. Then

$$\overline{(\mathbb{1}-R)(\mathbb{1}+R)^{-1}\theta} = -(\mathbb{1}-\overline{R})(\mathbb{1}+\overline{R})^{-1}\theta$$
(9.7)

$$= -(\mathbb{1} - R^{-1})(\mathbb{1} + R^{-1})^{-1}\theta = (\mathbb{1} - R)(\mathbb{1} + R)^{-1}\theta.$$
(9.8)

Hence, $c(R)\theta \in \text{Sym}(\mathbb{R}^{2d})$.

(4) Clearly,

$$\lambda \in]-1,1[$$
 iff $\frac{1-\lambda}{1+\lambda} \in]0,\infty[$.

Therefore,

$$\sigma(A\theta) \subset]-1,1[$$
 iff $\sigma(c(A\theta)) \subset]0,\infty[.$

Then we use the characterization of $\operatorname{Sym}_{p}^{\operatorname{qnd}}(\mathbb{R}^{2d})$ given in Proposition 11.

Proof of Proposition 14. Let $R \in Sp_{p}(\mathbb{C}^{2d})$. By Theorem 18(4),

$$c(R)\theta \in \operatorname{Sym}_{p}^{\operatorname{qnd}}(\mathbb{R}^{2d}).$$

Proposition 11 implies that $c(R)\theta \in \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{R}^{2d})$. Now Theorem 18(2) shows that $R = c((c(R)\theta)\theta) \in Sp_{++}(\mathbb{C}^{2d})$.

Proof of Proposition 15. Let $R \in Sp_p(\mathbb{C}^{2d})$.

Functional calculus of operators is invariant with respect to similarity transformations. Therefore, $R^{\#(-1)} = \theta R \theta^{-1}$ implies $R^{\#(-t)} = \theta R^t \theta^{-1}$. Hence $R^t \in Sp(\mathbb{C}^{2d})$.

$$\overline{R} = R^{-1} \text{ implies } \overline{R}^t = (R^t)^{-1}. \text{ Hence, } R^t \in Sp_h(\mathbb{C}^{2d}).$$

$$\sigma(R) \subset]0, \infty[\text{ implies } \sigma(R^t) \subset]0, \infty[. \text{ Hence } R^t \in Sp_p(\mathbb{C}^{2d}).$$

Proof of Proposition 16. Theorem 18(2) assures us that we can find a matrix $A \in \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{R}^{2d})$, such that $c(A\theta) = R$. By Theorem 13(2), $\overline{A} \# A \in \operatorname{Sym}_{\mathrm{p}}^{\operatorname{qnd}}(\mathbb{R}^{2d})$. Now we may use Theorem 18(4) to see that $c(\overline{A} \# A \theta) \in \operatorname{Spp}(\mathbb{C}^{2d})$.

It is easy to check that $\overline{R}^{-1} = c(\overline{A}\theta)$. Moreover, by (9.4),

$$\overline{R}^{-1}R = c(\overline{A}\theta)c(A\theta) = c(\overline{A}\#A\theta).$$
(9.9)

Therefore, $\overline{R}^{-1}R \in Sp_{p}(\mathbb{C}^{2d}).$

Proof of Proposition 17. By Proposition 16, we have $\overline{R}^{-1}R \in Sp_p(\mathbb{C}^{2d})$, while Proposition 15 yields $S := \sqrt{\overline{R}^{-1}R} \in Sp_p(\mathbb{C}^{2d})$. Clearly, $\overline{R} \in Sp(\mathbb{C}^{2d})$. Hence, $T := \overline{R}S \in Sp(\mathbb{C}^{2d})$.

$$\overline{T} = \overline{\overline{RS}} = RS^{-1} = RS^{-2}S = RR^{-1}\overline{R}S = T.$$
(9.10)

Therefore, $T := \overline{RS} \in Sp(\mathbb{R}^{2d}).$

Theorem 19. The map

$$\operatorname{Osc}_{++}^{\operatorname{nor}}(\mathbb{C}^{2d}) \ni \pm \sqrt{\operatorname{det}(\mathbb{1} + A\theta)} \operatorname{Op}(\mathrm{e}^{-A}) \mapsto c(A\theta) \in Sp_{++}(\mathbb{C}^{2d})$$

is a 2–1 epimorphism of semigroups.

Proof. We use Proposition 9 and Theorem 18(2).

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10. Metaplectic group

It is easy to see that if $C \in \text{Sym}(\mathbb{R}^{2d})$, then $c(C\omega) \in Sp(\mathbb{R}^{2d})$. In fact, elements of this form constitute an open dense subset of $Sp(\mathbb{R}^{2d})$.

We define $Mp(\mathbb{R}^{2d})$, called the metaplectic group in dimension 2d, to be the group generated by operators of the form

$$\pm \sqrt{\det(\mathbb{1} + C\omega)} \operatorname{Op}(\mathrm{e}^{-\mathrm{i}C}), \quad C \in \operatorname{Sym}(\mathbb{R}^{2d}).$$
(10.1)

The theory of the metaplectic group is well known, see, e.g., [11, Sect. 10.3.1]. We assume that the reader is familiar with its basic elements. Actually, we have already used it in our proof of Proposition 10(3).

The theory of the metaplectic group can be summed up by the following theorem:

Theorem 20. The metaplectic group consists of unitary operators. Operators of the form (10.1) constitute an open and dense subset of $Mp(\mathbb{R}^{2d})$. The map

$$\pm \sqrt{\det(\mathbb{1} + C\omega)} \operatorname{Op}(e^{-iC}) \mapsto c(C\omega)$$
(10.2)

extends by continuity to a 2-1 epimorphism $Mp(\mathbb{R}^{2d}) \to Sp(\mathbb{R}^{2d})$

Remark 1. For completeness, one should mention some other natural semigroups closely related to $\text{Osc}_{++}(\mathbb{C}^{2d})$:

- 1. Osc₊(\mathbb{C}^{2d}) generated by operators $aOp(e^{-A})$ with $A \in Sym_+(\mathbb{C}^{2d}), a \in \mathbb{C}$;
- 2. $\operatorname{Osc}_{+}^{\operatorname{nor}}(\mathbb{C}^{2d})$ generated by operators of the form $\pm \sqrt{\det(\mathbb{1} + A\theta)}\operatorname{Op}(e^{-A})$ with $A \in \operatorname{Sym}_{+}(\mathbb{C}^{2d})$.

11. Polar decomposition

For an operator V, its *absolute value* is defined as

$$|V| := \sqrt{V^* V}.\tag{11.1}$$

The following theorem provides a formula for the absolute value of elements of the oscillator semigroup.

Theorem 21. Let $A \in \text{Sym}_{++}^{\text{qnd}}(\mathbb{C}^{2d})$. Then

$$\left|\operatorname{Op}(\mathrm{e}^{-A})\right| = \frac{\sqrt[4]{\det\left(\mathbbm{1} + (B\theta)^2\right)}}{\sqrt[4]{\det(\mathbbm{1} + \overline{A}\theta A\theta)}} \operatorname{Op}(\mathrm{e}^{-B}), \qquad (11.2)$$

where

$$B = c \left(\sqrt{c(\overline{A}\theta)c(A\theta)} \right) \theta.$$
(11.3)

 $Besides, \ the \ function$

$$\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d}) \ni A \mapsto \left|\operatorname{Op}(\mathrm{e}^{-A})\right|$$

is smooth.

Proof. By Proposition 16, $c(\overline{A}\theta)c(A\theta) = \overline{c(A\theta)}^{-1}c(A\theta) \in Sp_p(\mathbb{C}^{2d})$. Hence, by Proposition 15, we can define $\sqrt{c(\overline{A}\theta)c(A\theta)} \in Sp_p(\mathbb{C}^{2d})$. Therefore, *B* defined in (11.3) belongs to $Sym_p^{qnd}(\mathbb{R}^{2d})$ and satisfies $\overline{A}\#A = B\#B$.

We have

$$Op(e^{-B})^2 = \frac{1}{\sqrt{\det(\mathbb{1} + (B\theta)^2)}} Op(e^{-B\#B}).$$
 (11.4)

Hence,

$$Op(e^{-A})^*Op(e^{-A}) = \frac{\sqrt{\det(\mathbb{1} + (B\theta)^2)}}{\sqrt{\det(\mathbb{1} + \overline{A}\theta A\theta)}}Op(e^{-B})^2.$$
(11.5)

Besides, $\operatorname{Op}(e^{-B}) \ge 0$. Therefore, $|\operatorname{Op}(e^{-A})|$ is given by (11.2).

Now the square root is a smooth function on the set of invertible matrices (and obviously on the set of nonzero numbers). In the formula (11.3) for $A \in \text{Sym}_{++}^{\text{qnd}}(\mathbb{C}^{2d})$, we never need to take roots of zero or of non-invertible matrices, because $\mathbb{1} \pm A\theta$ and $\mathbb{1} \pm \overline{A}\theta$ are invertible. Therefore,

$$\operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d}) \ni A \mapsto \sqrt{c(\overline{A}\theta)c(A\theta)}$$
(11.6)

is smooth. Therefore, the map $A\mapsto B$ is smooth

For $A \in \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$, $\overline{A}, B \in \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$. Therefore, by Proposition 5.10, $\mathbb{1} + \overline{A}\theta A\theta$ and $\mathbb{1} + (B\theta)^2$ are invertible. Hence, the prefactors of (11.2) are smooth. This ends the proof of the smoothness of (11.2).

Let V be a closed operator such that $\text{Ker}V = \text{Ker}V^* = \{0\}$. Then it is well known that there exists a unique unitary operator U such that we have the identity

$$V = U|V|. \tag{11.7}$$

called the *polar decomposition*.

Theorem 22. Let $A \in \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^{2d})$. Let $B \in \operatorname{Sym}_{p}^{\operatorname{qnd}}(\mathbb{C}^{2d})$ be defined as in (11.3). Then

$$\sqrt{\det(\mathbb{1} + A\theta)} \operatorname{Op}(e^{-A}) \Big| = \sqrt{\det(\mathbb{1} + B\theta)} \operatorname{Op}(e^{-B}), \quad (11.8)$$

and the unitary operator U that appears in the polar decomposition

$$\sqrt{\det(\mathbb{1} + A\theta)} \operatorname{Op}(e^{-A}) = U\sqrt{\det(\mathbb{1} + B\theta)} \operatorname{Op}(e^{-B})$$
(11.9)

belongs to $Mp(\mathbb{R}^{2d})$. Besides, if

$$iC := A \# (-B)$$
 (11.10)

is well defined, then

$$U = \epsilon \sqrt{\det(\mathbb{1} + C\omega)} \operatorname{Op}(\mathrm{e}^{-\mathrm{i}C}), \qquad (11.11)$$

where $\epsilon = 1$ or $\epsilon = -1$.

Proof. By (5.10),

$$1 + \overline{A}\theta A\theta = (1 + \overline{A}\theta)(1 + \overline{A}\#A\theta)^{-1}(1 + A\theta), \qquad (11.12)$$

$$1 + B\theta B\theta = (1 + B\theta)(1 + B\#B\theta)^{-1}(1 + B\theta), \qquad (11.13)$$

Besides, $\overline{A}#A = B#B$. This together with (11.2) implies (11.8).

Assume now that iC := A # (-B) is well defined. Then clearly

$$\sqrt{\det(\mathbb{1} + A\theta)\operatorname{Op}(e^{-A})} = \epsilon \sqrt{\det(\mathbb{1} + B\theta)}\operatorname{Op}(e^{-B})\sqrt{\det(\mathbb{1} + iC\theta)}\operatorname{Op}(e^{-iC}).$$
(11.14)

It remains to show that iC is purely imaginary.

$$\overline{A\#(-B)} = (-B)\#\overline{A} = (-B)\#\overline{A}\#A(-A)$$
(11.15)

$$= (-B)\#B\#B\#(-A) \tag{11.16}$$

$$= B\#(-A) = -A\#(-B).$$
(11.17)

12. Trace and the trace norm

Suppose we have an operator K on $L^2(\mathbb{R}^d)$. As proven in [13] (for a more general setting, see [4, 5]), if K has a continuous kernel K(x, y) belonging to $L^2(\mathbb{R}^d \times \mathbb{R}^d)$ and $x \mapsto K(x, x)$ is in $L^1(\mathbb{R}^d)$, then

$$\operatorname{Tr} K = \int K(x, x) \,\mathrm{d}x. \tag{12.1}$$

In the case of Weyl–Wigner quantization, for a symbol k we get

Tr Op(k) =
$$\int Op(k)(x, x) dx = (2\pi)^{-d} \int k(x, \xi) dx d\xi.$$
 (12.2)

This easily implies the following proposition:

Proposition 23. The trace of operator $Op(e^{-A})$ with $A \in Sym_{++}(\mathbb{C}^{2d})$ is

$$\operatorname{Tr}\operatorname{Op}(\mathrm{e}^{-A}) = \frac{1}{2^d\sqrt{\det A}} = \frac{1}{2^d\sqrt{\det A\theta}}.$$
(12.3)

(Note that det $\theta = 1$, hence we could insert θ in (12.3)).

One can also compute the trace of the absolute value of elements of the oscillator semigroup, the so-called trace norm.

Theorem 24. The trace norm of $Op(e^{-A})$, where $A \in Sym_{++}(\mathbb{C}^{2d})$, is

$$\operatorname{Tr} \left| \operatorname{Op}(\mathrm{e}^{-A}) \right| = \frac{\sqrt{2}}{2^d \sqrt{\det \left| (\mathbb{1} + A\theta) (\mathbb{1} - \sqrt{c(A^*\theta)c(A\theta)}) \right|}}.$$
 (12.4)

Proof. Equations (12.3) and (11.2) imply

$$\operatorname{Tr} \left| \operatorname{Op}(\mathrm{e}^{-A}) \right| = \frac{\sqrt[4]{\det\left(\mathbbm{1} + (B\theta)^2\right)}}{2^d \sqrt[4]{\det(\mathbbm{1} + \overline{A}\theta A\theta)(B\theta)^2}}.$$
(12.5)

Now, easy algebra shows that

$$\frac{\det\left(\mathbbm{1} + (B\theta)^2\right)}{\det(\mathbbm{1} + \overline{A}\theta A\theta)(B\theta)^2} = \frac{2\det\left(\mathbbm{1} + c(\overline{A}\theta)c(A\theta)\right)}{\det(\mathbbm{1} + \overline{A}\theta A\theta)(\mathbbm{1} - \sqrt{c(\overline{A}\theta)c(A\theta)})^2} = \frac{4}{\det(\mathbbm{1} + \overline{A}\theta)(\mathbbm{1} + A\theta)(\mathbbm{1} - \sqrt{c(\overline{A}\theta)c(A\theta)})^2} = \frac{2^2}{\left(\det\left|(\mathbbm{1} + A\theta)\left(\mathbbm{1} - \sqrt{c(\overline{A}\theta)c(A\theta)}\right)\right|\right)^2}.$$

Corollary 25. The trace norm of $Op(e^{-B})$, where $B \in Sym_{++}(\mathbb{R}^{2d})$, is

$$\operatorname{Tr} \left| \operatorname{Op}(\mathrm{e}^{-B}) \right| = \frac{\sqrt{2}}{2^d \sqrt{\det \left| |\mathbb{1} + B\theta| - |\mathbb{1} - B\theta| \right|}}.$$
 (12.6)

Thus, if we diagonalize simultaneously B and $\omega,$ as in the proof of Proposition 10, then

$$\operatorname{Tr} \left| \operatorname{Op} \left(e^{-B} \right) \right| = \frac{\sqrt{2}}{4^d \prod_{\lambda_i < 1} \lambda_i}.$$
(12.7)

13. Operator norm

Proposition 26. Let $B \in \text{Sym}_{++}(\mathbb{R}^{2d})$. Then

$$\left\|\operatorname{Op}\left(\mathrm{e}^{-B}\right)\right\| = \frac{1}{\sqrt{\det(\mathbb{1} + \sqrt{B\theta B\theta})}}.$$
(13.1)

Proof. First, using (1.2), we check that in the case of one degree of freedom we have

$$\left\|\operatorname{Op}\left(\mathrm{e}^{-\lambda(x^{2}+p^{2})}\right)\right\| = \frac{1}{1+\lambda}.$$
(13.2)

An arbitrary B we can diagonalize together with θ , as in the proof of Proposition 10(3), and then we obtain

$$\|\operatorname{Op}(e^{-B})\| = \prod_{i=1}^{d} \frac{1}{1+\lambda_i}.$$
 (13.3)

Now the right-hand side of (13.3) can be rewritten as the right-hand side of (13.1). $\hfill \Box$

Using (11.8), we obtain an identity for an arbitrary element of the oscillator semigroup. A closely related result is described in [21, Theorem 5.2].

Theorem 27. Let $A \in \text{Sym}_{++}(\mathbb{C}^{2d})$. Then

$$\left\|\sqrt{\det(\mathbb{1}+A\theta)}\operatorname{Op}(e^{-A})\right\| = \frac{\sqrt{\det\left(\mathbb{1}+c\left(\sqrt{c(\overline{A}\theta)c(A\theta)}\right)\right)}}{\sqrt{\det\left(\mathbb{1}+\sqrt{c\left(\sqrt{c(\overline{A}\theta)c(A\theta)}\right)c\left(\sqrt{c(\overline{A}\theta)c(A\theta)}\right)}\right)}}.$$
(13.4)

14. One degree of freedom

In the case of one degree of freedom we have a complete characterization of quantum nondegenerate symmetric matrices.

Theorem 28. Let $A \in \text{Sym}(\mathbb{C}^2)$. Then $A \in \text{Sym}^{\text{qnd}}(\mathbb{C}^2)$ iff det $A \neq 1$.

Proof. We easily compute that for $A \in \text{Sym}(\mathbb{C}^2)$,

$$\det(\mathbb{1} + A\theta) = 1 - \det A.$$

Next we describe the quantum degenerate case for one degree of freedom on the level of the oscillator group.

Theorem 29. Elements of $Osc_{++}(\mathbb{C}^2)$ that are not proportional to an element of $Osc_{++}^{nor}(\mathbb{C}^2)$ are proportional to a projection. They have the integral kernel of the form

$$ce^{-(ax^2+by^2)},$$
 (14.1)

where $a, b, c \in \mathbb{C}$, $\operatorname{Re} a, \operatorname{Re} b > 0$. The Weyl symbol of the operator with the kernel (14.1) is

$$c\frac{2\sqrt{\pi}}{\sqrt{a+b}}\,\mathrm{e}^{-A},\tag{14.2}$$

where

$$A = \frac{1}{(a+b)} \begin{bmatrix} 4ab & i(-a+b) \\ i(-a+b) & 1 \end{bmatrix}.$$
 (14.3)

Matrices of the form (14.3) with $\operatorname{Re} a, \operatorname{Re} b > 0$ are precisely all matrices in

$$\operatorname{Sym}_{++}(\mathbb{C}^2)\backslash \operatorname{Sym}_{++}^{\operatorname{qnd}}(\mathbb{C}^2).$$
(14.4)

15. Application to the boundedness of pseudo-differential operators

Cordes proved the following result [10]:

Theorem 30. Suppose $k \in \mathscr{S}'(\mathbb{R}^d \times \mathbb{R}^d)$ and $s > \frac{d}{2}$. Then there exists a constant $c_{d,s}$ such that

$$\|Op(k)\| \leq c_{d,s} \|(1 - \Delta_x)^s (1 - \Delta_p)^s k\|_{\infty}.$$
 (15.1)

The above result can be called the *Calderón and Vaillancourt Theorem for* the Weyl quantization. (The original result of Calderón and Vaillancourt [9] concerned the x - p quantization, known also as the standard or Kohn-Nirenberg quantization).

Note that Theorem 30 is not optimal with respect to the number of derivatives. The optimal bound on the number of derivatives for the Weyl quantization is $s > \frac{d}{4}$. It was discovered by A. Boulkhemair [3] and it requires a different proof than the one developed by Cordes.

In what follows we will describe a proof of Theorem 30 which gives an estimate of $c_{d,s}$. We will follow the ideas of Cordes and Kato ([10] and [18]), who however do not give an explicit bound on the constant $c_{d,s}$. The estimate (1.4) for the trace norm of operators with Gaussian symbols plays an important role in our proof.

We start with the following proposition.

Proposition 31. For $s > \frac{d}{2}$, define the functions

$$\psi_s(\xi) := (2\pi)^{-d} \int d\zeta \, (1+\zeta^2)^{-s} e^{i\zeta\xi},$$
(15.2)

$$P_s(x,p) := \psi_s(x)\psi_s(p).$$
 (15.3)

Then $Op(P_s)$ is of trace class and

$$\operatorname{Tr} \left| \operatorname{Op}(P_s) \right| \le \frac{\Gamma(s)^2 + \Gamma(s - \frac{d}{2})^2}{(2\pi)^d \Gamma(s)^2}.$$
(15.4)

Proof. Let us use the so-called Schwinger parametrization

$$X^{-s} = \frac{1}{\Gamma(s)} \int_0^\infty e^{-tX} t^{s-1} dt$$
 (15.5)

to get

$$\psi_s(\xi) = \frac{1}{\Gamma(s)(2\pi)^d} \int_0^\infty dt \int d\zeta \, \mathrm{e}^{-t(1+\zeta^2)} t^{s-1} \mathrm{e}^{\mathrm{i}\zeta\xi}$$
$$= \frac{1}{\pi^{\frac{d}{2}} 2^d \Gamma(s)} \int_0^\infty dt \, t^{s-\frac{d}{2}-1} \mathrm{e}^{-t-\frac{\xi^2}{4t}}.$$
(15.6)

Now

$$P_s(x,p) = \frac{1}{\pi^d 2^{2d} \Gamma^2(s)} \int_0^\infty \mathrm{d}u \int_0^\infty \mathrm{d}v \mathrm{e}^{-u-v-\frac{x^2}{4u}-\frac{p^2}{4v}} (uv)^{s-\frac{d}{2}-1}.$$
 (15.7)

By (1.4), we have

$$\operatorname{Tr} \left| \operatorname{Op} \left(e^{-\alpha x^2 - \beta p^2} \right) \right| = \begin{cases} \frac{1}{(2\sqrt{\alpha\beta})^d}, & \alpha\beta \le 1, \\ \frac{1}{2^d}, & 1 \le \alpha\beta. \end{cases}$$
(15.8)

Hence,

$$\operatorname{Tr} \left| \operatorname{Op}(P_{s}) \right| \\
\leq \frac{1}{2^{2d} \pi^{d} \Gamma^{2}(s)} \int_{0}^{\infty} \mathrm{d}u \int_{0}^{\infty} \mathrm{d}v e^{-u-v} \operatorname{Tr} \left| \operatorname{Op} \left(e^{-\frac{x^{2}}{4u} - \frac{p^{2}}{4v}} \right) \right| (uv)^{s-\frac{d}{2}-1} \\
\leq \frac{1}{2^{d} \pi^{d} \Gamma^{2}(s)} \left(\int_{4 \leq uv, \ u,v > 0} \mathrm{d}u \int_{0}^{d} \mathrm{d}v e^{-u-v} (uv)^{s-1} + \int_{uv \leq 4, \ u,v > 0} \mathrm{d}u \int_{0}^{d} \mathrm{d}v e^{-u-v} (uv)^{s-\frac{d}{2}-1} \right) \quad (15.9) \\
\leq \frac{\Gamma(s)^{2} + \Gamma(s - \frac{d}{2})^{2}}{2^{d} \pi^{d} \Gamma^{2}(s)}.$$

Proposition 32. Let B be a self-adjoint trace class operator and $h \in L^{\infty}(\mathbb{R}^{2d})$. Then

$$C := \frac{1}{(2\pi)^d} \int \mathrm{d}y \int \mathrm{d}w h(y, w) \mathrm{e}^{-\mathrm{i}y\hat{p} + \mathrm{i}w\hat{x}} B \mathrm{e}^{\mathrm{i}y\hat{p} - \mathrm{i}w\hat{x}}$$
(15.10)

 $is \ bounded \ and$

$$||C|| \le \operatorname{Tr} |B| ||h||_{\infty}.$$
 (15.11)

Proof. For $\Phi \in L^2(\mathbb{R}^d)$, $\|\Phi\| = 1$, define $T_{\Phi} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^{2d})$ by

$$T_{\Phi}\Theta(y,w) := (2\pi)^{-\frac{d}{2}} \left(\Phi | \mathrm{e}^{\mathrm{i}y\hat{p} - \mathrm{i}w\hat{x}}\Theta \right), \quad \Theta \in L^2(\mathbb{R}^{2d}).$$
(15.12)

We check that T_{Φ} is an isometry. This implies that for $\Phi, \Psi \in L^2(\mathbb{R}^d)$ of norm one

$$\frac{1}{(2\pi)^d} \int \mathrm{d}y \int \mathrm{d}w h(y,w) \mathrm{e}^{-\mathrm{i}y\hat{p}+\mathrm{i}w\hat{x}} |\Phi) (\Psi| \mathrm{e}^{\mathrm{i}y\hat{p}-\mathrm{i}w\hat{x}}$$
(15.13)

is bounded and its norm is less than $||h||_{\infty}$. Indeed, (15.13) can be written as the product of three operators

$$T_{\Phi}^* h T_{\Psi}, \tag{15.14}$$

where h is meant to be the operator of the multiplication by the function h on the space $L^2(\mathbb{R}^{2d})$. Now it suffices to write

$$B = \sum_{i=1}^{\infty} \lambda_i |\Phi_i\rangle (\Psi_i|, \qquad (15.15)$$

where Φ_i, Ψ_i are normalized, $\lambda_i \ge 0$ and $\operatorname{Tr} |B| = \sum_{i=1}^{\infty} \lambda_i$.

Proof of Theorem 30. Set

$$h := (1 - \Delta_x)^s (1 - \Delta_p)^s k.$$
(15.16)

Then

$$k(x,p) = (1 - \Delta_x)^{-s} (1 - \Delta_p)^{-s} h(x,p)$$

= $\int dy \int dw P_s(x - y, p - w) h(y,w).$ (15.17)

Hence

$$Op(k) = \int dy \int dw Op(P_s(x - y, p - w))h(y, w)$$

= $\frac{1}{(2\pi)^d} \int dy \int dw h(y, w) e^{-iy\hat{p} + iw\hat{x}} Op(P_s) e^{iy\hat{p} - iw\hat{x}}.$ (15.18)

Therefore, by Proposition 32,

$$\|\operatorname{Op}(k)\| \le \operatorname{Tr} |\operatorname{Op}(P_s)| \|h\|_{\infty}.$$
(15.19)

Thus we can set

$$c_{d,s} = \operatorname{Tr} |\operatorname{Op}(P_s)|, \qquad (15.20)$$

 \square

which is finite by Proposition 31.

Proposition 31 yields an explicit estimate for $c_{d,s}$ given by the right-hand side of (15.4). Actually, in the proof of Proposition 31 we have an even better, although more complicated explicit estimate given by (15.9).

16. Complex symplectic Lie algebra

The well known symplectic Lie algebra in dimension 2d is defined as the set of $R \in L(\mathbb{R}^{2d})$ satisfying

$$R^{\#}\omega + \omega R = 0. \tag{16.1}$$

Similarly, the set of $R \in L(\mathbb{C}^{2d})$ satisfying (16.1) is called the *complex symplectic* Lie algebra in dimension 2d and denoted $sp(\mathbb{C}^{2d})$. As usual in the complex case, we usually prefer to replace ω in (16.1) with θ .

We define

$$sp_+(\mathbb{C}^{2d}) := \{ D \in sp(\mathbb{C}^{2d}) \mid D^*\theta + \theta D \ge 0 \},$$

$$(16.2)$$

$$sp_{++}(\mathbb{C}^{2d}) := \{ D \in sp(\mathbb{C}^{2d}) \mid D^*\theta + \theta D > 0 \}.$$
 (16.3)

We also introduce

$$sp_{\rm h}(\mathbb{C}^{2d}) := \{ D \in sp(\mathbb{C}^{2d}) \mid \overline{D} = -D \},$$
(16.4)

$$sp_{p}(\mathbb{C}^{2d}) := \{ D \in sp_{h}(\mathbb{C}^{2d}) \mid \theta D > 0 \}.$$
 (16.5)

Proposition 33. (1) Let $D \in sp(\mathbb{C}^{2d})$. Then $e^{-D} \in Sp(\mathbb{C}^{2d})$. (2) Let $D \in sp_{++}(\mathbb{C}^{2d})$. Then $e^{-D} \in Sp_{++}(\mathbb{C}^{2d})$. (3) Let $D \in sp_{\rm h}(\mathbb{C}^{2d})$. Then $e^{-D} \in Sp_{\rm h}(\mathbb{C}^{2d})$. (4) Let $D \in sp_{\rm p}(\mathbb{C}^{2d})$. Then $e^{-D} \in Sp_{\rm p}(\mathbb{C}^{2d})$.

Proof. Claims (1) and (3) are obvious corollaries from the definitions.

(2) Integrating

$$\frac{d}{dt} (e^{-tD})^* \theta e^{-tD} = -(e^{-tD})^* (D^*\theta + \theta D) e^{-tD} < 0,$$
(16.6)

we obtain $(e^{-D})^* \theta e^{-D} < \theta$.

(4) We can write

 $e^{-D} = e^{-\theta(\theta D)}$.

We diagonalize simultaneously the positive form θD and θ . In the diagonalizing basis, the matrices θ and θD commute, the former has eigenvalues ± 1 , the latter has positive eigenvalues. Hence e^{-D} has positive eigenvalues.

17. Hamiltonians

Let $H \in \text{Sym}(\mathbb{C}^{2d})$. As usual, the quadratic form $\mathbb{R}^{2d} \ni y \mapsto y^{\#}Hy \in \mathbb{C}$ will be also denoted by H. Let us briefly recall the properties of quantum quadratic Hamiltonians Op(H) and their relationship to the metaplectic group. We will use [11] as the basic reference, although most of these facts are well known.

Set

$$D := 2H\omega^{-1}.\tag{17.1}$$

Clearly, $D \in sp(\mathbb{C}^{2d})$. We will say that D is the symplectic generator associated with the Hamiltonian H.

First assume that $H \in \text{Sym}(\mathbb{R}^{2d})$. It is well known that then Op(H) is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^d)$ (see, e.g., [11, Theorem 10.21]). Moreover, $e^{itOp(H)} \in Mp(\mathbb{R}^{2d})$ (see, e.g., [11, Theorem 10.36]). Under the epimorphism 10.2, $e^{itOp(H)}$ is mapped onto e^{tD} , where $D \in sp(\mathbb{R}^{2d})$ is defined by (17.1) (see, e.g., [11, Theorem 10.22]). Finally, if $e^{tD} \in Sp^{reg}(\mathbb{R})$ and $C_t := c(e^{tD})\omega^{-1}$,

$$e^{itOp(H)} = \sqrt{\det(1+C_t\omega)}Op(e^{-iC_t}), \qquad (17.2)$$

see, e.g., [11, Theorem 10.35].

Next consider $H \in \text{Sym}_{++}(\mathbb{C}^{2d})$. It is easy to show that Op(H) extends from $\mathcal{S}(\mathbb{R}^d)$ to a maximal accretive operator (see, e.g., [11, Theorem 10.21]). Moreover, $e^{-t\text{Op}(H)} \in \text{Osc}_{++}^{\operatorname{nor}}(\mathbb{C}^{2d})$. In fact, if D is defined as in (17.1), then $-iD \in sp_{++}(\mathbb{C}^{2d})$, and hence by Proposition 33(2), $e^{itD} \in Sp_{++}(\mathbb{C}^{2d})$. Moreover, under the epimorphism (6.7), $e^{-t\text{Op}(H)}$ is mapped onto e^{itD} . Finally, if we set $A_t := c(e^{itD})\theta$, then

$$e^{-tOp(H)} = \sqrt{\det(\mathbb{1} + A_t\theta)}Op(e^{-A_t}), \qquad (17.3)$$

see, e.g., in [11, Theorem 10.35].

18. Holomorphic 1-parameter subsemigroups

Let $H \in \text{Sym}_{++}(\mathbb{C}^{2d})$. As we recalled above, Op(H) is maximally accretive, and hence

$$[0,\infty[\ni t \mapsto e^{-tOp(H)}$$
(18.1)

is a well defined subsemigroup of $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$. One can ask whether it can be extended to a larger subsemigroup if we replace real t with a complex parameter.

If H is real, then the answer is obvious and simple. Then Op(H) is a positive self-adjoint operator and we have a well defined semigroup

$$\{z \in \mathbb{C} \mid \operatorname{Re} z \ge 0\} \ni z \mapsto e^{-z\operatorname{Op}(H)}$$
(18.2)

inside $\operatorname{Osc}_+(\mathbb{C}^{2d})$. For $\operatorname{Re} z > 0$, (18.2) is in $\operatorname{Osc}_{++}(\mathbb{C}^{2d})$.

If ${\cal H}$ is not real, then the answer can be more complicated.

Let $D \in sp_{++}(\mathbb{C}^{2d})$ correspond to H as in (17.1). Clearly

$$\mathbb{C} \ni z \mapsto e^{izD} \in Sp(\mathbb{C}^{2d}) \tag{18.3}$$

is a holomorphic subgroup of $Sp(\mathbb{C}^{2d})$. However, not all elements of the complex symplectic group correspond to (bounded) operators on the Hilbert space. Motivated by this, we define

$$\mathcal{A}_{+}(H) := \{ z \in \mathbb{C} \mid e^{izD} \in Sp_{+}(\mathbb{C}^{2d}) \},$$
(18.4)

$$\mathcal{A}_{++}(H) := \{ z \in \mathbb{C} \mid e^{izD} \in Sp_{++}(\mathbb{C}^{2d}) \}.$$
(18.5)

From the definition it is obvious that $\mathcal{A}_+(H)$ is a closed subsemigroup of \mathbb{C} and $\mathcal{A}_{++}(H)$ is an open subsemigroup of $\mathcal{A}_+(H)$.

If $z \in \mathcal{A}_{++}(H)$, then we define

$$A_{z} := c(\mathrm{e}^{\mathrm{i}zD})\theta \in \mathrm{Sym}_{++}(\mathbb{C}^{2d}), \qquad (18.6)$$

$$e^{-z\operatorname{Op}(H)} := \sqrt{\det(\mathbb{1} + A_z\theta)}\operatorname{Op}(e^{-A_z}).$$
(18.7)

(The definition of (18.7) is consistent with the usual definition of $e^{-zOp(H)}$ for real positive z).

The shapes of $\mathcal{A}_+(H)$ and $\mathcal{A}_{++}(H)$ can be quite curious. This is already seen in the simplest nontrivial example, known under the name of the *Davies harmonic oscillator*, as shown in [1], see also [21]. In this example, $\psi \in \left] -\frac{\pi}{2}, \frac{\pi}{2} \right]$ is a parameter, the classical and quantum Hamiltonians and the generator are

$$H_{\psi} := e^{i\psi}x^2 + e^{-i\psi}p^2, \qquad (18.8)$$

$$\hat{H}_{\psi} := \operatorname{Op}(H_{\psi}) = \mathrm{e}^{\mathrm{i}\psi}\hat{x}^2 + \mathrm{e}^{-\mathrm{i}\psi}\hat{p}^2,$$
 (18.9)

$$D_{\psi} := 2 \begin{bmatrix} 0 & -e^{i\psi} \\ e^{-i\psi} & 0 \end{bmatrix}.$$
(18.10)

The proposition below reproduces the result of Aleman and Viola (see (1.2) of [1]).

Proposition 34. Let H_{ψ} be the Davies' harmonic oscillator, as above. Then

$$\mathcal{A}_{+}(H_{\psi}) = \left\{ z \in \mathbb{C} \mid \operatorname{Re}\left(z\right) \ge 0 \text{ and } |\operatorname{arg} \tanh z| + |\psi| \leqslant \frac{\pi}{2} \right\}, \qquad (18.11)$$

$$\mathcal{A}_{++}(H_{\psi}) = \left\{ z \in \mathbb{C} \mid \operatorname{Re}(z) > 0 \text{ and } |\operatorname{arg} \tanh z| + |\psi| < \frac{\pi}{2} \right\}.$$
(18.12)

Proof. iD_{ψ} generates a holomorphic group in $Sp(\mathbb{C}^{2d})$, which can be computed using $D_{\psi}^2 = -41$ as

$$e^{izD_{\psi}} = \begin{bmatrix} \cosh 2z & ie^{i\psi} \sinh 2z \\ -ie^{-i\psi} \sinh 2z & \cosh 2z \end{bmatrix}.$$
 (18.13)

Now

$$A_{\psi,z} = c(\mathrm{e}^{\mathrm{i}zD_{\psi}})\theta = 2\tanh z \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\psi} & 0\\ 0 & \mathrm{e}^{\mathrm{i}\psi} \end{bmatrix}.$$
 (18.14)

Let us denote $t := \arg \tanh z$. $A_{\psi,z}$ belongs to $\operatorname{Sym}_{++}(\mathbb{C}^{2d})$ iff $\operatorname{Re}(z) > 0$ and

$$\begin{cases} |t + \psi| < \frac{\pi}{2}, \\ |t - \psi| < \frac{\pi}{2}. \end{cases}$$
(18.15)

The above pair of inequalities is equivalent to

$$|t| + |\psi| < \frac{\pi}{2}.$$
 (18.16)

By Theorem 18(2), $A_{\psi,z} \in \text{Sym}_{++}(\mathbb{C}^{2d})$ iff $e^{izD_{\psi}} \in Sp_{++}(\mathbb{C}^{2d})$. The proof for $\mathcal{A}_{+}(H_{\psi})$ is analogous.

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