QUANTUM MECHANICS IN PHASE SPACE

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Abstract. This paper concerns the generalized Segal-Bargmann transform for compact Lie groups, which I introduced in [H1]. Firstly, I wish to describe the history of this transform and some related results by a variety of authors. Secondly, I wish to discuss the physical interpretation of this transform as providing a "phase space Hilbert space" for a quantum particle whose configuration space is a compact Lie group. This interpretation is strongly supported by the results of [H2, H3]. Thirdly, I wish to announce some new results concerning Toeplitz operators in the group setting.

In Section 1 I briefly recap the classical Segal-Bargmann transform for $\mathbb{R}^n$, and then discuss the origins in the work of L. Gross of the generalized Segal-Bargmann transform for compact groups. I mention several results which clarify and extend my results and those of Gross. In Section 2 I set some notation and describe two different versions of the generalized Segal-Bargmann transform. I discuss the relative merits of each version of the transform.

In Section 3 I explain how to identify the target manifold of the transform with "phase space," that is, with the cotangent bundle of the compact group. This identification is essential to the desired interpretation of the transform and involves some deep issues.

In Section 4 I describe an inversion formula for the generalized Segal-Bargmann transform which says, roughly, that the position wave function can be obtained from the phase space wave function by integrating out the momentum variables. In Section 5 I discuss the general notion of a phase space probability density, and define such a density in the context of a compact Lie group. I then give a uniform bound on the phase space probability density. This bound limits the phase space concentration of states and thus is a form of the uncertainty principle.

In Section 6 I discuss Toeplitz operators, and announce some new results. The main result is that the quantum mechanically important operators, including Schrödinger operators, can be represented in the phase space Hilbert space as Toeplitz operators. Finally, in Section 7, I compare the Hilbert space constructed in the generalized Segal-Bargmann transform to the Hilbert space constructed by means of geometric quantization.

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1. History and background

In studying quantum mechanics of a particle moving in $\mathbb{R}^n$, one can represent the Hilbert space in at least three ways: the "position" representation, the symmetric tensor representation, and the Segal-Bargmann holomorphic function representation. The first Hilbert space is the space of square-integrable functions on $\mathbb{R}^n$, with respect to either Lebesgue measure or Gauss measure. (One can convert easily from one measure to the other via the so-called ground state transform.) The second Hilbert space is the completion, with respect to a suitable inner product, of the symmetric tensor algebra over $\mathbb{R}^n$. The third Hilbert space is the space of holomorphic functions on $\mathbb{C}^n$ which are square-integrable with respect to Gauss measure. There is some confusion in the terminology–both the second and third Hilbert spaces are commonly called "Fock space." In my opinion Fock's name is more properly attached to the symmetric tensor space, and Segal and Bargmann's names to the holomorphic function space.

Each of these three Hilbert spaces has an intrinsically-defined set of creation and annihilation operators, and a natural ground state (or vacuum state). Between any two of the three spaces there is a unique unitary map which takes ground state to ground state and which intertwines the creation and annihilation operators. The intertwining map from the position representation to the holomorphic function representation is called the Segal-Bargmann transform [B, S1, S2, S3]. All three spaces and the associated operators and intertwining maps carry over to the infinite-dimensional setting ($n \to \infty$) of quantum field theory.

In [Gr1] L. Gross developed an analog of the symmetric tensor representation for a particle whose configuration space is an arbitrary simply-connected compact Lie group K, and constructed a unitary intertwining map between this space and the position Hilbert space. (See also the partly expository paper [Gr2], and further results in [Gr3].) As it turns out, the tensor space does not consist of symmetric tensors; instead it is a completion of the universal enveloping algebra of $\mathrm{Lie}(K)$. The Gross isomorphism is the unique unitary map taking ground state to ground state and intertwining the relevant creation and annihilation operators. Gross' results came out of the study of the infinite-dimensional set of paths in K, and the proof made use of stochastic analysis.

Motivated by these results of Gross, I constructed in [H1] a holomorphic function representation of the Hilbert space, and an associated unitary isomorphism of this space with the position Hilbert space. This isomorphism is to be viewed as a generalization of the classical Segal-Bargmann transform. The proof was in terms of Lie group theory and did not involve stochastic analysis. Thus the whole "triad" of spaces from the classical setting generalizes to the setting of a simply-connected compact Lie group.

I should point out that there is at least one important physical system whose configuration space is a compact Lie group, namely a rotor. That is, if you consider the rotational degrees of freedom of a rigid body, then the configuration space is the compact rotation group $\mathsf{SO}(3)$. Of course $\mathsf{SO}(3)$ is not simply-connected, but much of the analysis is applicable anyway. Specifically, the generalized Segal-Bargmann transform works perfectly well for non-simply-connected groups.

O. Hijab [Hi2, Hi2] gave a direct, non-probabilistic proof of the Gross isomorphism. B. Driver [D] gave a direct proof of the unitarity of the map from the holomorphic function space to the completed universal enveloping algebra, which was previously proved by combining my results with those of Gross. Driver also gave a new proof of the unitarity of the generalized Segal-Bargmann transform.

Going in the opposite direction, Gross and P. Malliavin [GM] have recently given a new probabilistic proof of the unitarity of the generalized Segal-Bargmann transform for K. This proof is by the authors' admission harder than either my proof or Driver's, but it gives an interesting connection between the generalized Segal-Bargmann transform and the original stochastic-analytical setting of Gross. Gross and Malliavin's proof makes use of the *infinite-dimensional classical* version of the Segal-Bargmann transform. In fact, the whole triad of spaces for a compact group can be embedded into the infinite-dimensional classical triad, using the Itô mapping. Here "infinite-dimensional" means that the underlying configuration space is infinite-dimensional.

The role played by $\mathbb{C}^n$ in the classical theory is played in the generalized theory by the "complexification" of the compact group K. Driver and Gross [DG] have further generalized one leg of the triad to the setting of an arbitrary simply-connected complex Lie group G, one that is not necessarily the complexification of a compact group. They give a unitary map from a certain Hilbert space of holomorphic functions on G to a certain completion of the universal enveloping algebra of $\mathrm{Lie}(G)$, which as usual is the unique unitary map taking ground state to ground state and intertwining the creation and annihilation operators. See also [Gr4].

A. Ashtekar, J. Lewandowski, D. Marolf, J. Mourão, and T. Thiemann [A] have given an infinite-dimensional extension of my generalized Segal-Bargmann transform, in which the compact group K is replaced by a certain space of connections-modulo-gauge-transformations. Specifically, given a manifold M and a principal K-bundle over M they describe a unitary transform whose domain is L^2 (connections/gauge) with respect to a suitable measure, and whose range is a certain L^2-space of holomorphic functions. According to the authors, this extension of the generalized Segal-Bargmann transform "is expected to play a key role in a non-perturbative, canonical approach to quantum gravity in 4 dimensions." R. Loll [L] has also used my generalized Segal-Bargmann transform in the context of quantum gravity. Loll's approach is distinct from but conceptually similar to that of Ashtekar *et al.*

Finally, P. Biane [Bi] has given an analog of the generalized Segal-Bargmann transform in the setting of free probability in the sense of Voiculescu.

2. The holomorphic function representation

In passing from the Segal-Bargmann transform on $\mathbb{R}^n$ to the generalized Segal-Bargmann transform on a compact Lie group K, one simply replaces each of the Gaussians in the classical transform by its natural geometric analog: a heat kernel. No fewer than three heat kernels appear in the generalized transform: the heat kernel on the configuration space, the heat kernel on the phase space, and the heat kernel on the "momentum space."

The set-up is as follows [H1]. Let K be an arbitrary connected compact Lie group. Unlike the Gross isomorphism, the generalized Segal-Bargmann transform does not require that K be simply-connected. In particular the physically interesting case $K = \mathsf{SO}(3)$ is permitted.

Let $\mathfrak{k}$ be the real Lie algebra of K. Fix an inner product $\langle\ ,\ \rangle$ on $\mathfrak{k}$ which is invariant under the adjoint action of K. The choice of an invariant inner product on $\mathfrak{k}$ gives rise to a bi-invariant Riemannian metric on K. Let Δ be the Laplace-Beltrami operator for this metric. Algebraically, Δ is the Casimir element of the universal enveloping algebra of $\mathfrak{k}$. For example, if

$$K = \mathsf{SU}(2) = \left\{ \left(\begin{array}{cc} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{array} \right) \middle| \, |\alpha|^2 + |\beta|^2 = 1 \right\},$$

then there is up to a constant exactly one invariant inner product on $\mathfrak{k}$. With the associated bi-invariant metric, $\mathsf{SU}(2)$ is isometric to a standard three-sphere. The operator Δ is then the standard spherical Laplacian on S^3.

Let $K_{\mathbb{C}}$ be the complexification of K. This is defined by a universal property (see [H1]), and satisfies the following two properties: 1) the Lie algebra $\mathfrak{k}_{\mathbb{C}}$ of $K_{\mathbb{C}}$ is the complexification of $\mathfrak{k}$, and 2) $K_{\mathbb{C}}$ contains K as a subgroup. For example, if $K = \mathsf{SU}(n)$, then $K_{\mathbb{C}} = \mathsf{SL}(n;\mathbb{C})$. Let $\rho_t(x)$ denote the heat kernel on K, that is, the fundamental solution at the identity of the heat equation

$$\frac{d\rho}{dt} = \frac{1}{2}\Delta\rho_t.$$

This is a smooth positive function on K which can be accurately estimated by means of the Poisson summation formula of Urakawa. (See [H3, U].) As proved in [H1], ρ_t has a unique analytic continuation from K to $K_{\mathbb{C}}$.

The choice of an inner product on $\mathfrak{k}$ determines a real-valued inner product on $\mathfrak{k}_{\mathbb{C}}$ given by $\langle X_1 + iY_1, X_2 + iY_2 \rangle = \langle X_1, X_2 \rangle + \langle Y_1, Y_2 \rangle$, where X_1, X_2, Y_1, Y_2 are in $\mathfrak{k}$. This inner product on $\mathfrak{k}_{\mathbb{C}}$ is Ad-K-invariant but *not* Ad-$K_{\mathbb{C}}$-invariant, unless K is commutative. This inner product on $\mathfrak{k}_{\mathbb{C}}$ gives rise to a left-invariant (but not right-invariant) Riemannian metric on $K_{\mathbb{C}}$ and thus to a left-invariant Laplace-Beltrami operator $\Delta_{K_{\mathbb{C}}}$. Let μ_t denote the heat kernel on $K_{\mathbb{C}}$, that is, the fundamental solution at the identity of the equation

$$\frac{d\mu}{dt} = \frac{1}{4}\Delta_{K_{\mathbb{C}}}\mu_t.$$

For convenience I have normalized the heat equation differently on K and on $K_{\mathbb{C}}$.

Finally, let ν_t be the function on $K_{\mathbb{C}}$ given by

$$\nu_t(g) = \int_K \mu_t(gx)\, dx, \qquad g \in K_{\mathbb{C}}.$$

This function can be interpreted as the heat kernel on the Riemannian symmetric space $K_{\mathbb{C}}/K$. The function ν_t (but unfortunately not the function μ_t) has an explicit formula, due to Gangolli. (See [H3, Eq. 11, Ga].)

So we have three different heat kernels on $K_{\mathbb{C}}$: the holomorphic function ρ_t which is the analytic continuation of the heat kernel on K; the real positive function μ_t which is the heat kernel on $K_{\mathbb{C}}$; and the real, positive, function ν_t which is the heat kernel on $K_{\mathbb{C}}/K$, viewed as a K-invariant function on $K_{\mathbb{C}}$. In the context of the one-dimensional classical Segal-Bargman transform, these would all be functions on $\mathbb{C}$, given by

$$\begin{aligned} \rho_t(z) &= \frac{1}{\sqrt{2\pi t}} e^{-z^2/2t}, \\ \mu_t(z) &= \frac{1}{\pi t} e^{-|z|^2/t}, \\ \nu_t(z) &= \frac{1}{\sqrt{\pi t}} e^{-(\mathrm{Im} z)^2/t}. \end{aligned}$$

In all that we do the real positive number t will be a parameter that plays the role of Planck's constant ($\hbar$).

There are two versions of the generalized Segal-Bargmann transform for K. The first is the "Gaussian" version. Let dx denote Haar measure on K and $\mathcal{H}(K_{\mathbb{C}})$ the space of holomorphic functions on $K_{\mathbb{C}}$. Define

$$B_t : L^2(K, \rho_t(x)\ dx) \to \mathcal{H}(K_{\mathbb{C}})$$

by the formula

$$B_t f(g) = \int_K \rho_t\left(gx^{-1}\right) f(x)\ dx \qquad g \in K_{\mathbb{C}}.$$

Here ρ_t refers to the analytic continuation of ρ_t from K to $K_{\mathbb{C}}$. Since ρ_t is the heat kernel, we see that

$$B_t f = \text{ analytic continuation of } e^{t\Delta/2} f.$$

Theorem 2.1. *For each $t > 0$, B_t is an isometric isomorphism of $L^2(K, \rho_t(x)\ dx)$ onto the space of holomorphic functions in $L^2(K_{\mathbb{C}}, \mu_t(g)\ dg)$, where dg is Haar measure on $K_{\mathbb{C}}$.*

This is the Gaussian version of the transform, in which the measures on both K and $K_{\mathbb{C}}$ are as Gaussian as possible (that is, heat kernels). The result is Theorem 1′ of [H1]. It is this version of the transform that connects directly with the Gross isomorphism. Note that the Hilbert spaces and the transform depend on the parameter t, which is to be interpreted as Planck's constant.

The "invariant" version of the transform is the map

$$C_t : L^2(K, dx) \to \mathcal{H}(K_{\mathbb{C}})$$

given by

$$C_t f(g) = \int_K \rho_t\left(gx^{-1}\right) f(x)\ dx \qquad g \in K_{\mathbb{C}}.$$

Note that C_t is the same map as B_t, except that we are using a different inner product on the domain space.

Theorem 2.2. *For each $t > 0$, C_t is an isometric isomorphism of $L^2(K, dx)$ onto the space of holomorphic functions in $L^2(K_{\mathbb{C}}, \nu_t(g)\ dg)$.*

This result is Theorem 2 of [H1].

The chief advantage of this version of the generalized Segal-Bargmann transform is that it is more invariant than the Gaussian version. The measure dx on K is invariant under the left- and right-action of K, as is the measure $\nu_t(g)\ dg$ on $K_{\mathbb{C}}$, and the transform commutes with the left- and right-action of K. Of course, sometimes one may not want to work invariantly; in the stochastic set-up of Gross the identity is a distinguished point and it is natural to work with a measure like $\rho_t(x)\ dx$ which is concentrated near the identity. Nevertheless, if one thinks simply of quantum mechanics for a particle with configuration space K, it is natural to make things as invariant as possible. As explained in the appendix of [H1], all of this makes little difference in the $\mathbb{R}^n$ case. But in the compact group case there is a significant difference between the two versions of the transform.

A more subtle advantage of the invariant version of the transform lies in my desire to interpret $C_t f$ as the "phase space wave function" corresponding to the "position wave function" f. Looking at the $\mathbb{R}^n$ case, you will see that this interpretation is natural because the "coherent state" with parameter z has mean position $\mathrm{Re}z$ and mean momentum $\mathrm{Im}z$. By contrast, to get this interpretation in the $\mathbb{R}^n$ case for B_t, one needs to replace $z \in \mathbb{C}^n$ by $z/2$. (See the appendix of [H1].) The analogous operation in $K_{\mathbb{C}}$ would be to replace g by $\sqrt{g}$, an unpleasant and ill-defined operation!

Finally, at a practical level, the invariant transform C_t is simply easier to calculate with. The reproducing kernel, for example, has a much nicer form in the invariant case, and this leads to results which seem unattainable in the Gaussian case.

All of this being said, the Gaussian version of the transform, and the associated measure μ_t, play a vital role in the results of Section 6.

A phase space Hilbert space is a natural setting for a semiclassical analysis of quantum mechanics, simply because it brings quantum mechanics closer to classical mechanics, which takes place in phase space. This idea has been developed on a non-rigorous level by A. Voros [V], who gives a simple and natural derivation of the Bohr-Sommerfeld quantization condition by expressing the WKB method in the Segal-Bargmann representation. Specifically, the Segal-Bargmann representation avoids the problem of turning points in the WKB method. Rigorous developments along these lines have been made by T. Paul and A. Uribe [PU], S. Graffi and Paul [GP], and L. Thomas and S. Wassell [TW].

3. The complex group as phase space

Physically, I wish to interpret the complex group $K_{\mathbb{C}}$ as the phase space corresponding to the configuration space K. (See Section 3 of [H3].) To this end, I wish to identify $K_{\mathbb{C}}$ with the customary phase space, namely the cotangent bundle of K. We identify the cotangent bundle $T^*(K)$ with $K \times \mathfrak{k}^*$ via left-translation, and then with $K \times \mathfrak{k}$ via the inner product on $\mathfrak{k}$. We then consider the map $\Phi : K \times \mathfrak{k} \to K_{\mathbb{C}}$ given by

$$\Phi(x, Y) = xe^{iY} \qquad x \in K,\ Y \in \mathfrak{k}.$$

This map is a diffeomorphism of $K \times \mathfrak{k} = T^*(K)$ with $K_{\mathbb{C}}$. For example, if $K = \mathsf{SU}(n)$ and $K_{\mathbb{C}} = \mathsf{SL}(n;\mathbb{C})$, then $Y \in \mathsf{su}(n)$ is skew (and trace zero), so that iY is self-adjoint and e^{iY} is self-adjoint and positive. Thus $xe^{iY} = UP$ is the ordinary polar decomposition for a matrix in $\mathsf{SL}(n;\mathbb{C})$. Physically, x represents position and Y momentum.

Although the map between $T^*(K)$ and $K_{\mathbb{C}}$ apparently favors left over right, this is an illusion. You could just as well identify $T^*(K)$ with $K \times \mathfrak{k}^*$ via right translation, then with $K \times \mathfrak{k}$ via the inner product, and then with $K_{\mathbb{C}}$ via the map $(x, Y) \to e^{iY}x$. It is easy to check that the resulting map from $T^*(K)$ to $K_{\mathbb{C}}$ is the same as the "left" one.

Theorem 3.1. *If we identify the symplectic manifold $T^*(K)$ with the complex manifold $K_{\mathbb{C}}$ as above, then we obtain a Kähler manifold.*

As explained in [H3], this result follows from the theory of adapted complex structures, as developed by Lempert and Szöke [LS, Sz] and by Guillemin and Stenzel [GS1, GS2].

Let ω denote the symplectic 2-form on $T^*(K)$, and let J denote the complex structure on $K_{\mathbb{C}}$, which can be viewed as living on $T^*(K)$ because of our identification. The Kähler condition means that

$$\begin{aligned} \omega(JX, JY) &= \omega(X, Y), \\ \omega(X, JX) &\geq 0 \end{aligned}$$

for all tangent vectors X and Y. The first condition implies that the Poisson bracket of two holomorphic functions is always zero.

Except in the case where K is commutative, $K_{\mathbb{C}}$ is *not* a homogeneous Kähler manifold. In particular the symplectic structure on $K_{\mathbb{C}}$ obtained via identification with $T^*(K)$ is neither left- nor right-invariant.

4. An inversion formula

In position-momentum coordinates, the measure $\nu_t(g)\,dg$ decomposes as follows

$$\nu_t(g)\,dg = dx\,\widetilde{\nu}_t(Y)\,dY$$

where dx is Haar measure on K, dY is Lebesgue measure on $\mathfrak{k}$, and $\widetilde{\nu}_t$ is an appropriate density on $\mathfrak{k}$. See Section 7 for an explicit formula for $\widetilde{\nu}_t$. In this notation we have the following inversion formula [H2, Theorem 1].

Theorem 4.1. *If $F = C_t f$, then*

$$f(x) = \int_{\mathfrak{k}} F\left(xe^{2iY}\right)\widetilde{\nu}_{t/2}(Y)\,dY \qquad x \in K. \tag{4.1}$$

Note the factors of two!

This formula says that one can recover the position wave function from the phase space wave function by integrating out the momentum variables, with respect to a suitable measure. Now, as explained in [H2], the integral (4.1) may not be absolutely convergent. Strictly speaking, the inversion should be accomplished by integrating over the set $|Y| \leq R$ and then taking a limit in $L^2(K, dx)$ as $R \to \infty$. In fact, the integral *cannot* always be convergent, because f is an arbitrary L^2 function on K, which may be infinite at certain points. However [H2, Theorem 3], if f is sufficiently smooth, then (4.1) is absolutely convergent and the inversion formula may be taken literally.

Note also that because B_t and C_t are the same transform (but with different inner products), (4.1) may also be regarded as an inversion formula for the Gaussian version of the transform. Since the transform is just the heat operator, followed by analytic continuation, (4.1) may be regarded as a formula for the *inverse* heat operator for K.

In the $\mathbb{R}^n$ case, $\widetilde{\nu}_t$ is just a Gaussian, and (4.1) becomes

$$f(x) = 2^n(2\pi t)^{-n/2}\int_{\mathbb{R}^n} F(x + 2iy)\,e^{-2y^2/t}dy.$$

Making the change of variable $\widetilde{y} = 2y$ this is equivalent to

$$f(x) = (2\pi t)^{-n/2}\int_{\mathbb{R}^n} F(x + i\widetilde{y})\,e^{-\widetilde{y}^2/2t}d\widetilde{y}. \tag{4.2}$$

We can now see how to verify the inversion formula in the $\mathbb{R}^n$ case. Fix a holomorphic function F on $\mathbb{C}^n$, and consider the right side of (4.2). Note that $(2\pi t)^{-n/2}\,e^{-\widetilde{y}^2/2t}$ is the heat kernel on $\mathbb{R}^n$. Thus differentiating with respect to t, integrating by parts, and using Cauchy-Riemann, we see that the right side of (4.2) satisfies the *inverse* heat equation. Furthermore, letting $t \to 0$, the right side of (4.2) converges to $F(x)$. So the right side of (4.2) is nothing but the *inverse* heat operator applied to $F(x)$. Since C_t is just the forward heat operator (followed by analytic continuation), the right side of (4.2) is $C_t^{-1}F$.

In the non-commutative case, the proof is largely the same, using the fact that ν_t is the heat kernel for $K_{\mathbb{C}}/K$. One simply needs to verify an identity [H2, Theorem 5] which relates the Laplacian for $K_{\mathbb{C}}/K$ to the Laplacian for K, using the Cauchy-Riemann equations. This identity works only with the factors of two the way they are in the theorem. The $\mathbb{R}^n$ case is special because in that case a re-scaling of the space variable in the heat kernel can be absorbed by an appropriate re-scaling of the time variable; no such result holds for the symmetric space $K_{\mathbb{C}}/K$.

5. An uncertainty principle

Let $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$ denote the space of holomorphic functions on $K_{\mathbb{C}}$ which are square-integrable with respect to the measure $\nu_t(g)\,dg$. Take $F \in \mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$ with $\|F\| = 1$. This means that

$$\int_{K_{\mathbb{C}}} |F(g)|^2\,\nu_t(g)\,dg = 1. \tag{5.1}$$

Now let dL denote the Liouville "phase volume" measure on $T^*(K)$, which we think of as a measure on $T^*(K)$ via our identification of $T^*(K)$ and $K_{\mathbb{C}}$. Then (5.1) can be rewritten as

$$\int_{K_{\mathbb{C}}} |F(g)|^2\,\nu_t(g)\,\sigma(g)\,dL = 1, \tag{5.2}$$

where σ is the "Jacobian" of the map Φ, given explicitly in [H3, Lemma 5].

I wish to think of $|F(g)|^2\,\nu_t(g)\,\sigma(g)$ as the phase space probability density associated to the state F. Now, according to (5.2), $|F(g)|^2\,\nu_t(g)\,\sigma(g)$ is a probability density, that is, a positive function which integrates to one. What is less clear is the sense in which this is *the* density associated to the state F.

In general one should have a different definition of phase space probability density for each quantization scheme. By a quantization scheme I mean a map Q from functions on phase space to operators on a Hilbert space. In specifying such a map some choice must be made (implicitly or explicitly) as to how to order non-commuting operators. Given such a map Q and a unit vector F in the corresponding Hilbert space, we can try to define a probability density p_F by the condition that

$$\int \phi(m)\,p_F(m)\,dL(m) = \langle F, Q(\phi)\,F\rangle \tag{5.3}$$

for all functions ϕ on phase space. Here $\langle\ ,\ \rangle$ denotes the inner product in the quantum Hilbert space. The condition (5.3) serves to define p_F as a distribution, provided that $Q(\phi)$ is a bounded operator whenever ϕ is a C^∞ function of compact support. In general there is no reason that p_F should be a positive function. For example, if Q is the Weyl quantization of $\mathbb{R}^{2n}$, then p_F is the famous Wigner function. (See Chap. 1, Sec. 8 and Chap. 2, Sec. 1 of [F].) The Wigner function may or may not be positive, depending on F.

As we shall see in the next section, the density $|F(g)|^2\,\nu_t(g)\,\sigma(g)$ satisfies the condition (5.3) if Q is the Berezin-Toeplitz quantization, which is a generalization of anti-Wick ordering. The fact that this density is always positive reflects the fact that the Berezin-Toeplitz quantization associates positive operators to positive functions. In the $\mathbb{R}^{2n}$ case, the Berezin-Toeplitz density can be obtained from the Wigner function by convolving with an appropriate Gaussian [F, Chap. 2, Sec. 7]. It is interesting that the Wigner function convolved with this Gaussian is always positive, even when the Wigner function itself is not.

By the way, it is worthwhile to contrast the $\mathbb{R}^n$ case of the inversion formula of Section 4 with a standard result concerning the Wigner function. It is well known that the position *probability density* $|f(x)|^2$ can be obtained (in the $\mathbb{R}^n$ case) by taking the Wigner function and integrating out the momentum variables. (This follows from the relationship between the Wigner function and the Weyl quantization.) By contrast, our inversion formula says that the position *wave function* $f(x)$ can be obtained from the phase space wave function by suitably integrating out the momentum variables.

In the $\mathbb{R}^n$ case, the probability density defined with respect to the Segal-Bargmann transform has the disadvantage that it is defined in terms of the Berezin-Toeplitz quantization instead of the more physically natural Weyl quantization. However, the Segal-Bargmann density has several advantages. First, it is always positive, while the Wigner function is not. Second, it is defined in terms of a phase space wave function, which allows you to take all of your operators and wave functions in phase space (as in [V]), and then simply to take the absolute value squared to get the phase space probability density. Last, the Segal-Bargmann density can be defined for systems with configuration space K, whereas (so far as I know) the Wigner function can be defined only for $\mathbb{R}^n$. For small Planck's constant (in $\mathbb{R}^n$), there is very little difference between the Wigner function and the Segal-Bargmann probability density.

Any result which gives a bound on the concentration of a state in phase space should be regarded as a form of the Heisenberg uncertainty principle. In the context of the generalized Segal-Bargmann transform for K we have the following such result [H3, Theorem 1].

Theorem 5.1. *For all $F \in \mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$ with $\|F\| = 1$ the phase space probability density satisfies*

$$|F(g)|^2 \nu_t(g)\, \sigma(g) \leq a_t (2\pi t)^{-n}.$$

Here $n = \dim K$ and a_t is a constant (independent of F and g) which tends to one exponentially fast as t tends to zero.

This bound is sharp in a sense described in [H3]. In the $\mathbb{R}^n$ case $\sigma \equiv 1$ and we may take $a_t = 1$.

Recalling that $t = \hbar$ (Planck's constant), we can recognize the quantity $(2\pi t)^n$ as the volume of a semiclassical cell in phase space. Thus the above result says that if E is a region of phase space whose volume is small compared to the volume of a semiclassical cell, then the probability of a particle being found in E is small, with estimates independent of the state F of the particle. Thus Theorem 5.1 is a physically natural bound on the phase space concentration.

It is easy to see that there is a bound on $|F(g)|^2 \nu_t(g)\, \sigma(g)$ which is independent of F, for F with $\|F\| = 1$. However, since $K_{\mathbb{C}}$ is not a homogeneous Kähler manifold, there is no *a priori* reason that there should exist bounds independent of g. In fact, amazing cancelations occur to give this independence, suggesting that there is something "right" about this set-up.

6. Toeplitz operators

As on any reasonable L^2-space of holomorphic functions, we may define Toeplitz operators on $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$. Let Π_t denote the orthogonal projection operator from $L^2(K_{\mathbb{C}}, \nu_t)$ onto the holomorphic subspace, which is a closed subspace. Then for ϕ a bounded measurable function on $K_{\mathbb{C}}$ we may define

$$T_t(\phi) : \mathcal{H}L^2(K_{\mathbb{C}}, \nu_t) \to \mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$$

by the formula

$$T_t(\phi) F = \Pi_t(\phi F).$$

The projection is necessary because ϕ is not assumed holomorphic. Because of the projection, two Toeplitz operators need not commute–this, of course, is the whole point!

We can think of $T_t(\phi)$ as an operator on the full L^2-space $L^2(K_{\mathbb{C}}, \nu_t)$ by making it zero on the orthogonal complement of the holomorphic subspace. Then

$$T_t(\phi) = \Pi_t M_\phi \Pi_t \tag{6.1}$$

where M_ϕ denotes multiplication by ϕ. Writing things in this way it is clear that

$$T_t(\overline{\phi}) = T_t(\phi)^* \tag{6.2}$$

and that

$$\|T_t(\phi)\| \leq \|\phi\|_{L^\infty}.$$

In particular, if ϕ is real then $T_t(\phi)$ is self-adjoint.

If ϕ is an unbounded but with moderate growth, then $T_t(\phi)$ will be a densely-defined operator on $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$. Because of domain issues, the adjoint identity (6.2) may not hold in the unbounded case. Some of these domain issues will be addressed in certain cases in [H4].

In general,

$$T_t(\phi_1) \cdots T_t(\phi_n) = \Pi_t M_{\phi_1} \Pi_t \cdots \Pi_t M_{\phi_n} \Pi_t.$$

Now, if the ϕ's all happen to be holomorphic, then all the projections except the first and last are unnecessary, so

$$\begin{aligned} T_t(\phi_1) \cdots T_t(\phi_n) &= \Pi_t M_{\phi_1} \cdots M_{\phi_n} \Pi_t \\ &= T_t(\phi_1 \cdots \phi_n). \end{aligned}$$

(There are no non-constant bounded holomorphic functions on $K_{\mathbb{C}}$, so there are some domain issues here, which I will ignore.) Taking the adjoint of this identity gives a similar formula in the case where all the ϕ's are anti-holomorphic. Finally, if ϕ is anti-holomorphic and ψ is holomorphic, then

$$\begin{aligned} T_t(\phi) T_t(\psi) &= \Pi_t M_\phi \Pi_t M_\psi \Pi_t \\ &= \Pi_t M_\phi M_\psi \Pi_t \\ &= T_t(\phi\psi). \end{aligned}$$

Note that this argument does not work with the order of ϕ and ψ reversed on the left! That is, the Toeplitz operator associated to the holomorphic function must be on the right.

In the $\mathbb{C}^1$ case this means that

$$\begin{aligned} T_t\left(\overline{z}^n z^m\right) &= T_t\left(\overline{z}^n\right) T_t\left(z^m\right) \\ &= T_t\left(\overline{z}\right)^n T_t\left(z\right)^m . \end{aligned}$$

Since $T_t(z)$ is (unitarily equivalent to) the creation operator and $T_t(\overline{z})$ is the annihilation operator, this corresponds to "anti-Wick ordering." Properties of the classical Wick and anti-Wick orderings, and connections with Toeplitz operators, are given in Chap. 2, Sec. 7 of [F].

If you compute a matrix entry of a Toeplitz operator between two holomorphic functions then the projections in (6.1) are unnecessary. Thus

$$\langle F, T_t(\phi) F\rangle = \int_{K_{\mathbb{C}}} \phi(g) \left|F(g)\right|^2 \nu_t(g)\ dg,$$

or, in the notation of Section 5,

$$\langle F, T_t(\phi) F\rangle = \int_{K_{\mathbb{C}}} \phi(g) \left|F(g)\right|^2 \nu_t(g) \sigma(g)\ dL.$$

Thus the expectation value of $T_t(\phi)$ in the state F is equal to the integral of ϕ against the probability density $\left|F(g)\right|^2 \nu_t(g)\sigma(g)$.

It is natural to regard the map $\phi \to T_t(\phi)$ as a quantization map, that is, a map from functions on the classical phase space $K_{\mathbb{C}} = T^*(K)$ to operators on a Hilbert space, with the parameter t playing the role of Planck's constant. In light of the above properties, this quantization should be thought of as a generalization of the anti-Wick ordering. The idea of using Toeplitz operators as a means of quantization began with Berezin. Toeplitz operators have been studied as a quantization map for various symplectic manifolds by various authors, including: Klimek and Lesniewski [KL1, KL2], for the disk and other Riemann surfaces; Coburn [Co], for $\mathbb{C}^n$; Borthwick, Lesniewski, and Upmeier [BLU], for bounded symmetric domains; and Bordemann, Meinrenken, and Schlichenmaier [BMS], for arbitrary compact Kähler manifolds. In all of these examples the Kähler manifolds studied are either compact or homogeneous. The case of $K_{\mathbb{C}} = T^*(K)$ is thus of interest because it is non-compact and (unless K is commutative) non-homogeneous.

I am not going to discuss general properties of Toeplitz operators on $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$, beyond the simple remarks above. Instead I am going to describe how certain quantum-mechanically important operators on $L^2(K, dx)$, including Schrödinger operators, can be represented as Toeplitz operators. I hope that this will lead to a semiclassical analysis of Schrödinger operators on $L^2(K, dx)$, using the phase space Hilbert space $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$. The results of this section are from the forthcoming paper [H4].

¿From the point of view of quantum mechanics the most important operators on $L^2(K, dx)$ are the momentum operators, the kinetic energy operator, and the multiplication (potential energy) operators. I want to conjugate each of these operators by the generalized Segal-Bargmann transform C_t to obtain operators on $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$, and to express these new operators as Toeplitz operators.

Let $\{X_k\}$ be an orthonormal basis for $\mathfrak{k}$ with respect to our chosen inner product. Define momentum operators $\{P_k\}$ by the formula

$$P_k f(x) = it \left.\frac{d}{ds}\right|_{s=0} f\left(xe^{sX_k}\right).$$

These are left-invariant first-order differential operators, the natural analogs of the operators $it\frac{\partial}{\partial x_k}$ on $L^2(\mathbb{R}^n, dx)$. Define the kinetic energy operator by the formula

$$\frac{1}{2}\sum_k P_k^2 = -\frac{t^2}{2}\Delta.$$

This is a bi-invariant operator on K. The momentum and kinetic energy operators are essentially self-adjoint on $C^\infty(K)$. Finally, define multiplication operators $M_V f = Vf$ for any function V on K. Each of these operators, when conjugated by C_t produces an operator on $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$.

Theorem 6.1. *For all $t > 0$,*

$$C_t P_k C_t^{-1} = T_t(\phi_k)$$

where

$$\phi_k\left(xe^{iY}\right) = \langle Y, X_k\rangle + tf_k(Y)$$

and where $f_k(Y)$ is a bounded function which is independent of t. If K is commutative then $f_k \equiv 0$.

For all $t > 0$,

$$C_t\left(-\frac{t^2}{2}\Delta\right)C_t = T_t(\phi)$$

where

$$\phi\left(xe^{iY}\right) = \frac{|Y|^2}{2} - \frac{n}{4}t - \frac{t^2}{2}|\rho|^2.$$

Here $n = \dim K$ and ρ is half the sum of the positive roots.

See [H3] for information on the roots. I have been a bit vague about domain issues here. In the case of the kinetic energy operator, the natural domain of the Toeplitz operator $T_t(\phi)$ coincides with the image under C_t of the self-adjoint domain of Δ. However, the corresponding statement for the momentum operators seems to be false. So a more precise statement is that $C_t P_k C_t^{-1}$ is equal to the closure of $T_t(\phi_k)$, where P_k is the self-adjoint version of the momentum operator.

Note that the function ϕ_k (the "Toeplitz symbol" of the operator P_k) is equal to the kth component of the classical momentum Y, plus a bounded term of order t. Similarly, the Toeplitz symbol of the kinetic energy operator is the classical kinetic energy function plus order t corrections, which happen to be constants. These corrections are to be expected because we are mixing two different quantization schemes.

For example, in the $\mathbb{R}^n$ case, the Toeplitz symbol of the kinetic energy operator is

$$\frac{|Y|^2}{2} - \frac{n}{4}t,$$

because $\rho = 0$ in that case. Now, $-\left(t^2/2\right)\Delta$ is the Weyl quantization of the classical kinetic energy function, and we are then taking not the Weyl symbol but the Toeplitz (anti-Wick) symbol of $-\left(t^2/2\right)\Delta$. But the Toeplitz symbol is obtained from the Weyl symbol by applying $e^{-t\Delta/4}$, which gives precisely the correction term $-nt/4$. (See [F, Prop. 2.96, 2.97].)

Theorem 6.2. *Suppose V is of the form $V = e^{t\Delta/2}\widetilde{V}$, for some function $\widetilde{V}$. Then*

$$C_t M_V C_t^{-1} = T_t\left(\phi_V\right)$$

where

$$\phi_V\left(g\right) = \frac{\int_K \mu_t\left(gy^{-1}\right)\widetilde{V}\left(y\right)\,dy}{\nu_t\left(g\right)}.$$

Recall that μ_t is the full heat kernel on $K_{\mathbb{C}}$, ν_t is the heat kernel for $K_{\mathbb{C}}/K$, and that the two functions are related by the formula $\nu_t\left(g\right) = \int_K \mu_t\left(gx\right)\,dx$. In particular, if $V \equiv 1$ then $\phi_V \equiv 1$. If K is commutative, then the heat kernel μ_t factors as $\mu_t\left(xe^{iY}\right) = \rho_{t/2}\left(x\right)\nu_t\left(e^{iY}\right)$. The factor of two is a result of the different normalizations of the heat kernel on K and on $K_{\mathbb{C}}$. Thus in the commutative case the above reduces to

$$\begin{aligned}
\phi_V\left(xe^{iY}\right) &= \int_K \rho_{t/2}\left(xy^{-1}\right)\widetilde{V}\left(y\right)\,dy \\
&= e^{-t\Delta/4}V\left(x\right),
\end{aligned}$$

provided that $e^{-t\Delta/4}V$ exists. In the non-commutative case, $\phi_V\left(xe^{iY}\right)$ will depend non-trivially on both x and Y.

Note that the theorem assumes that V can be expressed in the form $e^{t\Delta/2}\widetilde{V}$. This is more restrictive than necessary; according to [H4], ϕ_V exists provided only that V is of the form $e^{t\Delta/4}\widehat{V}$. However, I believe that in general $C_t M_V C_t^{-1}$ simply cannot be expressed as a Toeplitz operator, not even if you allowed ϕ_V to be a distribution.

Since Toeplitz quantization is a generalization of anti-Wick ordering, the map $V \to \phi_V$ could be viewed as a generalization of Wick ordering. For example, in the $\mathbb{R}^1$ case, if $V\left(x\right) = x^4$, then $\phi_V\left(x+iy\right) = x^4 - 3tx^2 + \frac{3}{4}t^2$, which is just the Wick ordering of x^4. Note that if K is non-commutative then the map $V \to \phi_V$ takes a function of x only and produces a function of both x and Y.

7. Comparison with geometric quantization

As we have noted the identification of $T^*(K)$ with $K_{\mathbb{C}}$ makes $K_{\mathbb{C}}$ into a Kähler manifold. This Kähler manifold admits a global Kähler potential given by

$$f\left(xe^{iY}\right) = \left|Y\right|^2.$$

(See [LS, Theorem 5.6, Sz] or [GS1, GS2].) The theory of geometric quantization thus provides a way of constructing a Hilbert space, using the "Kähler polarization." After suitable identifications, and writing t for $\hbar$, the Hilbert space is

$$\mathcal{H}L^2\left(K_{\mathbb{C}}, \gamma_t\right),$$

where γ_t is the measure given by

$$d\gamma_t = b_t e^{-f/t} dL.$$

(See [W, Eq. 5.7.11].) Here b_t is a constant which is conventionally taken to be $(2\pi t)^{-n}$. Now in terms of x, Y coordinates, the Liouville measure is just Haar measure dx times Lebesgue measure dY. (See [H3, Lemma 4].) So

$$d\gamma_t\left(x, Y\right) = b_t e^{-\left|Y\right|^2/t}\,dx\,dY.$$

Let us compare this to the Hilbert space $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$. According to [H3, Eq. 11, Lemma 5], the measure $\nu_t(g)\,dg$ satisfies

$$\nu_t(g)\;dg = c_t\,u(Y)\,e^{-|Y|^2/t}\,dx\,dY. \tag{7.1}$$

Here c_t is a constant (given explicitly in [H3]) and u is a function independent of x and t. Note that (7.1) reflects both the formula for ν_t and the conversion factor σ between Haar measure on $K_{\mathbb{C}}$ and Liouville measure. In the case $K = \mathsf{SU}(2)$, and with a suitable inner product on $\mathfrak{k}$, u is given by the formula

$$u(Y) = \frac{\sinh|Y|}{|Y|}.$$

In general, $u(Y)$ is Ad-K-invariant and is given explicitly on a maximal abelian subabalgebra of $\mathfrak{k}$ by the formula

$$u(Y) = \prod_{\alpha\in R^+}\frac{\sinh\alpha(Y)}{\alpha(Y)}.$$

Here R^+ is the set of positive roots.

If K is commutative, then $u \equiv 1$, and the two Hilbert spaces are the same, except for an irrelevant constant. If K is non-commutative, then the two Hilbert spaces are not the same, although they differ only by a relatively small factor, which is t-independent.

I do not fully understand at present the difference between these two spaces. However, from a certain point of view "my" space $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$ is preferable to the geometric quantization space $\mathcal{H}L^2(K_{\mathbb{C}}, \gamma_t)$. My point of view is that a phase space Hilbert space is not so much a new way of quantizing $T^*(K)$ as it is a handy unitary transform that may be useful in studying operators in the conventional position Hilbert space $L^2(K, dx)$. From this point of view the "goodness" of a phase space Hilbert space is measured by how well it is related to the position Hilbert space and by how easy it is to calculate with.

The generalized Segal-Bargmann space seems to be better related to the position Hilbert space than the geometric quantization space. While there is a unitary transform, say D_t, from $L^2(K, dx)$ onto $\mathcal{H}L^2(K_{\mathbb{C}}, \gamma_t)$ (see [H1, Sec. 10]), this transform will not be given in terms of the heat operator, and it seems difficult to understand its kernel. Moreover, it seems unlikely that there could be an inversion formula for D_t of the sort we have for the generalized Segal-Bargmann transform. Finally, many of the results about Toeplitz operators would fail if D_t replaces C_t. In particular, I do not see how to express $D_t M_V D_t^{-1}$ as a Toeplitz operator.

The generalized Segal-Bargmann space also seems easier to calculate with than the geometric quantization space. For example, the reproducing kernel for $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$ is known fairly explicitly [H1, Theorem 6, H3], whereas the reproducing kernel for $\mathcal{H}L^2(K_{\mathbb{C}}, \gamma_t)$ would be given by a complicated series expansion. Our knowledge of the reproducing kernel in $\mathcal{H}L^2(K_{\mathbb{C}}, \nu_t)$ leads to sharp pointwise bounds and to the uncertainty principle of Section 5, results which seem unattainable for $\mathcal{H}L^2(K_{\mathbb{C}}, \gamma_t)$.

Further study is merited to understand the difference between the generalized Segal-Bargmann space and the geometric quantization space.

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