# PSEUDODIFFERENTIAL OPERATORS, COVARIANT QUANTIZATION, THE INESCAPABLE VAN VLECK–MORETTE DETERMINANT, AND THE $\frac{R}{6}$ CONTROVERSY

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### WHAT IS A PSEUDODIFFERENTIAL OPERATOR?
(and why should a physicist care?)

The important point is that physicists *already know* about pseudodifferential operators. In essence, a pseudodifferential operator ($\Psi$DO) is nothing other than what is called in quantum mechanics *a function of both position* ($\mathbf{x}$) *and momentum* ($-i\hbar \frac{\partial}{\partial \mathbf{x}}$). This generalizes two familiar classes of operators:
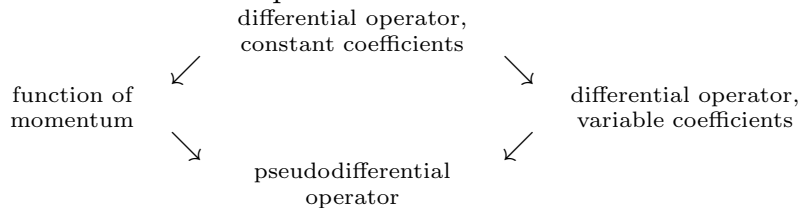


A polynomial function of momentum is just a differential operator (although if the coefficients depend on $\mathbf{x}$, this "quantization" is afflicted by the notorious *factor ordering ambiguity*, about which more later). A nonpolynomial function of momentum *alone* can be defined by the Fourier transform. But what operator corresponds to a *general* (smooth) function, $a(\mathbf{x}, \mathbf{p})$? The simplest answer to this question is given by the *conventional $\Psi DO$ calculus*:

**Semiformal Definition:** A *pseudodifferential operator* is one whose action on functions $\psi(\mathbf{x})$ can be expressed in the form

$$[A\psi](\mathbf{x}) = (2\pi\hbar)^{-\frac{d}{2}} \int_{\mathbf{R}^d} d\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\, a(\mathbf{x}, \mathbf{p})\, \hat{\psi}(\mathbf{p})$$

for some function $a(\mathbf{x}, \mathbf{p})$ on the phase space $\mathbf{R}^{2d}$. The Fourier transform here is defined by

$$\hat{\psi}(\mathbf{p}) \equiv (2\pi\hbar)^{-\frac{d}{2}} \int_{\mathbf{R}^d} d\mathbf{x}\, e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}\, \psi(\mathbf{x}).$$

The function $a$ is called the *symbol* of the operator $A$.

This definition is only "semiformal" because, in the mathematical literature [e.g., 15, 16, 27, 29], the term *pseudodifferential operator* is confined to the results of applying this construction to symbols satisfying certain technical conditions. Roughly speaking, the standard $\Psi$DOs include all differential operators and also the inverses of elliptic differential operators, but not the inverses of hyperbolic ones. Thus we have the usual situation

that what is easy to do rigorously in Euclidean manifolds becomes harder in Lorentzian manifolds.

To make the formulas simpler, I shall now adopt units in which $\hbar = 1$ and hence $2\pi = h$.

If $a(\mathbf{x}, \mathbf{p})$ is a polynomial in $\mathbf{p}$, such as $e^x p$ in dimension 1, then $A$ is the corresponding differential operator, with the $\mathbf{x}$-dependent coefficients standing on the left of the derivatives: $-i\, e^x \frac{d}{dx}$.

Another way of writing the definition of $A$ is

$$[A\psi](\mathbf{x}) = \int_{\mathbf{R}^d} d\mathbf{y}\, \mathcal{A}(\mathbf{x}, \mathbf{y})\, \psi(\mathbf{y}),$$

where

(S $\rightarrow$ K) $$\mathcal{A}(\mathbf{x}, \mathbf{y}) = h^{-d} \int_{\mathbf{R}^d} d\mathbf{p}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\, a(\mathbf{x}, \mathbf{p}).$$

(In general, the *kernel* $\mathcal{A}$ is a distribution, not a genuine function.) Inverting the Fourier transform, we get

(K $\rightarrow$ S) $$a(\mathbf{x}, \mathbf{p}) = \int_{\mathbf{R}^d} d\mathbf{y}\, e^{i\mathbf{p}\cdot(\mathbf{y}-\mathbf{x})}\, \mathcal{A}(\mathbf{x}, \mathbf{y}).$$

These two kernel $\leftrightarrow$ symbol formulas will be the focus of our discussion of possible refinements and generalizations of the $\Psi$DO formalism.

This conventional symbolic calculus for $\Psi$DOs has two glaring deficiencies, especially for physical applications:

1. Real symbols do not generally correspond to self-adjoint operators. ($\mathbf{x}$ and $\mathbf{y}$ are treated asymmetrically. Derivatives are arbitrarily put on the right of coefficient functions. The symplectic structure of phase space is not properly revealed.) This is remedied by the *Weyl calculus* (the mathematician's name for the operator half of the Wigner–Weyl–Moyal formulation of quantum mechanics) [20, 29].

2. The formalism is not geometrically covariant. (The conventional symbol is not intrinsically defined as a function on $T^*(M)$ (the cotangent bundle of the configuration space).) Even in flat space, it is not gauge-invariant when a vector potential is present. The problem is that already in the symbol of a *differential* operator, only the leading term transforms as a tensor. The coefficients of the lower-degree terms become tensors only after coordinate derivatives are replaced by covariant derivatives. The counterpart of this step for $\Psi$DOs is performed by the *intrinsic calculus* developed by Bokobza, Widom, and Drager.

Unfortunately, the Weyl formalism and the intrinsic formalism are orthogonal improvements at best; in some ways they actually seem to work at cross purposes. We set ourselves the goal of finding the *common generalization* of the Weyl and Widom calculi:

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conventional

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Weyl                  intrinsic

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?

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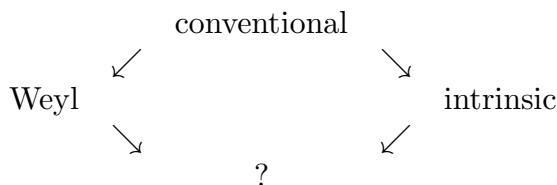
Even on the formal level this turns out to be far from trivial.

## The Weyl Calculus

In the Weyl calculus, the conventional relations between kernel and symbol are replaced by the more symmetrical formulas (I redisplay the conventional formulas for comparison)

$$(S \to K) \qquad \mathcal{A}(\mathbf{x}, \mathbf{y}) = h^{-d} \int_{\mathbf{R}^d} d\mathbf{p} \, e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \, a\left( \frac{\mathbf{x} + \mathbf{y}}{2}, \mathbf{p} \right)$$

$$\left( \text{was} \quad \mathcal{A}(\mathbf{x}, \mathbf{y}) = h^{-d} \int_{\mathbf{R}^d} d\mathbf{p} \, e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \, a(\mathbf{x}, \mathbf{p}) \quad \right)$$

and

$$(K \to S) \qquad a(\mathbf{q}, \mathbf{p}) = \int_{\mathbf{R}^d} d\mathbf{v} \, e^{-i\mathbf{p} \cdot \mathbf{v}} \, \mathcal{A}\left( \mathbf{q} + \frac{\mathbf{v}}{2}, \mathbf{q} - \frac{\mathbf{v}}{2} \right)$$

$$\left( \text{was} \quad a(\mathbf{x}, \mathbf{p}) = \int_{\mathbf{R}^d} d\mathbf{y} \, e^{i\mathbf{p} \cdot (\mathbf{y} - \mathbf{x})} \, \mathcal{A}(\mathbf{x}, \mathbf{y}) \quad \right).$$

Thus the classical position variable $\mathbf{q}$ is associated with the midpoint of the straight line segment joining $\mathbf{x}$ and $\mathbf{y}$, and the Fourier variable conjugate to $\mathbf{p}$ is the vectorial difference between $\mathbf{x}$ and $\mathbf{y}$.

Other definitions of Weyl quantization are more common in the physics literature:

1. **Weyl's definition:** If

$$a(\mathbf{q}, \mathbf{p}) = \int_{\mathbf{R}^{2d}} d\mathbf{u} \, d\mathbf{v} \, \hat{a}(\mathbf{u}, \mathbf{v}) \, e^{i(\mathbf{u} \cdot \mathbf{q} - \mathbf{v} \cdot \mathbf{p})},$$

then

$$A = \int_{\mathbf{R}^{2d}} d\mathbf{u} \, d\mathbf{v} \, \hat{a}(\mathbf{u}, \mathbf{v}) \, e^{i(\mathbf{u} \cdot \mathbf{Q} - \mathbf{v} \cdot \mathbf{P})},$$

where $\mathbf{Q}$ and $\mathbf{P}$ are the quantum operators.

2. **McCoy's formula:** The quantization of $q^n p^m$ is (in one dimension)

$$\frac{1}{2^n} \sum_{l=0}^{n} \binom{n}{l} Q^{n-l} P^m Q^l.$$

These two constructions are equivalent to the Fourier-transform definition I have stated. Both of them, of course, were developed to resolve the factor ordering ambiguity in the passage from commuting to noncommuting variables.

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When applied to a momentum polynomial $a(\mathbf{q}, \mathbf{p}) = A_\alpha(\mathbf{q})\mathbf{p}^\alpha$, Weyl quantization gives

$$A\psi(\mathbf{x}) = (-i\partial_\mathbf{y})^\alpha \left[ A_\alpha \left( \frac{\mathbf{x} + \mathbf{y}}{2} \right) \psi(\mathbf{y}) \right]_{\mathbf{y}=\mathbf{x}}.$$

(Here $\alpha$ is a *multiindex*, running over all the independent (unordered) choices of the indices of a totally symmetric tensor.) Working this out for the example $A^{\mu\nu}(\mathbf{q})\mathbf{p}_\mu\mathbf{p}_\nu$, we get the differential operator

$$A = -A^{\mu\nu}(\mathbf{x})\partial_\mu\partial_\nu - \left( \partial_\mu A^{\mu\nu}(\mathbf{x}) \right)\partial_\nu - \tfrac{1}{4}\partial_\mu\partial_\nu\left( A^{\mu\nu}(\mathbf{x}) \right)$$
$$= \tfrac{1}{2}P_\mu A^{\mu\nu}(\mathbf{Q})P_\nu + \tfrac{1}{4}P_\mu P_\nu A^{\mu\nu}(\mathbf{Q}) + \tfrac{1}{4}A^{\mu\nu}(\mathbf{Q})P_\mu P_\nu .$$

This result is Hermitian, but it is not uniquely determined by the requirement of Hermiticity. (In general, real-valued symbols (phase-space observables) correspond to Hermitian operators, as one would expect of any decent quantum-mechanical formalism.)

In the Wigner–Weyl–Moyal formulation of quantum mechanics [e.g., 23, 24], the expectation value of the observable $A$ is the phase-space integral

$$\langle \psi | A | \psi \rangle = \int_{\mathbf{R}^{2d}} d\mathbf{q}\, d\mathbf{p}\, a(\mathbf{q}, \mathbf{p})\, W(\mathbf{q}, \mathbf{p}),$$

where $W$ is the *Wigner function* of the quantum state $\psi$. The Wigner function is obtained from the density matrix of the state by a formula just like the Weyl K $\to$ S formula, except for the normalization constant:

$$W(\mathbf{q}, \mathbf{p}) = h^{-d} \int_{\mathbf{R}^d} d\mathbf{v}\, e^{-i\mathbf{p}\cdot\mathbf{v}}\, \psi\left( \mathbf{q} + \frac{\mathbf{v}}{2} \right) \psi\left( \mathbf{q} - \frac{\mathbf{v}}{2} \right)^*.$$

Having said this, I should emphasize that the Weyl calculus of $\Psi$DOs is not limited to situations where the elements of the domain of the operators are interpreted as quantum wave functions. It can be useful when these functions are relativistic quantum fields, or quantities in classical continuum mechanics, or any things satisfying partial differential equations or integral equations.

### The Intrinsic Symbolic Calculus

Now, what must be done to make the conventional $\Psi$DO calculus covariant? I shall consider a Riemannian manifold $M$ equipped with the usual covariant differentiation operation (Levi-Civita connection) and another connection that tells us how to differentiate the fields or wave functions $\psi$ (which are sections of some vector bundle over $M$). These connections define *parallel transport* of objects along curves. Following DeWitt [8], I denote by $I(x, y)$ the parallel transport (in the bundle) along a geodesic from $y$ to $x$. (Other references on the geometrical formalism used here include [11, 12, 26].)

I adopt the convention that the density $\sqrt{g}$ is part of the integration element, not part of the fields nor part of the kernels. Thus a kernel defines an operator via

$$[A\psi](x) = \int_M dy\, \sqrt{g(y)}\, \mathcal{A}(x, y)\, \psi(y).$$

The analogue of the straight line between two points is a geodesic segment connecting them. Such a segment exists and is effectively unique if the points are "sufficiently close". More precisely, given a base point $x$, the geodesic flow (or *exponential map*) sets up a (local) correspondence between points in the manifold and tangent vectors at $x$: Given $\mathbf{u} \in T_x(M)$, solve the geodesic equation with initial point $x$ and initial direction $\mathbf{u}$, and travel along it to the point with geodesic parameter $\xi = 1$; this other endpoint of the geodesic segment is $y \equiv \exp_x(\mathbf{u})$; the geodesic distance between $x$ and $y$ is the length of $\mathbf{u}$. Conversely, given $x$ and $y$ sufficiently close, we can solve the two-point boundary value problem for the geodesic equation, choosing the shortest solution in case of nonuniqueness, and find the corresponding tangent vector $\mathbf{u} \equiv \exp_x^{-1}(y)$. Several other notations are used in this situation:

1. The *Synge–DeWitt world function* $\sigma(x, y)$ is half the square of the geodesic distance from $x$ to $y$. Equivalently, $\sigma$ is the action for the geodesic equation regarded as a dynamical system. Then the gradient of $\sigma$ with respect to $x$ is essentially $\mathbf{u}$. Precisely,

$$\mathbf{u} \equiv \exp_x^{-1}(y) = -(\nabla_x \sigma)^\sharp : \qquad u^\mu = -g(x)^{\mu\nu} \partial_{x^\nu} \sigma(x, y).$$

In the physics literature the gradient is itself denoted by sigma:

$$\sigma_\mu \equiv \sigma_{;\mu} \equiv \nabla_{x^\mu} \sigma.$$

2. Choose a coordinate system (basis) for $T_x(M)$. Then the corresponding labeling of the points $y$ is a *normal coordinate system* based at $x$. The coefficients in a Taylor series with respect to normal coordinates are the covariant derivatives of the subject function, evaluated at the expansion point. In other words, *ordinary derivatives with respect to normal coordinates are equivalent in the coincidence limit to symmetrized covariant derivatives.*

In general, there will be a *caustic* around $x$, beyond which the geodesics begin to cross each other and the exponential map is no longer smooth and invertible. For today's formal considerations I shall simply ignore caustics; I pretend that all the constructions are meaningful globally, with the understanding that in a rigorous development, cutoff functions will be inserted to keep the supports of all the integrands inside the normal neighborhoods where the necessary exponential maps are defined. (This is closely related to the other big piece of business I left unfinished earlier, the technical condition characterizing admissible symbols. For the standard classes of $\Psi$DOs studied by mathematicians, the kernels $\mathcal{A}(x, y)$ are smooth functions except possibly at $x = y$. Therefore, putting in a cutoff function changes the kernel by a totally smooth function, corresponding to a symbol that falls off faster than any power of $\mathbf{p}$ and hence can be ignored in the asymptotic calculations that are the hallmark of applied $\Psi$DO calculus. One should not forget that there are certain to be major complications when applying pseudodifferential methods to manifolds with indefinite metric, or (say in Wigner–Weyl theory) to generic phase-space functions.)

In the DeWitt notation, the *Van Vleck–Morette determinant* is

$$\Delta(x, y) \equiv g(x)^{-1/2} g(y)^{-1/2} \det\left[-\sigma_{\mu\nu'}\right]$$

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(where the prime indicates differentiation with respect to $y$). It is a scalar function, symmetric in its arguments. Nevertheless, its primary geometrical importance is in a very nonsymmetrical role: The Jacobian relation needed to pass from integration over the tangent space to integration over the manifold is

$$\sqrt{g(x)}\,d\mathbf{u} = \Delta(x,y)\,\sqrt{g(y)}\,dy \qquad \left(\mathbf{u} = \exp_x^{-1}(y)\right).$$

The intrinsic, or covariant, $\Psi$DO calculus was defined (in minor variations) by Bokobza [4], Widom [31–32], and Drager [10]; it was developed and used by Kennedy and me [13–14] and by Gusynin and coworkers [18–19] to calculate heat kernels for operators that do not yield to the usual Schwinger–DeWitt ansatz. I shall present the basic formulas in the kernel $\leftrightarrow$ symbol form, with an extra bit of freedom in the role of the Van Vleck–Morette determinant that has not been discussed in the literature previously.

Given a symbol, one defines a kernel (and hence an operator) by

(S $\rightarrow$ K) $$\qquad \mathcal{A}(x,y) = h^{-d}\Delta(x,y)^\gamma \int_{T_x^*} \frac{d\mathbf{p}}{\sqrt{g(x)}}\, e^{-i\mathbf{p}\cdot\mathbf{u}}\, a(x,\mathbf{p})I(x,y)$$

$$\left(\text{was} \quad \mathcal{A}(\mathbf{x},\mathbf{y}) = h^{-d}\int_{\mathbf{R}^d} d\mathbf{p}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\, a(\mathbf{x},\mathbf{p}) \quad\right),$$

where $\mathbf{u} = \exp_x^{-1}(y)$ (the negative of the Synge–DeWitt sigma vector) and $\gamma$ is a parameter. The Fourier inversion of this formula can be written

(K $\rightarrow$ S) $$\qquad a(x,\mathbf{p}) = \int_M dy\,\sqrt{g(y)}\, e^{i\mathbf{p}\cdot\mathbf{u}}\, \mathcal{A}(x,y)I(y,x)\,\Delta(x,y)^{1-\gamma}$$

$$\left(\text{was} \quad a(\mathbf{x},\mathbf{p}) = \int_{\mathbf{R}^d} d\mathbf{y}\, e^{i\mathbf{p}\cdot(\mathbf{y}-\mathbf{x})}\, \mathcal{A}(\mathbf{x},\mathbf{y}) \quad\right).$$

(Again, I have shown the conventional flat-space formulas for comparison.)

We observe that the S $\rightarrow$ K formula is simplest if one chooses $\gamma = 0$, but the K $\rightarrow$ S formula is simplest if one chooses $\gamma = 1$. Both definitions were, in effect, studied by Drager [10]:

$$\gamma = 0 \longleftrightarrow \text{``parallel-translation symbol''},$$
$$\gamma = 1 \longleftrightarrow \text{``covariant-derivative symbol''}.$$

He, and most other authors, have settled on $\gamma = 1$ as preferable, because of what it does to differential operators:

$$\text{If} \quad a(x,\mathbf{p}) = A_\alpha(x)\mathbf{p}^\alpha, \quad \text{then} \quad A = A_\alpha(x)(-i\nabla)^\alpha \quad \text{(when } \gamma = 1\text{)}.$$

That is, *the "quantization rule" is exactly the same as in the conventional Fourier analysis, except that coordinate derivatives are replaced by covariant derivatives.* (Since covariant differentiation operators do not commute among themselves, it is important to insist here that $A_\alpha(x)$ be a *symmetric* tensor.) Any other choice of $\gamma$ would modify this correspondence by terms coming from the covariant Taylor expansion of $\Delta$.

## A Proposal for a Covariant Weyl Calculus

One of the reasons why quantum gravity is so hard is that relativity often pulls the mathematics of physics in one direction while quantum theory pulls it in a different direction. That is true here. In the intrinsic calculus, calculations leading from operators to symbols tend to be simple, while those going from symbols to operators are relatively arcane; in the Weyl calculus, precisely the reverse is true. So, the project of constructing a covariant analogue of the Weyl calculus is likely to run into obstacles no matter which way we turn.

At this point I should pause to mention some physical motivations for that project.

1. Recent papers of Osborn and Molzahn [22, 25] have demonstrated that the Weyl formalism can be very helpful in constructing elegant semiclassical approximations to quantum dynamics, in either the Schrödinger or the Heisenberg picture. When external gravitational or gauge fields are present, however, manifest covariance is lost in these constructions. On the other hand, abandoning the Weyl symmetrization obscures equally the symplectic structure of mechanics. Therefore, a pseudodifferential calculus that preserves both of these crucial geometrical structures is highly desired.

2. Naive perturbation theory with respect to a weak external gravitational field leads to technical difficulties because the perturbation is a differential operator of the same order as the unperturbed one. Pseudodifferential thinking, however, suggests that one might write the operator as the sum of an "unperturbed" *pseudodifferential* operator and a perturbation of lower order (also pseudodifferential), such that the unperturbed problem can be solved exactly. In particular, is there a $\Psi$DO whose propagator equals *exactly* the leading term of the famous Schwinger–DeWitt series? (These thoughts were inspired by a paper of Gurarie [17], who proved a theorem on the asymptotic behavior of resolvent kernels by similar reasoning.) This heuristic point of view turns out to be an oversimplification, but the general approach remains promising. I call it *covariant perturbation theory with soft, almost local perturbations*; I hope that it will prove to be simply related to the covariant perturbation theory of Barvinsky and Vilkovisky [2–3] and will help resolve some of the uncertainty about the global aspects of the latter. Surely, the best prospects in this venture are for a formalism that displays both covariance and the Weyl symmetry.

To mimic the Weyl calculus on a manifold, the obvious starting point is the following. Given $x$ and $y$ in $M$, sufficiently close that the geodesic construction works, define $q$ to be the midpoint of the geodesic segment joining them, and define $\mathbf{v} \in T_q$ by

$$\mathbf{v} \equiv 2 \exp_q^{-1}(x) = -2 \exp_q^{-1}(y).$$
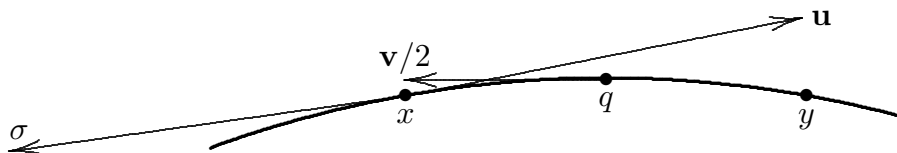
Then I propose to merge the Weyl and intrinsic $S \to K$ formulas this way:

$$(S \to K) \qquad \mathcal{A}(x, y) = h^{-d} \Delta(x, y)^\gamma \int_{T_q^*} \frac{d\mathbf{p}}{\sqrt{g(q)}} \, e^{i\mathbf{p}\cdot\mathbf{v}} \, I(x, q) a(q, \mathbf{p}) I(q, y)$$

$$\left( \text{was} \quad \mathcal{A}(\mathbf{x}, \mathbf{y}) = h^{-d} \int_{\mathbf{R}^d} d\mathbf{p} \, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \, a\left( \frac{\mathbf{x}+\mathbf{y}}{2}, \mathbf{p} \right) \right.$$

$$\left. \text{or} \quad \mathcal{A}(x, y) = h^{-d} \Delta(x, y)^\gamma \int_{T_x^*} \frac{d\mathbf{p}}{\sqrt{g(x)}} \, e^{-i\mathbf{p}\cdot\mathbf{u}} \, a(x, \mathbf{p}) I(x, y) \right).$$

In inverting this Fourier transform we must think of $q$ and $\mathbf{v}$ as the independent variables and define

$$x = \exp_q\left( +\frac{\mathbf{v}}{2} \right), \qquad y = \exp_q\left( -\frac{\mathbf{v}}{2} \right).$$

We get

$$(K \to S) \qquad a(q, \mathbf{p}) = \int_{T_q} d\mathbf{v} \, \sqrt{g(q)} \, e^{-i\mathbf{p}\cdot\mathbf{v}} \, I(q, x) \mathcal{A}(x, y) I(y, q) \Delta(x, y)^{-\gamma}$$

$$\left( \text{was} \quad a(\mathbf{q}, \mathbf{p}) = \int_{\mathbf{R}^d} d\mathbf{v} \, e^{-i\mathbf{p}\cdot\mathbf{v}} \, \mathcal{A}\left( \mathbf{q} + \frac{\mathbf{v}}{2}, \mathbf{q} - \frac{\mathbf{v}}{2} \right) \right.$$

$$\text{or} \quad a(x, \mathbf{p}) = \int_M dy \, \sqrt{g(y)} \, e^{i\mathbf{p}\cdot\mathbf{u}} \, \mathcal{A}(x, y) I(y, x) \, \Delta(x, y)^{1-\gamma}$$

$$\left. = \int_{T_x} d\mathbf{u} \, \sqrt{g(x)} \, e^{i\mathbf{p}\cdot\mathbf{u}} \, \mathcal{A}(x, y) I(y, x) \, \Delta(x, y)^{-\gamma} \right).$$

Note that converting the integral over the tangent-space vector $\mathbf{v}$ into an integral over the manifold would destroy the symmetry between $x$ and $y$ that we are working so hard to maintain.

Since both of the basic formulas contain the factor $\Delta^\gamma$, it may seem that $\gamma = 0$ is the only natural choice. I shall argue, however, that there are two other choices that are better.

Consider first the passage from a momentum polynomial to a differential operator. This requires a rather complicated calculation, in which a Jacobian $\Delta^{-1}$ arises. The conclusion is just like that in the usual intrinsic calculus: *Covariant Weyl quantization with $\gamma = 1$ is exactly the same as conventional Weyl quantization, except that coordinate derivatives are replaced by symmetrized covariant derivatives.* Any other choice of $\gamma$ modifies the correspondence by terms coming from the covariant Taylor expansion of $\Delta$. This is a strong argument in favor of $\gamma = 1$. (Cf. (3.48) of Avramidi [1].)

On the other hand, let's contemplate the possibility of a covariant Wigner function. Presumably it should satisfy the fundamental equation

$$\langle \psi | A | \psi \rangle = \int_{T^*(M)} dq \, d\mathbf{p} \, a(q, \mathbf{p}) \, W(q, \mathbf{p}).$$

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(The symplectic measure on the cotangent bundle is covariant, without any $\sqrt{g}$ factors.) If we assume that the formula for the Wigner function in terms of the density matrix is essentially the same as the covariant Weyl K → S formula,

$$W(q, \mathbf{p}) = h^{-d} \int_{T_q} d\mathbf{v} \sqrt{g(q)}\, e^{-i\mathbf{p}\cdot\mathbf{v}}\, \psi(x)\psi(y)^* \Delta(x, y)^{-\gamma},$$

then a bit of Fourier analysis shows that $\gamma$ must equal $\frac{1}{2}$ for consistency! Any other choice of $\gamma$ used in both halves of the Wigner–Weyl–Moyal transformation will replace the fundamental phase-space integral by a *nonlocal* formula (i.e., one involving another layer of integration).

Of course, one could simply accept a Wigner transform that is different from the Weyl transform. (These are all just definitions, after all.) The local formula for the expectation value is consistent with any pair of exponents satisfying

$$\gamma_{\text{Weyl}} + \gamma_{\text{Wigner}} = 1.$$

However, there is another argument for choosing $\gamma = \frac{1}{2}$. Recall that I proposed doing covariant perturbation theory around the so-called WKB propagator (the leading term of the Schwinger–DeWitt series),

$$\mathcal{U}_0(x, y) = (4\pi t)^{-d/2} e^{i\sigma(x,y)/2t} \Delta(x, y)^{1/2} I(x, y).$$

On the other hand, if the perturbation theory is to be conducted in Fourier space, then we would expect the covariant symbol of the unperturbed operator to be simply

$$u_0(q, \mathbf{p}) = e^{-it g^{\mu\nu}(q) p_\mu p_\nu}.$$

From this latter, the covariant Weyl S → K formula yields

$$\mathcal{U}_0(x, y) = (4\pi t)^{-d/2} e^{i\sigma(x,y)/2t} \Delta(x, y)^{\gamma} I(x, y).$$

So, perhaps we should come down midway between the two obvious candidates, 0 and 1.

Let us take a closer look at the covariant Weyl quantization of polynomials. For the generic second-order case,

$$a(q, \mathbf{p}) = A^{\mu\nu}(q) p_\mu p_\nu,$$

one gets the operator

$$A = -A^{\mu\nu}\nabla_\mu\nabla_\nu - A^{\mu\nu}{}_{;\mu}\nabla_\nu - \frac{1}{4} A^{\mu\nu}{}_{;\mu\nu} - \frac{\gamma - 1}{3} A^{\mu\nu} R_{\mu\nu}.$$

In the special case $A^{\mu\nu} = g^{\mu\nu}$, this is

$$A = -g^{\mu\nu}\nabla_\mu\nabla_\nu - \frac{\gamma - 1}{3} R \equiv \Delta - \frac{\gamma - 1}{3} R,$$

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where $\Delta$ is the Laplace–Beltrami operator and $R$ is the scalar curvature. Now, this equation has a long history! If one thinks of $\frac{1}{2}\, g^{\mu\nu} p_\mu p_\nu$ as the classical Hamiltonian of a free particle (of unit mass) on a manifold, then our equation says:

1. If $\gamma = 1$, then the quantum Hamiltonian is just $\frac{1}{2}\Delta$.

2. If $\gamma = 0$, the quantum Hamiltonian is $\frac{1}{2}\Delta + \frac{1}{6}R$ (times $\hbar^2$, suppressed by my choice of units).

3. If $\gamma = \frac{1}{2}$, the curvature term is $\frac{1}{12}R$.

For decades, people have been calculating different values for this curvature coefficient, depending on how they do their path integrals [e.g., 5–6, 7, 9, 34]. (The factor $\hbar^2$ indicates that the term is part of the factor ordering ambiguity.) I believe that they have often been asking the wrong question. Seventy years after the discovery of quantum mechanics, we should no longer be asking how to quantize a given classical Hamiltonian. We should think in the other direction! The Schrödinger equation of a system is a given, to be determined by experiment. The appropriate question is, "What definitions help us to elucidate the behavior of this system in the semiclassical limit?" *A definition is not true or false. On the other hand, some definitions are more useful or more elegant than others.* So spend some time deciding which is the best $\gamma$ for your problem, but do not wage a holy war to convince the world that yours is the One True $\gamma$!

With that, I must close this brief account by an incomplete list of previous related work. In the physics literature one finds various papers on "covariant Wigner functions" (notably Winter [33]) that state (in effect) my K $\rightarrow$ S formula with $\gamma = 0$. In the mathematics literature, papers that attempt to combine geometrical covariance and symplectic symmetry in something like the present spirit are those of Underhill [30], Liu and Qian [21], and Safarov [28]. The last of these is an especially thorough and rigorous piece of work, though it considers only $\gamma = 0$.

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ADDENDUM: THE PRODUCT FORMULA

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In many applications of pseudodifferential operators a central role is played by a formula for the symbol of the product of two operators (say $C = AB$) in terms of the symbols of the factors. In each variant of the $\Psi$DO calculus there are two such formulas. One is a ($4d$-fold) multiple integral obtained by substituting the S $\rightarrow$ K formulas for $A$ and $B$ into the K $\rightarrow$ S formula for $C$; this is exact (at least if the symbols decay fast enough at infinity to make the integrals converge without cutoffs) but very cumbersome for calculations. The other is a purely local series expansion in successively higher derivatives of the symbols $a$ and $b$. This one makes sense only if at least one of the symbols is a smooth function, and even then only asymptotically — unless the series happens to terminate, as it does in the important special case of polynomials in $\mathbf{p}$, which dominate both quantum mechanics and the theory of partial differential equations.

In the standard Weyl calculus the series formula is

$$c(\mathbf{q}, \mathbf{p}) = e^{\frac{i}{2}\left(\frac{\partial}{\partial \mathbf{q}_1} \cdot \frac{\partial}{\partial \mathbf{p}_2} - \frac{\partial}{\partial \mathbf{p}_1} \cdot \frac{\partial}{\partial \mathbf{q}_2}\right)} \left[ a(\mathbf{q}_1, \mathbf{p}_1) b(\mathbf{q}_2, \mathbf{p}_2) \right]_{\substack{\mathbf{q}_1 = \mathbf{q}_2 = \mathbf{q} \\ \mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p}}}$$

$$= \sum_{\alpha, \beta} \frac{i^{|\beta| - |\alpha|}}{\alpha! \, \beta! \, 2^{|\alpha| + |\beta|}} \, \partial_\mathbf{q}^\beta \partial_\mathbf{p}^\alpha a(\mathbf{q}, \mathbf{p}) \, \partial_\mathbf{q}^\alpha \partial_\mathbf{p}^\beta b(\mathbf{q}, \mathbf{p}).$$

When the units are put back in, this is a Taylor series in $\hbar$; the leading term gives "classical theory" (i.e., $c(\mathbf{q}, \mathbf{p}) = a(\mathbf{q}, \mathbf{p})b(\mathbf{q}, \mathbf{p})$), and (for scalar observables) the leading term in the commutator $[A, B]$ is $i\hbar$ times the Poisson bracket $\{a, b\}$. (There may still be some quantum mechanics texts that state the principal axiom of quantization as "Replace all Poisson brackets by commutators". That is correct for the $\mathbf{q}$s and $\mathbf{p}$s themselves and many other important special cases, but *wrong* for general observables, because it neglects all the higher-order terms in this series.)

The corresponding formula [32, 10, 14, 28] in the Widom intrinsic calculus is much more complicated, bristling with coincidence limits of derivatives of the world function $\sigma$ (which can in principle be expressed in terms of the Riemann tensor). In the special case of flat space, but with a (possibly non-Abelian) external gauge field, it reduces to

$$c(\mathbf{x}, \mathbf{p}) = e^{i\left(\frac{\partial}{\partial \mathbf{z}} \cdot \frac{\partial}{\partial \mathbf{p}_2} - \frac{\partial}{\partial \mathbf{p}_1} \cdot \frac{\partial}{\partial \mathbf{x}_2}\right)} \left[ a(\mathbf{x}, \mathbf{p}_1) I(\mathbf{x}, \mathbf{x}_2) \right.$$

$$\left. \times b(\mathbf{x}_2, \mathbf{p}_2) I(\mathbf{x}_2, \mathbf{x} + \mathbf{x}_2 - \mathbf{z}) I(\mathbf{x} + \mathbf{x}_2 - \mathbf{z}, \mathbf{x}) \right]_{\substack{\mathbf{x}_2 = \mathbf{z} = \mathbf{x} \\ \mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p}}}$$

$$= \sum_{\alpha, \beta, \gamma} \frac{(-i)^{|\alpha| + |\beta| + |\gamma|}}{\alpha! \, \beta! \, \gamma!} \, \partial_\mathbf{p}^{\alpha + \beta} a(\mathbf{x}, \mathbf{p}) \, \nabla^\gamma \partial_\mathbf{p}^\beta b(\mathbf{x}, \mathbf{p}) \, \nabla^\alpha \nabla^\beta I(\mathbf{x}, \mathbf{x}).$$

(In the last factor, the parallel-transport operator is covariantly differentiated with respect to its first argument before the arguments are set equal.) To the best of my knowledge, the exponential version of this formula is published here for the first time.

All this is prologue to the announcement that although I have been unable to reduce the product formula for the covariant Weyl calculus to a tractable form in the general case, I can present here the formulas for flat space. I hope to publish elsewhere the details of the derivation and applications of the result.

Since the kernel of $C$ is the matrix product of the kernels of $A$ and $B$, substituting the S $\to$ K formulas for $A$ and $B$ into the K $\to$ S formula for $C$ yields the exact integral formula

$$c(\mathbf{q}, \mathbf{p}) = h^{-2d} \int d\mathbf{v} \int d\mathbf{y} \int d\mathbf{k} \int d\mathbf{l} \, e^{i(\mathbf{k} \cdot \mathbf{v}'' + \mathbf{l} \cdot \mathbf{v}' - \mathbf{p} \cdot \mathbf{v})}$$

$$\times I(\mathbf{q}, \mathbf{x}) I(\mathbf{x}, \mathbf{q}'') a(\mathbf{q}'', \mathbf{k}) I(\mathbf{q}'', \mathbf{y}) I(\mathbf{y}, \mathbf{q}') b(\mathbf{q}', \mathbf{l}) I(\mathbf{q}', \mathbf{z}) I(\mathbf{z}, \mathbf{q}),$$

where
$$\mathbf{x} = \mathbf{q} + \frac{\mathbf{v}}{2}, \quad \mathbf{z} = \mathbf{q} - \frac{\mathbf{v}}{2}, \quad \mathbf{v}'' = \mathbf{q} - \mathbf{y} + \frac{\mathbf{v}}{2}, \quad \mathbf{v}' = \mathbf{y} - \mathbf{q} + \frac{\mathbf{v}}{2},$$

$$\mathbf{q}'' = \frac{1}{2}\left(\mathbf{y} + \mathbf{q} + \frac{\mathbf{v}}{2}\right), \quad \mathbf{q}' = \frac{1}{2}\left(\mathbf{y} + \mathbf{q} - \frac{\mathbf{v}}{2}\right).$$

The strategy of the asymptotic calculation now is: Expand $a$ and $b$ as power series in $\mathbf{k} - \mathbf{p}$ and $\mathbf{l} - \mathbf{p}$; realize the powers of the momentum differences as derivatives of the exponential factor with respect to spatial variables; integrate by parts to move the derivatives off the exponentials; evaluate the momentum integrals as delta functions; evaluate the now trivial coordinate integrals. The result can be written

$$c(\mathbf{q}, \mathbf{p}) = e^{\frac{i}{2}\left(\frac{\partial}{\partial \mathbf{q}_1} \cdot \frac{\partial}{\partial \mathbf{p}_2} - \frac{\partial}{\partial \mathbf{p}_1} \cdot \frac{\partial}{\partial \mathbf{q}_2}\right)}\Big[\mathcal{I}(\mathbf{q}, \mathbf{q}_1; \mathbf{q}_2)a(\mathbf{q}_1, \mathbf{p}_1)\mathcal{I}(\mathbf{q}_1, \mathbf{q}_2; \mathbf{q})$$
$$\times\, b(\mathbf{q}_2, \mathbf{p}_2)\mathcal{I}(\mathbf{q}_2, \mathbf{q}; \mathbf{q}_1)\Big]_{\substack{\mathbf{q}_1 = \mathbf{q}_2 = \mathbf{q} \\ \mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p}}},$$

where $\mathcal{I}(\mathbf{x}, \mathbf{y}; \mathbf{z}) = I(\mathbf{x}, \mathbf{x} + \mathbf{y} - \mathbf{z})I(\mathbf{x} + \mathbf{y} - \mathbf{z}, \mathbf{y})$. Expanding the derivatives in terms of covariant derivatives of the factors, and using the properties of $I$, one gets the alternative form

$$c(\mathbf{q}, \mathbf{p}) = \sum_{\alpha, \ldots, \tau} \frac{i^{|\beta| + |\kappa| + |\rho| + |\sigma| - |\alpha| - |\lambda| - |\mu| - |\nu| - |\tau|}}{\alpha!\, \beta!\, \kappa!\, \lambda!\, \mu!\, \nu!\, \rho!\, \sigma!\, \tau!\, 2^{|\alpha| + \cdots + |\tau|}} \tilde{\nabla}^\rho \tilde{\nabla}^\kappa I(\mathbf{q}, \mathbf{q})\, \nabla^\beta \partial_{\mathbf{p}}^{\alpha + \kappa + \lambda + \mu + \nu} a(\mathbf{q}, \mathbf{p})$$
$$\times\, \nabla^\sigma \nabla^\lambda \tilde{\nabla}^\mu I(\mathbf{q}, \mathbf{q})\, \nabla^\alpha \partial_{\mathbf{p}}^{\beta + \rho + \sigma + \tau} b(\mathbf{q}, \mathbf{p})\, \nabla^\nu \nabla^\tau I(\mathbf{q}, \mathbf{q}).$$

Here $\tilde{\nabla}$ represents a derivative that acts on the second argument of $I$ before the arguments are set equal. All the derivatives of $I$ at equal arguments can be expressed in terms of the gauge field strength tensor.

Since $a$ or $b$ is a matrix-valued function, the "Christoffel" part of its covariant derivative is a commutator with the gauge potential. In particular, in the Abelian case the derivatives of $a$ and $b$ reduce to ordinary derivatives.

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