GEOMETRIC PSEUDODIFFERENTIAL CALCULUS
WITH APPLICATIONS TO QFT
ON CURVED SPACETIMES

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BALANCED GEOMETRIC WEYL QUANTIZATION

The usual Weyl quantization of $b \in \mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d)$ is the operator $\text{Op}(b) : \mathcal{S}(\mathcal{X}) \to \mathcal{S}'(\mathcal{X})$ with the kernel

$$\text{Op}(b)(x, y) := \int b\left(\frac{x + y}{2}, p\right) e^{i(y-x)p} \frac{dp}{(2\pi)^d}.$$ 

Hilbert-Schmidt operators correspond to square integrable symbols:

$$(2\pi)^{-d} \text{Tr} \text{Op}(a)^* \text{Op}(b) = \int a(z, p) b(z, p) dz dp.$$
Consider a (pseudo-)Riemannian manifold $M$. Let $x \in M$ and $u \in T_x M$. We will write
\[ x + u := \exp_x(u). \]
There exists a geodesic neighborhood $\Omega \subset M \times M$ of the diagonal with the property that every pair $(x, y) \in \Omega$ is joined by a unique geodesics $[0, 1] \ni \tau \mapsto \gamma_{x,y}(\tau)$ such that $\gamma_{x,y} \times \gamma_{x,y} \subset \Omega$. 
Let \((x, y) \in \Omega\).

\(y - x\) will denote the unique vector in \(T_xM\) tangent to the geodesics \(\gamma_{x,y}\) such that
\[x + (y - x) = y.\]

\((y - x)_\tau\) will denote the vector in \(T_{x+\tau(y-x)}M\) such that
\[(x + \tau(y - x)) + (1 - \tau)(y - x)_\tau = y.\]
The Van Fleck–Morette determinant is defined as

\[ \Delta(x, y) := \left| \frac{\partial(y - x)}{\partial y} \right| \frac{|g(x)|^{1/2}}{|g(y)|^{1/2}}. \]

Note that

\[ \Delta(x, y) = \Delta(y, x), \quad \Delta(x, x) = 1. \]
If $B$ is an operator $C^\infty_c(M) \to \mathcal{D}'(M)$ then its kernel is a distribution in $\mathcal{D}'(M \times M)$ such that

$$\langle f | B g \rangle = \int f(x) B(x, y) g(y) dx dy, \quad f, g \in C^\infty_c(M).$$

We will treat elements of $C^\infty_c(M)$ not as scalar functions, but as half-densities. With this convention, the kernel of an operator is a half-density on $M \times M$. 
Assume for simplicity that $\Omega = M \times M$. Consider
\[ T^* M \ni (z, p) \ni b(z, p) \]
Its balanced geometric Weyl quantization, denoted $\text{Op}(b)$, is the operator with the kernel
\[
\text{Op}(b)(x, y) := \Delta(x, y)^{1/2} \frac{|g(x)|^{1/4} |g(y)|^{1/4}}{|g(z)|^{1/2}} 
\times \int b(z, p) e^{iup} \frac{dp}{(2\pi)^d},
\]
where
\[ z := x + \frac{y - x}{2}, \quad u := (y - x)^{1/2}. \]
Note that $T^*M$ possesses a natural density, hence there is a natural identification of scalars with half-densities.

Up to a coefficient, the quantization that we defined is unitary from $L^2(T^*M)$ to operators on $L^2(M)$ equipped with the Hilbert-Schmidt scalar product:

$$\frac{1}{(2\pi)^d} \int_{T^*M} \overline{c(x, p)}b(x, p)dx dp = \text{TrOp}(c)^*\text{Op}(b).$$
Define the star product

\[ \operatorname{Op}(a \star b) = \operatorname{Op}(a)\operatorname{Op}(b). \]

Its asymptotic expansion in Planck’s constant:

\[
(a \star b) \sim ab
+ \frac{i}{2} (a_\alpha b^\alpha - a^\alpha b_\alpha)
- \frac{1}{8} (a_{\alpha_1\alpha_2} b^{\alpha_1\alpha_2} - 2a_{\alpha_1} b^{\alpha_1} + a^{\alpha_1\alpha_2} b_{\alpha_1\alpha_2}) + \frac{1}{12} R_{\alpha_1\alpha_2} a^{\alpha_2} b^{\alpha_1}
- \frac{1}{24} R^\beta_{\alpha_1\alpha_2\alpha_3} p_\beta (a^{\alpha_2} b^{\alpha_1\alpha_3} + a^{\alpha_1\alpha_3} b^{\alpha_2}) + \ldots
\]

where lower indices denote horizontal derivatives (in spatial directions) and upper indices denote vertical derivatives (in momentum directions).
Consider a symbol quadratic in the momenta, with the principal part given by the Riemannian metric:
\[ k(z, p) = g^{\mu\nu}(z)(p_\mu - A_\mu(z))(p_\nu - A_\nu(z)) + Y(z). \]
Its quantization is a magnetic Schrödinger operator
\[
K := \text{Op}(k) = |g|^{-\frac{1}{4}}(D_\mu - A_\mu)|g|^\frac{1}{2}g^{\mu\nu}(D_\nu - A_\nu)|g|^{-\frac{1}{4}} + \frac{1}{6}R + Y.
\]
$K$ is a self-adjoint operator on $L^2(M)$. We are interested in the corresponding

heat semigroup $W(t) := e^{-tK}$, $\text{Re} t > 0$

and Green’s operator (inverse) $G := \frac{1}{K}$.

They are closely related:

$$G = \int_0^\infty W(t)dt.$$
We would like to compute the asymptotics of their kernels around the diagonal. We make the ansatz

\[ W(t) = Op(w(t)), \]

\[ w(t, z, p) \simeq e^{-tk(z, p)} \sum_{n=0}^{\infty} \frac{t^n}{n!} w_n(z, p), \]

\[ w_0(z, p) = 1. \]
By applying the geometric pseudodifferential calculus one can iteratively find $w_n$ and show that

$$w_n(z, p) \simeq \sum_{|\alpha| \leq \frac{3}{2}n} w_{n, \alpha}(z) (p - A(z))^\alpha.$$ 

Note that the naive bound would be $|\alpha| \leq 2n$, however one can improve it to $|\alpha| \leq \frac{3}{2}n$. 
From this one obtains

\[ W(t, x, y) \simeq t^{-\frac{d}{2}} C(x, y) \exp \left( -\frac{1}{4t} u g^{-1}(z) u - t Y(z) \right) \]

\[ \times \sum_{-|\beta| \leq 3k} t^k u^\beta W_{k, \beta}(z) e^{-iuA(z)}, \]

where \( C(x, y) \) is a geometric factor. As usual,

\[ z := x + \frac{y - x}{2}, \quad u := (y - x)^{\frac{1}{2}}. \]
Assume that $Y > 0$. By integrating the heat kernel we obtain a representation of Green’s operator:

$$G(x, y) \simeq 2C(x, y) \sum_{-|\beta| \leq 3k} u^\beta \mathcal{W}_{k, \beta}(z) e^{-iuA(z)}$$

$$\times K_{k+1-\frac{d}{2}} \left( \sqrt{ug^{-1}(z)uY(z)} \right) \left( \frac{ug^{-1}(z)u}{4Y(z)} \right)^{k+1-\frac{d}{2}},$$

where $K_m$ are the MacDonald functions.
Using the well-known expansions of the MacDonald functions we obtain

\[ G(x, y) \simeq 2C(x, y)e^{-iuA(z)} \]

\[ \times \left( \left( \frac{ug^{-1}(z)u}{4Y(z)} \right)^{1-d/2} \sum_{\alpha} u^\alpha w_\alpha(z) \right) \]

\[ + \log \left( \frac{ug^{-1}(z)u}{4Y(z)} \right) \sum_{\alpha} u^\alpha v_\alpha(z) \right). \]

(In odd dimensions the term with the logarithm is absent).
Assume now that $\mathcal{M}$ is a globally hyperbolic Lorentzian manifold.

The operator $K$, formally defined by the same expression as before,

$$ K := |g|^{-\frac{1}{4}}(D_{\mu} - A_{\mu})|g|^\frac{1}{2}g^{\mu\nu}(D_{\nu} - A_{\nu})|g|^{-\frac{1}{4}} + Y $$

is then called a Klein-Gordon operator. Its mathematical theory is much more complicated than that of a Schrödinger operator.
We say that $G$ is a **bisolution** of $K$ if

$$GK = KG = 0.$$  

We say that $G$ is an **inverse** (**Green’s function** or a **fundamental solution**) if

$$GK = KG = 1.$$  

Let us discuss **distinguished** bisolutions and inverses. We will call them **propagators**. (This word is often used in this context in quantum field theory).
On the Minkowski space:

the forward/backward or advanced/retarded propagator
\[ G^{\vee/\wedge}(p) := \frac{1}{(p^2 + m^2 \mp i0 \text{sgn} p^0)}, \]

the Feynman/anti-Feynman propagator
\[ G^{F/F}(p) := \frac{1}{(p^2 + m^2 \mp i0)}, \]

the Pauli-Jordan propagator
\[ G^{PJ}(p) := \text{sgn}(p^0) \delta(p^2 + m^2), \]

and the positive/negative frequency bisolution
\[ G^{(+)/(−)}(p) := \theta(±p^0) \delta(p^2 + m^2). \]
In QFT textbooks, the Pauli-Jordan propagator expresses commutation relations of fields, and hence it is often called the commutator function.

The positive frequency bisolution is the vacuum 2-point function.

The Feynman propagator is the expectation value of time-ordered products of fields and is used to evaluate Feynman diagrams.
It is well-known that on an arbitrary globally hyperbolic spacetime one can define the forward propagator (inverse) $G^\vee$ and the backward propagator (inverse) $G^\wedge$.

Their difference is a bisolution called sometimes the Pauli-Jordan propagator (bisolution)

$$G^{PJ} := G^\vee - G^\wedge.$$ 

All of them have a causal support. We will jointly call them classical propagators. They are relevant for the Cauchy problem.
We are however more interested in “non-classical propagators”, typical for quantum field theory. They are less known to pure mathematicians and more difficult to define on curved spacetimes:

- the **Feynman propagator** $G^F$,
- the **anti-Feynman propagator** $G^{\overline{F}}$,
- the **positive frequency bisolution** $G^{(+)}$,
- the **negative frequency bisolutions** $G^{(-)}$. 
There exists a well-known paper of Duistermat-Hörmander, which defined Feynman parametrices (a parametrix is an approximate inverse in appropriate sense).

There exists a large literature devoted to the so-called Hadamard states, which can be interpreted as bisolutions with approximately positive frequencies. These are however large classes of bisolutions. We would like to have distinguished choices.
It is helpful to introduce a time variable $t$, so that the spacetime is $M = \mathbb{R} \times \Sigma$. Assume that there are no time-space cross terms so that the metric can be written as

$$-g_{00}(t, \vec{x})d^2t + g_{ij}(t, \vec{x})dx^i dx^j.$$

By conformal rescaling we can assume that $g_{00} = 1$, so that, setting $V := A^0$, we have

$$K = -(i\partial_t + V)^2 + L,$$

$$L = -|g|^{-\frac{1}{4}}(i\partial_i + A_i)|g|^\frac{1}{2} g^{ij}(i\partial_j + A_j)|g|^{-\frac{1}{4}} + Y.$$
We rewrite the Klein-Gordon equation as a 1st order equation given by

$$\partial_t + iB(t),$$

where

$$B(t) := \begin{pmatrix} W(t) & 1 \\ L(t) & \overline{W(t)} \end{pmatrix},$$

$$W(t) := V(t) + \frac{i}{4}|g|(t)^{-1}\partial_t|g|(t).$$
Denote by $U(t, t')$ the dynamics defined by $B(t)$, that is

\[
\partial_t U(t, t') = -i B(t) U(t, t'),
\]

\[U(t, t) = 1.\]

Note that if $E = \begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix}$ is a bisolution/inverse of $\partial_t + i B(t)$, then $E_{12}$ is a bisolution/inverse of $K$. 
The classical propagators can be easily expressed in terms of the dynamics:

\[
E^{\text{PJ}}(t, t') := U(t, t') , \quad E^{\text{PJ}}_{12} = -iG^{\text{PJ}};
\]

\[
E^{\vee}(t, t') := \theta(t - t') U(t, t') , \quad E^{\vee}_{12} = -iG^{\vee};
\]

\[
E^{\wedge}(t, t') := -\theta(t' - t) U(t, t') , \quad E^{\wedge}_{12} = -iG^{\wedge}.
\]
We introduce the charge matrix
\[ Q := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \]

and the classical Hamiltonian
\[ H(t) := QB(t) = \begin{pmatrix} L(t) & \overline{W}(t) \\ W(t) & 1 \end{pmatrix}. \]

We will assume that \( H(t) \) is positive and invertible. (Existence of a mass gap).
Assume now for a moment that the problem is static, so that $L, V, B, H$ do not depend on time $t$. Clearly,

$$U(t, t') = e^{-i(t-t')B}.$$ 

The quadratic form $H$ defines the so-called energy scalar product. It is easy to see that $B$ can be interpreted as a self-adjoint operator with a gap in its spectrum around 0. Let $\Pi^{(\pm)}$ be the projections onto the positive/negative part of the spectrum of $B$. 
We define the positive and negative frequency bisolutions and the Feynman and anti-Feynman inverse on the level of $\partial_t + iB(t)$:

\[
E^{(\pm)}(t, t') := \pm e^{-i(t-t')B} \Pi^{(\pm)} ,
\]

\[
E^{F}(t, t') := \theta(t - t') e^{-i(t-t')B} \Pi^{(+)} - \theta(t' - t) e^{-i(t-t')B} \Pi^{(-)} ,
\]

\[
E^{\overline{F}}(t, t') := \theta(t - t') e^{-i(t-t')B} \Pi^{(-)} - \theta(t' - t) e^{-i(t-t')B} \Pi^{(+)} .
\]
They lead to corresponding propagators on the level of $K$:

\[ G^{(\pm)} := E^{(\pm)}_{12}, \]
\[ G^{F} := -iE^{F}_{12}, \]
\[ G^{\bar{F}} := -iE^{\bar{F}}_{12}. \]

They satisfy the relations

\[ G^{F} - G^{\bar{F}} = iG^{(+)} + iG^{(-)}, \]
\[ G^{F} + G^{\bar{F}} = G^{\vee} + G^{\wedge}. \]
In the static case in QFT there is a distinguished state given by the vacuum $\Omega$. The nonclassical propagators are often called 2-point functions, because they are vacuum expectation values of free fields:

$$G^{(+)}(x, y) = \langle \Omega | \hat{\phi}(x)\hat{\phi}(y)\Omega \rangle,$$
$$G^{F}(x, y) = -i \langle \Omega | T(\hat{\phi}(x)\hat{\phi}(y))\Omega \rangle.$$

$G^{F}$ is used to evaluate Feynman diagrams.
It is easy to see that on a general spacetime the Klein-Gordon operator $K$ is Hermitian (symmetric) on $C_c^\infty(M)$ in the sense of the Hilbert space $L^2(M)$.

**Theorem.** [D., Siemssen] Assume the spacetime is static.

1. $K$ is essentially self-adjoint on $C_c^\infty(M)$.
2. For $s > \frac{1}{2}$, the operator $G^F$ is bounded from the space $\langle t \rangle^{-s}L^2(M)$ to $\langle t \rangle^sL^2(M)$. Besides, in the sense of these spaces,

$$s- \lim_{\epsilon \searrow 0} (K - i\epsilon)^{-1} = G^F.$$
Can one generalize non-classical propagators to non-static spacetimes? We will assume that the spacetime is close to being static and for large times it approaches a static spacetime sufficiently fast.

In the non-static case we do not have a single energy space, because the Hamiltonian depends on time. We make technical assumptions that make possible to define a Hilbertizable energy space in which the dynamics is bounded.
One can define the incoming positive/negative frequency bisolution by cutting the phase space with the projections \( \Pi_{\pm} \) onto the positive/negative part of the spectrum of \( B(-\infty) \). \( \Pi_{(+)} \) defines the vacuum state in the distant past given by a vector \( \Omega_- \). It corresponds to a preparation of an experiment.
Analogously, one can define the **outgoing positive/negative bisolutions** by using the projections $\Pi_+^{(\pm)}$ onto the positive/negative part of the spectrum of $B(\infty)$. They correspond to the vacuum state in the remote future given by a vector $\Omega_+$. This vector is related to the future measurements.
The projection $\Pi_{(+)}$ can be transported by the dynamics to any time $t$, obtaining the projection $\Pi_{(+)}^{(t)}$. Similarly we obtain the projection $\Pi_{(-)}^{(t)}$. Using the fact that the dynamics is symplectic, one can show that for a large class of spacetimes for all $t$ the subspaces

$$\text{Ran}\Pi_{(-)}^{(t)}, \quad \text{Ran}\Pi_{(+)}^{(t)}$$

are complementary.
Define $\Pi_{\text{can}}^{(+)}(t), \Pi_{\text{can}}^{(-)}(t)$ to be the unique pair of projections corresponding to the pair of spaces

$$\text{Ran}\Pi_{-}^{(+)}(t), \text{Ran}\Pi_{+}^{(-)}(t)$$

The canonical Feynman propagator is defined as

$$E^F(t_2, t_1) := \theta(t_2 - t_1)U(t_2, t_1)\Pi_{\text{can}}^{(+)}(t_1)$$

$$-\theta(t_1 - t_2)U(t_2, t_1)\Pi_{\text{can}}^{(-)}(t_1),$$

$$G^F := -iE^F_{12}.$$
In a somewhat different setting, in the case of massless Klein-Gordon operator $G^F$ was considered before by A.Vasy et al. A similar construction can be found in a recent paper of Gerard-Wrochna.

Here is the physical meaning of the canonical Feynman propagator: it is the expectation value of the time-ordered product of fields between the in-vacuum and the out-vacuum:

$$G^F(x, y) = \frac{(\Omega_+|T(\hat{\phi}(x)\hat{\phi}(y))\Omega_-)}{(\Omega_+|\Omega_-)}.$$
Thus for a large class of asymptotically static spacetimes one can show the existence of a distinguished Feynman propagator. One can make a stronger conjecture:

**Conjecture.** On a large class of spacetimes (e.g. for compactly supported perturbations of static spacetimes) the Klein-Gordon operator $K$ is essentially self-adjoint on $C^\infty_c(M)$ and in the sense $\langle t \rangle^{-s} L^2(M) \to \langle t \rangle^s L^2(M)$,

$$s- \lim_{\epsilon \searrow 0} (K - i\epsilon)^{-1} = G^F.$$

In a recent paper of A. Vasy this conjecture is proven for asymptotically Minkowskian spaces. This is also true on a large class of cosmological spacetimes.
ASYMPTOTICS OF PROPAGATORS AROUND THE DIAGONAL

In the Lorentzian case, even if we can interpret $K$ as self-adjoint, the heat semigroup does not exists and instead one should consider the so-called proper time dynamics $W(it) = e^{-itK}$. 
One can apply the geometric pseudodifferential calculus to find the asymptotics of $W(it)$ around the diagonal.

$$W(it, x, y) \simeq (it)^{-\frac{d}{2}} C(x, y) \exp \left( -\frac{1}{4it} u g^{-1}(z) u - it Y(z) \right)$$
$$\times \sum_{-|\beta| \leq 3k} (it)^k u^\beta \mathcal{W}_{k, \beta}(z) e^{-iuA(z)}.$$
One can obtain the Feynman and the anti-Feynman propagator by integration:

\[
G_F := (K - i0)^{-1} = i \int_0^\infty W(it)dt,
\]

\[
G_{\overline{F}} := (K + i0)^{-1} = -i \int_0^\infty W(-it)dt.
\]
Here is the asymptotics of the Feynman and anti-Feynman propagator:

\[ G_{F/F}^F(x,y) \]
\[ \simeq 2C(x,y) \sum_{-|\beta| \leq 3k} u^\beta \mathcal{W}_{k,\beta}(z)e^{-iuA(z)} \]
\[ \times \pm iK_{k+1-\frac{d}{2}} \left( \sqrt{ug^{-1}(z)uY(z) \pm i0} \right) \left( \frac{ug^{-1}(z)u \pm i0}{4Y(z)} \right)^{\frac{k+1-\frac{d}{2}}{2}}. \]

Note that for spacelike \( u \) we can drop \( \pm i0 \).
For timelike $u$ the propagators are obtained by an appropriate analytic continuation. In particular, instead of the MacDonald function

$$\pm 2iK_{k+1-\frac{d}{2}}\left(\sqrt{ug^{-1}(z)uY(z)} \pm i0\right),$$

we put

$$-\pi H^\pm_{k+1-\frac{d}{2}}\left(\sqrt{-ug^{-1}(z)uY(z) \mp i0}\right),$$

where $H^\pm_m$ are the Hankel functions of the first and second kind.
Note that the asymptotic expansion of \( \frac{1}{2}(G_F + G_{-F}) \) vanishes for spacelike separated points. The same property is shared by \( \frac{1}{2}(G^\vee + G^\wedge) \). Indeed, on the level of full asymptotic expansions we have

\[
G_F + G_{-F} \simeq G^\vee + G^\wedge.
\]

Let us stress that this does not imply

\[
G_F + G_{-F} = G^\vee + G^\wedge,
\]

except for some special spacetimes.
We can compute the asymptotics of the retarded and advanced propagators:

\[ G^{\vee/\wedge}(x, y) \simeq \pi C(x, y) \sum_{-|\beta| \leq 3k} u^\beta \mathcal{W}_{k,\beta}(z)e^{-iuA(z)} \]

\[ \times J_{k+1-d/2} \left( \sqrt{ug^{-1}(z)uY(z)} \right) \left( \frac{ug^{-1}(z)u}{4Y(z)} \right)^{k+1-d/2}, \]

\[ u^2 \leq 0, \quad \pm u^0 \geq 0, \]

where \( J_m \) are the Bessel functions.
We will say that a pair of positive bisolutions $G^{(+)/(−)}$ of the Klein-Gordon equation satisfies the quasi-vacuum condition if

$$G^{(+)} - G^{(−)} = iG^{PJ}$$

and its asymptotics around the diagonal is given by

$$G^{(+)/(−)} = -iG^{F} + iG^{V/\wedge}.$$ 

It is easy to show that such bisolutions exist. For instance, if our spacetime has a static period, then the bisolutions defined by the positive/negative frequency projections inside this period will satisfy this condition.
The behavior around the diagonal of quasi-vacuum bispersions is fully determined by the geometry:

\[ G^{(+)/(-)}(x, y) \simeq 2C(x, y) \sum_{-|\beta| \leq 3k} u^\beta \mathcal{W}_{k, \beta}(z) e^{-iuA(z)} \]

\[ \times \pm iK_{k+1-d/2} \left( \sqrt{ug^{-1}(z)uY(z) \pm \text{isgn}(u^0)0} \right) \]

\[ \times \left( \frac{ug^{-1}(z)u \pm \text{isgn}(u^0)0}{4Y(z)} \right)^{k+1-d/2}. \]
In the contemporary mathematical community the concept which is viewed as the standard one is the so-called Hadamard condition, where the requirement about the asymptotics around the diagonal is replaced by a condition on the wave front set. This condition is much broader: it includes various kinds of temperature states, which may have a different behavior around the diagonal.

The class of quasi-vacuum states is more narrow. One can argue that they are the most natural states for QFT on curved spacetimes.