

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 $\text{Op}(b) : \mathcal{S}(\mathcal{X}) \rightarrow \mathcal{S}'(\mathcal{X})$ 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:

$$(2\pi)^{-d} \text{Tr} \text{Op}(a)^* \text{Op}(b) = \int \overline{a(z, p)} b(z, p) dz dp.$$

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 $T_x M$ 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

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

Note that

$$\Delta(x, y) = \Delta(y, x), \quad \Delta(x, x) = 1.$$

If B is an operator $C_c^\infty(M) \rightarrow \mathcal{D}'(M)$ then its **kernel** is a distribution in $\mathcal{D}'(M \times M)$ such that

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

We will treat elements of $C_c^\infty(M)$ 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

$$\begin{aligned} \text{Op}(b)(x, y) := & \Delta(x, y)^{\frac{1}{2}} \frac{|g(x)|^{\frac{1}{4}} |g(y)|^{\frac{1}{4}}}{|g(z)|^{\frac{1}{2}}} \\ & \times \int b(z, p) e^{iup} \frac{dp}{(2\pi)^d}, \end{aligned}$$

where

$$z := x + \frac{y - x}{2}, \quad u := (y - x)_{\frac{1}{2}}.$$

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**

$$\text{Op}(a \star b) = \text{Op}(a)\text{Op}(b).$$

Its asymptotic expansion in Planck's constant:

$$\begin{aligned} (a \star b) &\sim ab \\ &+ \frac{i}{2}(a_\alpha b^\alpha - a^\alpha b_\alpha) \\ &- \frac{1}{8}(a_{\alpha_1\alpha_2} b^{\alpha_1\alpha_2} - 2a_{\alpha_1}^{\alpha_2} b_{\alpha_2}^{\alpha_1} + a^{\alpha_1\alpha_2} b_{\alpha_1\alpha_2}) + \frac{1}{12}R_{\alpha_1\alpha_2} a^{\alpha_2} b^{\alpha_1} \\ &- \frac{1}{24}R^\beta_{\alpha_1\alpha_2\alpha_3} p_\beta (a^{\alpha_2} b^{\alpha_1\alpha_3} + a^{\alpha_1\alpha_3} b^{\alpha_2}) + \dots \end{aligned}$$

where lower indices denote **horizontal derivatives** (in spatial directions) and upper indices denote **vertical derivatives** (in momentum directions).

SCHRÖDINGER OPERATORS ON A RIEMANNIAN MANIFOLD—THE ASYMPTOTICS OF THEIR INVERSE AROUND THE DIAGONAL

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

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

$$\begin{aligned} W(t) &= \text{Op}(w(t)), \\ w(t, z, p) &\simeq e^{-tk(z,p)} \sum_{n=0}^{\infty} \frac{t^n}{n!} w_n(z, p), \\ w_0(z, p) &= 1. \end{aligned}$$

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

$$W(t, x, y) \simeq t^{-\frac{d}{2}} C(x, y) \exp \left(-\frac{1}{4t} u g^{-1}(z) u - t Y(z) \right) \\ \times \sum_{-|\beta| \leq 3k} t^k u^\beta \mathcal{W}_{k, \beta}(z) e^{-i u A(z)},$$

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:

$$G(x, y) \simeq 2C(x, y) \sum_{-|\beta| \leq 3k} u^\beta \mathcal{W}_{k, \beta}(z) e^{-iuA(z)} \\ \times K_{k+1-\frac{d}{2}} \left(\sqrt{ug^{-1}(z)uY(z)} \right) \left(\frac{ug^{-1}(z)u}{4Y(z)} \right)^{\frac{k+1-\frac{d}{2}}{2}},$$

where K_m are the **MacDonald functions**.

Using the well-known expansions of the MacDonald functions we obtain

$$G(x, y) \simeq 2C(x, y)e^{-iuA(z)} \\ \times \left(\left(\frac{ug^{-1}(z)u}{4Y(z)} \right)^{1-\frac{d}{2}} \sum_{\alpha} u^{\alpha} w_{\alpha}(z) \right. \\ \left. + \log \left(\frac{ug^{-1}(z)u}{4Y(z)} \right) \sum_{\alpha} u^{\alpha} v_{\alpha}(z) \right).$$

(In odd dimensions the term with the logarithm is absent).

KLEIN-GORDON OPERATORS, THEIR INVERSES AND BISOLUTIONS (PROPAGATORS)

Assume now that 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

$$G^{\vee/\wedge}(p) := \frac{1}{(p^2 + m^2 \mp i0 \operatorname{sgn} p^0)},$$

the **Feynman/anti-Feynman** propagator

$$G^{\mathrm{F}/\overline{\mathrm{F}}}(p) := \frac{1}{(p^2 + m^2 \mp i0)},$$

the **Pauli-Jordan** propagator

$$G^{\mathrm{PJ}}(p) := \operatorname{sgn}(p^0) \delta(p^2 + m^2),$$

and the **positive/negative frequency** bisolution

$$G^{(+)/(-)}(p) := \theta(\pm p^0) \delta(p^2 + m^2).$$

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)**

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

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 $G^{\bar{F}}$,
- the positive frequency bisolution $G^{(+)}$,
- the negative frequency bisolutions $G^{(-)}$.

There exists a well-known paper of Duistermaat-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

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

$$L = -|g|^{-\frac{1}{4}}(\mathrm{i}\partial_i + A_i)|g|^{\frac{1}{2}}g^{ij}(\mathrm{i}\partial_j + A_j)|g|^{-\frac{1}{4}} + Y.$$

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

$$\begin{aligned}\partial_t U(t, t') &= -\mathrm{i}B(t)U(t, t'), \\ U(t, t) &= 1.\end{aligned}$$

Note that if

$$E = \begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix}$$

is a bisolution/inverse of $\partial_t + \mathrm{i}B(t)$, then E_{12} is a bisolution/inverse of K .

The classical propagators can be easily expressed in terms of the dynamics:

$$\begin{aligned}
 E^{\text{PJ}}(t, t') &:= U(t, t'), & E_{12}^{\text{PJ}} &= -iG^{\text{PJ}}; \\
 E^{\vee}(t, t') &:= \theta(t - t') U(t, t'), & E_{12}^{\vee} &= -iG^{\vee}; \\
 E^{\wedge}(t, t') &:= -\theta(t' - t) U(t, t'), & E_{12}^{\wedge} &= -iG^{\wedge}.
 \end{aligned}$$

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 $\partial_t + iB(t)$:

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

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

$$E^{\overline{\text{F}}}(t, t') := \theta(t - t') e^{-i(t-t')B} \Pi^{(-)} - \theta(t' - t) e^{-i(t-t')B} \Pi^{(+)}.$$

They lead to corresponding propagators on the level of K :

$$\begin{aligned}G^{(\pm)} &:= E_{12}^{(\pm)}, \\G^F &:= -iE_{12}^F, \\G^{\bar{F}} &:= -iE_{12}^{\bar{F}}.\end{aligned}$$

They satisfy the relations

$$\begin{aligned}G^F - G^{\bar{F}} &= iG^{(+)} + iG^{(-)}, \\G^F + G^{\bar{F}} &= G^\vee + G^\wedge.\end{aligned}$$

In the static case in QFT there is a distinguished state given by the vacuum Ω . The nonclassical propagators are often called **2-point functions**, because they are vacuum expectation values of free fields:

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

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 $\langle t \rangle^s L^2(M)$. Besides, in the sense of these spaces,

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

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 Ω_{-} . 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 Ω_{+} . 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

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

The **canonical Feynman propagator** is defined as

$$\begin{aligned} E^{\text{F}}(t_2, t_1) &:= \theta(t_2 - t_1)U(t_2, t_1)\Pi_{\text{can}}^{(+)}(t_1) \\ &\quad - \theta(t_1 - t_2)U(t_2, t_1)\Pi_{\text{can}}^{(-)}(t_1), \\ G^{\text{F}} &:= -\text{i}E_{12}^{\text{F}}. \end{aligned}$$

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 $C_c^\infty(M)$ and in the sense $\langle t \rangle^{-s} L^2(M) \rightarrow \langle t \rangle^s L^2(M)$,

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

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 exist 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:

$$\begin{aligned}
 & G^{\text{F}/\overline{\text{F}}}(x, y) \\
 & \simeq 2C(x, y) \sum_{-|\beta| \leq 3k} u^\beta \mathcal{W}_{k, \beta}(z) e^{-i u A(z)} \\
 & \times \pm i K_{k+1-\frac{d}{2}} \left(\sqrt{u g^{-1}(z) u Y(z)} \pm i0 \right) \left(\frac{u g^{-1}(z) u \pm i0}{4Y(z)} \right)^{\frac{k+1-\frac{d}{2}}{2}}.
 \end{aligned}$$

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

where H_m^{\pm} are the **Hankel functions** of the first and second kind.

Note that the asymptotic expansion of $\frac{1}{2}(G_F + G_{\overline{F}})$ 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

$$G_F + G_{\overline{F}} \simeq G^\vee + G^\wedge.$$

Let us stress that this does not imply

$$G_F + G_{\overline{F}} = G^\vee + G^\wedge,$$

except for some special spacetimes.

We can compute the asymptotics of the **retarded** and **advanced propagators**:

$$G^{\vee/\wedge}(x, y) \simeq \pi C(x, y) \sum_{-|\beta| \leq 3k} u^\beta \mathcal{W}_{k, \beta}(z) e^{-i u A(z)} \\ \times J_{k+1-\frac{d}{2}} \left(\sqrt{u g^{-1}(z) u Y(z)} \right) \left(\frac{u g^{-1}(z) u}{4 Y(z)} \right)^{\frac{k+1-\frac{d}{2}}{2}}, \\ u^2 \leq 0, \quad \pm u^0 \geq 0,$$

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

$$G^{(+)} - G^{(-)} = iG^{\text{PJ}}$$

and its asymptotics around the diagonal is given by

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

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 bisolutions is fully determined by the geometry:

$$\begin{aligned}
G^{(+)/(-)}(x, y) &\simeq 2C(x, y) \sum_{-|\beta| \leq 3k} u^\beta \mathcal{W}_{k,\beta}(z) e^{-iuA(z)} \\
&\times \pm i K_{k+1-\frac{d}{2}} \left(\sqrt{ug^{-1}(z)uY(z) \pm i \operatorname{sgn}(u^0)0} \right) \\
&\times \left(\frac{ug^{-1}(z)u \pm i \operatorname{sgn}(u^0)0}{4Y(z)} \right)^{\frac{k+1-\frac{d}{2}}{2}}.
\end{aligned}$$

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.