

COVARIANT WEYL QUANTIZATION, SYMBOLIC CALCULUS,
AND THE PRODUCT FORMULA

A Dissertation

by

KAMIL SERKAN GÜNTÜRK

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

May 2006

Major Subject: Physics

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Approved by:

Chair of Committee,	Stephen A. Fulling
Committee Members,	Christopher Pope
	Ergin Sezgin
	James T. White
	Guy Battle
Head of Department,	Edward Fry

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ABSTRACT

Covariant Weyl Quantization, Symbolic Calculus,
and the Product Formula. (May 2006)

Kamil Serkan Güntürk, B.S., Istanbul Technical University;
M.S., Boğaziçi University

Chair of Advisory Committee: Dr. Stephen A. Fulling

A covariant Wigner-Weyl quantization formalism on the manifold that uses pseudo-differential operators is proposed. The asymptotic product formula that leads to the symbol calculus in the presence of gauge and gravitational fields is presented. The new definition is used to get covariant differential operators from momentum polynomial symbols. A covariant Wigner function is defined and shown to give gauge-invariant results for the Landau problem. An example of the covariant Wigner function on the 2-sphere is also included.

To my family

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CHAPTER I

INTRODUCTION

Hermann Weyl, in his *Symmetry* [1], relates a brief account of the early 18th century rather theological controversy between Leibniz and Clarke¹ on the relative concepts of position and direction, whether God had a *sufficient reason* to favor right over left in the beginning of creation. Although the details of this debate and Weyl’s personal resolution to it can be considered off topic for this dissertation, the remarks made by the great mathematician, philosopher and physicist of the last century – despite his acknowledgment of not being a member of the physics community to Sommerfeld in 1922 [2]– upon the importance of the *asymmetries* which are secondary in nature, but “superimposed on the basic bilateral-symmetrically built ground plan” are worthy of quoting here. He wrote:

If nature were all lawfulness then every phenomenon would share the full symmetry of the universal laws of nature as formulated by the theory of relativity. The mere fact that this is not so proves that *contingency* is an essential feature of the world. ([1], *emph. in orig.*)

Interestingly enough, one among the dozens of beautiful illustrations he chose for his book is the *human heart*, an asymmetric screw.

Nevertheless, by the end of the 1920’s he had become one of the main contributors to the newly discovered theory of Quantum Mechanics by introducing *symmetry* to this novel way of understanding of the “ground plan” [3]. Much later, in 1958, Wolfgang Pauli would call this period the “preliminary end” of the “initial phase”:

The journal model is *IEEE Transactions on Automatic Control*.

¹A “clergyman acting as the spokesman for Newton” according to Weyl [1].

The last decisive turning point of quantum theory came with de Broglie's hypothesis of matter waves, Heisenberg's discovery of matrix mechanics, and Schrodinger's wave equation, the last establishing the relationship between the first two sets of ideas. With Heisenberg's uncertainty principle and Bohr's fundamental discussions thereon the initial phase of development of the theory came to a preliminary end. ([4], p. 1.)

One should note that this humble list excludes some other prominent figures like Dirac, Wigner and the discoverer of the *exclusion principle* himself.

Classical mechanics had no problem with position and momentum being *scalar* quantities (or so called c-numbers) and the idea that the two can be measured simultaneously with a precision that had no limits, at least in principle. The new mechanics though, introduced an alien concept of measurement into this deterministic world where observables were now represented by *operators* (or q-numbers) which did not necessarily commute. The quantum state $|\psi\rangle$ describing the system before the measurement collapses to the *eigenstate* of the operator \hat{O} that represents the observable. Thus a subsequent measurement of a different observable has to be described by the corresponding operator \hat{O}' acting on that particular eigenstate. Unless the two operators share eigenstates, in other words $\hat{O}\hat{O}' = \hat{O}'\hat{O}$, the outcome of this second measurement is unrelated to the pre-collapsed quantum state. There was no such concept as the order of measurements in classical mechanics. The case for *simultaneous* measurement is quite similar. Since \hat{Q} and \hat{P} do not commute it is impossible to have definite simultaneous values for position and momentum.

The process of finding the quantum operators corresponding to classical observables is called *quantization* [5]. This usually involves the quantization of not only position and momentum but any given function (also called the *symbol*) of these variables

such as the classical Hamiltonian. In mathematics, the result is called a *pseudodifferential operator* (ψ DO). Obviously as these functions get complicated this process becomes ambiguous, for instance, the ordering of non-commuting operators becomes a matter of choice. In some problems terms like $\sum_k [\hat{A}_k(Q)\hat{P}_k + \hat{P}_k\hat{A}_k(Q)]$ are needed in the Hamiltonian so that Hermiticity is preserved² ([4], pp. 37–39), and certain schemes like Weyl quantization, or McCoy’s formula, where $\frac{1}{2^n} \sum_{l=0}^n \binom{n}{l} \hat{Q}^{n-l} \hat{P}^l \hat{Q}^l$ is the quantization of $q^n p^m$ in one dimension, can produce Hermitian operators that possess a natural (preferred) operator ordering [6], [7].

It is interesting to note here that it would be wrong to say that quantum mechanics is just classical mechanics under some sort of operation or *deformation*, when we do not even have a rigorous proof that the *self-adjoint* operator \hat{H} which determines the time evolution should be the quantum mechanical analogue of the classical Hamiltonian! [5]. The fact that equations of motion are similar if the *Poisson bracket* (with the classical Hamiltonian) is replaced by i times the commutator (with the Hamiltonian operator) should not lead us to the assumption that this replacement is a quantization because this connection is not total. In Weyl quantization it is possible to write a formula for the symbol of the product of two operators, $\text{Sym}(\hat{A}\hat{B})$, in terms of the symbols of these operators, $\text{Sym}(\hat{A})$ and $\text{Sym}(\hat{B})$. In the physics literature this is referred to as the star, twisted, or Weyl product. In fact the Poisson bracket is only one of the low order terms in the *Moyal bracket*, which is an anti-symmetrization of the Weyl product [7].

Weyl quantization tells us only how symbols define operators; it is the *Wigner transform* that gives the unique real phase space function for each quantum observable. This transform can be regarded as the *inverse* of Weyl quantization (only up

²If \hat{H}_1 and \hat{H}_2 are linear Hermitian operators, so is $\hat{H}_1\hat{H}_2 + \hat{H}_2\hat{H}_1$.

to a factor, to be precise [8]). This formulation has its roots in statistical mechanics where one has to deal with systems of very large degrees of freedom and a phase space probabilistic approach is needed. All one needs is a *density function* ρ which carries information about the energy of the system by means of the Hamiltonian function. Then the average value (or the expectation value) $\langle A \rangle$ of any observable $A(q, p)$ is found by integrating $A(q, p)\rho(q, p)$ over the phase space [9]. Landau and von Neumann (see [10], p. 328) observed that there should be a quantum mechanical analogue of the density function (called the *density matrix* $\hat{\rho}$) such that the average of a function of position and momentum operators can be written as $\langle \hat{A} \rangle = \text{Tr}(\hat{A}\hat{\rho})$. Wigner's contribution was to show that $\langle \hat{A} \rangle$ could also be obtained from a phase space distribution function, which is essentially the Wigner transform of the density matrix. In 1949, the Jerusalem-born Australian electrical engineer, statistician, mathematician and theoretical physicist Jose Enrique Moyal established the above mentioned "Wigner-Weyl correspondence" [7], [10], [11]. One should note here that at the heart of this formalism lies the faithful companion of physicists, the Fourier transform, and the mathematical interest on the issue has led to some elegant formulations including the Heisenberg translation operator and *quantizer*³ methods [12]. One can also find group-theoretical aspects in [13], [14].

Recalling the dangers of false interpretations of the quantization process, we should be careful when trying to interpret the reverse process of "dequantization" [5]. Many quantum systems are found to have a discrete energy spectrum, whereas their classical counterparts are allowed to take any value for energy. Some quantum mechanical observables do not even have any classical analogues. The famous way of explaining these physical phenomena is to set up a *classical limit* of quantum

³Also called the *Stratonovich* quantizer.

mechanics by taking the formal limit $\hbar \rightarrow 0$. One must ensure that this limit is mathematically well-defined and physically makes sense⁴. There are other methods like Bohr's correspondence principle (the limit of large quantum numbers) and Ehrenfest Theorem. The former does not refer to dynamics and fails to work in certain physical systems like the harmonic oscillator [15], while the latter is restricted to special forms of potential [5].

Another method for obtaining the classical limit is the insertion of $\psi(x, t) = \exp[iS(x, t)/\hbar]$ into the Schrodinger equation to find the *Hamilton-Jacobi equation* for $S(x, t)$, provided that certain asymptotics exist. This is the celebrated Wentzel-Kramers-Brillouin (WKB) method and despite its weakness of incompatibility with the superposition principle of quantum mechanics [15], it has been fruitful in semiclassical calculation of wavefunctions [16]. In physics literature one can find several WKB type expansion methods under the name of Schwinger-DeWitt, Wigner-Kirkwood (large mass limit), Birkhoff-VanVleck series and varieties [17], [18]. Molzahn and Osborn showed that the Weyl formalism could be used as a foundation for semiclassical analysis in either the Schrödinger [19] or the Heisenberg [7] evolution picture. While [19] demonstrates an ansatz-free derivation of the Schrödinger propagator's WKB expansion, the Heisenberg-Weyl description of evolution presented in [7] is advantageous over the WKB approximation for propagators, since it does not involve singularities, multiple trajectories, caustics or Maslov indices. Their work is also of great mathematical interest for employing cluster expansions, which have a graph-combinatorial structure and also arise in quantum transport equation solutions [20]. For a detailed analysis of graph representations and semiclassical expansions one should also refer to [17], [21] and [22].

⁴For instance, the *fine structure constant* $\alpha = e^2/\hbar c$ gives rise to a divergence as $\hbar \rightarrow 0$ if the other constants are fixed [15].

It is well known that in classical electrodynamics, the physical fields \mathbf{E} and \mathbf{B} are unchanged under a *gauge transformation*⁵ of the scalar (ϕ) and magnetic (\mathbf{A}) potentials. When the wave function simultaneously goes under a *phase* transformation of the second kind $\psi(\mathbf{x}, t) \rightarrow e^{\frac{ie}{\hbar c}\theta(\mathbf{x}, t)}\psi(\mathbf{x}, t)$, the Schrödinger equation is covariant provided that the ordinary derivative operators are replaced⁶ by $\nabla - i(e/\hbar c)\mathbf{A}$ [24]. It is easy to check that the *canonical* momentum operator is not gauge invariant; therefore, it cannot represent a physical observable. On the other hand the operator representing the *kinetic* momentum $\vec{\pi} = \mathbf{p} - (e/c)\mathbf{A}$ turns out to be gauge independent and therefore physical. In the conventional symbol-operator correspondence this covariance issue is addressed in various ways. In the quantizer approach of Weyl formalism one includes gauge invariance by replacing the canonical momentum appearing in the definitions by the kinetic momentum [25], [26], [27], [28]. Recently, Karasev and Osborn developed a gauge invariant symbol calculus based on their “magnetic product” \star_F , where F stands for the electromagnetic Faraday 2-form $F = \frac{1}{2}F_{jk}(q)dq^k \wedge dq^j$, which is used to modify the usual symplectic form ω [29].

Since covariant derivatives are also used in physics in order to explain the coupling of matter to gravitational fields [24], one may argue that a general geometrical framework is needed to establish a covariant operator-symbol correspondence. Indeed, the components of the electromagnetic vector potential (or Yang-Mills potential) are the *connection coefficients* w_μ on the vector bundle, just like Christoffel symbols $\Gamma_{\nu\lambda}^\mu$ represent a connection on the tangent bundle of the manifold. *Parallel transport* defined by a connection is one of the basic notions in Riemannian geometry and is required for a geometrically covariant, or *intrinsic*, formalism. One

⁵ $\phi \rightarrow \phi - \frac{1}{c}\frac{\partial}{\partial t}\theta(\mathbf{x}, t)$ and $\mathbf{A} \rightarrow \mathbf{A} + \nabla\theta(\mathbf{x}, t)$.

⁶This is often called a “minimal substitution” [23].

of the first attempts⁷ to apply the operator-symbol correspondence to manifolds came from Gilkey in 1975 [31], where he calculated the coefficients in the expansion $K(t, x, x) \sim (4\pi t)^{-d/2} \sum_{n=0}^{\infty} E_n(x) t^{n/2}$ for the kernel function that defines the operator e^{-tH} on a d -dimensional Riemannian manifold where H is a second order differential operator. Only the leading term of the symbol of H is an invariant; the lower order terms depend upon the local system chosen. The E_n are complicated combinations of the covariant objects like $R_{\mu\nu\lambda\rho}$ (the Riemann curvature tensor), and $W_{\mu\nu} = \partial_\mu w_\nu - \partial_\nu w_\mu + [w_\mu, w_\nu]$, the curvature of the bundle (or the gauge field strength) and covariant derivatives⁸ of these.

An intrinsic pseudo-differential calculus needs to be covariant from the start; the symbol should be defined as a function on $T^*(M)$, the cotangent bundle of the configuration space [6]. The credit here goes to Bokobza-Haggiag [30], Widom [32] and Drager [33]. In this formalism, the geodesic flow $y = \exp_x(\mathbf{u})$ that arises from a given connection, plays the major role. The symbol, now a function of the “momentum variable” $\in T_x^*(M)$ and \mathbf{u} , is accompanied by τ^E (which will be renamed I later in this dissertation), the parallel transport with respect to a given connection on the vector bundle E . The formula for the symbol of a product, the application of the intrinsic calculus to the asymptotic expansion of the symbol of a *resolvent parametrix*⁹, and reduction to the conventional calculus upon specialization to flat connections can be found in [35].

Despite its success in establishing a manifestly covariant quantization, intrinsic calculus lacks the symmetry of conventional Weyl calculus. With the physical motiva-

⁷The earliest seems to be the paper by Juliane Bokobza-Haggiag [30] in 1969.

⁸Note that in the most general case, the covariant derivative of the covector $\nabla_\mu \phi$ is $\nabla_\nu \nabla_\mu \phi = \partial_\nu (\nabla_\mu \phi) + w_\nu \nabla_\mu \phi - \Gamma_{\nu\mu}^\rho \nabla_\rho \phi$.

⁹The symbol of the operator $(\hat{A} - \lambda)^{-1}$, roughly speaking [34].

tions presented in [7] and [19] in mind, one may ask the question of how to construct a covariant analogue of the Weyl calculus. Fulling proposed such a formalism in 1998 where an operator is covariantly obtained from the symbol function that is symmetric in the points on the manifold [6]. This can be considered to be the first systematic discussion of the conventional, Weyl and Widom ψ DO formalisms (and the fusion of them) from both a mathematical and a physical point of view. A covariant Wigner function which may be of interest for relativistic quantum field theorists (see [36], [37], [38], [39]) is also provided. For a generic second-order momentum polynomial $A^{\mu\nu}(q)p_\mu p_\nu$ case, one gets a second-order covariant differential operator with intrinsic coefficients, *i.e.*, the covariant derivatives of the tensor $A^{\mu\nu}$ and the curvature tensor $R_{\mu\nu}$. In the special case of $A^{\mu\nu} = g^{\mu\nu}$, which can be thought of as a case where the symbol becomes the classical Hamiltonian of a free particle of unit mass on a manifold, one gets the *Laplace-Beltrami operator* $\Delta = -g^{\mu\nu}\nabla_\mu\nabla_\nu$ plus a parameter-dependent Ricci scalar curvature term.

The product formula in this new formalism is found by Fulling in the special case of flat space [6] (the paper also includes an exponential version of the asymptotic product rule in Widom calculus, which is published for the first time). The asymptotic expansion for the product formula for the general case (manifold) is not known. This was the motivation for the work in this dissertation. The integrals used in the definition of operator \rightleftharpoons symbol relations are over $T_x(M)$ and $T_x^*(M)$. The difficulty arises from the fact that the steps towards an expression for the symbol of $\hat{C} = \hat{A}\hat{B}$ necessitate the handling of such integrals on the tangent and cotangent spaces of more than one point, which cannot be carried out by brute force calculations. I try to solve the problem by modifying the operator \rightleftharpoons symbol formulae by introducing a fiducial point on the manifold where all integrations are to be carried out. With this approach I was able to obtain an asymptotic product formula on the manifold. Some of the

point separation techniques given in [40], [41], [42] and [43] are used in analyzing the product rule and testing the formalism in the case of momentum polynomial symbols. The related covariant Wigner function is defined and its application to a) the Landau problem (charged particle moving in a magnetic field) in flat space with gauge invariance and b) a test function on the 2-sphere subject to a rotation by $\pi/2$, are discussed as examples.

CHAPTER II

PRELIMINARIES

Physicists commonly refer to covariance in the context of the mathematical concept of form invariance. If the written form of an equation describing a physical law does not change under a particular transformation of a certain kind, it is said to be covariant under that transformation. A quantity that is invariant under such a change may also be called covariant (in that case it is also an observable). Apart from the physical motivations, it is sometimes the beauty factor that attracts theoreticians to covariance. It is often stated that “a theoretical physicist who had never heard of magnetism might be led to predict its existence, on the basis of the purely aesthetic requirement that quantum mechanics be invariant under the local phase transformations” ([24], p. 161). This reverse logic actually is responsible for some of the major discoveries in science, especially in the field of high energy physics [44].

A. Gauge Invariance

1. Classical Electromagnetism

The discovery of the vector potential \mathbf{A} and its connection to the magnetic field

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{2.1}$$

and the induced electromotive force, in the form $c\mathbf{E} = -d\mathbf{A}/dt$, goes all the way back to Carl Friedrich Gauss¹⁰. Later Helmholtz and Maxwell noticed the arbitrariness in

¹⁰He did not publish his handwritten notes of 1835 until 1867, and the credit went to Wilhelm Weber (1846), Franz E. Neumann (1847), Gustav Kirchhoff (1857) and Hermann von Helmholtz (1870) [45].

the choice of this potential¹¹, and stated that the physical fields \mathbf{B} and

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} \quad (2.2)$$

are invariant under the transformation

$$\mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla\theta. \quad (2.3)$$

Maxwell did not mention the accompanying transformation of the scalar potential

$$\phi \rightarrow \phi' = \phi - \frac{1}{c}\frac{\partial\theta}{\partial t} \quad (2.4)$$

in his 1873 paper, although a few years earlier, in 1867, the Danish physicist Ludvig Valentin Lorenz had stated this fact indirectly with the introduction of his *retarded potentials* [45]. Lorenz also established that these potentials are solutions of the wave equation and satisfy¹²

$$\nabla \cdot \mathbf{A} + \frac{1}{c}\frac{\partial\phi}{\partial t} = 0. \quad (2.5)$$

2. Motion in an Electromagnetic Field

The force on a particle with charge e and mass m in the presence of electric and magnetic fields is

$$\begin{aligned} \frac{d}{dt}(m\mathbf{v}) &= e\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right) \\ &= e\left[-\nabla\left(\phi - \frac{\mathbf{v} \cdot \mathbf{A}}{c}\right) - \frac{1}{c}\frac{d\mathbf{A}}{dt}\right] \end{aligned} \quad (2.6)$$

¹¹Maxwell used three different expressions for this quantity: Electro-tonic intensity, electromagnetic momentum and electrokinetic momentum [45]

¹²This condition is often erroneously attributed to the more famous Dutch physicist Hendrik Antoon Lorentz.

where \mathbf{v} is the particle's velocity. This force equation can be derived from the Lagrangian [46]

$$L = \frac{1}{2}mv^2 + \frac{e}{c} \mathbf{v} \cdot \mathbf{A} - e\phi. \quad (2.7)$$

Then the momentum $\mathbf{p} = \partial L / \partial \mathbf{v}$ is related to the *kinetic* momentum $\mathbf{k} = m\mathbf{v}$ through

$$\mathbf{p} = m\mathbf{v} + \frac{e}{c} \mathbf{A}. \quad (2.8)$$

Using (2.7) and (2.8) one can write the Hamiltonian function as

$$\begin{aligned} H &= \mathbf{p} \cdot \mathbf{v} - L \\ &= \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + e\phi. \end{aligned} \quad (2.9)$$

Then the canonical equations are

$$\frac{d\mathbf{p}}{dt} = -e\nabla \left(\phi - \frac{\mathbf{v} \cdot \mathbf{A}}{c} \right) \quad \text{and} \quad \mathbf{v} = \frac{1}{m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right), \quad (2.10)$$

which are identical with eqs. (2.6) and (2.8), respectively [46]. One can easily check¹³ that (2.6) is covariant under the transformations given by (2.3) and (2.4).

3. The Relativistic Problem

The kinetic term in the Lagrangian given in (2.7) does not impose any limit on the magnitude of \mathbf{v} , in contrast to special relativity where it is impossible to accelerate beyond the speed of light. One needs an action which is also Lorentz invariant. In special relativity [47], it is postulated that there should be a quantity, defined in terms of time and space intervals between two events, that is invariant under the

¹³Using $d\theta(\mathbf{r}, t)/dt = \partial\theta/\partial t + \nabla\theta \cdot \mathbf{v}$

transformation $(ct, \mathbf{r}) \rightarrow (ct', \mathbf{r}')$. This invariant is defined as

$$\Delta s^2 = (c\Delta t)^2 - (\Delta x^1)^2 - (\Delta x^2)^2 - (\Delta x^3)^2 \quad (2.11)$$

or

$$ds^2 = (cdt)^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2 \quad (2.12)$$

for infinitesimal intervals. Any change of coordinates that leaves ds^2 invariant, *i.e.*,

$$ds^2 = ds'^2 \quad (2.13)$$

is called a Lorentz transformation (examples are: Linear boost¹⁴ along the x direction, rotations etc.). For timelike infinitesimal intervals, $ds^2 > 0$ and $ds \equiv \sqrt{ds^2}$. In the special case of $d\mathbf{r} = 0$, the quantity ds/c is called the *proper time* which is a good candidate for the action. With a little arrangement to get the dimension right (energy \times time) and an appropriate choice of sign¹⁵, the relativistic action should look like

$$S = -mc^2 \int ds + \text{e.m. terms.} \quad (2.14)$$

Therefore the relativistic Lagrangian for the particle in an electromagnetic field (see [47] and [48]) is

$$\mathcal{L} = -mc^2 \sqrt{1 - \frac{v^2}{c^2}} + \frac{e}{c} \mathbf{v} \cdot \mathbf{A} - e\phi. \quad (2.15)$$

Some textbooks [49] also include an additional term mc^2 in (2.15) so that one gets the classical Lagrangian (2.7) in the $v \ll c$ limit, which does not affect the equations of motion. Using (2.15) and $\mathbf{p} = \gamma m\mathbf{v} + e\mathbf{A}/c$ one writes the relativistic Hamiltonian function as

$$\mathcal{H} = c\sqrt{m^2c^2 + (\mathbf{p} - e\mathbf{A}/c)^2} + e\phi \quad (2.16)$$

¹⁴ $x' = \gamma(x - vt)$ and $ct' = \gamma(ct - vx/c)$ where $\gamma \equiv (1 - v^2/c^2)^{-1/2}$.

¹⁵Negative for consistency with $E^2 = p^2c^2 + m^2c^4$ (free particle case).

and find the equations of motion

$$\frac{d\mathbf{p}}{dt} = -e\nabla\left(\phi - \frac{\mathbf{v} \cdot \mathbf{A}}{c}\right) \quad \text{and} \quad \mathbf{v} = \frac{c(\mathbf{p} - \frac{e}{c}\mathbf{A})}{\sqrt{m^2c^2 + (\mathbf{p} - e\mathbf{A}/c)^2}}. \quad (2.17)$$

4. Quantum-Mechanical Problem

In a paper submitted to *Annalen der Physik* in June 1926 [50], Erwin Schrödinger presented the wave equation for the relativistic particle in an electromagnetic field [45]. Following his footsteps, we state that the Hamilton-Jacobi equation

$$\mathcal{H}\left(q_i, \frac{\partial S}{\partial q_i}\right) + \frac{\partial S}{\partial t} = 0, \quad (2.18)$$

where S is the modern conventional notation for his contemporaries' *Wirkungsfunktion*, applied to (2.16) reads

$$c\sqrt{m^2c^2 + (\nabla S - e\mathbf{A}/c)^2} + e\phi + \frac{\partial S}{\partial t} = 0. \quad (2.19)$$

The square of (2.19), after a little manipulation, is

$$\left(\frac{1}{c}\frac{\partial S}{\partial t} + \frac{e}{c}\phi\right)^2 - \left(\nabla S - \frac{e}{c}\mathbf{A}\right)^2 - m^2c^2 = 0. \quad (2.20)$$

The magical replacement of $\partial S/\partial t$ and ∇S by the operators

$$\pm \frac{\hbar}{2\pi i} \frac{\partial}{\partial t} \quad \text{and} \quad \pm \frac{\hbar}{2\pi i} \nabla$$

and letting the resultant operator act on the wavefunction ψ , leads to

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} \mp \frac{2ie}{\hbar c}\left(\frac{\phi}{c}\frac{\partial\psi}{\partial t} + \mathbf{A} \cdot \nabla\psi\right) + \frac{e^2}{\hbar^2c^2}\left(\phi^2 - \mathbf{A}^2 - \frac{m^2c^4}{e^2}\right)\psi = 0 \quad (2.21)$$

where $\hbar \equiv h/2\pi$. In obtaining (2.21), Schrödinger used the Loren(t)z condition given in (2.5).

Also in June of the same year, Vladimir Aleksandrovich Fock submitted a paper

[51] to *Zeitschrift für Physik* where he solved the wave equations for the “Kepler problem¹⁶ in a magnetic field” and the “relativistic Kepler problem” [45]. The method he used to derive these equations begins with the Hamilton-Jacobi equation (2.19) as Schrödinger did, and then makes the following pair of substitutions:

$$\frac{\partial S}{\partial t} \longrightarrow -E = -E \frac{(\partial\psi/\partial t)}{(\partial\psi/\partial t)}, \quad (2.22)$$

$$\frac{\partial S}{\partial q_i} \longrightarrow -E \frac{(\partial\psi/\partial q_i)}{(\partial\psi/\partial t)}, \quad (2.23)$$

where E is the energy constant of the system. After multiplication by $(\frac{\partial\psi}{\partial t})^2$, he moves on to deriving the wave equations from a variational principle using the quadratic form obtained.

In his succeeding paper submitted in July [48], he studied the wave mechanics of the problem described by the Lagrangian (2.15). Independently from Schrödinger ([50] was published in September), Fock also ended up with the wave equation (2.21) for ψ except his version included a term with

$$\nabla \cdot \mathbf{A} + \frac{1}{c} \frac{\partial\phi}{\partial t} \quad (2.24)$$

which he kept there for a reason! In this article gauge invariance in quantum mechanics was explicitly introduced for the first time [45].

The new *Ansätze* are

$$\nabla S = \frac{\nabla\psi}{(\partial\psi/\partial\mathbf{p})}, \quad (2.25)$$

$$\frac{\partial S}{\partial t} = \frac{(\partial\psi/\partial t)}{(\partial\psi/\partial\mathbf{p})}, \quad (2.26)$$

where \mathbf{p} is a parameter with a dimension matching that of the action. Then one

¹⁶Motion under the influence of the potential $U = -e^2/r$.

considers varying the integral of the quadratic form

$$\begin{aligned} \mathcal{Q} = & (\nabla\psi)^2 - \frac{1}{c^2} \left(\frac{\partial\psi}{\partial t} \right)^2 - \frac{2e}{c} \left(\mathbf{A} \cdot \nabla\psi + \frac{\phi}{c} \frac{\partial\psi}{\partial t} \right) \left(\frac{\partial\psi}{\partial \mathbf{p}} \right) \\ & + \left[m^2 c^2 + \frac{e^2}{c^2} (\mathbf{A}^2 - \phi^2) \right] \left(\frac{\partial\psi}{\partial \mathbf{p}} \right)^2. \end{aligned} \quad (2.27)$$

in five dimensions¹⁷ with

$$ds^2 = c^2 dt^2 - dx^2 - dy^2 - dz^2 - (d\Omega)^2 \quad (2.28)$$

where

$$d\Omega = \frac{e}{mc} \phi dt - \frac{e}{mc^2} (A_x dx + A_y dy + A_z dz) - \frac{1}{mc} d\mathbf{p}. \quad (2.29)$$

Fock stated that the variation related to (2.27) and the linear differential form in (2.29) are invariant under the transformations

$$\mathbf{A} = \mathbf{A}_1 + \nabla\theta \quad (2.30)$$

$$\phi = \phi_1 - \frac{1}{c} \frac{\partial\theta}{\partial t} \quad (2.31)$$

$$\mathbf{p} = \mathbf{p}_1 - \frac{e}{c} \theta \quad (2.32)$$

where $\theta = \theta(\mathbf{r}, t)$ is an arbitrary function. The invariance of the former can be verified by employing the identity

$$e^{\pm(e\theta/c)\partial/\partial\mathbf{p}} \psi(\mathbf{p}) = \psi\left(\mathbf{p} \pm \frac{e}{c} \theta\right). \quad (2.33)$$

Using the well-known techniques of variation and integration by parts, the following Laplace equation for ψ is obtained:

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{2e}{c} \left(\mathbf{A} \cdot \nabla \frac{\partial\psi}{\partial \mathbf{p}} + \frac{\phi}{c} \frac{\partial^2 \psi}{\partial t \partial \mathbf{p}} \right)$$

¹⁷The identical results of a similar five-dimensional general-relativistic formalism by Oscar Klein were published 10 days before Fock submitted his work [45] (also see the footnote in [48] p. 226).

$$-\frac{e}{c}\left(\nabla \cdot \mathbf{A} + \frac{1}{c}\frac{\partial\phi}{\partial t}\right)\left(\frac{\partial\psi}{\partial\mathbf{p}}\right) + \left[m^2c^2 + \frac{e^2}{c^2}(\mathbf{A}^2 - \phi^2)\right]\left(\frac{\partial^2\psi}{\partial\mathbf{p}^2}\right) = 0. \quad (2.34)$$

At this point, if ψ is assumed to have the form

$$\psi = \psi_0 e^{i\mathbf{p}/\hbar}, \quad (2.35)$$

(2.34) reduces to

$$\begin{aligned} \nabla^2\psi_0 - \frac{1}{c^2}\frac{\partial\psi_0}{\partial t^2} - \frac{2ie}{\hbar c}\left(\mathbf{A} \cdot \nabla\psi_0 + \frac{\phi}{c}\frac{\partial\psi_0}{\partial t}\right) - \frac{ie}{\hbar c}\left(\nabla \cdot \mathbf{A} + \frac{1}{c}\frac{\partial\phi}{\partial t}\right)\psi_0 \\ - \frac{1}{\hbar^2}\left[m^2c^2 + \frac{e^2}{c^2}(\mathbf{A}^2 - \phi^2)\right]\psi_0 = 0 \end{aligned} \quad (2.36)$$

which is identical to (2.21). Now the presence of the (2.24) term in (2.36) is the guarantor for invariance under the transformations (2.3) and (2.4), provided that one makes the simultaneous substitution

$$\psi_0 \rightarrow \psi'_0 = e^{ie\theta(\mathbf{r},t)/\hbar c}\psi_0. \quad (2.37)$$

For the first time this fact was referred to as the “principle of gauge invariance” by Weyl. The use of the term *gauge* arose from the desire to establish contact with his 1919 attempt to unify electromagnetism and gravitation, which was invariant under a scale change of the metric tensor [45].

Note that gauge invariance exists in the non-relativistic Schrödinger equation for matter-electromagnetic field coupling also. As a matter of fact modern textbooks use this as an introduction to the subject of covariant derivatives [24]. A phase transformation of the second kind in the form of (2.37) has no effect on the probability density, however the expected value of the canonical momentum in the transformed state is gauge dependent (unlike the kinetic momentum, which is an invariant observable).

The Schrödinger equation is covariant under (2.37) only in the form

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\nabla - \frac{ie}{\hbar c}\mathbf{A}\right)^2\psi + e\phi\psi \quad (2.38)$$

as the potentials \mathbf{A} and ϕ change according to (2.3) and (2.4), respectively¹⁸.

B. Some Useful Geometrical Apparatus

In this section we will summarize the tools of differential geometry that will be used in the remainder of this dissertation. Our approach is going to be practical, rather than formal. A lemma-theorem-proof fashion mathematical rigor with heavy jargon will be avoided, although an introductory level familiarity with objects like the *metric tensor* or *Christoffel symbols* is assumed.

1. The Covariant Derivative of ψ

Let's begin with setting $\hbar = c = 1$, and rewrite equation (2.38) in a generic way as

$$i\left(\frac{\partial}{\partial t} + ie\phi\right)\psi = -\frac{1}{2m}\left[\left(\frac{\partial}{\partial x^1} - ieA^1\right)^2 + \left(\frac{\partial}{\partial x^2} - ieA^2\right)^2 + \dots\right]\psi. \quad (2.39)$$

As usual, we will treat time as the zeroth member of the $(d+1)$ -dimensional generalized coordinate system x^μ (*i.e.* $x^0 = t$), and use the shorthand $\partial_\mu \equiv \partial/\partial x^\mu$. Upon redefining the potentials in (2.39) as $A^0 = e\phi$ and $eA^j \rightarrow A^j$ (for $j = 1, \dots, d$), we get

$$i(\partial_0 + iA^0)\psi = -\frac{1}{2m}\sum_{j=1}^d(\partial_j - iA^j)^2\psi. \quad (2.40)$$

¹⁸This equation may be obtained from the classical Hamiltonian (2.9) using the “quantum correspondence rules”: $\mathbf{p} \rightarrow -i\hbar\nabla$ and $E \rightarrow i\hbar\frac{\partial}{\partial t}$ in the equation $\hat{H}\psi = E\psi$.

To resolve the discrepancy between sub and superscripts, and also to fix the relative signs of the derivatives and components of the potential, we introduce the following rule of lowering the indices:

$$A_0 = A^0 \text{ and } A_j = -A^j, \quad j = 1, \dots, d. \quad (2.41)$$

Finally we define

$$\nabla_\mu \psi(x) = [\partial_\mu + iA_\mu(x)]\psi(x) \quad (2.42)$$

as the covariant derivative of the complex-valued wave function ψ and write the gauge-invariant Schrödinger equation in the form

$$i\nabla_0 \psi = -\frac{1}{2m} \sum_{j=1}^d \nabla_j^2 \psi. \quad (2.43)$$

The components of the generalized potential, A_μ , are called the connection coefficients and the gauge transformations of (2.3) and (2.4) are summarized by the single substitution formula $A_\mu \rightarrow A_\mu - \partial_\mu \theta$.

2. The Intrinsic Meaning of ∇_μ and Parallel Transport

Now we will try to give a geometrical meaning to the connection coefficients. Let the (complex) number $a = \psi(x)$ be an element of a vector space called the *fiber*¹⁹ at x . In this vector space, it is possible to introduce a basis $\{\mathbf{e}_j\}_{j=1}^r$ in each x [24], such that

$$\psi(x) = \sum_{j=1}^r \psi^j(x) \mathbf{e}_j(x). \quad (2.44)$$

¹⁹Technically, the inverse image of a set with exactly one element is called a fiber. Example: In \mathbb{R}^2 , $f^{-1}[\{9\}]$ is the fiber at $x = (\sqrt{6}, \sqrt{3})$ which is a circle of radius = 3 about the origin where $f(x^1, x^2) = (x^1)^2 + (x^2)^2$.

If we change to a new basis given by $\mathbf{e}'_j(x) = (U^{-1})^k{}_j \mathbf{e}_k(x)$, the components ψ^j should transform²⁰ according to $\psi'^k(x) = U^k{}_j \psi^j(x)$ so that the function ψ , which is called a *section* in this context, remains invariant:

$$\psi \rightarrow U^k{}_j \psi^j (U^{-1})^l{}_k \mathbf{e}_l = \delta^l{}_j \psi^j \mathbf{e}_l = \psi. \quad (2.45)$$

Here the change of basis *is* the gauge transformation, so there should be a link between this and the covariant differentiation of (2.42) in the intrinsic sense. The $\nabla_\mu \psi$ should be considered as a mapping of ordinary sections to covector-valued sections and the connection coefficients w_μ (previously iA_μ) are now defined by

$$\nabla_\mu \mathbf{e}_k \equiv (w_\mu)^j{}_k \mathbf{e}_j \quad (2.46)$$

and they are matrices. If we include coordinate transformations in a manifold²¹ of dimension n into this general framework (the principle of gauge invariance is broadened to include gravity), the covariant derivative of the covector $v_\mu \equiv \nabla_\mu \psi$ is given by

$$\nabla_\nu v_\mu = \partial_\nu v_\mu - \Gamma^\rho{}_{\mu\nu} v_\rho + w_\nu v_\mu \quad (2.47)$$

where the connection coefficients on the manifold are Christoffel symbols [52]. Higher order combinations of these non-commutative derivatives will involve other objects such as the *curvature* (see next section) or the *torsion* (see [24]). But first, let us briefly explain the concept of parallel transport.

Parallel transport is the act of moving a vector (or a section) along a curve without changing it. In a flat world this is something we do all the time, but on a manifold (like our universe) it is meaningless to compare (add, subtract, etc.) two

²⁰From now on we will suppress the summation sign \sum whenever summation must be made over an index that occurs twice, once as a superscript and once as a subscript.

²¹A manifold is a space that looks, locally, like an Euclidean space.

vectors living in different tangent spaces. One needs to carry the vector in $T_{x'}$ to the other tangent space T_x while keeping it constant along the selected curve $x(\lambda)$ that joins x' and x . The requirement is that the *absolute derivative* of ψ , $\nabla_\mu\psi$, or any tensor of higher rank should be equal to zero:

$$\frac{dx^\mu}{d\lambda}\nabla_\mu(\cdot) = 0. \quad (2.48)$$

This operation will be connection dependent as well as path dependent since the definition is given in terms of the covariant derivative. When applied to sections and vectors, (2.48) reads

$$\frac{d\psi}{d\lambda} + \frac{dx^\mu}{d\lambda}w_\mu\psi = 0 \quad \text{“gauge”} \quad (2.49)$$

and

$$\frac{dv^\nu}{d\lambda} + \frac{dx^\mu}{d\lambda}\Gamma_{\rho\mu}^\nu v^\rho = 0 \quad \text{“gravitational”}. \quad (2.50)$$

In general (2.49) is a system of differential equations since the connection coefficients include matrices (Yang-Mills theory). If $\psi(\lambda)$ is the solution of (2.49) with the initial value $\psi(0)$, then suppose $\psi(1)$ is given by

$$\psi(1) = I(x, x')\psi(0) \quad (2.51)$$

where $x' = x(0)$ and $x = x(1)$. $I(x, x')$ is called the *parallel displacement matrix* (see [24], [40] p. 151) and satisfies

$$\lim_{x' \rightarrow x} I = \text{unit matrix}. \quad (2.52)$$

Let us leave the discussion of the second case (2.50) aside for now (we will come back to it later) and work out the electromagnetic parallel transport for Abelian gauge fields $A_\mu = -iw_\mu$. One may multiply both sides of (2.49), which is now a first order

differential equation, by $d\lambda/\psi$ and integrate to get

$$\psi(1) = \exp\left(-i \int_{x'}^x A_\mu(\bar{x}) d\bar{x}^\mu\right) \psi(0) \quad (2.53)$$

where the line integral is along the curve $\bar{x} = x(\lambda)$ [24].

3. Geodesics and Curvature

If the curve $x(\lambda)$ of the previous section parallel transports its own tangent vector, it is called a *geodesic*. In other words, it is the solution of

$$\frac{d^2 x^\nu}{d\lambda^2} + \Gamma_{\rho\mu}^\nu \frac{dx^\mu}{d\lambda} \frac{dx^\rho}{d\lambda} = 0, \quad (2.54)$$

which is equation (2.50) with the special choice $v^\nu = dx^\nu/d\lambda$. Alternatively, one may consider the variation of the (proper time) action integral of (2.14) introduced in section A-3 to find the shortest-distance path:

$$\delta \int ds = \delta \int \sqrt{g_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}} d\lambda. \quad (2.55)$$

The $g_{\mu\nu}(x)$ is the *metric tensor*, which provides a generalization of (2.12). The resulting equation is identical to (2.54) if the metric satisfies the compatibility condition

$$\nabla_\rho g_{\mu\nu} = 0, \quad (2.56)$$

and the parameter λ turns out to be the proper time itself (actually, any other parameter related to the proper time in a linear fashion²² works just fine). The coincidence of these two notions tell us that, quoting [53], the “straightest curve” is also the “shortest curve”.

Geodesics can also be used in mapping the tangent space at a point x' to a local

²²They are called *affine* parameters.

neighborhood of x' . Given an arbitrary vector $\mathbf{u} \in T_{x'}(M)$, one can solve the geodesic equation (2.54) with the initial conditions

$$x^\mu(0) = x'^\mu \quad \text{and} \quad \frac{dx^\mu(0)}{d\lambda} = \mathbf{u}^\mu \quad (2.57)$$

and find the point y on the geodesic where the parameter is equal to 1. This is the definition of the *exponential map* or the “geodesic flow”

$$y = \exp_{x'}(\mathbf{u}), \quad (2.58)$$

which is invertible:

$$\mathbf{u} = \exp_{x'}^{-1}(y). \quad (2.59)$$

This definition makes sense only locally; spacetimes in general relativity usually have singularities which geodesics may “fall” into. A converse definition is as follows: If two points on M are “sufficiently close”, then there is a tangent vector given by (2.59) which can be found after solving the two-point boundary problem (2.54) for the shortest distance [6].

Now let us consider an example regarding parallel transport which may be intuitive. Due to the fact that parallel transport is a path-dependent operation in curved space, the results of parallel transporting a vector from point A to a nearby point B along two distinct paths, let’s say along the edges of a “rectangle” (*i.e.*, along some ACB and ADB), are expected to be different. Similarly, if the vector is brought back to the starting point along the *other* path, therefore completing the loop, it will be transformed to a new vector. Since it is the curved nature of space that we blame, one may attempt to quantitatively express the change experienced by this vector in terms of the total curvature enclosed by the loop; or even better, may consider an infinitesimal loop and associate a local curvature to point A . If the above mentioned

path dependence and the anti-symmetry attached to it²³ are taken into account, the goal is to find a geometrical object of the form

$$R^\alpha{}_{\beta\mu\nu} = -R^\alpha{}_{\beta\nu\mu}. \quad (2.60)$$

The formula for this tensor in terms of the connection coefficients can be found by computing the commutator of covariant derivatives, therefore finding the difference between parallel transporting along paths ACB and ADB :

$$[\nabla_\mu, \nabla_\nu]v^\alpha = R^\alpha{}_{\beta\mu\nu}v^\beta, \quad (2.61)$$

where we assumed $\Gamma^\alpha_{\mu\nu} = \Gamma^\alpha_{\nu\mu}$ (no torsion). Then [24],

$$R^\alpha{}_{\beta\mu\nu} \equiv \nabla_\mu\Gamma^\alpha_{\beta\nu} - \nabla_\nu\Gamma^\alpha_{\beta\mu} + \Gamma^\alpha_{\gamma\mu}\Gamma^\gamma_{\beta\nu} - \Gamma^\alpha_{\gamma\nu}\Gamma^\gamma_{\beta\mu}, \quad (2.62)$$

which is called the *Riemann curvature tensor*.

We have not mentioned what happens in the bundle in this context, but the situation is very similar. The commutator of the covariant derivatives of a section ψ is

$$[\nabla_\mu, \nabla_\nu]\psi = Y_{\mu\nu}\psi, \quad (2.63)$$

where

$$Y_{\mu\nu} \equiv \partial_\mu w_\nu - \partial_\nu w_\mu + [w_\mu, w_\nu] \quad (2.64)$$

is the curvature tensor of the bundle (electromagnetic field strength tensor in the Abelian case). In the same fashion as (2.47), the general formula is [24]

$$[\nabla_\nu, \nabla_\rho]\nabla_\mu\psi = R^\alpha{}_{\mu\nu\rho}\nabla_\alpha\psi + Y_{\nu\rho}\nabla_\mu\psi. \quad (2.65)$$

²³A loop can be completed clockwise or counterclockwise.

4. More on Geodesic Theory

Let s be the geodesic distance between $x' = x(0)$ and $x = x(1)$. Using (2.55), this is

$$s = \int_0^1 \sqrt{g_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}} d\lambda. \quad (2.66)$$

Let us again assume that the points are close and there is only one geodesic connecting them. In other words, x is closer than first *caustic* we would meet. The *Synge-deWitt world function* is defined by (see [6], [24], [40], [41], [42], [43])

$$\sigma(x', x) \equiv \frac{1}{2} s^2. \quad (2.67)$$

The *bi-scalar* $\sigma(x', x)$ is a symmetric function of x and x' , and can be considered as related to an action²⁴ (different from (2.55)) that produces the geodesic equation in a dynamic way [40]:

$$S = \frac{1}{2} \int_{\lambda'}^{\lambda} g_{\mu\nu} \frac{dx^\mu}{d\tilde{\lambda}} \frac{dx^\nu}{d\tilde{\lambda}} d\tilde{\lambda} = \frac{\sigma(y', y)}{\lambda - \lambda'}, \quad (2.68)$$

where $y' = x(\lambda')$ and $y = x(\lambda)$. The advantage of this formal approach over the prominent definition (2.67) becomes apparent when one realizes that the Hamilton-Jacobi equation based on this action can be written in the form

$$\frac{1}{2} g^{\mu\nu} \nabla_\mu \sigma \nabla_\nu \sigma = \sigma. \quad (2.69)$$

The abundance of occurrence of these derivatives of σ in calculations made the following notation customary among physicists:

$$\sigma_\mu \equiv \nabla_\mu \sigma \quad \text{or} \quad \sigma^\mu \equiv g^{\mu\nu} \nabla_\nu \sigma. \quad (2.70)$$

²⁴The two actions give the same extremal curve when the parameter $\tilde{\lambda}$ grows *linearly* with arc-length (or proper time for a timelike geodesic) [54].

Note that (2.69) can be equivalently written in terms of covariant derivatives with respect to the other end point x' . From now on we will adopt the notation of putting primes on the indices that live in x' , and keep in mind that an inattentive look at the total number of mixed indices can be misleading²⁵. The Hamilton-Jacobi equation at x' is

$$\frac{1}{2}\sigma_{\mu'}\sigma^{\mu'} = \sigma, \quad (2.71)$$

where

$$\sigma^{\mu'} = g^{\mu'\nu'}(x')\nabla_{\nu'}\sigma. \quad (2.72)$$

The significance of (2.69) and (2.71) is better understood if σ^μ ($\sigma^{\mu'}$) is associated with the tangent vector at x (x') of length equal to the geodesic distance. Technically, σ^μ ($\sigma^{\mu'}$) is a vector that points *away* from x' (x) (see Fig. 1), therefore the following notation [24] will be used frequently:

$$\hat{\sigma}^{\mu'} \equiv -\sigma^{\mu'}. \quad (2.73)$$

In terms of the exponential map introduced in the previous section, we may write

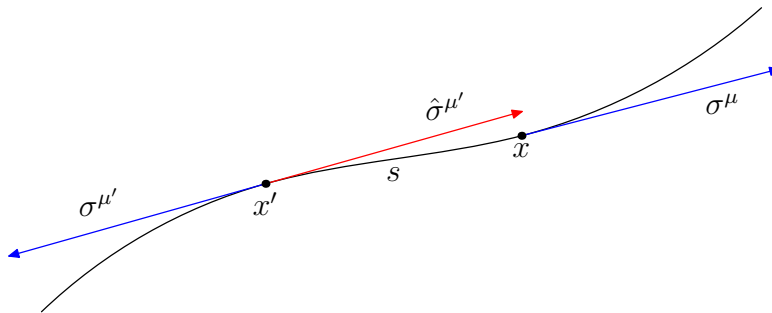


Fig. 1. The tangent vectors on the geodesic.

²⁵For instance, the *bi-vector* $b^\mu{}_{\nu'}(x, x')$ is an object that transforms as a vector, not a tensor of rank 2.

this vector as

$$\hat{\sigma}^{\mu'}(x', x) = \exp_{x'}^{-1}(x^\mu). \quad (2.74)$$

Since the vectors $\hat{\sigma}^{\mu'}$ and σ^μ are self-parallel by definition, there should be a *parallel transport bi-vector* $g^{\mu'}{}_\nu(x', x)$, which is the solution of (2.50), or in the new notation

$$\sigma^\mu \nabla_\mu g^{\nu'}{}_\alpha = 0, \quad (2.75)$$

and satisfies

$$-\sigma^{\mu'} = g^{\mu'}{}_\nu \sigma^\nu, \quad -\sigma_{\mu'} = g_{\mu'}{}^\nu \sigma_\nu. \quad (2.76)$$

The boundary conditions for the world function, tangent vectors and the parallel transport are

$$[\sigma] = [\sigma^\mu] = [\sigma^{\mu'}] = 0, \quad [g^{\mu'}{}_\nu] = \delta^\mu{}_\nu, \quad (2.77)$$

where $[\cdot]$ stands for the *coincidence limit* $x' \rightarrow x$. By differentiating (2.69) twice and using (2.77), one finds

$$[\nabla_\rho \sigma^\mu] = \delta^\mu{}_\rho. \quad (2.78)$$

Similarly, differentiation of (2.76) yields $[\nabla_\rho \sigma^{\mu'}] = -\delta^\mu{}_\rho$. One needs to take the derivative of (2.75), and employ (2.77) to get

$$[\nabla_\kappa g^{\nu'}{}_\alpha] = 0. \quad (2.79)$$

Considering higher order derivatives in a similar fashion, the following coincidence limits of *symmetrized* derivatives of $g^{\nu'}{}_\alpha$ and σ^ν are found:

$$[\nabla_{(\mu_1} \dots \nabla_{\mu_n)} g^{\nu'}{}_\alpha] = 0, \quad (2.80)$$

and

$$[\nabla_{(\mu_1} \dots \nabla_{\mu_n)} \sigma^\nu] = [\nabla_{(\mu_1} \dots \nabla_{\mu_n)} \sigma^{\nu'}] = 0. \quad (2.81)$$

One has (see Appendix A, [41], [43])

$$[\nabla_\alpha \nabla_\beta g^{\mu'}{}_\nu] = \frac{1}{2} R^\mu{}_{\nu\beta\alpha} \quad \text{and} \quad [\nabla_\tau \nabla_\sigma \nabla_\nu \sigma^\mu] = -\frac{1}{3} (R^\mu{}_{\sigma\nu\tau} + R^\mu{}_{\tau\nu\sigma}). \quad (2.82)$$

Two other significant objects are $\eta^{\mu'}{}_\nu \equiv \nabla_\nu \sigma^{\mu'}$ and its inverse $\eta^{-1} \equiv \gamma = \{\gamma^\mu{}_{\nu'}\}$. These will be used frequently later when we need to make a change of variables from the tangent vectors to the geodesic flow or vice versa, *i.e.*,

$$\partial_{\sigma^{\mu'}(x',x)} f(x) = \gamma^\nu{}_{\mu'}(x',x) \nabla_\nu f(x), \quad (2.83)$$

and

$$\nabla_\mu g(\sigma^{\mu'}(x',x)) = \eta^{\nu'}{}_\mu(x',x) \partial_{\sigma^{\nu'}(x',x)} g(\sigma^{\mu'}(x',x)). \quad (2.84)$$

The coincidence limits of these matrices and their derivatives are straightforward:

$$[\eta^{\nu'}{}_\mu] = [\gamma^\nu{}_{\mu'}] = -\delta^\nu{}_\mu, \quad [\nabla_\mu \gamma^\nu{}_{\beta'}] = 0, \quad \text{etc.} \quad (2.85)$$

The matrix $D_{\mu\nu'} \equiv -\nabla_{\nu'} \sigma_\mu$ (or its inverse) may be used as a measure of how much x^μ varies as a result of the variation of the tangent vector $\sigma_{\nu'}$ [40],

$$\delta x^\mu = -D^{-1\mu\nu'} \delta \sigma_{\nu'} \quad (2.86)$$

and the Jacobian

$$\frac{\partial(\sigma_{\nu'}, x'^\tau)}{\partial(x^\mu, x'^\rho)} = -\det(D_{\mu\nu'}) \quad (2.87)$$

describes the rate at which geodesics emanating from a point diverge (or conversely, one may consider a point where they start converging). This is called the *VanVleck-Morette determinant* and we will be using it in the more common form

$$\Delta(x', x) \equiv g(x')^{-1/2} \det(D_{\mu\nu'}) g(x)^{-1/2} \quad (2.88)$$

where $g(x) = \det[g_{\mu\nu}(x)]$. This determinant is employed in the Jacobian one needs

when passing from integrals²⁶ over the tangent space to integrals on the manifold (or vice versa) [6]

$$\int_{T_{x'}} \sqrt{g(x')} d\hat{\sigma}(x', x) \dots \Leftrightarrow \int_M \Delta(x', x) \sqrt{g(x)} dx \dots, \quad (2.89)$$

and it satisfies [43]

$$\Delta^{-1/2}(\sigma^\mu \nabla_\mu \Delta^{1/2}) = \frac{1}{2}(d - \square\sigma) \quad (2.90)$$

where $\square\sigma \equiv \nabla_\mu \nabla^\mu \sigma$ and d is the dimension of the manifold. Some of the coincidence limits are (see Appendix A for derivation)

$$[\Delta] = 1, \quad [\nabla_\mu \Delta] = 0, \quad [\nabla_\mu \nabla_\nu \Delta] = \frac{1}{3} R_{\mu\nu}, \quad (2.91)$$

$$[\Delta^{1/2}] = 1, \quad [\nabla_\mu \Delta^{1/2}] = 0, \quad [\nabla_\mu \nabla_\nu \Delta^{1/2}] = \frac{1}{6} R_{\mu\nu}, \quad (2.92)$$

where $R_{\mu\nu} = R^\alpha{}_{\mu\alpha\nu}$ is the *Ricci tensor*. Before we finish this section let us note that the coincidence limits of the parallel displacement matrix $I(x', x)$ of (2.51) will include the gauge strength (bundle curvature) $Y_{\mu\nu}$ in analogy with (2.82).

²⁶The reader should keep in mind that the exponential map and $\hat{\sigma}(x', x)$ are not globally defined because of caustics. Therefore, our spatial integrals are not globally defined either. One has to put in cutoff functions and argue that the contribution from distant points are rather unimportant contributions.

CHAPTER III

CLASSICAL WEYL-WIGNER FORMALISM

In this chapter we discuss the “non-covariant” Weyl quantization in the classical sense, both in the standard pseudo-differential form [6] [8], and in quantizer schemes [12]. After a brief introduction to Wigner distribution functions we will derive the classical product formula for the symbol of the operator $\hat{C} = \hat{A}\hat{B}$.

A. Pseudo-Differential Operators

1. The Operator Ordering Problem

The classical \mapsto quantum correspondence relation $p_j = -i\hbar\partial/\partial q_j$ of Schrödinger inevitably leads to a non-commutative character for the operators representing position and momentum. The quantization of a phase space function of the form $a(q, p) = q^m p^n$ has an ambiguity in the ordering of these operators. One may push all \hat{P} 's to the right of \hat{Q} 's,

$$q^m p^n \mapsto \hat{Q}^m \hat{P}^n \quad (3.1)$$

or vice versa:

$$q^m p^n \mapsto \hat{P}^n \hat{Q}^m. \quad (3.2)$$

A common way of ordering called *McCoy's formula* is the association [6], [7]

$$q^m p^n \mapsto \sum_{l=0}^m \binom{m}{l} \hat{Q}^{m-l} \hat{P}^n \hat{Q}^l, \quad (3.3)$$

which is a symmetrization of (3.1) and (3.2). It is also possible to assume a *momentum polynomial* of the form

$$a(\mathbf{q}, \mathbf{p}) = A_0(\mathbf{q}) + A_1^i(\mathbf{q})p_i + A_2^{ij}(\mathbf{q})p_i p_j + \dots \quad (3.4)$$

in $2d$ -dimensional phase space and work out the symmetrized quantum operator ordering. For instance, the third term in (3.4) will yield [6]

$$A_2^{ij}(\mathbf{q})p_i p_j \mapsto \frac{1}{4}\hat{P}_i \hat{P}_j A_2^{ij}(\hat{Q}) + \frac{1}{2}\hat{P}_i A_2^{ij}(\hat{Q}) \hat{P}_j + \frac{1}{4}A_2^{ij}(\hat{Q}) \hat{P}_i \hat{P}_j. \quad (3.5)$$

The result is a second order *differential operator*.

These generalizations are not limited to momentum polynomials, of course. The quantum mechanical problem may involve the quantization of a function of practically any form. The proper mathematical term for such an operator is a *pseudo-differential operator* or ψ DO for short. The phase space function is called a *symbol*.

2. The Multi-Index Notation

Before we move further, let us introduce the *multi-index* notation. In an expression such as (3.4), one frequently encounters clusters of the n_i th power of the i th component where $i \leq d$, therefore a handy notation which would summarize lengthy expansions is needed. A d -tuple of nonnegative integers $(\alpha_1, \alpha_2, \dots, \alpha_d)$ will be called the multi-index α when the index i occurs α_i times in the cluster. For example in $d = 3$ dimensions, terms factored around $p_1(p_2)^2 p_3$ in (3.4) are represented by only one index, which is $(1, 2, 0, 1)$. This allows us to write that expansion as a single sum

$$a(\mathbf{q}, \mathbf{p}) = \sum_{\alpha} A_{\alpha}(\mathbf{q}) p^{\alpha} \quad (3.6)$$

where the coefficients now represent the sum of redundant terms in (3.4). For instance,

$$A_{(1,2,0,1)} = A_4^{1224} + A_4^{2124} + \text{etc} \dots \quad (3.7)$$

Note that in the case of multi-indices, we will not be using the Einstein summation convention of the previous chapter. Also the regular p -subscript q -superscript indexing will be swapped to emphasize multi-indices. There are two numbers associated

to a multi-index, which are quite practical:

$$|\alpha| \equiv \alpha_1 + \cdots + \alpha_d \quad (\text{the length of } \alpha), \quad (3.8)$$

and

$$\alpha! \equiv \alpha_1! \cdots \alpha_d!. \quad (3.9)$$

Finally, note the following notation for partial derivatives (with respect to \mathbf{p}):

$$\partial_{\mathbf{p}}^{\alpha} \equiv \frac{\partial^{|\alpha|}}{\partial p_1^{\alpha_1} \cdots \partial p_d^{\alpha_d}}. \quad (3.10)$$

3. ψ DO Formulae

In general the action of an operator \hat{A} on a function Ψ can be given in the form of an integral

$$[\hat{A}\Psi](\mathbf{x}) = \int_{\mathbf{R}^d} d^d y \mathcal{A}(\mathbf{x}, \mathbf{y}) \Psi(\mathbf{y}), \quad (3.11)$$

where $\mathcal{A}(\mathbf{x}, \mathbf{y})$ is called the *integral kernel*. In general, $\mathcal{A}(x, y)$ is a distribution, not a function (as in the case of differential operators). If it is a ψ DO, studying the $\mathbf{p} \mapsto -i\hbar\nabla$ example and *Fourier transform* techniques, one may intuitively decide that the definition involves the symbol of \hat{A} and the Fourier transform of Ψ :

$$[\hat{A}\Psi](\mathbf{x}) = (2\pi)^{-d/2} \int_{\mathbf{R}^d} d^d p e^{i\mathbf{p}\cdot\mathbf{x}} a(\mathbf{x}, \mathbf{p}) \tilde{\Psi}(\mathbf{p}). \quad (3.12)$$

Using (3.11), (3.12) and the definition of the d -dimensional Fourier transform

$$\tilde{\Psi}(\mathbf{p}) = (2\pi)^{-d/2} \int_{\mathbf{R}^d} d^d y e^{-i\mathbf{p}\cdot\mathbf{y}} \Psi(\mathbf{y}), \quad (3.13)$$

the kernel can be expressed in terms of the symbol as

$$\mathcal{A}(\mathbf{x}, \mathbf{y}) = (2\pi)^{-d} \int_{\mathbf{R}^d} d^d p e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} a(\mathbf{x}, \mathbf{p}), \quad (3.14)$$

which is a Fourier transform itself. Inverting this, one gets the “kernel to symbol” formula

$$a(\mathbf{x}, \mathbf{p}) = \int_{\mathbf{R}^d} d^d y e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \mathcal{A}(\mathbf{x}, \mathbf{y}). \quad (3.15)$$

Note that it may be necessary to cutoff the contribution from widely separated argument points of $\mathcal{A}(x, y)$ because of caustics²⁷.

B. Weyl-Wigner Correspondence

1. Weyl Quantization and Wigner Transform

The following interpretation of Weyl quantization follows the *symbol* \rightleftharpoons *kernel* style of the previous section and [6]. Weyl’s original definition (see [3], [5], [7] and [8]) will be discussed separately.

The equations that are to be modified in the Weyl calculus are (3.14) and (3.15). The basic idea is to symmetrize x and y in the definitions by introducing a “new” variable q , the classical position, which turns out to be equally far from each point. The easiest way to do this is to take the midpoint $(\mathbf{x}+\mathbf{y})/2$, therefore the new “symbol to kernel” formula becomes

$$\mathcal{A}(\mathbf{x}, \mathbf{y}) = (2\pi)^{-d} \int_{\mathbf{R}^d} d^d p e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} a[(\mathbf{x} + \mathbf{y})/2, \mathbf{p}]. \quad (3.16)$$

To invert this formula one defines a difference vector $\mathbf{v} \equiv \mathbf{x} - \mathbf{y}$ and works out the solutions for \mathbf{x} and \mathbf{y} in terms of \mathbf{v} and \mathbf{q} :

$$\mathbf{x} \rightarrow \mathbf{q} + \frac{\mathbf{v}}{2}, \quad \mathbf{y} \rightarrow \mathbf{q} - \frac{\mathbf{v}}{2}. \quad (3.17)$$

²⁷A differential operator is an excellent example where the cutoff is unnecessary, since derivatives of delta functions have support on the diagonal!

Therefore,

$$a(\mathbf{q}, \mathbf{p}) = \int_{\mathbf{R}^d} d^d v e^{-i\mathbf{p}\cdot\mathbf{v}} \mathcal{A}(\mathbf{q} + \mathbf{v}/2, \mathbf{q} - \mathbf{v}/2). \quad (3.18)$$

This is also called the *Wigner transform* [7] [11], and usually written as

$$\text{Sym}(\hat{A})(\mathbf{q}, \mathbf{p}) \equiv \int_{\mathbf{R}^d} d^d v e^{-i\mathbf{p}\cdot\mathbf{v}} \langle \mathbf{q} + \mathbf{v}/2 | \hat{A} | \mathbf{q} - \mathbf{v}/2 \rangle. \quad (3.19)$$

Sometimes the Wigner transform is defined as (3.19) divided by $(2\pi)^d$ [8] and (3.19) is referred as the inverse Weyl transform. It follows from (3.19) that

$$\text{Sym}(\hat{A}) = \text{Sym}(\hat{A}^\dagger)^* \quad (3.20)$$

and in the case of Hermitian operators, the symbols are real.

In order to demonstrate the symmetry of the definition (3.16), let us try to find the operator corresponding to the symbol

$$a(\mathbf{q}, \mathbf{p}) = b^{\mu\nu}(\mathbf{q}) p_\mu p_\nu + c^\mu(\mathbf{q}) p_\mu + d(\mathbf{q}). \quad (3.21)$$

Plugging the definition of the kernel (3.16) into (3.11) one gets

$$[\hat{A}\Psi](\mathbf{x}) = (2\pi)^{-d} \int d^d y \Psi(\mathbf{y}) \int d^d p e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} a(\mathbf{q}, \mathbf{p}). \quad (3.22)$$

If multi-index notation is used in the symbol this is

$$\begin{aligned} [\hat{A}\Psi](\mathbf{x}) &= (2\pi)^{-d} \sum_{\alpha} \int d^d y \Psi(\mathbf{y}) \int d^d p e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} A_{\alpha}(\mathbf{q}) \mathbf{p}^{\alpha} \\ &= (2\pi)^{-d} \sum_{\alpha} \int d^d y \Psi(\mathbf{y}) \int d^d p A_{\alpha}(\mathbf{q}) (-i\partial_{\mathbf{y}})^{\alpha} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}, \end{aligned} \quad (3.23)$$

and integration by parts yields

$$[\hat{A}\Psi](\mathbf{x}) = (2\pi)^{-d} \sum_{\alpha} \int d^d p \int d^d y e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} (+i\partial_{\mathbf{y}})^{\alpha} \left[A_{\alpha} \left(\frac{\mathbf{x} + \mathbf{y}}{2} \right) \Psi(\mathbf{y}) \right]. \quad (3.24)$$

If one employs the definition of *Dirac delta-function*

$$\delta(\mathbf{x} - \mathbf{y}) \equiv (2\pi)^{-d} \int d^d p e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \quad (3.25)$$

and

$$f(\mathbf{x}) = \int d^d y \delta(\mathbf{x} - \mathbf{y}) f(\mathbf{y}), \quad (3.26)$$

(3.24) becomes

$$[\hat{A}\Psi](\mathbf{x}) = \sum_{\alpha} (+i\partial_{\mathbf{y}})^{\alpha} \left[A_{\alpha} \left(\frac{\mathbf{x} + \mathbf{y}}{2} \right) \Psi(\mathbf{y}) \right] \Big|_{\mathbf{y}=\mathbf{x}}. \quad (3.27)$$

Now the terms in (3.21) correspond to the $|\alpha| = 2$, $|\alpha| = 1$ and $|\alpha| = 0$ terms above, for example,

$$[\text{Op}(b^{\mu\nu} p_{\mu} p_{\nu})\Psi](\mathbf{x}) = -\partial_{\mu} \partial_{\nu} \left[b^{\mu\nu} \left(\frac{\mathbf{x} + \mathbf{y}}{2} \right) \Psi(\mathbf{y}) \right] \Big|_{\mathbf{y}=\mathbf{x}}. \quad (3.28)$$

Upon taking the derivatives and setting $\mathbf{y} = \mathbf{x}$ one finds

$$-\left[\frac{1}{4} (\partial_{\mu} \partial_{\nu} b^{\mu\nu}) \Psi + \partial_{\nu} b^{\mu\nu} \partial_{\mu} \Psi + b^{\mu\nu} \partial_{\mu} \partial_{\nu} \Psi \right](\mathbf{x}), \quad (3.29)$$

or after a rearrangement of the terms,

$$-\left[\frac{1}{4} \partial_{\mu} \partial_{\nu} (b^{\mu\nu} \Psi) + \frac{1}{2} \partial_{\nu} (b^{\mu\nu} \partial_{\mu} \Psi) + \frac{1}{4} b^{\mu\nu} \partial_{\mu} \partial_{\nu} \Psi \right](\mathbf{x}), \quad (3.30)$$

which has the manifest symmetry of (3.5).

2. Product Rule

The symbol representation of quantum mechanics is practically useful if there is a symbol calculus. On many occasions one needs to consider the product of operators or commutators of these. The simplest problem is to write the symbol of operator

$\hat{C} = \hat{A}\hat{B}$ in terms of the symbols of \hat{A} and \hat{B} . The starting point is the equation

$$[\hat{C}\Psi](\mathbf{x}) = \int d^d z \mathcal{C}(\mathbf{x}, \mathbf{z})\Psi(\mathbf{z}), \quad (3.31)$$

which may also be written as

$$\begin{aligned} [\hat{A}(\hat{B}\Psi)](\mathbf{x}) &= \int d^d y \mathcal{A}(\mathbf{x}, \mathbf{y})[\hat{B}\Psi](\mathbf{y}) \\ &= \int d^d y \mathcal{A}(\mathbf{x}, \mathbf{y}) \int d^d z \mathcal{B}(\mathbf{y}, \mathbf{z})\Psi(\mathbf{z}). \end{aligned} \quad (3.32)$$

Comparing (3.31) and (3.32),

$$\mathcal{C}(\mathbf{x}, \mathbf{z}) = \int d^d y \mathcal{A}(\mathbf{x}, \mathbf{y})\mathcal{B}(\mathbf{y}, \mathbf{z}). \quad (3.33)$$

Then one has

$$\begin{aligned} c(\mathbf{q}, \mathbf{p}) &= \int d^d v e^{-i\mathbf{p}\cdot\mathbf{v}} \mathcal{C}(\mathbf{q} + \mathbf{v}/2, \mathbf{q} - \mathbf{v}/2) \\ &= \int d^d v e^{-i\mathbf{p}\cdot\mathbf{v}} \int d^d y \mathcal{A}(\mathbf{q} + \mathbf{v}/2, \mathbf{y})\mathcal{B}(\mathbf{y}, \mathbf{q} - \mathbf{v}/2) \end{aligned} \quad (3.34)$$

The kernels on the right hand side of (3.34) can be written in terms of their symbols as follows:

$$\mathcal{A}(\mathbf{q} + \mathbf{v}/2, \mathbf{y}) = (2\pi)^{-d} \int d^d p'_1 e^{i\mathbf{p}'_1 \cdot (\mathbf{q} + \frac{\mathbf{v}}{2} - \mathbf{y})} a\left(\frac{\mathbf{q} + \frac{\mathbf{v}}{2} + \mathbf{y}}{2}, \mathbf{p}'_1\right), \quad (3.35)$$

$$\mathcal{B}(\mathbf{y}, \mathbf{q} - \mathbf{v}/2) = (2\pi)^{-d} \int d^d p'_2 e^{i\mathbf{p}'_2 \cdot (\mathbf{y} - \mathbf{q} + \frac{\mathbf{v}}{2})} b\left(\frac{\mathbf{y} + \mathbf{q} - \frac{\mathbf{v}}{2}}{2}, \mathbf{p}'_2\right). \quad (3.36)$$

Using (3.35) and (3.36) in (3.34) and passing from $(\mathbf{v}, \mathbf{y}, \mathbf{p}'_1, \mathbf{p}'_2)$ to $(\mathbf{q}_1, \mathbf{q}_2, \mathbf{p}_1, \mathbf{p}_2)$ in the resulting integral, via

$$\mathbf{p}'_1 = \mathbf{p}_1 + \mathbf{p} \quad (3.37)$$

$$\mathbf{p}'_2 = \mathbf{p}_2 + \mathbf{p} \quad (3.38)$$

$$\mathbf{y} = \mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q} \quad (3.39)$$

$$\mathbf{v} = 2(\mathbf{q}_1 - \mathbf{q}_2) \quad (3.40)$$

one obtains the 4-tuple integral

$$\begin{aligned} c(\mathbf{q}, \mathbf{p}) &= (\pi)^{-2d} \int d^d \mathbf{q}_1 \int d^d \mathbf{q}_2 \int d^d \mathbf{p}_1 \int d^d \mathbf{p}_2 e^{2i(\mathbf{p}_2 \cdot \mathbf{q}_1 - \mathbf{q}_2 \cdot \mathbf{p}_1)} \\ &\quad \times a(\mathbf{q}_1 + \mathbf{q}, \mathbf{p}_1 + \mathbf{p}) b(\mathbf{q}_2 + \mathbf{q}, \mathbf{p}_2 + \mathbf{p}), \end{aligned} \quad (3.41)$$

which is called the *twisted product* [8]. Other names include star or Weyl product [7]. This is an exact identity, but the asymptotic expansion of it is more popular. If the symbols a and b are expanded as power series in \mathbf{p}_1 and \mathbf{p}_2 , respectively, as

$$a(\mathbf{q}_1 + \mathbf{q}, \mathbf{p}_1 + \mathbf{p}) = \sum_{\alpha} \frac{1}{\alpha!} \partial_{\mathbf{p}}^{\alpha} a(\mathbf{q}_1 + \mathbf{q}, \mathbf{p}) \mathbf{p}_1^{\alpha} \quad (3.42)$$

$$b(\mathbf{q}_2 + \mathbf{q}, \mathbf{p}_2 + \mathbf{p}) = \sum_{\beta} \frac{1}{\beta!} \partial_{\mathbf{p}}^{\beta} b(\mathbf{q}_2 + \mathbf{q}, \mathbf{p}) \mathbf{p}_2^{\beta} \quad (3.43)$$

and put into (3.41), one realizes that

$$\mathbf{p}_1^{\alpha} \mathbf{p}_2^{\beta} e^{2i(\mathbf{p}_2 \cdot \mathbf{q}_1 - \mathbf{q}_2 \cdot \mathbf{p}_1)} = \left(-\frac{i}{2} \partial_{\mathbf{q}_1} \right)^{\beta} \left(+\frac{i}{2} \partial_{\mathbf{q}_2} \right)^{\alpha} e^{2i(\mathbf{p}_2 \cdot \mathbf{q}_1 - \mathbf{q}_2 \cdot \mathbf{p}_1)}. \quad (3.44)$$

The partial integration that comes after this shifts the derivatives onto the symbols:

$$\begin{aligned} c(\mathbf{q}, \mathbf{p}) &= (\pi)^{-2d} \int d^d \mathbf{q}_1 \int d^d \mathbf{q}_2 \int d^d \mathbf{p}_1 \int d^d \mathbf{p}_2 \sum_{\alpha, \beta} \frac{1}{\alpha! \beta!} \frac{i^{|\alpha| - |\beta|}}{2^{|\alpha| + |\beta|}} \\ &\quad \times e^{2i(\mathbf{p}_2 \cdot \mathbf{q}_1 - \mathbf{q}_2 \cdot \mathbf{p}_1)} \partial_{\mathbf{q}_1}^{\beta} \partial_{\mathbf{p}}^{\alpha} a(\mathbf{q}_1 + \mathbf{q}, \mathbf{p}) \partial_{\mathbf{q}_2}^{\alpha} \partial_{\mathbf{p}}^{\beta} b(\mathbf{q}_2 + \mathbf{q}, \mathbf{p}). \end{aligned} \quad (3.45)$$

The final step is to replace the following integrals by Dirac deltas,

$$(\pi)^{-d} \int d^d \mathbf{p}_2 e^{2i(\mathbf{p}_2 \cdot \mathbf{q}_1)} \rightarrow \delta(\mathbf{q}_1), \quad (3.46)$$

$$(\pi)^{-d} \int d^d \mathbf{p}_1 e^{-2i(\mathbf{p}_1 \cdot \mathbf{q}_2)} \rightarrow \delta(\mathbf{q}_2), \quad (3.47)$$

and integrate over \mathbf{q}_1 and \mathbf{q}_2 to get

$$c(\mathbf{q}, \mathbf{p}) = \sum_{\alpha, \beta} \frac{1}{\alpha! \beta!} \frac{i^{|\alpha| - |\beta|}}{2^{|\alpha| + |\beta|}} \partial_{\mathbf{q}}^{\beta} \partial_{\mathbf{p}}^{\alpha} a(\mathbf{q}, \mathbf{p}) \partial_{\mathbf{q}}^{\alpha} \partial_{\mathbf{p}}^{\beta} b(\mathbf{q}, \mathbf{p}). \quad (3.48)$$

The exponential version of (3.48) [6] [8],

$$c(\mathbf{q}, \mathbf{p}) = \exp \left[\frac{i}{2} \left(\frac{\partial}{\partial \mathbf{q}_1} \cdot \frac{\partial}{\partial \mathbf{p}_2} - \frac{\partial}{\partial \mathbf{p}_1} \cdot \frac{\partial}{\partial \mathbf{q}_2} \right) \right] a(\mathbf{q}_1, \mathbf{p}_1) b(\mathbf{q}_2, \mathbf{p}_2) \Big|_{(\mathbf{q}, \mathbf{p})} \quad (3.49)$$

is known as *Groenewold's formula* [7].

3. The Wigner Function

This function has a long history in physics (see [11] and references therein). For brevity we will only concern ourselves with the fact that it is proportional to the Wigner transform of the *density matrix*,

$$W(\mathbf{q}, \mathbf{p}) = (2\pi)^{-d} \int_{\mathbf{R}^d} d^d v e^{-i\mathbf{p} \cdot \mathbf{v}} \Psi(\mathbf{q} + \mathbf{v}/2) \Psi(\mathbf{q} - \mathbf{v}/2)^*, \quad (3.50)$$

and the expectation value of \hat{A} is found in terms of the Wigner distribution function as

$$\langle \hat{A} \rangle = \int_{\mathbf{R}^d} d^d q d^d p a(\mathbf{q}, \mathbf{p}) W(\mathbf{q}, \mathbf{p}). \quad (3.51)$$

4. Weyl's Original Definition

Weyl's method for quantization was very straightforward but beautiful at the same time. If one cannot simply replace all the p 's and q 's in a function (symbol) by their quantum counterparts \hat{P} and \hat{Q} to get the corresponding quantum operator, he should first take the Fourier transform of the symbol and *then* perform this substitution in the inverse transform. This necessitates the employment of an auxiliary symbol called

\tilde{a} :

$$a(\mathbf{q}, \mathbf{p}) = \int d^d s \int d^d t e^{-i(\mathbf{s} \cdot \mathbf{q} + \mathbf{t} \cdot \mathbf{p})} \tilde{a}(\mathbf{s}, \mathbf{t}). \quad (3.52)$$

Then the quantum operator that corresponds to the function $a(\mathbf{q}, \mathbf{p})$ is²⁸

$$\hat{A} = \int d^d s \int d^d t e^{-i(\mathbf{s} \cdot \hat{\mathbf{Q}} + \mathbf{t} \cdot \hat{\mathbf{P}})} \tilde{a}(\mathbf{s}, \mathbf{t}) \quad (3.53)$$

where

$$\hat{\mathbf{Q}}\Psi(\mathbf{x}) = \mathbf{x}\Psi(\mathbf{x}), \quad \hat{\mathbf{P}}\Psi(\mathbf{x}) = -i\nabla\Psi(\mathbf{x}), \quad [\hat{\mathbf{Q}}, \hat{\mathbf{P}}] = \hat{\mathbf{1}} \quad (3.54)$$

as usual. It can be shown by using (3.11) and the *Baker-Campbell-Hausdorff formula* (BCH)²⁹

$$e^{\hat{A} + \hat{B}} = e^{-[\hat{A}, \hat{B}]/2} e^{\hat{A}} e^{\hat{B}} \quad (3.55)$$

and the identity

$$e^{-i\hat{\mathbf{P}} \cdot \mathbf{t}} \Psi(\mathbf{x}) = \Psi(\mathbf{x} - \mathbf{t}) \quad (3.56)$$

that the integral kernel of \hat{A} can be written in terms of the auxiliary symbol $\tilde{a}(\mathbf{s}, \mathbf{t})$ as

$$\mathcal{A}(\mathbf{x}, \mathbf{y}) = \int d^d s e^{-i\mathbf{s} \cdot (\mathbf{x} + \mathbf{y})/2} \tilde{a}(\mathbf{s}, \mathbf{x} - \mathbf{y}) \quad (3.57)$$

after a change of variables $\mathbf{y} = \mathbf{x} - \mathbf{t}$.

Finally, if one inverts (3.52) and plugs it in (3.53), we have the (alternative³⁰) “symbol to operator” relation

$$\hat{A} = (2\pi)^{-2d} \int d^d q \int d^d p \int d^d s \int d^d t a(\mathbf{q}, \mathbf{p}) e^{i(\mathbf{s} \cdot \mathbf{q} + \mathbf{t} \cdot \mathbf{p})} e^{-i(\mathbf{s} \cdot \hat{\mathbf{Q}} + \mathbf{t} \cdot \hat{\mathbf{P}})}. \quad (3.58)$$

For completeness let us also give the formulae for the auxiliary symbol in terms of

²⁸Recall that we are using units where $\hbar = 1$. In this choice of units, h just means 2π (see Chapter V).

²⁹refer to [8], pp. 7–8 for a derivation of BCH.

³⁰In comparison with the form $[\hat{A}\Psi](\mathbf{x})$ that one gets after putting (3.16) in (3.11).

the symbol and the kernel:

$$\tilde{a}(\mathbf{s}, \mathbf{t}) = (2\pi)^{-2d} \int d^d q \int d^d p e^{i(\mathbf{s}\cdot\mathbf{q}+\mathbf{t}\cdot\mathbf{p})} a(\mathbf{q}, \mathbf{p}), \quad (3.59)$$

$$\tilde{a}(\mathbf{s}, \mathbf{v}) = (2\pi)^{-2d} \int d^d q e^{i\mathbf{s}\cdot\mathbf{q}} \mathcal{A}(\mathbf{q} + \mathbf{v}/2, \mathbf{q} - \mathbf{v}/2). \quad (3.60)$$

A summary of these relations is given in Fig. 2, where the factors by the arrows are to be placed in the integrand along with functions of the proper set of variables.

5. Operator Bases and the Quantizer

The definitions of the previous section give the motivation to establish a notion of operator basis. The *Heisenberg translation operators* defined by [12] [26]

$$\hat{T} \equiv \exp[i(\mathbf{s} \cdot \hat{\mathbf{Q}} + \mathbf{t} \cdot \hat{\mathbf{P}})], \quad (3.61)$$

which satisfy

$$\text{Tr}[\hat{T}(\mathbf{s}, \mathbf{t})] \equiv \int d^d x \langle x | \hat{T}(\mathbf{s}, \mathbf{t}) | x \rangle = (2\pi)^d \delta(\mathbf{s}) \delta(\mathbf{t}), \quad (3.62)$$

form a basis called the *Weyl basis*. The product of two Heisenberg operators can be expressed as a single Heisenberg operator with a phase factor:

$$\hat{T}(\mathbf{s}, \mathbf{t}) \hat{T}(\mathbf{s}', \mathbf{t}') = e^{(i/2)(\mathbf{t}\cdot\mathbf{s}' - \mathbf{t}'\cdot\mathbf{s})} \hat{T}(\mathbf{s} + \mathbf{s}', \mathbf{t} + \mathbf{t}'), \quad (3.63)$$

which is called the *duplication formula*. Taking the the trace of the product in (3.63),

$$\text{Tr}[\hat{T}(\mathbf{s}, \mathbf{t}) \hat{T}(\mathbf{s}', \mathbf{t}')] = (2\pi)^d \delta(\mathbf{s} - \mathbf{s}') \delta(\mathbf{t} - \mathbf{t}'), \quad (3.64)$$

one finds the inverse of the basis $\hat{T}(\mathbf{s}, \mathbf{t})$ as $(2\pi)^{-d} \hat{T}(-\mathbf{s}, -\mathbf{t})$.

Another common basis which we can extract from (3.58) is the operator con-

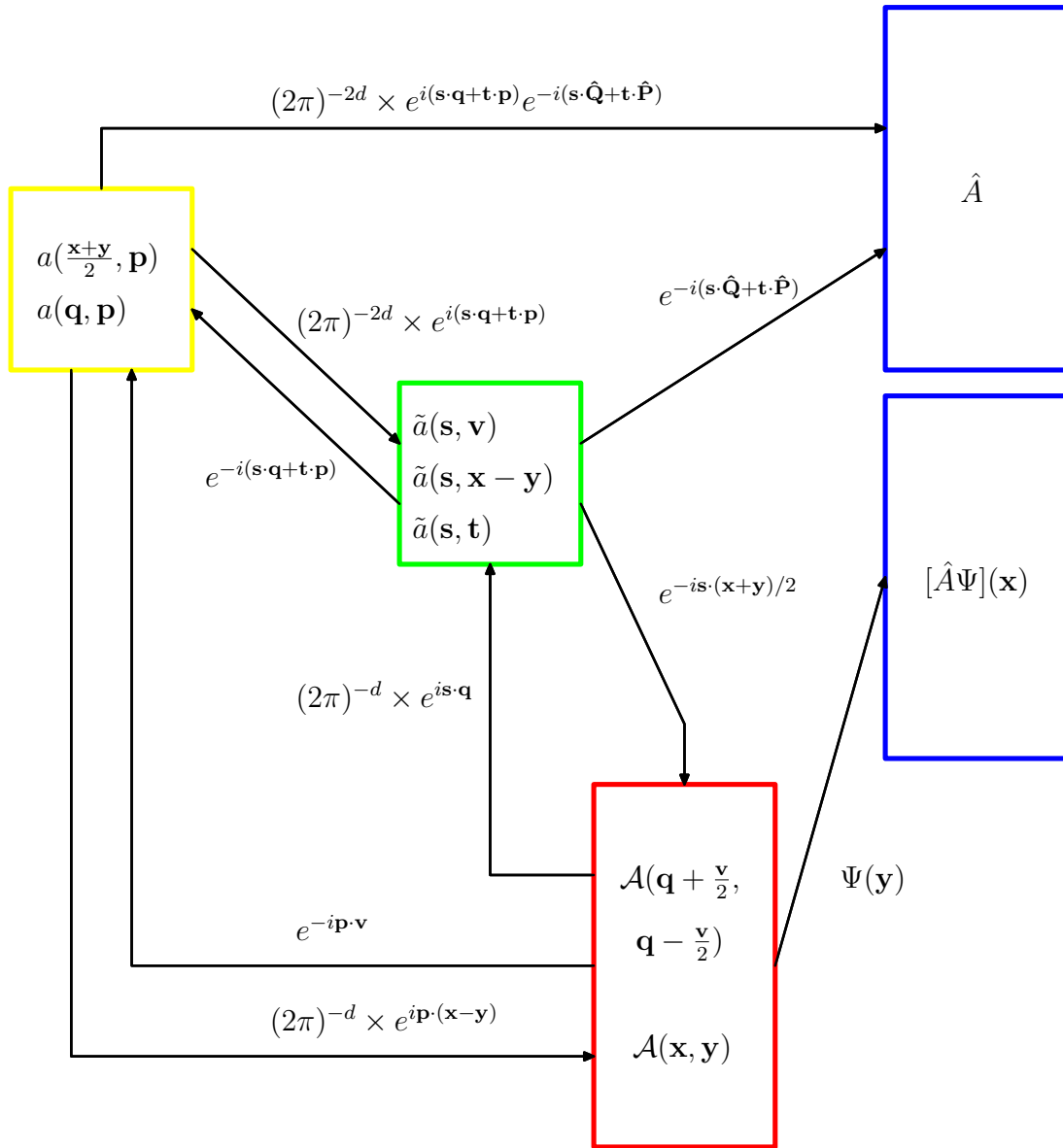


Fig. 2. The integral machinery in the symbol-kernel-operator formalism.

structed from $\hat{T}(\mathbf{s}, \mathbf{t})$ in the form

$$\hat{\Delta}(\mathbf{q}, \mathbf{p}) = (2\pi)^{-d} \int d^d s \int d^d t e^{i(\mathbf{s}\cdot\mathbf{q}+\mathbf{t}\cdot\mathbf{p})} \hat{T}(-\mathbf{s}, -\mathbf{t}). \quad (3.65)$$

This is called *Wigner's basis* [12] or the *quantizer* [55] [27]. These operators satisfy

$$\text{Tr} \hat{\Delta}(\mathbf{q}, \mathbf{p}) = \hat{\mathbf{1}}, \quad (3.66)$$

$$\text{Tr}[\hat{\Delta}(\mathbf{q}, \mathbf{p}) \hat{\Delta}(\mathbf{q}', \mathbf{p}')] = (2\pi)^d \delta(\mathbf{q} - \mathbf{q}') \delta(\mathbf{p} - \mathbf{p}'). \quad (3.67)$$

Therefore the inverse base to $\hat{\Delta}(\mathbf{q}, \mathbf{p})$ is $(2\pi)^{-d} \hat{\Delta}(\mathbf{q}', \mathbf{p}')$. There is no simple duplication formula for $\hat{\Delta}$'s; the analogue of (3.63) is that the product of two operators is a combination of an infinite number of $\hat{\Delta}$'s [12]:

$$\hat{\Delta}(\mathbf{q}, \mathbf{p}) \hat{\Delta}(\mathbf{q}', \mathbf{p}') = \left(\frac{2}{\pi}\right)^d \int d^d \bar{q} \int d^d \bar{p} e^{2i\varphi} \hat{\Delta}(\bar{\mathbf{q}}, \bar{\mathbf{p}}), \quad (3.68)$$

where the 'phase factor' φ is given by

$$\varphi = (\mathbf{q} - \mathbf{q}') \cdot (\mathbf{p}' - \bar{\mathbf{p}}) - (\mathbf{p} - \mathbf{p}') \cdot (\mathbf{q}' - \bar{\mathbf{q}}). \quad (3.69)$$

In obtaining this, one uses (3.65), (3.63) and

$$\bar{\mathbf{s}} = \mathbf{s} + \mathbf{s}' \quad (3.70)$$

$$\bar{\mathbf{t}} = \mathbf{t} + \mathbf{t}' \quad (3.71)$$

$$\bar{\mathbf{q}} = \mathbf{q}' + \mathbf{t}/2 \quad (3.72)$$

$$\bar{\mathbf{p}} = \mathbf{p}' - \mathbf{s}/2 \quad (3.73)$$

Using Fig. 2 and the definitions (3.61) and (3.65), one can write an arbitrary operator \hat{A} in both Weyl and Wigner bases as

$$\hat{A} = \int d^d s \int d^d t \tilde{a}(\mathbf{s}, \mathbf{t}) \hat{T}(-\mathbf{s}, -\mathbf{t}), \quad (3.74)$$

and

$$\hat{A} = (2\pi)^{-d} \int d^d q \int d^d p a(\mathbf{q}, \mathbf{p}) \hat{\Delta}(\mathbf{q}, \mathbf{p}). \quad (3.75)$$

Conversely, it can be shown that the symbols \tilde{a} and a can be expressed in terms of the operator \hat{A} in the following way:

$$\tilde{a}(\mathbf{s}, \mathbf{t}) = (2\pi)^{-d} \text{Tr}[\hat{T}(-\mathbf{s}, -\mathbf{t})\hat{A}], \quad (3.76)$$

$$a(\mathbf{q}, \mathbf{p}) = \text{Tr}[\hat{\Delta}(\mathbf{q}, \mathbf{p})\hat{A}]. \quad (3.77)$$

By these relations one completes (see Fig. 3) the ‘symbol-kernel-operator’ chart. For completeness let us also give the representations of \hat{T} and $\hat{\Delta}$ in the coordinate basis [12] that are needed to derive the trace formulas in this section:

$$\langle \mathbf{x} | \hat{T}(\mathbf{s}, \mathbf{t}) | \mathbf{x}' \rangle = \delta(\mathbf{x} - \mathbf{x}' + \mathbf{t}) \exp[i\mathbf{s} \cdot (\mathbf{x} + \mathbf{x}')/2], \quad (3.78)$$

and

$$\langle \mathbf{x} | \hat{\Delta}(\mathbf{q}, \mathbf{p}) | \mathbf{x}' \rangle = \delta\left(\frac{\mathbf{x} + \mathbf{x}'}{2} - \mathbf{q}\right) \exp[i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')]. \quad (3.79)$$

Let us finish this chapter with the following remarks: First, if one replaces the arbitrary operator in (3.77) by the density matrix and evaluates the trace using (3.79) the result is the Wigner function multiplied by $(2\pi)^d$. Secondly, it can be shown that the product formula in the exponential form (Groenewold’s formula) is easily obtained in this formalism as a consequence of the duplication relation of the Heisenberg translation operators [7] [12]. Finally, as we will see in the next chapter, the gauge invariant versions of the Weyl calculus are mostly based on the ‘magnetic’ analogue of (3.63) (see [26]), and we will present our version of a covariant representation of the quantizer in a form similar to (3.79).

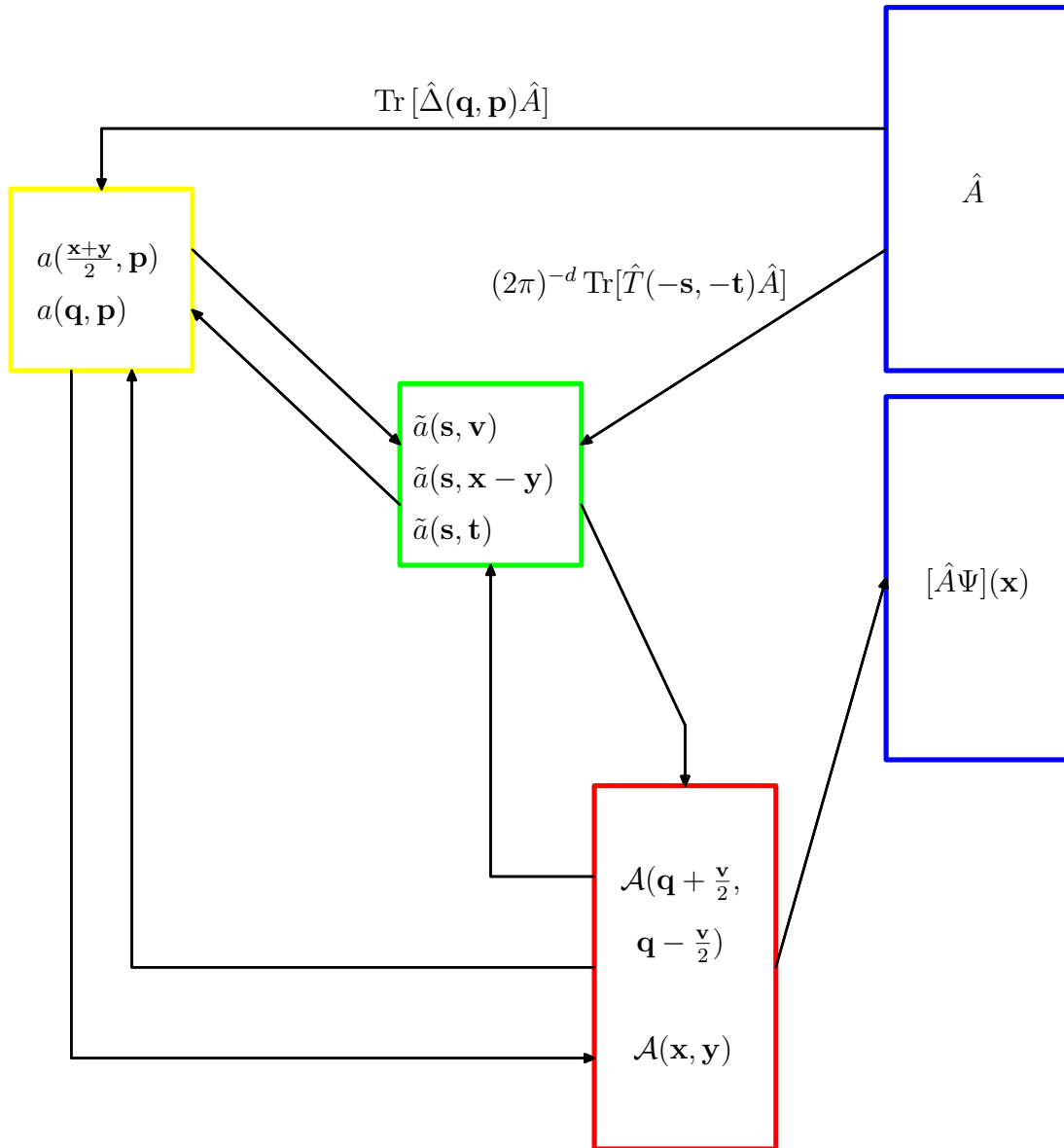


Fig. 3. The trace formulas for obtaining the symbols.

CHAPTER IV

INTRINSIC SYMBOLS OF ψ DO'S AND WEYL SYMMETRY

A. The Electromagnetic Case

The problem of semiclassically describing the motion of a charged particle interacting with an electromagnetic field has attracted much attention in past years due to its vast area of applications. Some of these areas include plasma physics, accelerator physics and quantum Hall effect (see [25], [26] and references therein). Gauge invariant Wigner functions may be used in \hbar expansions to study photon recoil effects [56] on an atom and the center of mass motion of an ion trapped in a travelling light wave [57]. In a recent paper [26], Müller derived a product rule for gauge invariant Weyl symbols using the quantizer approach, which is a generalization of the *Moyal bracket* defined by [7]

$$i\hbar\{a, b\}_{\mathcal{M}} \equiv a * b - b * a \quad (4.1)$$

for the symbols a and b . The $*$ product was defined in the previous chapter by (3.41) and (3.48), in the form of a 4-tuple integral and a multi-index summation, respectively. Karasev and Osborn, from a more elegant geometric point of view, developed a gauge invariant quantization over a linear phase space endowed with the electromagnetic 2-form $F = \frac{1}{2}F_{jk}(q)dq^k \wedge dq^j$ in addition to the usual *symplectic* canonical 2-form $w = \frac{1}{2}J_{jk}dx^k \wedge dx^j$ which generates Hamilton's equations of motion³¹ [29].

³¹Here, J is a skew-symmetric matrix equal to $\begin{bmatrix} 0 & \hat{1} \\ -\hat{1} & 0 \end{bmatrix}$ and $x = (q, p)$ stands for a point in the $2d$ -dimensional phase space.

1. Gauge Invariant Symbols and the Magnetic Product

The gauge dependence of the canonical momentum $\hat{\mathbf{P}}$ causes the basis operators $\hat{\Delta}(\mathbf{q}, \mathbf{p})$ to be gauge dependent as well. Upon inspecting (3.58), (3.77) and (3.79), one concludes that a gauge invariant operator (Weyl symbol) leads to a gauge dependent Weyl symbol (operator). To remedy this problem one replaces the gauge³² dependent canonical momentum by the gauge independent kinetic momentum [26]:

$$\hat{\Pi}_i = \hat{P}_i - \frac{e}{c} A_i(\hat{\mathbf{Q}}) \quad (4.2)$$

and writes the new quantizer as

$$\hat{\Delta}_q(\mathbf{q}, \mathbf{p}) = (2\pi)^{-d} \int d^d s \int d^d t e^{i(\mathbf{s} \cdot \mathbf{q} + \mathbf{t} \cdot \hat{\pi})} \hat{T}_q(-\mathbf{s}, -\mathbf{t}), \quad (4.3)$$

where

$$\hat{T}_q \equiv \exp[i(\mathbf{s} \cdot \hat{\mathbf{Q}} + \mathbf{t} \cdot \hat{\mathbf{\Pi}})]. \quad (4.4)$$

The operator \rightleftharpoons symbol relations (3.74)-(3.77) are unchanged.

It can be shown [25] by studying the operator

$$\hat{T}(\mathbf{s}, \mathbf{t}; \tau) \equiv \exp[i\tau(\mathbf{s} \cdot \hat{\mathbf{Q}} + \mathbf{t} \cdot \hat{\mathbf{\Pi}})] \quad (4.5)$$

parametrized by τ and a (2.33)-type relation that

$$\exp[i(\mathbf{t} \cdot \hat{\mathbf{\Pi}})] = \exp\left[-i \frac{e}{c} \mathbf{t} \cdot \int_0^1 d\tau \mathbf{A}(\hat{\mathbf{Q}} + \tau \mathbf{t})\right] \exp[i(\mathbf{t} \cdot \hat{\mathbf{P}})]. \quad (4.6)$$

Using this and the BCH formula (3.55), the following duplication relation can be found [26]:

$$\hat{T}(\mathbf{s}, \mathbf{t}) \hat{T}(\mathbf{s}', \mathbf{t}') = e^{i\hat{\mathcal{Z}}(\mathbf{t}, \mathbf{A}, \mathbf{t}')} e^{(i/2)(\mathbf{t} \cdot \mathbf{s}' - \mathbf{t}' \cdot \mathbf{s})} \hat{T}(\mathbf{s} + \mathbf{s}', \mathbf{t} + \mathbf{t}'). \quad (4.7)$$

³²One may also include time dependent gauge fields [29].

(4.7) differs from the zero field duplication relation (3.63) by the factor $\exp[i\hat{\chi}(\mathbf{t}, \mathbf{A}, \mathbf{t}')]$ where

$$\begin{aligned} \hat{\chi}(\mathbf{t}, \mathbf{A}, \mathbf{t}') &= \frac{e}{c} \mathbf{t} \cdot \int_0^1 d\tau [\mathbf{A}(\hat{\mathbf{Q}} + \tau(\mathbf{t} + \mathbf{t}')) - \mathbf{A}(\hat{\mathbf{Q}} + \tau\mathbf{t})] \\ &\quad + \frac{e}{c} \mathbf{t}' \cdot \int_0^1 d\tau [\mathbf{A}(\hat{\mathbf{Q}} + \tau(\mathbf{t} + \mathbf{t}')) - \mathbf{A}(\hat{\mathbf{Q}} + \tau\mathbf{t}' + \mathbf{t})]. \end{aligned} \quad (4.8)$$

The resulting gauge independent symbol product formula analogous to (3.49) by Müller and its derivation are too long and technical to quote here (an elegant version can be found in [29] which also attempts to find an extended formula for the product of N operators) but let us stress one important result he obtained. The (3.41)-like integral formula of the twisted product for the *auxiliary* symbol in the electromagnetic case reads [26]

$$\begin{aligned} \tilde{c}(\mathbf{s}, \mathbf{t}) &= (2\pi)^{-d} \int d^d q \int d^d s' \int d^d t' \int d^d S e^{iF(\mathbf{t}, \mathbf{A}(\mathbf{q}), \mathbf{t}')} \tilde{a}(\mathbf{s}', \mathbf{t}') \tilde{b}(\mathbf{S} - \mathbf{s}', \mathbf{t} - \mathbf{t}') \\ &\quad \times \exp[i(\mathbf{S} - \mathbf{s}) \cdot \mathbf{q}] \exp\left[\frac{i}{2} \left((\mathbf{t} + \mathbf{t}') \cdot \mathbf{S} - \mathbf{t} \cdot (\mathbf{s} + \mathbf{s}') \right)\right], \end{aligned} \quad (4.9)$$

where

$$\begin{aligned} F(\mathbf{t}, \mathbf{A}(\mathbf{q}), \mathbf{t}') &\equiv \frac{e}{c} \mathbf{t}' \cdot \int_0^1 d\tau [\mathbf{A}(\mathbf{q} + (1 - \tau)\mathbf{t}' + \tau\mathbf{t}) - \mathbf{A}(\mathbf{q} + \tau\mathbf{t}')] \\ &\quad - \frac{e}{c} \mathbf{t} \cdot \int_0^1 d\tau [\mathbf{A}(\mathbf{q} + (1 - \tau)\mathbf{t}' + \tau\mathbf{t}) - \mathbf{A}(\mathbf{q} + \tau\mathbf{t})]. \end{aligned} \quad (4.10)$$

If (4.10) is expanded into a Taylor series in 3 dimensions, it is seen that the result

$$\begin{aligned} F\left(\mathbf{t}' + \mathbf{t}'', \mathbf{A}\left(\mathbf{q} - \frac{\mathbf{t}' + \mathbf{t}''}{2}\right), \mathbf{t}'\right) &= \sum_{n=1}^{\infty} \sum_{r,j,l=1}^3 \sum_{i_1, \dots, i_{n-1}=1}^3 \sum_{k=1}^n \aleph(n, k) \frac{\partial^{n-1} B_r}{\partial q_{i_1} \cdots \partial q_{i_{n-1}}} \\ &\quad \times \mathbf{t}''_l \mathbf{t}'_j \mathbf{t}'_{i_1} \cdots \mathbf{t}'_{i_{k-1}} \mathbf{t}''_{i_k} \cdots \mathbf{t}''_{i_{n-1}} \end{aligned} \quad (4.11)$$

is only a function of the derivatives of the *physical* magnetic field $\mathbf{B}(\mathbf{q})$. Here, $\aleph(n, k)$

is a combinatorial factor of the form

$$\aleph(n, k) = \frac{1}{n!} \left(-\frac{1}{2}\right)^{n+1} \frac{1}{(n+1)^2} \binom{n+1}{k}. \quad (4.12)$$

Therefore, the integrand in (4.9) is gauge independent. Finally, let us finish this section by quoting a gauge invariant Wigner function from [25],

$$\begin{aligned} W_g(\mathbf{q}, \vec{\pi}) &= (2\pi)^{-d} \int d^d t \langle \mathbf{q} - \frac{1}{2}\mathbf{t} | \hat{\rho} | \mathbf{q} + \frac{1}{2}\mathbf{t} \rangle \\ &\times \exp \left[i\mathbf{t} \cdot \left(\pi + \frac{e}{c} \int_{-1/2}^{1/2} d\tau \mathbf{A}(\mathbf{q} + \tau\mathbf{t}) \right) \right]. \end{aligned} \quad (4.13)$$

B. General Case

In this section we will briefly summarize the main results of the efforts to make ψ DO's and the Weyl calculus geometrically covariant, in the style of [6].

1. Intrinsic Widom Calculus

The covariant calculus of pseudo-differential operators was defined by Bokobza [30], Widom [32] and Drager [33] and developed for calculating *heat kernels* by Fulling and Kennedy [34] [35]. In this formalism the symbol is a function on the cotangent bundle; from the very start the calculations are to be kept manifestly covariant. If one wants to mimic the kernel \Rightarrow relations of Chapter III on the manifold³³, what would replace the vectorial difference $\mathbf{x} - \mathbf{y} = -(\mathbf{y} - \mathbf{x})$ in (3.14) and (3.15)? The most likely candidate is the negative tangent vector at x pointing in a direction that gives the point y as the solution of the geodesic equation. In the language of Chapter

³³From now on, the points on the manifold will be denoted by x, y, \dots , the vectors in the cotangent space by $\mathbf{p}, \mathbf{k}, \dots$, and vectors in the tangent space by $\hat{\sigma}, \vec{v}, \vec{u}, \dots$ etc.

III, this is the inverse exponential map

$$\hat{\sigma}(x, y) \equiv \exp_x^{-1} y. \quad (4.14)$$

Secondly, the parallel transport matrix on the bundle, $I(x, y)$, should accompany the symbol (and the kernel) to assure covariance:

$$\begin{aligned} T_x^*(M) \searrow_M & : e^{-i\mathbf{p} \cdot \hat{\sigma}(x, y)} a(x, \mathbf{p}) I(x, y) \dashrightarrow \mathcal{A}(x, y), \\ M \nearrow T_x^*(M) & : e^{-i\mathbf{p} \cdot \hat{\sigma}(x, y)} \mathcal{A}(x, y) I(y, x) \dashrightarrow a(x, \mathbf{p}). \end{aligned} \quad (4.15)$$

Finally, to make the integrals covariant, one needs to include the “ \sqrt{g} ” in the appropriate places, *i.e.*,

$$\int_M dx \sqrt{g(x)}, \quad \int_{T_x^*} \frac{d\mathbf{p}}{\sqrt{g(x)}}, \quad \int_{T_x} d\hat{\sigma}(x, y) \sqrt{g(x)} \quad \text{etc} \dots \quad (4.16)$$

Then, in the spirit of (3.15), the covariant symbol is defined as

$$a(x, \mathbf{p}) = \int_M dy \sqrt{g(y)} e^{i\mathbf{p} \cdot \hat{\sigma}(x, y)} \mathcal{A}(x, y) I(y, x). \quad (4.17)$$

In order to invert this Fourier transform, one multiplies both sides of (4.17) by $(2\pi)^{-d} \exp(-i\mathbf{p} \cdot \vec{v})$ and integrates over the cotangent space at x :

$$\begin{aligned} (2\pi)^{-d} \int_{T_x^*} \frac{d^d p}{\sqrt{g(x)}} e^{-i\mathbf{p} \cdot \vec{v}} a(x, \mathbf{p}) \\ = (2\pi)^{-d} \int_M dy \sqrt{g(y)} \int_{T_x^*} \frac{d^d p}{\sqrt{g(x)}} e^{i\mathbf{p} \cdot (\hat{\sigma} - \vec{v})} \mathcal{A}(x, y) I(y, x) \\ = \int_M dy \sqrt{g(y)} \delta(\hat{\sigma} - \vec{v}) \mathcal{A}(x, y) I(y, x). \end{aligned} \quad (4.18)$$

The integral over M can be converted to an integral over T_x by (2.89), and the right hand side of (4.18) becomes

$$\int_{T_x} \Delta^{-1}(x, \exp_x \hat{\sigma}) d\hat{\sigma}(x, y) \sqrt{g(x)} \delta(\hat{\sigma} - \vec{v}) \mathcal{A}(x, \exp_x \hat{\sigma}) I(\exp_x \hat{\sigma}, x)$$

$$= \Delta^{-1}(x, \exp_x \vec{v}) \mathcal{A}(x, \exp_x \vec{v}) I(\exp_x \vec{v}). \quad (4.19)$$

Upon renaming $\exp_x \vec{v}$ as y , and solving for $\mathcal{A}(x, y)$, the covariant ‘symbol to kernel’ formula can be written as

$$\mathcal{A}(x, y) = (2\pi)^{-d} \Delta(x, y) \int \frac{d^d p}{\sqrt{g(x)}} e^{-i\mathbf{p} \cdot \hat{\sigma}(x, y)} a(x, \mathbf{p}) I(x, y). \quad (4.20)$$

In [6], one reads (4.17) and (4.20) with parametrized Van Vleck-Morette determinants $\Delta^\gamma(x, y)$ and $\Delta^{1-\gamma}(x, y)$, respectively, for the purpose of comparison with Drager’s earlier work on the study of the choices $\gamma = 0$ and $\gamma = 1$ [33]. The latter choice has a clear advantage: If the symbol is taken to be a momentum polynomial $A_\alpha(x) \mathbf{p}^\alpha$, the resulting operator, which can now in general be found from the kernel by

$$[\hat{A}\psi](x) = \int_M dy \sqrt{g(y)} \mathcal{A}(x, y) \psi(y), \quad (4.21)$$

is a *covariant* differential operator of the form $A_\alpha(x) (-i\nabla)^\alpha$ without any extra terms! In other words one just replaces the ordinary derivatives by covariant derivatives.

2. Covariant Weyl Formalism: Fulling’s Definition

Let x and y be two given points on a geodesic. By definition, the tangent vector to the geodesic at a point continues to be a tangent vector wherever on the geodesic it is parallel transported to. So if $\vec{u}_0 = \exp_x^{-1}(y)$ and $\vec{v}_0 = \exp_y^{-1}(x)$, then $\vec{u}_0 = -g(x, y)\vec{v}_0$ where $g(x, y)$ is the parallel transport bi-vector. Now pick an arbitrary point on this geodesic line segment and let $\vec{v} \in T_q$ and $\vec{u} \in T_q$ be the vectors that satisfy

$$y = \exp_q(\vec{u}/2), \quad (4.22)$$

$$x = \exp_q(\vec{v}/2). \quad (4.23)$$

If $\vec{u}/2 = -\vec{v}/2$ then q is called the ‘midpoint’. With this symmetrical choice at hand, the ‘symbol to kernel’ formula is defined as [6]

$$\mathcal{A}(x, y) = (2\pi)^{-d} \Delta^\gamma(x, y) \int_{T_q^*} \frac{d^d p}{\sqrt{g(q)}} e^{i\mathbf{p}\cdot\vec{v}} I(x, q) a(q, \mathbf{p}) I(q, y). \quad (4.24)$$

Here q and \vec{v} should be understood as the dependent variables (on x and y) and they should form a unique pair if x and y are sufficiently close (no caustics). To find the symbol in terms of the kernel, one should invert the Fourier transform to get

$$a(q, \mathbf{p}) = \int_{T_q} d\vec{v} \sqrt{g(q)} e^{-i\mathbf{p}\cdot\vec{v}} I(q, x) \mathcal{A}(x, y) I(y, q) \Delta^{-\gamma}(x, y), \quad (4.25)$$

where x and y are defined by

$$x \equiv \exp_q(\frac{1}{2}\vec{v}), \quad y \equiv \exp_q(-\frac{1}{2}\vec{v}). \quad (4.26)$$

The Weyl quantization of momentum polynomials in this case yields a symmetric operator of the form (3.30). For the second order case, in addition to the ‘ordinary derivatives replaced by covariant ones’ terms in (3.30), there is a γ dependent curvature term:

$$\hat{A} = -A^{\mu\nu} \nabla_\mu \nabla_\nu - (\nabla_\mu A^{\mu\nu}) \nabla_\nu - \frac{1}{4} (\nabla_{\mu\nu} A^{\mu\nu}) - \frac{\gamma - 1}{3} A^{\mu\nu} R_{\mu\nu}. \quad (4.27)$$

The special case of $A^{\mu\nu} = g^{\mu\nu}$ is related to the *Laplace-Beltrami operator* and is of interest from the quantum gravity point of view. The quantization of the relativistic action (2.55) using the Feynman path integral method results in a similar term in the Schrodinger equation:

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \frac{1}{\sqrt{g}} \frac{\partial}{\partial q^m} \left(\sqrt{g} g^{mn} \frac{\partial \psi}{\partial q^n} \right) + \frac{R}{6} \psi. \quad (4.28)$$

This curvature term could be taken care of, if one starts with a Lagrangian that compensates for it; but some authors [58] find it “contradictory to the spirit of Feynman’s

formulation of quantum dynamics”. The reader should refer to [6] for more about this controversy.

It is also possible to look at these definitions from the quantizer point of view. The coordinate representation (3.79) of $\hat{\Delta}(q, \mathbf{p})$ may now be written as

$$\langle x | \hat{\Delta}(q, \mathbf{p}) | y \rangle = g(q)^{-1/2} \Delta(x, y)^\gamma \delta(q - \exp_x(-\frac{1}{2}\mathbf{v})) e^{i\mathbf{p}\cdot\mathbf{v}} I(x, y) \quad (4.29)$$

for an Abelian gauge field. This can be used in the (covariant modification of) operator \Leftrightarrow symbol formulas (3.75) and (3.77) of Chapter III:

$$\hat{A} = (2\pi)^{-d} \int \sqrt{g(q)} dq \int \frac{dp}{\sqrt{g(q)}} a(q, \mathbf{p}) \hat{\Delta}(q, \mathbf{p}), \quad (4.30)$$

or

$$\langle x | \hat{A} | y \rangle = (2\pi)^{-d} \int \sqrt{g(q)} dq \int \frac{dp}{\sqrt{g(q)}} a(q, \mathbf{p}) \langle x | \hat{\Delta}(q, \mathbf{p}) | y \rangle, \quad (4.31)$$

and

$$a(q, \mathbf{p}) = \text{Tr}[\hat{\Delta}(q, \mathbf{p}) \hat{A}]. \quad (4.32)$$

(4.29) shows that the quantizer formalism has an advantage over the “Heisenberg translation” formalism, because it is far from obvious what are the proper covariant analogues of $\hat{\mathbf{Q}}$ and \hat{T} in a curved space. The formula (4.29) does not have an obvious generalization to a non-Abelian gauge field.

As a closing remark for this chapter let us note that a product formula for the symbols is not known in this case and quote Fulling’s definition of the covariant Wigner function:

$$W(q, \mathbf{p}) = (2\pi)^{-d} \int_{T_q} d\vec{v} \sqrt{g(q)} e^{-i\mathbf{p}\cdot\vec{v}} \Delta^{-\gamma}(x, y) \psi(x) \psi(y)^*. \quad (4.33)$$

One can find papers in the mathematics literature which deal with Weyl symmetry and geometrical covariance together; for a rigorous study the reader may refer to [59].

CHAPTER V

A COVARIANT WEYL CALCULUS

In this chapter we propose a new method to establish a covariant Weyl calculus. The motivation for such a task comes from the fact that an asymptotic product formula for the symbols could not be achieved using Fulling’s definition. The ‘midpoint’ q itself is the point where the tangent and cotangent space integrals are carried out. In the problem of constructing a symbol for $\hat{C} = \hat{A}\hat{B}$ in terms of a and b , one encounters a “geodesic triangle” and three pairs of integral domains to use in the operator \rightleftharpoons symbol relations. After the asymptotic expansions for the symbols about momenta living in these cotangent spaces are obtained, the problem of what to do with these integrals and how to get rid of them using Dirac delta distributions arises. In order to remedy this problematic situation, we introduce a fiducial point x' separate from the ‘midpoint’, which carries the responsibility of housing the ‘ $\hat{\sigma}$ ’s and ‘ \mathbf{p} ’s in its $T_{x'}$ and T_x^* . After defining the kernel \rightleftharpoons symbol relations we directly move on to the momentum polynomial test and work out the corresponding operators for $|\alpha| = 1$ and $|\alpha| = 2$. After taking the coincidence limits we obtain the familiar ‘ordinary derivatives replaced by covariant ones’ form.

A. Definitions

Operators are defined through integral kernels as usual:

$$[\hat{C}\psi](X) = \int_M dZ \sqrt{g(Z)} \mathcal{C}(X, Z) \psi(Z). \quad (5.1)$$

We define a ‘symbol to kernel’ formula in the following manner: Given points X and Z ,

$$\mathcal{C}(X, Z) = \Delta^\gamma(x', X)\Delta^\gamma(x', Z)h^{-d} \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{P}_{\mu'} V^{\mu'}} c(x'; Q, \mathbf{P}), \quad (5.2)$$

where

$$Q = \exp_{x'} \frac{1}{2} [\hat{\sigma}^{\mu'}(x', X) + \hat{\sigma}^{\mu'}(x', Z)] \quad (5.3)$$

$$V^{\mu'} = \hat{\sigma}^{\mu'}(x', X) - \hat{\sigma}^{\mu'}(x', Z) \quad (5.4)$$

$$\tilde{P}_{\mu'} = g_{\mu'\nu}(x', Q) P_\nu \quad (5.5)$$

Note that $\hat{\sigma}^{\mu'}(x', \cdot) \in T_{x'}$, $\tilde{P}_{\mu'} \in T_{x'}^*$ and $P_\mu \in T_Q^*$. γ is an arbitrary constant kept in for generality. For definitions of $\Delta(x', X)$ and $\hat{\sigma}(x', X)$, see (2.67)–(2.89). The schematic representation of (5.3)–(5.5) is given in Fig. 4. Note also that Q is not the exact midpoint of the geodesic joining X and Z , but it is “close” in the sense that the two merge in the limit when the local radii of curvature are large compared to the lengths in the point configuration. The inverse formula which lets one pass from the kernel to the symbol is given by:

$$c(x'; q, \mathbf{P}) = \int_{T_{x'}} d^d \xi^{\mu'} \sqrt{g(x')} \Delta^{-\gamma}(x', x) \Delta^{-\gamma}(x', z) e^{-i\tilde{p}_{\mu'} \xi^{\mu'}} \mathcal{C}(x, z) \quad (5.6)$$

where x and z are defined by

$$x = \exp_{x'} [\hat{\sigma}^{\mu'}(x', q) + \frac{1}{2} \xi^{\mu'}] \quad (5.7)$$

$$z = \exp_{x'} [\hat{\sigma}^{\mu'}(x', q) - \frac{1}{2} \xi^{\mu'}]. \quad (5.8)$$

Here $p_{\mu'} \in T_q^*$ and $\tilde{p}_{\mu'} \in T_{x'}^*$ are related by means of the parallel transport:

$$\tilde{p}_{\mu'} = g_{\mu'\nu}(x', q) p_\nu \quad (5.9)$$

Relations (5.7)–(5.9) are summarized in Fig. 5. The addition of gauge fields in this

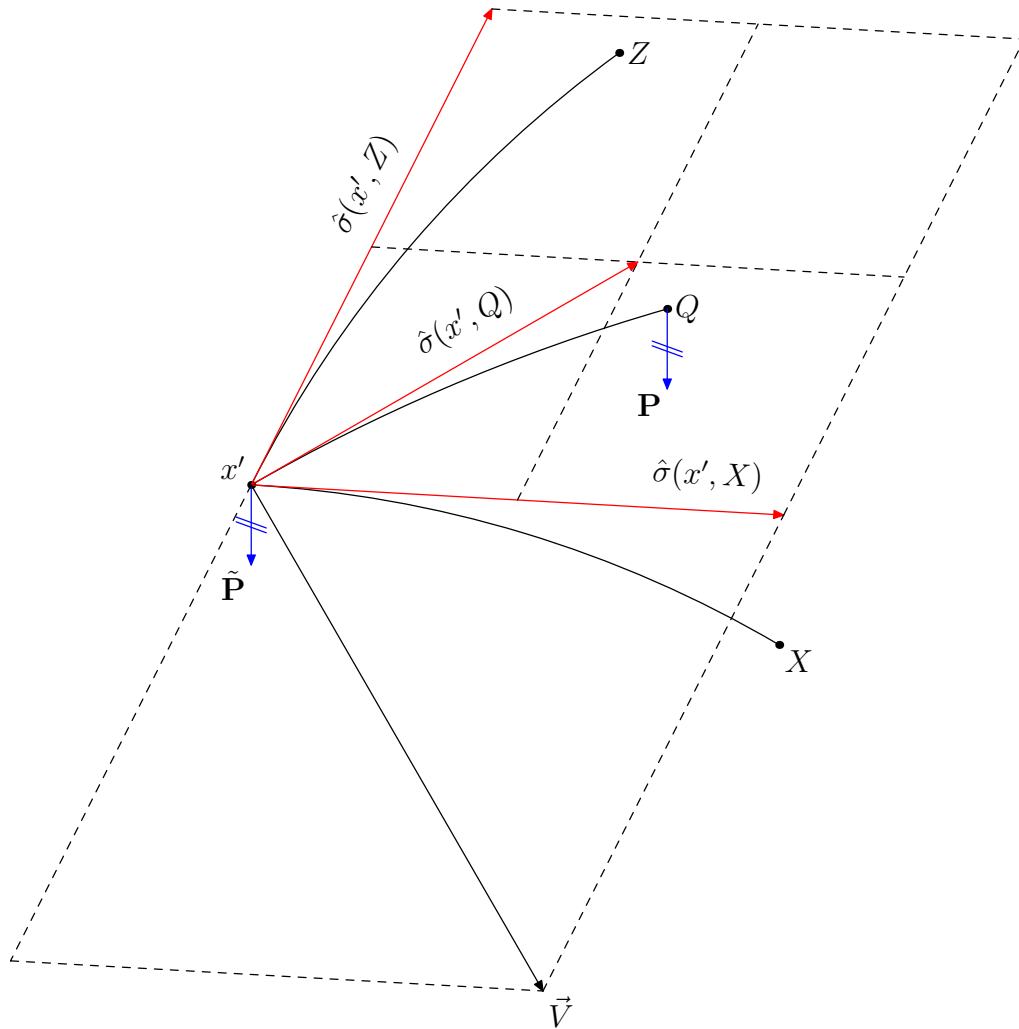


Fig. 4. The points used in symbol \mapsto kernel formula.

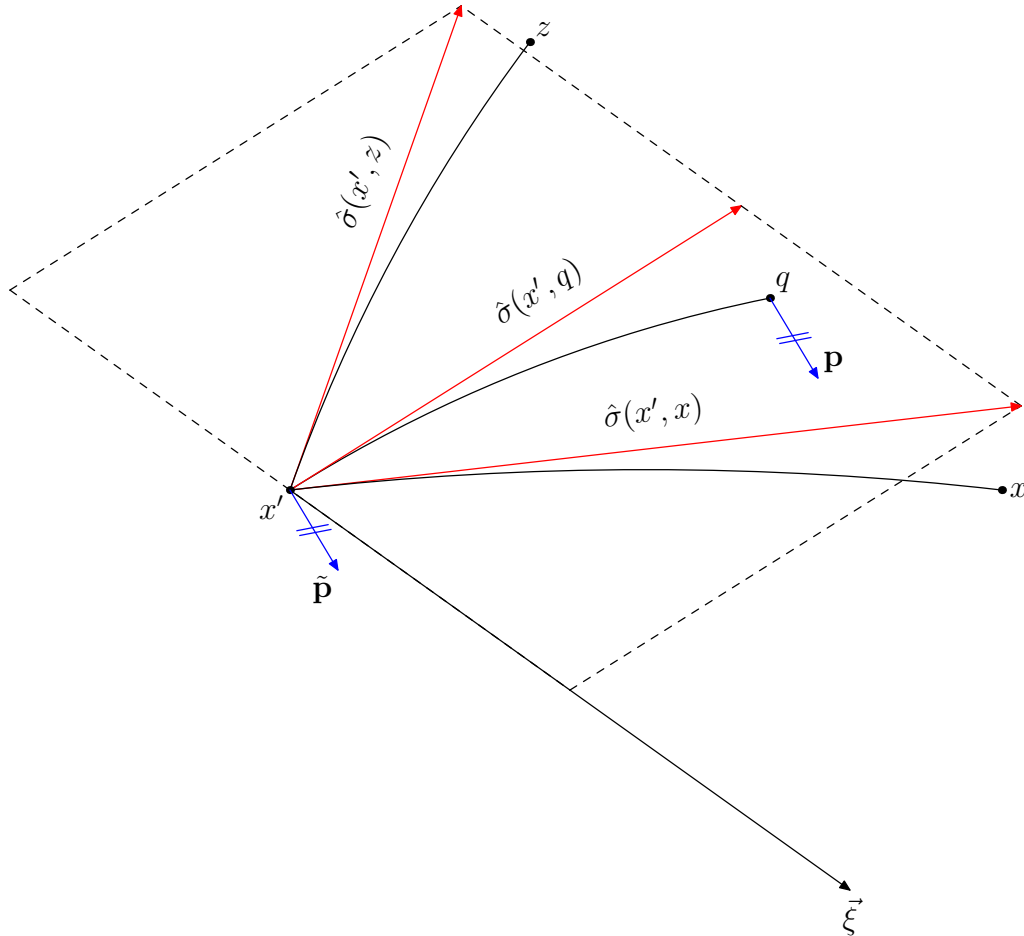


Fig. 5. The points used in kernel \mapsto symbol formula.

formalism will be in the style of (4.24) and (4.25) as follows:

$$\begin{aligned} \mathcal{C}(X, Z) &= \Delta^\gamma(x', X)\Delta^\gamma(x', Z)h^{-d} \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{P}_{\mu'} V^{\mu'}} \\ &\quad \times I(X, x')I(x', Q)c(x'; Q, \mathbf{P})I(Q, x')I(x', Z), \end{aligned} \quad (5.10)$$

and

$$\begin{aligned} c(x'; q, \mathbf{p}) &= \int_{T_{x'}} d^d \xi^{\mu'} \sqrt{g(x')} \Delta^{-\gamma}(x', x)\Delta^{-\gamma}(x', z) e^{-i\tilde{p}_{\mu'} \xi^{\mu'}} \\ &\quad \times I(q, x')I(x', x)\mathcal{C}(x, z)I(z, x')I(x', x). \end{aligned} \quad (5.11)$$

B. Differential Operators

Since we already know from classical Weyl formalism that symbols in the form of momentum polynomials produce differential operators, the next task is to see whether we get covariant derivatives in the general case. Before we begin to analyze the polynomial symbol, let us list the coincidence limits for some of the geometrical objects that we will need most. These are already defined and calculated in Chapter II and some details are in Appendix A.

The derivatives with respect to tangent vectors and points on the manifold are related by:

$$\partial_{\sigma^{\mu'}(x', x)} = \gamma^\nu_{\mu'}(x', x)\nabla_\nu, \quad (5.12)$$

and

$$\nabla_\mu = \eta^{\nu'}_{\mu}(x', x)\partial_{\sigma^{\nu'}(x', x)}. \quad (5.13)$$

The coincidence limits of $\gamma^\mu_{\nu'}$ and its first derivative are

$$[\gamma^\mu_{\nu'}] = -\delta^\mu_{\nu'}, \quad (5.14)$$

$$[\nabla_\mu \gamma^\nu_{\beta'}] = 0; \quad (5.15)$$

the coincidence limits of the parallel transport bi-vector $g^{\nu'}_{\mu}$ and its derivative are

$$[g^{\nu'}_{\mu}] = \delta^{\nu}_{\mu}, \quad (5.16)$$

$$[\nabla_{\alpha} g^{\nu'}_{\mu}] = 0; \quad (5.17)$$

the coincidence limits of the Synge-deWitt world function σ and its first and second order derivatives are

$$[\sigma^{\mu}] = 0, \quad (5.18)$$

$$[\nabla_{\alpha} \sigma^{\mu}] = \delta^{\mu}_{\alpha}; \quad (5.19)$$

and finally, the coincidence limits of the Van Vleck-Morette determinant Δ and its derivatives are

$$[\Delta^{\gamma}] = 1, \quad (5.20)$$

$$[\nabla_{\mu} \Delta^{\gamma}] = 0, \quad (5.21)$$

for $\gamma = 1$ and $\gamma = 1/2$; and

$$[\nabla_{\beta} \nabla_{\varphi} \Delta^{\gamma}] = \left\{ \begin{array}{ll} \frac{1}{6} R_{\beta\varphi} & , \quad \gamma = \frac{1}{2} \\ 0 & , \quad \gamma = 0 \\ \frac{1}{3} R_{\beta\varphi} & , \quad \gamma = 1 \end{array} \right\}. \quad (5.22)$$

The covariant Fourier integral can be defined as [43]

$$f(x) = \int \frac{dk_{\mu'}}{(2\pi)^d} g^{-1/2}(x') \exp\left(-ik_{\mu'} \sigma^{\mu'}(x', x)\right) \tilde{f}(k; x). \quad (5.23)$$

The inverse transformation has the form

$$\tilde{f}(k; x) = \int dx g^{1/2}(x) \Delta(x', x) \exp\left(ik_{\mu'} \sigma^{\mu'}(x', x)\right) f(x). \quad (5.24)$$

The covariant Fourier integral for the delta function has the form [43]

$$\begin{aligned} \delta(x, y) &= g^{1/4}(x)g^{1/4}(y)\Delta^{1/2}(x', x)\Delta^{1/2}(x', y) \\ &\times \int \frac{dk_{\mu'}}{(2\pi)^d} g^{-1/2}(x') \exp\left(ik_{\mu'}\left(\sigma^{\mu'}(x', y) - \sigma^{\mu'}(x', x)\right)\right). \end{aligned} \quad (5.25)$$

The equation defining the action of the delta function is

$$f(x) = \int dy \delta(x, y)f(y). \quad (5.26)$$

1. First Order

Let

$$\begin{aligned} c(x'; Q, \mathbf{P}) &= C_1^\mu(Q)P_\mu, \\ &= C_1^\mu(Q)g^{\nu'}{}_\mu(x', Q)\tilde{P}_{\nu'}. \end{aligned} \quad (5.27)$$

Then

$$\begin{aligned} [\hat{C}\psi](X) &= \int_M dZ \sqrt{g(Z)} h^{-d} \Delta^\gamma(x', X)\Delta^\gamma(x', Z) \\ &\times \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} \psi(Z) C_1^\mu(Q) g^{\nu'}{}_\mu(x', Q) \tilde{P}_{\nu'} e^{i\tilde{\mathbf{P}} \cdot \vec{V}}. \end{aligned} \quad (5.28)$$

Rewrite the last two factors in the integrand as

$$\begin{aligned} \tilde{P}_{\nu'} e^{i\tilde{\mathbf{P}} \cdot \vec{V}} &= -i \partial_{V_{\nu'}} e^{i\tilde{\mathbf{P}} \cdot \vec{V}}, \\ &= -i \partial_{\sigma^{\nu'}(x', Z)} e^{i\tilde{\mathbf{P}} \cdot \vec{V}}, \\ &= -i \gamma^\alpha{}_{\nu'}(x', Z) \nabla_\alpha^{(Z)} e^{i\tilde{\mathbf{P}} \cdot \vec{V}}, \end{aligned} \quad (5.29)$$

where we used (5.12); then

$$[\hat{C}\psi](X) = -i \int_M dZ \sqrt{g(Z)} h^{-d} \Delta^\gamma(x', X)\Delta^\gamma(x', Z) \psi(Z)$$

$$\times \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} C_1^\mu(Q) g^{\nu'}{}_\mu(x', Q) \gamma^{\alpha \nu'}(x', Z) \nabla_\alpha^{(Z)} e^{i\tilde{\mathbf{P}} \cdot \tilde{\mathbf{V}}}. \quad (5.30)$$

Integrate by parts to get

$$\begin{aligned} [\hat{C}\psi](X) &= +i \int_M dZ \sqrt{g(Z)} h^{-d} \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{\mathbf{P}} \cdot \tilde{\mathbf{V}}} \\ &\quad \times \nabla_\alpha^{(Z)} \left[\Delta^\gamma(x', X) \Delta^\gamma(x', Z) \psi(Z) C_1^\mu(Q) g^{\nu'}{}_\mu(x', Q) \gamma^{\alpha \nu'}(x', Z) \right]. \end{aligned} \quad (5.31)$$

The Dirac delta is given by

$$\delta(X, Z) = g^{1/4}(X) g^{1/4}(Z) \Delta^{1/2}(x', X) \Delta^{1/2}(x', Z) h^{-d} \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{\mathbf{P}} \cdot \tilde{\mathbf{V}}}; \quad (5.32)$$

plug this into (5.31) to get

$$\begin{aligned} [\hat{C}\psi](X) &= i \int_M dZ \sqrt{g(Z)} g^{-1/4}(X) g^{-1/4}(Z) \Delta^{\gamma-1/2}(x', X) \Delta^{-1/2}(x', Z) \delta(X, Z) \\ &\quad \times \nabla_\alpha^{(Z)} \left[\Delta^\gamma(x', Z) \psi(Z) C_1^\mu(Q) g^{\nu'}{}_\mu(x', Q) \gamma^{\alpha \nu'}(x', Z) \right], \end{aligned} \quad (5.33)$$

or

$$\begin{aligned} [\hat{C}\psi](X) &= i \Delta^{\gamma-1}(x', X) \nabla_\alpha^{(Z)} \left[\Delta^\gamma(x', Z) \psi(Z) C_1^\mu(Q) g^{\nu'}{}_\mu(x', Q) \gamma^{\alpha \nu'}(x', Z) \right] \Big|_{Z=X} \\ &= K_1 + K_2, \end{aligned} \quad (5.34)$$

where K_1 and K_2 are defined as

$$\begin{aligned} K_1 &\equiv i \Delta^{\gamma-1}(x', X) C_1^\mu(Q) g^{\nu'}{}_\mu(x', Q) \nabla_\alpha^{(Z)} \left[\Delta^\gamma(x', Z) \psi(Z) \gamma^{\alpha \nu'}(x', Z) \right] \Big|_{Z=X} \\ &= i \Delta^{\gamma-1}(x', X) C_1^\mu(X) g^{\nu'}{}_\mu(x', X) \nabla_\alpha^{(X)} \left[\Delta^\gamma(x', X) \psi(X) \gamma^{\alpha \nu'}(x', X) \right] \end{aligned} \quad (5.35)$$

and

$$K_2 \equiv i \Delta^{2\gamma-1}(x', X) \gamma^{\alpha \nu'}(x', Z) \psi(Z) \nabla_\alpha^{(Z)} \left[C_1^\mu(Q) g^{\nu'}{}_\mu(x', Q) \right] \Big|_{Z=X}, \quad (5.36)$$

where we used the definition of Q given by (5.3) in (5.35). In order to express $\nabla^{(Z)}$ in terms of $\nabla^{(Q)}$ one starts with (5.13) and writes

$$\begin{aligned}\nabla_{\alpha}^{(Z)} &= \eta^{\mu'}_{\alpha}(x', Z) \partial_{\sigma^{\mu'}(x', Z)}, \\ &= \eta^{\mu'}_{\alpha}(x', Z) \frac{\partial \sigma^{\theta'}(x', Q)}{\partial \sigma^{\mu'}(x', Z)} \partial_{\sigma^{\theta'}(x', Q)};\end{aligned}$$

again using (5.3),

$$\begin{aligned}\nabla_{\alpha}^{(Z)} &= \eta^{\mu'}_{\alpha}(x', Z) \left(\frac{1}{2} \delta_{\mu'}^{\theta'}\right) \partial_{\sigma^{\theta'}(x', Q)}, \\ &= \frac{1}{2} \eta^{\mu'}_{\alpha}(x', Z) \partial_{\sigma^{\mu'}(x', Q)};\end{aligned}\tag{5.37}$$

as a final step one uses (5.12) again to write

$$\nabla_{\alpha}^{(Z)} = \frac{1}{2} \eta^{\mu'}_{\alpha}(x', Z) \gamma^{\beta}_{\mu'}(x', Q) \nabla_{\beta}^{(Q)}.\tag{5.38}$$

Therefore

$$\begin{aligned}K_2 &= \frac{i}{2} \Delta^{2\gamma-1}(x', X) \gamma^{\alpha}_{\nu'}(x', Z) \psi(Z) \\ &\quad \times \eta^{\mu'}_{\alpha}(x', Z) \gamma^{\beta}_{\mu'}(x', Q) \nabla_{\beta}^{(Q)} \left[C_1^{\mu}(Q) g^{\nu'}_{\mu}(x', Q) \right] \Big|_{Z=X}, \\ &= \frac{i}{2} \Delta^{2\gamma-1}(x', X) \gamma^{\alpha}_{\nu'}(x', X) \psi(X) \\ &\quad \times \eta^{\mu'}_{\alpha}(x', X) \gamma^{\beta}_{\mu'}(x', X) \nabla_{\beta}^{(X)} \left[C_1^{\mu}(X) g^{\nu'}_{\mu}(x', X) \right].\end{aligned}$$

Since γ is η^{-1} , we have

$$\eta^{\mu'}_{\alpha}(x', X) \gamma^{\beta}_{\mu'}(x', X) = \delta^{\beta}_{\alpha}\tag{5.39}$$

and

$$K_2 = \frac{i}{2} \Delta^{2\gamma-1}(x', X) \gamma^{\alpha}_{\nu'}(x', X) \psi(X) \nabla_{\alpha}^{(X)} \left[C_1^{\mu}(X) g^{\nu'}_{\mu}(x', X) \right].\tag{5.40}$$

Now let's try to see what K_1 and K_2 look like in the coincidence limit $x' \rightarrow X$.

Eq (5.35) has two terms with derivatives of Δ and $\gamma^{\alpha}_{\nu'}$ which will vanish in the

coincidence limit according to (5.21) and (5.15). The third term is

$$i\Delta^{\gamma-1}(x', X)C_1^\mu(X)g^{\nu'}{}_\mu(x', X)\Delta^\gamma(x', X)\gamma^\alpha{}_{\nu'}(x', X)\nabla_\alpha^{(X)}\psi(X). \quad (5.41)$$

The $x' \rightarrow X$ limit of the VanVleck-Morette determinant, the parallel transport and $\gamma^\alpha{}_{\nu'}$ are given in (5.20), (5.16) and (5.14), therefore

$$[K_1] = -i C_1^\mu(X)\nabla_\mu\psi(X). \quad (5.42)$$

Similarly, in equation (5.40), the term with $\nabla_\alpha g^{\nu'}{}_\mu$ should vanish because of (5.17) and

$$\frac{i}{2}\Delta^{2\gamma-1}(x', X)\gamma^\alpha{}_{\nu'}(x', X)\psi(X)g^{\nu'}{}_\mu(x', X)\nabla_\alpha^{(X)}C_1^\mu(X) \quad (5.43)$$

becomes

$$[K_2] = -\frac{i}{2}\psi(X)\nabla_\mu C_1^\mu(X). \quad (5.44)$$

Therefore

$$[\hat{C}\psi](X)\Big|_{x'\rightarrow X} = -i C_1^\mu(X)\nabla_\mu\psi(X) - \frac{i}{2}\psi(X)\nabla_\mu C_1^\mu(X). \quad (5.45)$$

The symbol (5.27) gives a differential operator of the first order. The Weyl symmetry is easily seen if one writes (5.45) in the following form:

$$-\frac{i}{2}\left(C_1^\mu\nabla_\mu\psi + \nabla_\mu(C_1^\mu\psi)\right) \quad (5.46)$$

or

$$\text{Op}\left(C_1^\mu(Q)P_\mu\right) = -\frac{i}{2}\left(C_1^\mu(\hat{Q})\hat{\nabla}_\mu + \hat{\nabla}_\mu C_1^\mu(\hat{Q})\right). \quad (5.47)$$

2. Second Order

The symbol is

$$c(x'; Q, \mathbf{P}) = C_2^{\mu\nu}(Q)P_\mu P_\nu. \quad (5.48)$$

The momenta $P_\mu \in T_Q^*$, and $C_2^{\mu\nu}(Q)$ is symmetric. Define

$$\mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) \equiv \frac{1}{2}(g^{\mu' \mu} g^{\nu' \nu} + g^{\mu' \nu} g^{\nu' \mu})(x', Q), \quad (5.49)$$

then

$$\begin{aligned} [\hat{C}\psi](X) &= \int_M dZ \sqrt{g(Z)} h^{-d} \Delta^\gamma(x', X) \Delta^\gamma(x', Z) \\ &\quad \times \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} \psi(Z) C_2^{\mu\nu}(Q) \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) \tilde{P}_{\mu'} \tilde{P}_{\nu'} e^{i\tilde{\mathbf{P}} \cdot \tilde{\mathbf{V}}}. \end{aligned} \quad (5.50)$$

With the help of (5.29),

$$\tilde{P}_{\mu'} \tilde{P}_{\nu'} e^{i\tilde{\mathbf{P}} \cdot \tilde{\mathbf{V}}} = -\gamma^\varphi_{\mu'}(x', Z) \nabla_\varphi^{(Z)} \{ \gamma^{\alpha \nu'}(x', Z) \nabla_\alpha^{(Z)} e^{i\tilde{\mathbf{P}} \cdot \tilde{\mathbf{V}}} \}; \quad (5.51)$$

plug (5.51) into (5.50) and integrate by parts to get

$$[\hat{C}\psi](X) = h^{-d} \int_M dZ \sqrt{g(Z)} \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} \gamma^{\alpha \nu'}(x', Z) \mathfrak{B}^{\nu'} \Delta^\gamma(x', X) \nabla_\alpha^{(Z)} e^{i\tilde{\mathbf{P}} \cdot \tilde{\mathbf{V}}} \quad (5.52)$$

where

$$\mathfrak{B}^{\nu'} = \nabla_\varphi^{(Z)} \left\{ \Delta^\gamma(x', Z) \psi(Z) C_2^{\mu\nu}(Q) \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) \gamma^\varphi_{\mu'}(x', Z) \right\}. \quad (5.53)$$

Integrate by parts again to obtain

$$[\hat{C}\psi](X) = -h^{-d} \int_M dZ \sqrt{g(Z)} \int_{T_{x'}^*} \frac{d^d \tilde{P}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{\mathbf{P}} \cdot \tilde{\mathbf{V}}} \Delta^\gamma(x', X) \nabla_\alpha^{(Z)} \left\{ \gamma^{\alpha \nu'}(x', Z) \mathfrak{B}^{\nu'} \right\} \quad (5.54)$$

and use the Dirac delta given in (5.32) to get

$$- \int_M dZ (g(Z)/g(X))^{1/4} \delta(X, Z) \Delta^{-1/2}(x', Z) \Delta^{\gamma-1/2}(x', X) \nabla_\alpha^{(Z)} \left\{ \gamma^{\alpha \nu'}(x', Z) \mathfrak{B}^{\nu'} \right\}; \quad (5.55)$$

therefore,

$$[\hat{C}\psi](X) = -\Delta^{\gamma-1}(x', X) \nabla_\alpha^{(Z)} \left\{ \gamma^{\alpha \nu'}(x', Z) \mathfrak{B}^{\nu'} \right\} \Big|_{Z=X}. \quad (5.56)$$

Using the Leibnitz rule,

$$[\hat{C}\psi](X) = -\Delta^{\gamma-1}(x', X) \left\{ \nabla_{\alpha}^{(X)} \gamma^{\alpha \nu'}(x', X) \mathfrak{B}^{\nu'} + \gamma^{\alpha \nu'}(x', X) \nabla_{\alpha}^{(Z)} \mathfrak{B}^{\nu'} \right\} \Big|_{Z=X}. \quad (5.57)$$

The first term in (5.57) will vanish in the coincidence limit due to (5.15). So we need to focus on the second term only, in particular:

$$\nabla_{\alpha}^{(Z)} \mathfrak{B}^{\nu'} = \nabla_{\alpha}^{(Z)} \nabla_{\varphi}^{(Z)} \left\{ \Delta^{\gamma}(x', Z) \psi(Z) C_2^{\mu\nu}(Q) \mathfrak{g}^{\mu' \nu'}_{\mu \nu}(x', Q) \gamma^{\varphi}_{\mu'}(x', Z) \right\}. \quad (5.58)$$

The derivatives in (5.58) are to be distributed over the factors in parantheses in a regular fashion. Let's group the resulting terms in four,

$$\nabla_{\alpha}^{(Z)} \mathfrak{B}^{\nu'} = \mathfrak{D}_1 + \mathfrak{D}_2 + \mathfrak{D}_3 + \mathfrak{D}_4 \quad (5.59)$$

and analyze these terms one by one. The first one is

$$\mathfrak{D}_1 = \nabla_{\alpha}^{(Z)} \nabla_{\varphi}^{(Z)} \left\{ \Delta^{\gamma}(x', Z) \psi(Z) \gamma^{\varphi}_{\mu'}(x', Z) \right\} \mathfrak{g}^{\mu' \nu'}_{\mu \nu}(x', Q) C_2^{\mu\nu}(Q). \quad (5.60)$$

The rule in this rather lengthy analysis is to ignore the terms which will vanish in the coincidence limit according to (5.15), (5.17) and (5.21). For instance in (5.60) these are the terms containing $\nabla_{\alpha} \gamma^{\mu \nu'}$ and $\nabla_{\alpha} \Delta^{\gamma}$. Then we are left with

$$\begin{aligned} \mathfrak{D}_1 = & \left\{ \nabla_{\alpha}^{(Z)} \nabla_{\varphi}^{(Z)} \Delta^{\gamma}(x', Z) \psi(Z) \gamma^{\varphi}_{\mu'}(x', Z) + \Delta^{\gamma}(x', Z) \nabla_{\alpha}^{(Z)} \nabla_{\varphi}^{(Z)} \psi(Z) \gamma^{\varphi}_{\mu'}(x', Z) \right. \\ & \left. + \psi(Z) \Delta^{\gamma}(x', Z) \nabla_{\alpha}^{(Z)} \nabla_{\varphi}^{(Z)} \gamma^{\varphi}_{\mu'}(x', Z) \right\} \mathfrak{g}^{\mu' \nu'}_{\mu \nu}(x', Q) C_2^{\mu\nu}(Q) \end{aligned} \quad (5.61)$$

Similarly,

$$\mathfrak{D}_2 = \nabla_{\varphi}^{(Z)} \left\{ \Delta^{\gamma}(x', Z) \psi(Z) \gamma^{\varphi}_{\mu'}(x', Z) \right\} \nabla_{\alpha}^{(Z)} \left\{ \mathfrak{g}^{\mu' \nu'}_{\mu \nu}(x', Q) C_2^{\mu\nu}(Q) \right\} \quad (5.62)$$

is reduced to

$$\mathfrak{D}_2 = \Delta^{\gamma}(x', Z) \nabla_{\varphi}^{(Z)} \psi(Z) \gamma^{\varphi}_{\mu'}(x', Z) \mathfrak{g}^{\mu' \nu'}_{\mu \nu}(x', Q) \nabla_{\alpha}^{(Z)} C_2^{\mu\nu}(Q). \quad (5.63)$$

Here we used the fact that $\nabla_\alpha^{(Z)} \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q)$ is zero in the coincidence limit. This is seen better if one writes $\nabla_\alpha^{(Z)}$ as $\frac{1}{2} \eta^{\alpha'}_\alpha(x', Z) \gamma^{\beta \alpha'}(x', Q) \nabla_\beta^{(Q)}$ as in (5.38) and uses (5.17) and the definition of $\mathbf{g}^{\mu' \nu'}_{\mu' \nu'}$ given in (5.53). The third term coming out of (5.58) is almost identical to \mathfrak{D}_2 except for the fact that α and φ derivatives are interchanged:

$$\mathfrak{D}_3 = \nabla_\alpha^{(Z)} \left\{ \Delta^\gamma(x', Z) \psi(Z) \gamma^\varphi_{\mu'}(x', Z) \right\} \nabla_\varphi^{(Z)} \left\{ \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) C_2^{\mu\nu}(Q) \right\} \quad (5.64)$$

and again it is enough to focus on

$$\mathfrak{D}_3 = \Delta^\gamma(x', Z) \nabla_\alpha^{(Z)} \psi(Z) \gamma^\varphi_{\mu'}(x', Z) \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) \nabla_\varphi^{(Z)} C_2^{\mu\nu}(Q) \quad (5.65)$$

only. Finally we have

$$\mathfrak{D}_4 = \Delta^\gamma(x', Z) \psi(Z) \gamma^\varphi_{\mu'}(x', Z) \nabla_\alpha^{(Z)} \nabla_\varphi^{(Z)} \left\{ \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) C_2^{\mu\nu}(Q) \right\} \quad (5.66)$$

which can be shortened to

$$\begin{aligned} \mathfrak{D}_4 = & \Delta^\gamma(x', Z) \psi(Z) \gamma^\varphi_{\mu'}(x', Z) \left\{ \nabla_\alpha^{(Z)} \nabla_\varphi^{(Z)} \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) C_2^{\mu\nu}(Q) \right. \\ & \left. + \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) \nabla_\alpha^{(Z)} \nabla_\varphi^{(Z)} C_2^{\mu\nu}(Q) \right\} \end{aligned} \quad (5.67)$$

since the first derivatives of the parallel transport are zero at the coincidence limit.

Now it is time to calculate the coincidence limit of (5.57). We are going to multiply each \mathfrak{D}_i by $-\Delta^{\gamma-1}(x', X) \gamma^{\alpha \nu'}(x', X)$, set $Z = X$ and see what happens when $x' \rightarrow X$. Let's introduce another variable for shorthand:

$$\mathfrak{M}_i \equiv -\Delta^{\gamma-1}(x', X) \gamma^{\alpha \nu'}(x', X) \mathfrak{D}_i \Big|_{Z=X}. \quad (5.68)$$

The interesting terms are the ones with the second derivatives of the parallel transport, $\gamma^{\alpha \nu'}$ and the VanVleck-Morette determinant. Manipulating the Kronecker deltas

that would arise in $[\mathfrak{M}_1]$ we get

$$[\mathfrak{M}_1] = -[\nabla_{(\mu}\nabla_{\nu)}\Delta^\gamma]\psi C_2^{\mu\nu} - \nabla_{(\mu}\nabla_{\nu)}\psi C_2^{\mu\nu} + \psi C_2^{\mu\nu}[\nabla_{(\mu}\nabla_{|\varphi|}\gamma^\varphi{}_{\nu')}]. \quad (5.69)$$

Here is where we meet the Riemann curvature tensor. The $R_{\mu\nu}$ arises in the first term of (5.69) according to (5.22) and the coefficient will depend on the parameter γ . (See Appendix A). In order to find an expression for $\frac{1}{2}\mathfrak{L}_{\mu\nu} \equiv [\nabla_{(\mu}\nabla_{|\varphi|}\gamma^\varphi{}_{\nu')}]$ in the third term of (5.69) we should evaluate $[\nabla_{(\mu}\nabla_{\theta)}\gamma^\varphi{}_{\nu'}]$ first. The matrix $\gamma^\varphi{}_{\nu'}$ satisfies the second order linear differential equation [43]

$$\mathcal{D}^2\gamma + \mathcal{D}\gamma + \mathcal{K} \cdot \gamma = 0 \quad (5.70)$$

where $\mathcal{D} \equiv \sigma^\mu\nabla_\mu$ and $\mathcal{K}^\varphi{}_\nu \equiv R^\varphi{}_{\alpha\nu\beta}\sigma^\alpha\sigma^\beta$. If we differentiate (5.70) twice,

$$\nabla_\theta\nabla_\mu\left\{\sigma^\lambda\nabla_\lambda(\sigma^\nu\nabla_\nu\gamma^\varphi{}_{\nu'}) + \sigma^\lambda\nabla_\lambda\gamma^\varphi{}_{\nu'} + R^\varphi{}_{\alpha\nu\beta}\sigma^\alpha\sigma^\beta\gamma^\nu{}_{\nu'}\right\} = 0 \quad (5.71)$$

and take the coincidence limit while keeping (5.18) and (5.19) in mind, we get

$$3[\nabla_{(\theta}\nabla_{\mu)}\gamma^\varphi{}_{\nu'}] = R^\varphi{}_{(\theta|\nu|\mu)}. \quad (5.72)$$

Now rewrite $\mathfrak{L}_{\mu\nu}$ as

$$\mathfrak{L}_{\mu\nu} = 2\left\{[\nabla_{(\mu}\nabla_{\varphi)}\gamma^\varphi{}_{\nu'}] + [\nabla_{(\nu}\nabla_{\varphi)}\gamma^\varphi{}_{\mu'}] - [\nabla_\varphi\nabla_{(\mu}\gamma^\varphi{}_{\nu')}] \right\}, \quad (5.73)$$

and use the fact that

$$\nabla_\varphi\nabla_\mu\gamma^\varphi{}_{\nu'} = \nabla_\mu\nabla_\varphi\gamma^\varphi{}_{\nu'} - R^\varphi{}_{\beta\mu\varphi}\gamma^\beta{}_{\nu'} \quad (5.74)$$

in the third term of (5.73). Take the coincidence limits according to (5.72) and (5.14) to get

$$\mathfrak{L}_{\mu\nu} = 2\left\{\frac{1}{3}R^\varphi{}_{(\mu|\nu|\varphi)} + \frac{1}{3}R^\varphi{}_{(\nu|\mu|\varphi)} - [\nabla_{(\mu}\nabla_{|\varphi|}\gamma^\varphi{}_{\nu')}] + R_{\mu\nu}\right\} \quad (5.75)$$

or

$$\mathfrak{L}_{\mu\nu} = \frac{2}{3}R_{\mu\nu}, \quad (5.76)$$

where we used the following symmetry property of the Riemann curvature tensor

$$R^\varphi_{\theta\nu\mu} = -R^\varphi_{\theta\mu\nu} \quad (5.77)$$

and the Ricci tensor $R_{\mu\nu} \equiv R^\varphi_{\mu\varphi\nu}$

$$R_{\mu\nu} = R_{\nu\mu}. \quad (5.78)$$

Thus the final term of (5.69) is also found to contain a curvature factor along with the first term, and the coefficient is 1/3. Now with this good luck and (5.22), we can rewrite (5.69) as

$$[\mathfrak{M}_1] = \left\{ \begin{array}{l} -\frac{1}{6} + \frac{1}{3} = \frac{1}{6} \quad , \quad \gamma = \frac{1}{2} \\ 0 + \frac{1}{3} = \frac{1}{3} \quad , \quad \gamma = 0 \\ -\frac{1}{3} + \frac{1}{3} = 0 \quad , \quad \gamma = 1 \end{array} \right\} \psi R_{\mu\nu} C_2^{\mu\nu} - C_2^{\mu\nu} \nabla_{(\mu} \nabla_{\nu)} \psi. \quad (5.79)$$

So the $\gamma = 1$ choice gets rid of the curvature term. The remaining terms are relatively easier to find. In a few steps one can show that

$$[\mathfrak{M}_2] = [\mathfrak{M}_3] = -\frac{1}{2} \nabla_{(\mu} \psi \nabla_{\nu)} C_2^{\mu\nu}. \quad (5.80)$$

The 1/2 pops up as a chain rule factor as in (5.38). In the fourth term, *i.e.*, $[\mathfrak{M}_4]$, one needs two of them so the coefficient is 1/4: $\nabla_\alpha^{(Z)} \nabla_\varphi^{(Z)} \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q)$ which is equal to

$$\frac{1}{2} \eta^{\kappa'}_{\alpha'}(x', Z) \gamma^{\psi}_{\kappa'}(x', Q) \nabla_\psi^{(Q)} \left\{ \frac{1}{2} \eta^{\beta'}_{\varphi'}(x', Z) \gamma^{\theta}_{\beta'}(x', Q) \nabla_\psi^{(Q)} \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', Q) \right\} \quad (5.81)$$

gives $\frac{1}{4} \nabla_\alpha^{(X)} \nabla_\varphi^{(X)} \mathbf{g}^{\mu' \nu'}_{\mu' \nu'}(x', X)$ when $Z \rightarrow X$. The $\nabla\gamma$ can be omitted since it will vanish in the coincidence limit. The final step in this analysis is to show that the

$[\nabla_\alpha \nabla_\varphi \mathbf{g}^{\mu' \nu'}_\mu]_{\nu'}$ term in (5.67) will have zero contribution to $[\mathfrak{M}_4]$. According to (5.68) and (5.49) this term is the [...] of

$$-\frac{1}{8} \Delta^{2\gamma-1} \psi C_2^{\mu\nu} \gamma^\alpha_{\nu'} \gamma^\varphi_{\mu'} \nabla_\alpha \nabla_\varphi (g^{\mu'}_\mu g^{\nu'}_\nu + g^{\mu'}_\nu g^{\nu'}_\mu). \quad (5.82)$$

It can easily be shown that (5.82) is proportional to

$$\psi C_2^{\nu\alpha} \delta^\varphi_{\mu'} [(\nabla_\alpha \nabla_\varphi + \nabla_\varphi \nabla_\alpha) g^{\mu'}_\nu]. \quad (5.83)$$

The coincidence limits of the symmetrized derivatives of $g^{\mu'}_\nu$ are zero (see Appendix A). However, the second term of (5.67) does have a non-zero contribution:

$$\mathfrak{M}_4 = -\frac{1}{4} \psi \nabla_{(\mu} \nabla_{\nu)} C_2^{\mu\nu} \quad (5.84)$$

Let us put together all the terms in (5.69), (5.80), and (5.84) and choose $\gamma = 1$:

$$\begin{aligned} [\hat{C}\psi](X) \Big|_{x' \rightarrow X} &= \mathfrak{M}_1 + \mathfrak{M}_2 + \mathfrak{M}_3 + \mathfrak{M}_4 \\ &= -C_2^{\mu\nu} \nabla_{(\mu} \nabla_{\nu)} \psi - \nabla_{(\mu} \psi \nabla_{\nu)} C_2^{\mu\nu} - \frac{1}{4} \psi \nabla_{(\mu} \nabla_{\nu)} C_2^{\mu\nu} \end{aligned} \quad (5.85)$$

One can again write this in the operator form, where the symmetry of the momentum and position operators is easy to see:

$$\text{Op}\left(C_2^{\mu\nu}(Q) P_\mu P_\nu\right) = -\frac{1}{4} \hat{\nabla}_\mu \hat{\nabla}_\nu C_2^{\mu\nu}(\hat{\mathbf{Q}}) - \frac{1}{4} C_2^{\mu\nu}(\hat{\mathbf{Q}}) \hat{\nabla}_\mu \hat{\nabla}_\nu - \frac{1}{2} \hat{\nabla}_\mu C_2^{\mu\nu}(\hat{\mathbf{Q}}) \hat{\nabla}_\nu. \quad (5.86)$$

We may even include the curvature term we found in (5.79) with a γ -dependent coefficient.

$$\begin{aligned} \text{Op}\left(C_2^{\mu\nu}(Q) P_\mu P_\nu\right) &= -\frac{1}{4} \hat{\nabla}_\mu \hat{\nabla}_\nu C_2^{\mu\nu}(\hat{\mathbf{Q}}) - \frac{1}{4} C_2^{\mu\nu}(\hat{\mathbf{Q}}) \hat{\nabla}_\mu \hat{\nabla}_\nu \\ &\quad - \frac{1}{2} \hat{\nabla}_\mu C_2^{\mu\nu}(\hat{\mathbf{Q}}) \hat{\nabla}_\nu - \frac{\gamma-1}{3} R_{\mu\nu}(\hat{\mathbf{Q}}) C_2^{\mu\nu}(\hat{\mathbf{Q}}). \end{aligned} \quad (5.87)$$

The reader may refer back to (3.30) for comparison with the classical case.

CHAPTER VI

PRODUCT RULE

A. Derivation of the Product Rule

Let the operator \hat{C} be equal to a product of two operators \hat{A} and \hat{B} :

$$\hat{C} = \hat{A}\hat{B} \quad (6.1)$$

where

$$[\hat{A}\psi](x) = \int_M dy \sqrt{g(y)} \mathcal{A}(x, y) \psi(y) \quad (6.2)$$

and

$$[\hat{B}\psi](y) = \int_M dz \sqrt{g(z)} \mathcal{B}(y, z) \psi(z). \quad (6.3)$$

Then the kernel $\mathcal{C}(x, z)$ can be written as

$$\mathcal{C}(x, z) = \int_M dy \sqrt{g(y)} \mathcal{A}(x, y) \mathcal{B}(y, z). \quad (6.4)$$

Here we note that the kernels \mathcal{A} and \mathcal{B} are also written in terms of the symbols of the operators \hat{A} and \hat{B} , respectively, in the following way:

$$\mathcal{A}(x, y) = \Delta^\gamma(x', x) \Delta^\gamma(x', y) h^{-d} \int_{T_{x'}^*} \frac{d^d \tilde{k}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{k}_{\mu'} w^{\mu'}} a(x'; r, \bar{\mathbf{k}}) \quad (6.5)$$

where

$$w^{\mu'} \equiv \hat{\sigma}^{\mu'}(x', x) - \hat{\sigma}^{\mu'}(x', y), \quad (6.6)$$

$$r \equiv \exp_{x'} \frac{1}{2} [\hat{\sigma}^{\mu'}(x', x) + \hat{\sigma}^{\mu'}(x', y)], \quad (6.7)$$

$$\tilde{k}_{\mu'} = g_{\mu'\nu}(x', r) \bar{k}_\nu, \quad (6.8)$$

and

$$\mathcal{B}(y, z) = \Delta^\gamma(x', y)\Delta^\gamma(x', z)h^{-d} \int_{T_{x'}^*} \frac{d^d \tilde{l}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{l}_{\mu'} u^{\mu'}} b(x'; s, \bar{\mathbf{I}}) \quad (6.9)$$

where

$$u^{\mu'} \equiv \hat{\sigma}^{\mu'}(x', y) - \hat{\sigma}^{\mu'}(x', z), \quad (6.10)$$

$$s \equiv \exp_{x'} \frac{1}{2} [\hat{\sigma}^{\mu'}(x', y) + \hat{\sigma}^{\mu'}(x', z)], \quad (6.11)$$

$$\tilde{l}_{\mu'} = g_{\mu'\nu}(x', s) \bar{l}_{\nu}. \quad (6.12)$$

1. Integral Formula

Our goal is to find a formula for c , the symbol of \hat{C} , in terms of a and b . Plugging (6.5) and (6.9) into (6.4),

$$\begin{aligned} \mathcal{C}(x, z) &= \int_M dy \sqrt{g(y)} \Delta^\gamma(x', x) \Delta^\gamma(x', y) h^{-d} \int_{T_{x'}^*} \frac{d^d \tilde{k}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{k}_{\mu'} w^{\mu'}} a(x'; r, \bar{\mathbf{k}}) \\ &\quad \times \Delta^\gamma(x', y) \Delta^\gamma(x', z) h^{-d} \int_{T_{x'}^*} \frac{d^d \tilde{l}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{l}_{\mu'} u^{\mu'}} b(x'; s, \bar{\mathbf{I}}) \end{aligned}$$

and converting the integration over the manifold to an integral over the tangent space at x' by

$$\int_M dy \sqrt{g(y)} \dots = \int_{T_{x'}} d^d \hat{\sigma}^{\mu'}(x', y) \sqrt{g(x')} \Delta^{-1}(x', y) \dots \quad (6.13)$$

one gets

$$\begin{aligned} \mathcal{C}(x, z) &= \int_{T_{x'}} d^d \hat{\sigma}^{\mu'}(x', y) \sqrt{g(x')} \Delta^{2\gamma-1}(x', y) \Delta^\gamma(x', x) \Delta^\gamma(x', z) h^{-2d} \\ &\quad \int_{T_{x'}^*} \frac{d^d \tilde{k}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{k}_{\mu'} w^{\mu'}} a(x'; r, \bar{\mathbf{k}}) \int_{T_{x'}^*} \frac{d^d \tilde{l}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{l}_{\mu'} u^{\mu'}} b(x'; s, \bar{\mathbf{I}}). \end{aligned} \quad (6.14)$$

Plug (6.14) into (5.6) to get:

$$\begin{aligned} c(x'; q, \mathbf{p}) &= h^{-2d} \int_{T_{x'}} d^d \xi^{\mu'} \sqrt{g(x')} \int_{T_{x'}^*} \frac{d^d \tilde{k}_{\mu'}}{\sqrt{g(x')}} \int_{T_{x'}} d^d \hat{\sigma}(x', y) \sqrt{g(x')} \int_{T_{x'}^*} \frac{d^d \tilde{l}_{\mu'}}{\sqrt{g(x')}} \\ &\quad \times \Delta^{2\gamma-1}(x', y) e^{i(\bar{\mathbf{k}} \cdot \bar{w} + \bar{\mathbf{I}} \cdot \bar{u} - \bar{\mathbf{p}} \cdot \bar{\xi})} a(x'; r, \bar{\mathbf{k}}) b(x'; s, \bar{\mathbf{I}}). \end{aligned} \quad (6.15)$$

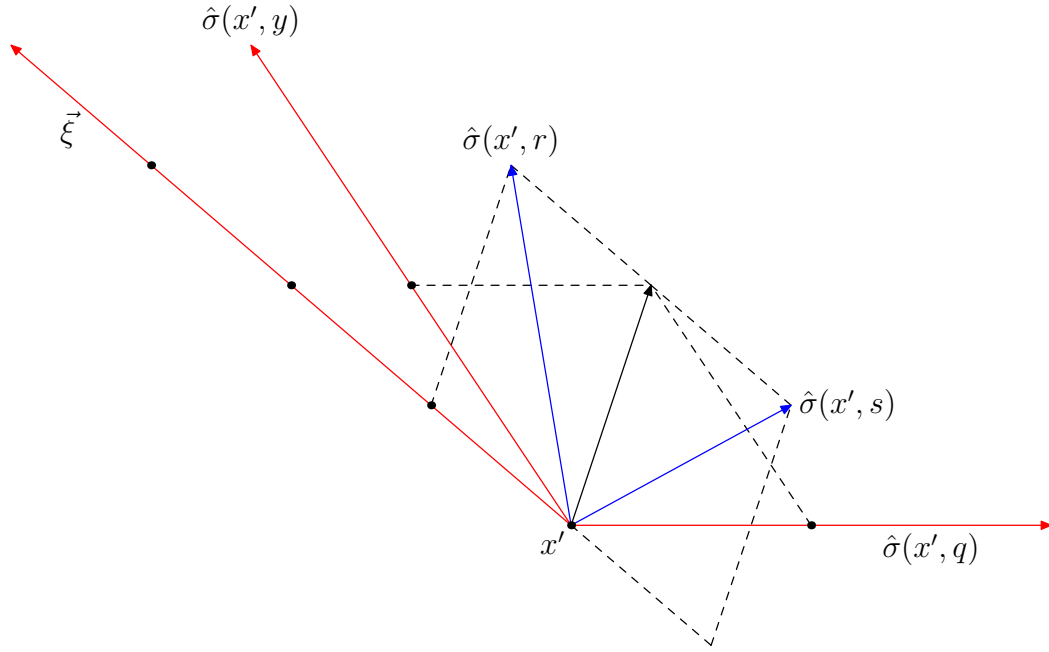


Fig. 6. The vectors $\hat{\sigma}(x', r)$ and $\hat{\sigma}(x', s)$ in (6.15).

In (6.15), r and s should be thought of as points determined by $\vec{\xi}$, $\hat{\sigma}(x', y)$ and $\hat{\sigma}(x', q)$ (see Fig. 6). If one writes (5.7) and (5.8) as

$$\hat{\sigma}^{\mu'}(x', x) = \hat{\sigma}^{\mu'}(x', q) + \frac{1}{2}\xi^{\mu'}, \quad (6.16)$$

$$\hat{\sigma}^{\mu'}(x', z) = \hat{\sigma}^{\mu'}(x', q) - \frac{1}{2}\xi^{\mu'}, \quad (6.17)$$

and uses the definitions (6.7) and (6.11), then

$$\hat{\sigma}^{\mu'}(x', r) = \frac{1}{2}[\hat{\sigma}^{\mu'}(x', q) + \hat{\sigma}^{\mu'}(x', y)] + \frac{1}{4}\xi^{\mu'}, \quad (6.18)$$

$$\hat{\sigma}^{\mu'}(x', s) = \frac{1}{2}[\hat{\sigma}^{\mu'}(x', q) + \hat{\sigma}^{\mu'}(x', y)] - \frac{1}{4}\xi^{\mu'}. \quad (6.19)$$

Now if we solve (6.16) and (6.17) for $\xi^{\mu'}$:

$$\xi^{\mu'} = \hat{\sigma}^{\mu'}(x', x) - \hat{\sigma}^{\mu'}(x', z). \quad (6.20)$$

Using (6.6) and (6.10) one sees that this is equal to

$$\xi^{\mu'} = w^{\mu'} + u^{\mu'}. \quad (6.21)$$

From (6.6) and (6.10)

$$w^{\mu'} - u^{\mu'} = \hat{\sigma}^{\mu'}(x', x) - 2\hat{\sigma}^{\mu'}(x', y) + \hat{\sigma}^{\mu'}(x', z) \quad (6.22)$$

and plugging in the expressions for $\hat{\sigma}^{\mu'}(x', x)$ and $\hat{\sigma}^{\mu'}(x', z)$ from (6.16) and (6.17), yields

$$w^{\mu'} - u^{\mu'} = 2\hat{\sigma}^{\mu'}(x', q) - 2\hat{\sigma}^{\mu'}(x', y). \quad (6.23)$$

Solve this for $\hat{\sigma}^{\mu'}(x', y)$:

$$\hat{\sigma}^{\mu'}(x', y) = \hat{\sigma}^{\mu'}(x', q) - \frac{1}{2}(w^{\mu'} - u^{\mu'}). \quad (6.24)$$

Using (6.21) and (6.24) one can switch from integrals over $\vec{\xi}$ and $\hat{\sigma}(x', y)$ to integrals over \vec{w} and \vec{u} with

$$d\vec{\xi}d\hat{\sigma}(x', y) = \left| \frac{\partial(\vec{\xi}, \hat{\sigma}(x', y))}{\partial(\vec{w}, \vec{u})} \right| d\vec{w} d\vec{u} \quad (6.25)$$

The Jacobian of this transformation is 1 and using (6.21) in the exponent, (6.15) can now be written as

$$\begin{aligned} c(x'; q, \mathbf{p}) &= h^{-2d} \int_{T_{x'}} d\vec{w} \sqrt{g(x')} \int_{T_{x'}^*} \frac{d\tilde{\mathbf{k}}}{\sqrt{g(x')}} \int_{T_{x'}} d\vec{u} \sqrt{g(x')} \int_{T_{x'}^*} \frac{d\tilde{\mathbf{l}}}{\sqrt{g(x')}} \\ &\times \Delta^{2\gamma-1}(x', y) e^{i(\tilde{\mathbf{k}}-\tilde{\mathbf{p}})\cdot\vec{w}} e^{i(\tilde{\mathbf{l}}-\tilde{\mathbf{p}})\cdot\vec{u}} a(x'; r, \tilde{\mathbf{k}}) b(x'; s, \tilde{\mathbf{l}}). \end{aligned} \quad (6.26)$$

(6.26) is an integral formula for $c(x'; q, \mathbf{p})$ in terms of the symbols $a(x'; r, \tilde{\mathbf{k}})$ and $b(x'; s, \tilde{\mathbf{l}})$. Note that y , r , and s are points defined in terms of \vec{w} , $\tilde{\mathbf{k}}$, $\tilde{\mathbf{l}}$ and \vec{u} as follows (see Fig. 7): we begin by rewriting (6.24) as

$$y = \exp_{x'}[\hat{\sigma}^{\mu'}(x', q) - \frac{1}{2}(w^{\mu'} - u^{\mu'})]. \quad (6.27)$$

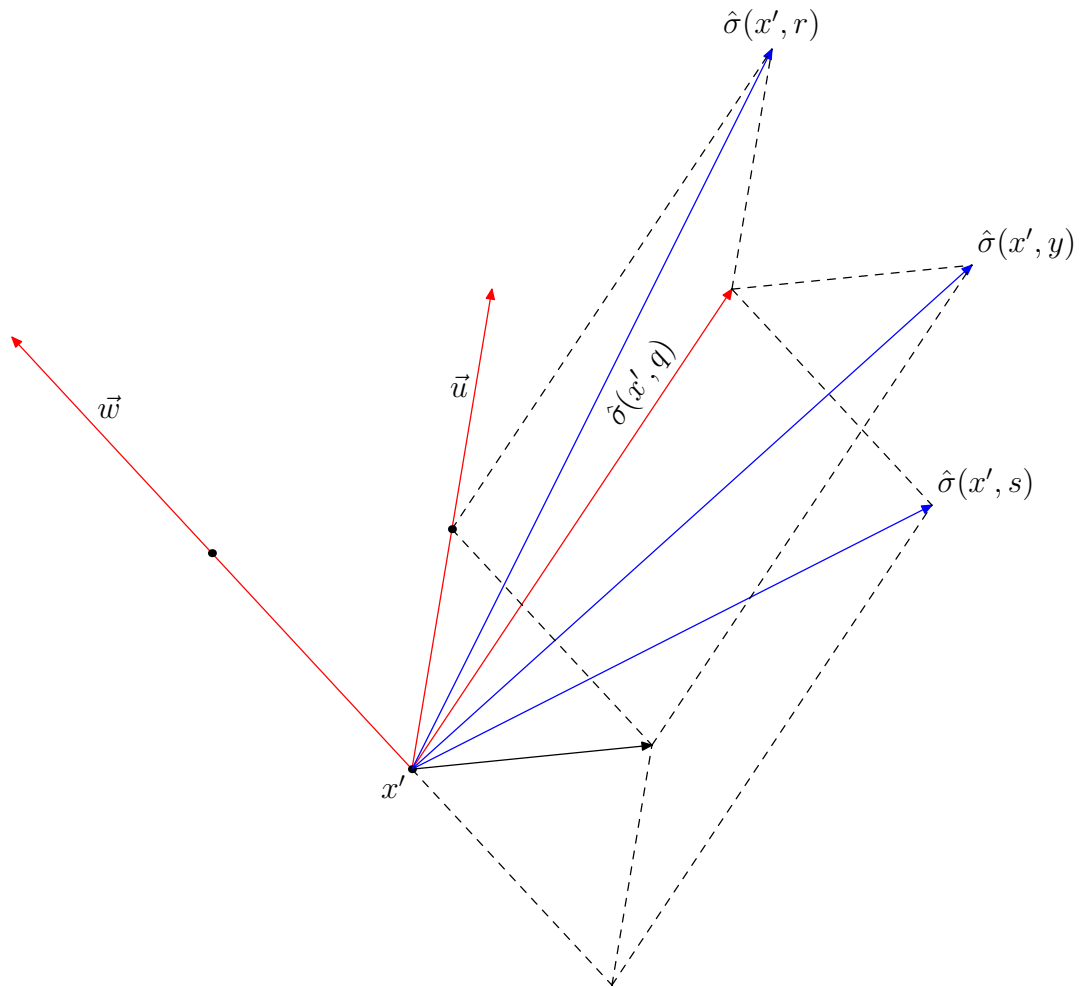


Fig. 7. The vectors $\hat{\sigma}(x', r)$, $\hat{\sigma}(x', y)$ and $\hat{\sigma}(x', s)$ in (6.26).

Using (6.21) for $\vec{\xi}$, write (6.16) as

$$\hat{\sigma}^{\mu'}(x', x) = \hat{\sigma}^{\mu'}(x', q) + \frac{1}{2}(w^{\mu'} + u^{\mu'}) \quad (6.28)$$

and plug (6.28) and (6.24) into (6.7) to get

$$r = \exp_{x'}[\hat{\sigma}^{\mu'}(x', q) + \frac{1}{2}u^{\mu'}]. \quad (6.29)$$

Similarly, (6.17) and (6.11) give

$$s = \exp_{x'}[\hat{\sigma}^{\mu'}(x', q) - \frac{1}{2}w^{\mu'}]. \quad (6.30)$$

Finally, we also note that the momenta $\mathbf{p} \in T_q^*$, $\bar{\mathbf{k}} \in T_r^*$, and $\bar{\mathbf{l}} \in T_s^*$ are related to $\tilde{\mathbf{p}}, \tilde{\mathbf{k}}, \tilde{\mathbf{l}} \in T_{x'}$ by parallel transport as in (5.9), (6.8), and (6.12).

2. Expansions and the Asymptotic Formula

Let $\mathbf{k} \in T_r^*$ be the momentum covector $\tilde{\mathbf{p}} \in T_{x'}^*$ parallel transported to the cotangent vector space at r :

$$k_\nu = g^{\mu'}{}_\nu(x', r)\tilde{p}_{\mu'} \quad (6.31)$$

We expand the symbol $a(x'; r, \bar{\mathbf{k}})$ into a Taylor series about $\mathbf{k} \in T_r^*$,

$$a(x'; r, \bar{\mathbf{k}}) = \sum_{\alpha} \frac{1}{\alpha!} \partial_{\mathbf{k}}^{\alpha} a(x'; r, \mathbf{k})(\bar{\mathbf{k}} - \mathbf{k})^{\alpha}. \quad (6.32)$$

Here $\alpha \equiv (\alpha_1, \alpha_2, \dots, \alpha_d)$ is a multi-index and $\mathbf{k}^{\alpha} = k_1^{\alpha_1} k_2^{\alpha_2} \dots k_d^{\alpha_d}$. The factorial is $\alpha! \equiv \alpha_1! \dots \alpha_d!$ and the derivative operator in (6.32) is given as

$$\partial_{\mathbf{k}}^{\alpha} = \frac{\partial^{|\alpha|}}{\partial k_1^{\alpha_1} \dots \partial k_d^{\alpha_d}}, \quad |\alpha| \equiv \alpha_1 + \dots + \alpha_d. \quad (6.33)$$

The formula corresponding to (6.31) in multi-index notation can be found from

$$\prod_{i=1}^d k_i^{\alpha_i} = \prod_{i=1}^d [g^{1'}_i \tilde{p}_{1'} + g^{2'}_i \tilde{p}_{2'} + \cdots + g^{d'}_i \tilde{p}_{d'}]^{\alpha_i} \quad (6.34)$$

or

$$\mathbf{k}^\alpha = \sum_{\beta'} G_{\beta'}^\alpha(x', r) \tilde{\mathbf{p}}^{\beta'} \quad (6.35)$$

where $|\alpha| = |\beta'|$. The factor $G_{\beta'}^\alpha$ is a product of parallel transport matrices.

Example: Let $\alpha = (0, 1, 2)$ and $\beta' = (1', 2', 0')$ so that

$$\mathbf{k}^{(0,1,2)} = k_2 k_3^2 = \cdots + G_{(1',2',0')}^{(0,1,2)} \tilde{p}_{1'} \tilde{p}_{2'}^2 + \cdots, \quad (6.36)$$

then

$$\begin{aligned} G_{(1',2',0')}^{(0,1,2)} &= g^{1'}_2 g^{2'}_3 g^{2'}_3 + \text{cyclic permutations of } 1', 2', 2' \\ &= g^{1'}_2 g^{2'}_3 g^{2'}_3 + 2g^{2'}_2 g^{1'}_3 g^{2'}_3. \end{aligned} \quad (6.37)$$

The non-primed multi-index $(0, 1, 2)$ tells us how to arrange the lower indices in the ‘ g ’ bundle on the right hand side: one 2, two 3’s and no 0’s. The number of g ’s multiplied is already determined to be $|\alpha| = 3$. Once the lower indices are fixed, we can add the distinct cyclic permutations of the primed indices to the product (note that this is not always needed, for example in the case of $\beta' = (3', 0', 0')$:

$$G_{(3',0',0')}^{(0,1,2)} = g^{1'}_2 g^{1'}_3 g^{1'}_3$$

since there are not any such permutations). Using (6.35) and (6.8), the expansion (6.32) can be rewritten as

$$a(x'; r, \bar{\mathbf{k}}) = \sum_{\alpha} \sum_{\beta'} \frac{1}{\alpha!} \partial_{\bar{\mathbf{k}}}^\alpha a(x'; r, \mathbf{k}) G_{\beta'}^\alpha(x', r) (\tilde{\mathbf{k}} - \tilde{\mathbf{p}})^{\beta'}. \quad (6.38)$$

A similar Taylor expansion for $b(x'; s, \bar{\mathbf{l}})$ about $l_\nu = g^{\mu'}{}_\nu(x', s)\tilde{p}_{\mu'}$ is as follows:

$$\begin{aligned} b(x'; s, \bar{\mathbf{l}}) &= \sum_{\theta} \frac{1}{\theta!} \partial_{\mathbf{l}}^{\theta} b(x'; s, \mathbf{l}) (\bar{\mathbf{l}} - \mathbf{l})^{\theta} \\ &= \sum_{\theta} \sum_{\delta'} \frac{1}{\theta!} \partial_{\mathbf{l}}^{\theta} b(x'; s, \mathbf{l}) G_{\delta'}{}^{\theta}(x', s) (\bar{\mathbf{l}} - \tilde{\mathbf{p}})^{\delta'}. \end{aligned} \quad (6.39)$$

As in the previous case, $G_{\delta'}{}^{\theta}(x', s)$ can be found by (6.12). Let us now plug (6.38) and (6.39) into (6.26) and rearrange the factors in the integrand,

$$\begin{aligned} c(x'; q, \mathbf{p}) &= h^{-2d} \sum_{\alpha, \theta, \beta', \delta'} \frac{1}{\alpha! \gamma!} \int \int \int \int d\tilde{w} d\tilde{u} d\tilde{\mathbf{k}} d\tilde{\mathbf{l}} \Delta^{2\gamma-1}(x', y) \\ &\quad \times \partial_{\mathbf{k}}^{\alpha} a(x'; r, \mathbf{k}) G_{\beta'}{}^{\alpha}(x', r) \partial_{\mathbf{l}}^{\theta} b(x'; s, \mathbf{l}) G_{\delta'}{}^{\theta}(x', s) \\ &\quad \times (\tilde{\mathbf{k}} - \tilde{\mathbf{p}})^{\beta'} e^{i(\tilde{\mathbf{k}} - \tilde{\mathbf{p}}) \cdot \tilde{w}} (\tilde{\mathbf{l}} - \tilde{\mathbf{p}})^{\delta'} e^{i(\tilde{\mathbf{l}} - \tilde{\mathbf{p}}) \cdot \tilde{u}}. \end{aligned} \quad (6.40)$$

For brevity, we suppressed the notation here:

$$d\tilde{w} d\tilde{u} d\tilde{\mathbf{k}} d\tilde{\mathbf{l}} = d\tilde{w} \sqrt{g(x')} d\tilde{u} \sqrt{g(x')} \frac{d\tilde{\mathbf{k}}}{\sqrt{g(x')}} \frac{d\tilde{\mathbf{l}}}{\sqrt{g(x')}}. \quad (6.41)$$

The next step will be integration by parts after modifying the ingredients of the last line a little bit:

$$(\tilde{\mathbf{k}} - \tilde{\mathbf{p}})^{\beta'} e^{i(\tilde{\mathbf{k}} - \tilde{\mathbf{p}}) \cdot \tilde{w}} = (-i\partial_{\tilde{w}})^{\beta'} e^{i(\tilde{\mathbf{k}} - \tilde{\mathbf{p}}) \cdot \tilde{w}} \quad (6.42)$$

$$(\tilde{\mathbf{l}} - \tilde{\mathbf{p}})^{\delta'} e^{i(\tilde{\mathbf{l}} - \tilde{\mathbf{p}}) \cdot \tilde{u}} = (-i\partial_{\tilde{u}})^{\delta'} e^{i(\tilde{\mathbf{l}} - \tilde{\mathbf{p}}) \cdot \tilde{u}}. \quad (6.43)$$

Then we have

$$\begin{aligned} c(x'; q, \mathbf{p}) &= h^{-2d} \sum_{\alpha, \theta, \beta', \delta'} \frac{1}{\alpha! \theta!} \int \int \int \int d\tilde{w} d\tilde{u} d\tilde{\mathbf{k}} d\tilde{\mathbf{l}} \Delta^{2\gamma-1}(x', y) \\ &\quad \times \partial_{\mathbf{k}}^{\alpha} a(x'; r, \mathbf{k}) G_{\beta'}{}^{\alpha}(x', r) \partial_{\mathbf{l}}^{\theta} b(x'; s, \mathbf{l}) G_{\delta'}{}^{\theta}(x', s) \\ &\quad \times (-i\partial_{\tilde{w}})^{\beta'} e^{i(\tilde{\mathbf{k}} - \tilde{\mathbf{p}}) \cdot \tilde{w}} (-i\partial_{\tilde{u}})^{\delta'} e^{i(\tilde{\mathbf{l}} - \tilde{\mathbf{p}}) \cdot \tilde{u}}, \end{aligned} \quad (6.44)$$

and

$$\begin{aligned}
c(x'; q, \mathbf{p}) &= h^{-2d} \sum_{\alpha, \theta, \beta', \delta'} \frac{i^{|\beta'|+|\delta'|}}{\alpha! \theta!} \int \int \int \int d\vec{w} d\vec{u} d\tilde{\mathbf{k}} d\tilde{\mathbf{l}} \\
&\quad \times e^{i(\tilde{\mathbf{k}}-\tilde{\mathbf{p}})\cdot\vec{w}} e^{i(\tilde{\mathbf{l}}-\tilde{\mathbf{p}})\cdot\vec{u}} \partial_{\vec{w}}^{\beta'} \partial_{\vec{u}}^{\delta'} \left[\Delta^{2\gamma-1}(x', y) \right. \\
&\quad \left. \times \partial_{\mathbf{k}}^\alpha a(x'; r, \mathbf{k}) G_{\beta'}^\alpha(x', r) \partial_1^\theta b(x'; s, \mathbf{l}) G_{\delta'}^\theta(x', s) \right]. \quad (6.45)
\end{aligned}$$

The Dirac delta can be written as the scalar

$$\delta(\vec{w}) = h^{-d} \int_{T_{x'}} \frac{d^d \tilde{\mathbf{k}}_{\mu'}}{\sqrt{g(x')}} e^{i\tilde{\mathbf{k}}\cdot\vec{w}}, \quad (6.46)$$

therefore,

$$\begin{aligned}
c(x'; q, \mathbf{p}) &= \sum_{\alpha, \theta, \beta', \delta'} \frac{i^{|\beta'|+|\delta'|}}{\alpha! \theta!} \int_{T_{x'}} d^d w^{\mu'} \sqrt{g(x')} \int_{T_{x'}} d^d u^{\mu'} \sqrt{g(x')} \delta(\vec{w}) \delta(\vec{u}) e^{-i\tilde{\mathbf{p}}\cdot(\vec{u}+\vec{w})} \\
&\quad \times \partial_{\vec{w}}^{\beta'} \partial_{\vec{u}}^{\delta'} \left[\Delta^{2\gamma-1}(x', y) \partial_{\mathbf{k}}^\alpha a(x'; r, \mathbf{k}) G_{\beta'}^\alpha(x', r) \partial_1^\theta b(x'; s, \mathbf{l}) G_{\delta'}^\theta(x', s) \right].
\end{aligned}$$

Carrying out the \vec{u} and \vec{w} integrals, we have

$$\begin{aligned}
c(x'; q, \mathbf{p}) &= \sum_{\alpha, \theta, \beta', \delta'} \frac{i^{|\beta'|+|\delta'|}}{\alpha! \theta!} \partial_{\vec{w}}^{\beta'} \partial_{\vec{u}}^{\delta'} \left[\Delta^{2\gamma-1}(x', y) \partial_{\mathbf{k}}^\alpha a(x'; r, \mathbf{k}) G_{\beta'}^\alpha(x', r) \right. \\
&\quad \left. \times \partial_1^\theta b(x'; s, \mathbf{l}) G_{\delta'}^\theta(x', s) \right]_{\vec{w}=0, \vec{u}=0}. \quad (6.47)
\end{aligned}$$

Now we need to apply the Leibniz rule for the derivative of a product for the multi-index case. The formula looks like

$$\partial^\alpha (FG) = \sum_{|\beta| \leq |\alpha|} \frac{\alpha!}{\beta! (\alpha - \beta)!} \partial^\beta F \partial^{\alpha - \beta} G \quad (6.48)$$

but we are going to use a slightly modified version of it by transforming $\alpha \rightarrow \alpha + \beta$ and then renaming α as β (and vice versa):

$$\sum_{\alpha} A_{\alpha} \partial^\alpha (FG) = \sum_{\alpha, \beta} \frac{(\alpha + \beta)!}{\alpha! \beta!} A_{\alpha + \beta} \partial^\alpha F \partial^\beta G. \quad (6.49)$$

From the definitions of y and r ((6.27) and (6.29)), we know that the \vec{u} derivative will be distributed over functions of y and r only, in (6.47):

$$c(x'; q, \mathbf{p}) = \sum_{\alpha, \theta, \beta', \delta', \kappa', \rho'} \frac{i^{|\beta'|+|\delta'+\kappa'+\rho'|} (\delta' + \kappa' + \rho')!}{\alpha! \theta! \delta'! \kappa'! \rho'!} \partial_{\vec{w}}^{\beta'} \left[\partial_{\vec{u}}^{\delta'} \Delta^{2\gamma-1}(x', y) \right. \\ \left. \times \partial_{\vec{u}}^{\kappa'} \partial_{\mathbf{k}}^{\alpha} a(x'; r, \mathbf{k}) \partial_{\vec{u}}^{\rho'} G_{\beta'}^{\alpha}(x', r) \partial_{\mathbf{1}}^{\theta} b(x'; s, \mathbf{1}) G_{\delta'+\kappa'+\rho'}^{\theta}(x', s) \right]_{\vec{w}=0, \vec{u}=0}.$$

Similarly, according to (6.27) and (6.30), it is enough to distribute the \vec{w} derivatives on functions of y and s only:

$$c(x'; q, \mathbf{p}) = \sum_{\alpha, \theta, \beta', \lambda', \phi', \delta', \kappa', \rho'} \frac{i^{|\beta'+\lambda'+\phi'|+|\delta'+\kappa'+\rho'|} (\delta' + \kappa' + \rho')! (\beta' + \lambda' + \phi')!}{\alpha! \theta! \delta'! \kappa'! \rho'! \beta'! \lambda'! \phi'!} \\ \times \partial_{\vec{w}}^{\beta'} \partial_{\vec{u}}^{\delta'} \Delta^{2\gamma-1}(x', y) \partial_{\vec{u}}^{\kappa'} \partial_{\mathbf{k}}^{\alpha} a(x'; r, \mathbf{k}) \partial_{\vec{u}}^{\rho'} G_{\beta'+\lambda'+\phi'}^{\alpha}(x', r) \\ \times \partial_{\vec{w}}^{\lambda'} \partial_{\mathbf{1}}^{\theta} b(x'; s, \mathbf{1}) \partial_{\vec{w}}^{\phi'} G_{\delta'+\kappa'+\rho'}^{\theta}(x', s) \Big|_{\vec{w}=0, \vec{u}=0}. \quad (6.50)$$

At this moment we have to stop and think about how to apply the \vec{u} and \vec{w} derivatives on functions of y , s , and r . For instance let us consider point s defined in equation (6.30) and the case of derivatives with regular covariant derivative indices (not multi-index). We start with the object

$$\eta^{\mu'}_v(x', s) = \nabla_{\nu} \sigma^{\mu'}(x', s). \quad (6.51)$$

This matrix is assumed to have an inverse

$$\eta^{-1} = \gamma = \{\gamma^{\nu}_{\mu'}(x', s)\} \quad (6.52)$$

which can be used as a ‘‘chain rule factor’’ in going from derivatives with respect to the tangent vector (technically it’s $-\hat{\sigma}$, see (2.73 and (2.76)) to derivatives with respect to the point given by the exponential map associated with that vector:

$$\partial_{\sigma^{\mu'}(x', s)} f(s) = \gamma^{\nu}_{\mu'}(x', s) \nabla_{\nu}^{(s)} f(s). \quad (6.53)$$

If we rewrite (6.30) as

$$\sigma^{\mu'}(x', s) = \sigma^{\mu'}(x', q) + \frac{1}{2}w^{\mu'} \quad (6.54)$$

we see that all we need is a 1/2 factor to get the result

$$\partial_{w^{\mu'}} f(s) = \frac{1}{2}\gamma^{\nu}{}_{\mu'}(x', s)\nabla_{\nu}^{(s)} f(s). \quad (6.55)$$

In a similar fashion, using (6.27) and (6.29) we get

$$\partial_{w^{\mu'}} f(r) = -\frac{1}{2}\gamma^{\nu}{}_{\mu'}(x', r)\nabla_{\nu}^{(r)} f(r) \quad (6.56)$$

and

$$\partial_{w^{\mu'}} f(y) = +\frac{1}{2}\gamma^{\nu}{}_{\mu'}(x', y)\nabla_{\nu}^{(y)} f(y) \quad (6.57)$$

$$\partial_{w^{\mu'}} f(y) = -\frac{1}{2}\gamma^{\nu}{}_{\mu'}(x', y)\nabla_{\nu}^{(y)} f(y). \quad (6.58)$$

One can apply this easily to higher order derivatives. For instance,

$$\begin{aligned} \partial_{w^{\mu'}} \partial_{w^{\nu'}} f(s) &= \frac{1}{2}\gamma^{\mu}{}_{\mu'}(x', s)\nabla_{\mu}^{(s)} \left(\frac{1}{2}\gamma^{\nu}{}_{\nu'}(x', s)\nabla_{\nu}^{(s)} f(s) \right) \\ &= \frac{1}{4}\gamma^{\mu}{}_{\mu'} \left((\nabla_{\mu}\gamma^{\nu}{}_{\nu'})\nabla_{\nu} f + \gamma^{\nu}{}_{\nu'}\nabla_{\mu}\nabla_{\nu} f \right) \end{aligned} \quad (6.59)$$

etc. It is obvious that in a sum over multi-indexed \vec{w} and \vec{v} derivatives we will see such mixed derivatives of any order

$$\sum_{\alpha'} a_{\alpha'} \partial_{\vec{w}}^{\alpha'} f(s) = a_0 f(s) + a_1^{\mu'} \partial_{w^{\mu'}} f(s) + a_2^{\mu'\nu'} \partial_{w^{\mu'}} \partial_{w^{\nu'}} f(s) + \dots, \quad (6.60)$$

therefore we need to consider a multi-index notation for the covariant derivatives of both $\gamma^{\mu}{}_{\mu'}(x', s)$ and $f(s)$. Since y , r and s are given by (6.27)–(6.30) we need to use the two-century old Faà di Bruno formula [60] [61] [62], but we need the multi-variate form of it.

3. The Multivariate Faà di Bruno Formula and the Product Rule

The Faà di Bruno formula is an explicit expression for the n th derivative of the composition $f(y)$, $y = g(x)$ at $x = \bar{x}$:

$$\left. \frac{d^n}{dx^n} f[g(x)] \right|_{\bar{x}} = \sum_{k=1}^n \left. \frac{d^k f}{dy^k} \right|_{\bar{y}} \sum_{p(n,k)} n! \prod_{j=1}^n \frac{1}{\lambda_j!} \left(\frac{1}{j!} \frac{d^j g}{dx^j} \right)^{\lambda_j} \Big|_{\bar{x}} \quad (6.61)$$

where

$$p(n, k) = \{(\lambda_1, \dots, \lambda_n) : \lambda_j \in \mathcal{N}_0, \sum_{j=1}^n \lambda_j = k, \sum_{j=1}^n j \lambda_j = n\} \quad (6.62)$$

and $\bar{y} = g(\bar{x})$ with \mathcal{N}_0 being the set of nonnegative integers.

The multivariate extension of this formula is as follows [63]. Let f be a composition of functions $f = f(y_1, \dots, y_m)$, $y_j = g^{(j)}(x_1, \dots, x_d)$ and $\bar{x} = (\bar{x}_1, \dots, \bar{x}_d)$. One can define $D_y^\lambda f$, the multi-indexed arbitrary derivative of f in a similar way as it is defined in (6.33):

$$D_y^\lambda f = \frac{\partial^{|\lambda|} f}{\partial y_1^{\lambda_1} \dots \partial y_m^{\lambda_m}} \quad (6.63)$$

with $|\lambda| = \lambda_1 + \dots + \lambda_m$ and $y = (y_1, \dots, y_m)$. Then the arbitrary partial derivative of

$$h(x_1, \dots, x_d) = f[g^{(1)}(x_1, \dots, x_d), \dots, g^{(m)}(x_1, \dots, x_d)] \quad (6.64)$$

is given by the formula

$$D_x^\nu h \Big|_{\bar{x}} = \sum_{1 \leq |\lambda| \leq |\nu|} D_y^\lambda f \Big|_{\bar{y}} \sum_{s=1}^{|\nu|} \sum_{p_s(\nu, \lambda)} \nu! \prod_{j=1}^s \frac{1}{k_j! (l_j!)^{|k_j|}} (D_x^{l_j} g)^{k_j} \Big|_{\bar{x}}. \quad (6.65)$$

Here $\nu = (\nu_1, \dots, \nu_d)$, $k_j = (k_{j1}, \dots, k_{jm})$, and $l_j = (l_{j1}, \dots, l_{jd})$ are multi-indices with $|\nu| = \nu_1 + \dots + \nu_d$, $k_j! = k_{j1}! \dots k_{jm}!$ and $l_j! = l_{j1}! \dots l_{jd}!$. Therefore

$$\begin{aligned} (D_x^{l_j} g)^{k_j} &= (D_x^{l_j} g^{(1)})^{k_{j1}} \dots (D_x^{l_j} g^{(m)})^{k_{jm}}, \\ D_x^{l_j} g^{(i)} &= \frac{\partial^{|\lambda_j|} g^{(i)}}{\partial x_1^{l_{j1}} \dots \partial x_d^{l_{jd}}}. \end{aligned} \quad (6.66)$$

The generalization of (6.62) is

$$p_s(\nu, \lambda) = \{(k_1, \dots, k_s; l_1, \dots, l_s) : |k_i| > 0, \bar{0} \prec l_1 \prec \dots \prec l_s, \\ \sum_{j=1}^s k_j = \lambda \text{ and } \sum_{j=1}^s |k_j| l_j = \nu\}. \quad (6.67)$$

Given $\mu = (\mu_1, \dots, \mu_d)$ and $\nu = (\nu_1, \dots, \nu_d)$ one writes $\mu \prec \nu$ if one of the following holds:

- (i) $|\mu| < |\nu|$;
- (ii) $|\mu| = |\nu|$ and $\mu_1 < \nu_1$; or
- (iii) $|\mu| = |\nu|$, $\mu_1 = \nu_1, \dots, \mu_k = \nu_k$ and $\mu_{k+1} < \nu_{k+1}$ for some $1 \leq k < d$.

In order to see how this applies to our case, let's consider one of the \vec{w} derivatives in (6.50):

$$\begin{aligned} \partial_{\vec{w}}^{\phi'} G_{\delta'+\kappa'+\rho'}^{\theta}(x', s) \Big|_{\vec{w}=0} &= \frac{1}{2^{|\phi'|}} \partial_{\sigma(x', s)}^{\phi'} G_{\delta'+\kappa'+\rho'}^{\theta}(x', s) \Big|_{\sigma(x', s)=0} \\ &= \frac{1}{2^{|\phi'|}} \sum_{1 \leq |\lambda| \leq |\phi'|} \nabla_{(s)}^{\lambda} G_{\delta'+\kappa'+\rho'}^{\theta}(x', s) S_{(\lambda)}^{\phi'} \Big|_{\sigma(x', s)=0}. \end{aligned} \quad (6.68)$$

Here $S_{(\lambda)}^{\phi'}$ is a shorthand for the sum

$$S_{(\lambda)}^{\phi'}(x', s) = \sum_{m=1}^{|\phi'|} \sum_{p_m(\phi', \lambda)} \phi'! \prod_{j=1}^m \frac{1}{\zeta_j! (\xi_j')^{|\zeta_j|}} (\partial_{\sigma(x', s)}^{\xi_j'} s)^{\zeta_j} \quad (6.69)$$

where

$$p_m(\phi', \lambda) = \{(\zeta_1, \dots, \zeta_m; \xi_1, \dots, \xi_m) : |\zeta_j| > 0, \bar{0} \prec \xi_1 \prec \dots \prec \xi_m, \\ \sum_{j=1}^m \zeta_j = \lambda \text{ and } \sum_{j=1}^m |\zeta_j| \xi_j' = \phi'\}. \quad (6.70)$$

$\partial_{\sigma(x', s)}^{\xi_j'}$ can be viewed as a higher order multivariate form of $\gamma^{\nu}_{\mu'}(x', s)$.

Then (6.50) becomes:

$$\begin{aligned}
c(x'; q, \mathbf{p}) &= \sum_{\alpha, \theta, \beta', \lambda', \phi', \delta', \kappa', \rho'} \frac{i^{|\beta'+\lambda'+\phi'|+|\delta'+\kappa'+\rho'|} (\delta' + \kappa' + \rho')! (\beta' + \lambda' + \phi')!}{\alpha! \theta! \delta'! \kappa'! \rho'! \beta'! \lambda'! \phi'!} \\
&\quad \times \partial_{\vec{w}}^{\beta'} \left(\frac{1}{(-2)^{|\delta'|}} \sum_{1 \leq |\psi| \leq |\delta'|} \nabla_{(y)}^{\psi} \Delta^{2\gamma-1}(x', y) S_{(\psi)}^{\delta'}(x', y) \right) \\
&\quad \times \frac{1}{(-2)^{|\kappa'|}} \sum_{1 \leq |\varphi| \leq |\kappa'|} \nabla_{(r)}^{\varphi} \partial_{\mathbf{k}}^{\alpha} a(x'; r, \mathbf{k}) S_{(\varphi)}^{\kappa'}(x', r) \\
&\quad \times \frac{1}{(-2)^{|\rho'|}} \sum_{1 \leq |\eta| \leq |\rho'|} \nabla_{(r)}^{\eta} G_{\beta'+\lambda'+\phi'}^{\alpha}(x', r) S_{(\eta)}^{\rho'}(x', r) \\
&\quad \times \frac{1}{2^{|\lambda'|}} \sum_{1 \leq |\Gamma| \leq |\lambda'|} \nabla_{(s)}^{\Gamma} \partial_{\mathbf{l}}^{\theta} b(x'; s, \mathbf{l}) S_{(\Gamma)}^{\lambda'}(x', s) \\
&\quad \times \frac{1}{2^{|\phi'|}} \sum_{1 \leq |\Omega| \leq |\phi'|} \nabla_{(s)}^{\Omega} G_{\delta'+\kappa'+\rho'}^{\theta}(x', s) S_{(\Omega)}^{\phi'}(x', s). \tag{6.71}
\end{aligned}$$

Note that the second line can also be written as

$$\frac{1}{(-2)^{|\delta'|}} \sum_{1 \leq |\psi| \leq |\delta'|} \frac{1}{2^{|\beta'|}} \sum_{1 \leq |\nu| \leq |\beta'|} \nabla_{(y)}^{\nu} \left(\nabla_{(y)}^{\psi} \Delta^{2\gamma-1}(x', y) S_{(\psi)}^{\delta'}(x', y) \right) S_{(\nu)}^{\beta'}(x', y)$$

or

$$\begin{aligned}
&\frac{1}{(-2)^{|\delta'|}} \sum_{1 \leq |\psi| \leq |\delta'|} \frac{1}{2^{|\beta'|}} \sum_{1 \leq |\nu+\mu| \leq |\beta'|} \frac{(\nu + \mu)!}{\nu! \mu!} \\
&\quad \times \nabla_{(y)}^{\nu} \nabla_{(y)}^{\psi} \Delta^{2\gamma-1}(x', y) \nabla_{(y)}^{\mu} S_{(\psi)}^{\delta'}(x', y) S_{(\nu+\mu)}^{\beta'}(x', y).
\end{aligned}$$

Arrange the factors a little bit to get

$$\begin{aligned}
&c(x'; q, \mathbf{p}) \\
&= \sum_{\alpha, \theta, \beta', \lambda', \phi', \delta', \kappa', \rho'} \frac{i^{|\beta'+\lambda'+\phi'|+|\delta'+\kappa'+\rho'|-2|\delta'|-2|\kappa'|-2|\rho'|} (\delta' + \kappa' + \rho')! (\beta' + \lambda' + \phi')!}{2^{|\delta'|+|\beta'|+|\kappa'|+|\rho'|+|\lambda'|+|\phi'|} \alpha! \theta! \delta'! \kappa'! \rho'! \beta'! \lambda'! \phi'!} \\
&\quad \times \sum_{1 \leq |\psi| \leq |\delta'|, 1 \leq |\nu+\mu| \leq |\beta'|, 1 \leq |\varphi| \leq |\kappa'|, 1 \leq |\eta| \leq |\rho'|, 1 \leq |\Gamma| \leq |\lambda'|, 1 \leq |\Omega| \leq |\phi'|} \\
&\quad \times \frac{(\nu + \mu)!}{\nu! \mu!} \nabla_{(y)}^{\nu} \nabla_{(y)}^{\psi} \Delta^{2\gamma-1}(x', y) \nabla_{(y)}^{\mu} S_{(\psi)}^{\delta'}(x', y) S_{(\nu+\mu)}^{\beta'}(x', y)
\end{aligned}$$

$$\begin{aligned}
& \times \nabla_{(r)}^\varphi \partial_{\mathbf{k}}^\alpha a(x'; r, \mathbf{k}) S_{(\varphi)}^{\kappa'}(x', r) \nabla_{(r)}^\eta G_{\beta'+\lambda'+\phi'}^\alpha(x', r) S_{(\eta)}^{\rho'}(x', r) \\
& \times \nabla_{(s)}^\Gamma \partial_{\mathbf{l}}^\theta b(x'; s, \mathbf{l}) S_{(\Gamma)}^{\lambda'}(x', s) \nabla_{(s)}^\Omega G_{\delta'+\kappa'+\rho'}^\theta(x', s) S_{(\Omega)}^{\phi'}(x', s) \Big|_{\vec{w}=0, \vec{u}=0}. \tag{6.72}
\end{aligned}$$

When $\vec{w} = 0$ and $\vec{u} = 0$, the points y , r , and s go to q as dictated by the definitions given in (6.27), (6.29), and (6.30). Similarly, the momenta \mathbf{k} and \mathbf{l} both go to \mathbf{p} according to (6.31) and (5.9). Therefore,

$$\begin{aligned}
& c(x'; q, \mathbf{p}) \\
& = \sum_{\alpha, \theta, \beta', \lambda', \phi', \delta', \kappa', \rho'} \frac{i^{|\beta'+\lambda'+\phi'|+|\delta'+\kappa'+\rho'|-2|\delta'|-2|\kappa'|-2|\rho'|} (\delta' + \kappa' + \rho')! (\beta' + \lambda' + \phi')!}{2^{|\delta'+|\beta'+|\kappa'+|\rho'+|\lambda'+|\phi'|} \alpha! \theta! \delta'! \kappa'! \rho'! \beta'! \lambda'! \phi'!} \\
& \times \sum_{\substack{1 \leq |\psi| \leq |\delta'|, 1 \leq |\nu+\mu| \leq |\beta'|, 1 \leq |\varphi| \leq |\kappa'|, 1 \leq |\eta| \leq |\rho'|, 1 \leq |\Gamma| \leq |\lambda'|, 1 \leq |\Omega| \leq |\phi'|}} \frac{(\nu + \mu)!}{\nu! \mu!} \\
& \times \nabla^\nu \nabla^\psi \Delta^{2\gamma-1}(x', q) \nabla^\mu S_{(\psi)}^{\delta'}(x', q) S_{(\nu+\mu)}^{\beta'}(x', q) \\
& \times \nabla^\varphi \partial_{\mathbf{p}}^\alpha a(x'; q, \mathbf{p}) S_{(\varphi)}^{\kappa'}(x', q) \nabla^\eta G_{\beta'+\lambda'+\phi'}^\alpha(x', q) S_{(\eta)}^{\rho'}(x', q) \\
& \times \nabla^\Gamma \partial_{\mathbf{p}}^\theta b(x'; q, \mathbf{p}) S_{(\Gamma)}^{\lambda'}(x', q) \nabla^\Omega G_{\delta'+\kappa'+\rho'}^\theta(x', q) S_{(\Omega)}^{\phi'}(x', q). \tag{6.73}
\end{aligned}$$

In principle, ∇G and S can be worked out in terms of the curvature tensor $R^\mu_{\nu\alpha\beta}$ in the coincidence limit according to the rules given in Chapter II. The coincidence limits of the desired order of derivatives of σ and $g^{\mu'}_{\nu'}$ can always be found using the basic defining relations (2.75) and (2.76) (also see Appendix A). We also point out that in (6.73), only α and θ are unrestricted. Because of the G factors we have $|\beta' + \lambda' + \phi'| = |\alpha|$ and $|\delta' + \kappa' + \rho'| = |\theta|$. The other multi-indices are explicitly restricted in the limits on the second sum sign. (6.73) is understood better if one identifies terms of the same order and considers the expansion parameters. Assuming “classical” behaviour of the symbols as functions of \mathbf{p} (i.e., each \mathbf{p} derivative increases the power of falloff at infinity by 1), we should group terms with the same number of \mathbf{p} derivatives, namely $|\alpha + \theta|$. Alternatively (but with the same result), one can count x derivatives (including derivatives of the metric tensor implicit in R), since

they are always paired with \mathbf{p} derivatives. Indeed, the total number of x derivatives is $|\nu + \psi + \mu + \phi + \eta + \Gamma + \Omega + (\text{derivatives implicit in } S \text{ factors})|$. Referring back to (6.68)–(6.70) we see that the first derivative of S yields $\gamma^\nu_{\mu'}$, whose coincidence limit is trivial and dimensionless. But further differentiations will yield (in principle) curvature tensors, so they need to be counted. Thus the number of derivatives in $\nabla^\xi S$ is $\xi - 1$, so the total in S^ϕ is (from (6.70)) $\sum \zeta(\xi - 1) = |\phi - \lambda|$. Applying this argument to the six S factors in (6.73) brings the total number of derivatives up to $|\beta' + \delta' + \kappa' + \rho' + \lambda' + \phi'| = |\alpha + \theta|$.

B. First Terms in the Expansion

The asymptotic product formula (6.73) results from the expression for $c(x'; q, \mathbf{p})$ at an earlier stage of the analysis given in the previous section, namely (6.47):

$$c(x'; q, \mathbf{p}) = \sum_{\alpha, \theta, \beta', \delta'} \frac{i^{|\beta'|+|\delta'|}}{\alpha! \theta!} \partial_{\vec{w}}^{\beta'} \partial_{\vec{u}}^{\delta'} \left[\Delta^{2\gamma-1}(x', y) \partial_{\mathbf{k}}^\alpha a(x'; r, \mathbf{k}) G_{\beta'^\alpha}(x', r) \right. \\ \left. \times \partial_1^\theta b(x'; s, \mathbf{l}) G_{\delta'^\theta}(x', s) \right]_{\vec{w}=0, \vec{u}=0}. \quad (6.74)$$

The sum is over the multi-indices α , β' , θ , and δ' . Our approach is to bring together terms with same length and therefore keep the sum of the order of derivatives constant in each step. The length of a multi-index is defined in (6.33). Once all possible derivatives are covered in a particular set, one can move to a higher step. Let

$$m \equiv |\alpha| + |\beta'| + |\theta| + |\delta'|.$$

The cases $m = 0$, $m = 1$, and $m = 2$ will be covered here. The presence of $G_{\beta'^\alpha}$ and $G_{\delta'^\theta}$ dictates that $|\alpha| = |\beta'|$ and $|\theta| = |\delta'|$. The parameter γ is chosen to be equal to one.

1. $m = 0$

This is when $|\alpha| = |\beta'| = |\theta| = |\delta'| = 0$. Neither the derivatives nor the parallel transport factors exist and we get

$$\Delta(x', y)a(x'; r, \mathbf{k})b(x'; s, \mathbf{l}) \Big|_{\vec{w}=0, \vec{u}=0} = \Delta(x', q)a(x'; q, \mathbf{p})b(x'; q, \mathbf{p}). \quad (6.75)$$

If we consider the coincidence limit again (*i.e.*, $x' \rightarrow q$), the first term in the expansion for $c(x'; q, \mathbf{p})$ becomes just

$$a(q, \mathbf{p})b(q, \mathbf{p}). \quad (6.76)$$

2. $m = 1$

There are two possibilities here, the first one being $|\alpha| = |\beta'| = 1$, $|\theta| = |\delta'| = 0$. The double sum associated with this case is

$$i \frac{\partial}{\partial w^{\nu'}} [\Delta(x', y) \frac{\partial a}{\partial k_\mu}(x'; r, \mathbf{k}) g^{\nu'}{}_\mu(x', r) b(x'; s, \mathbf{l})] \Big|_{\vec{w}=0, \vec{u}=0}. \quad (6.77)$$

The \vec{w} derivatives act on functions of y and s only, therefore one can rewrite (6.77) as

$$i \frac{\partial a}{\partial k_\mu}(x'; r, \mathbf{k}) g^{\nu'}{}_\mu(x', r) \left[\frac{\partial \Delta}{\partial w^{\nu'}}(x', y) b(x'; s, \mathbf{l}) + \Delta(x', y) \frac{\partial b}{\partial w^{\nu'}}(x'; s, \mathbf{l}) \right] \Big|_{\vec{w}=0, \vec{u}=0}.$$

One can use (6.57) and (6.55) to get

$$\begin{aligned} & \frac{i}{2} \frac{\partial a}{\partial k_\mu}(x'; r, \mathbf{k}) g^{\nu'}{}_\mu(x', r) \left[\gamma^\lambda{}_{\nu'}(x', y) \nabla_\lambda^{(y)} \Delta(x', y) b(x'; s, \mathbf{l}) \right. \\ & \quad \left. + \Delta(x', y) \gamma^\lambda{}_{\nu'}(x', s) \nabla_\lambda^{(s)} b(x'; s, \mathbf{l}) \right] \Big|_{\vec{w}=0, \vec{u}=0} \end{aligned}$$

which becomes

$$\frac{i}{2} \frac{\partial a}{\partial p_\mu}(x'; q, \mathbf{p}) g^{\nu'}{}_\mu(x', q) \left[\gamma^\lambda{}_{\nu'}(x', q) \nabla_\lambda^{(q)} \Delta(x', q) b(x'; q, \mathbf{p}) \right]$$

$$+ \Delta(x', q) \gamma^{\lambda}_{\nu'}(x', q) \nabla_{\lambda}^{(q)} b(x'; q, \mathbf{p}) \Big]. \quad (6.78)$$

With the help of (5.16), (5.14), and (5.21), the coincidence limit of (6.78) is found to be

$$-\frac{i}{2} \frac{\partial a}{\partial p_{\mu}}(q, \mathbf{p}) \nabla_{\mu} b(q, \mathbf{p}). \quad (6.79)$$

The reason we look at the coincidence limit is again to see if the presence of the fiducial point in the definitions had any effect on some of the expected results (remember the classical Poisson bracket analogue).

The second possibility for case $m = 1$ is $|\alpha| = |\beta'| = 0$, $|\theta| = |\delta'| = 1$. Summation (6.74) is reduced to

$$i \frac{\partial}{\partial u^{\nu'}} \left[\Delta(x', y) a(x'; r, \mathbf{k}) \frac{\partial b}{\partial l_{\mu}}(x'; s, \mathbf{l}) g^{\nu'}_{\mu}(x', s) \right]_{\vec{w}=0, \vec{u}=0}. \quad (6.80)$$

This time we use (6.56) and (6.58), keeping in mind that s has no \vec{u} dependence and write

$$\begin{aligned} -\frac{i}{2} \frac{\partial b}{\partial l_{\mu}}(x'; s, \mathbf{l}) g^{\nu'}_{\mu}(x', s) \left[\gamma^{\lambda}_{\nu'}(x', y) \nabla_{\lambda}^{(y)} \Delta(x', y) a(x'; r, \mathbf{k}) \right. \\ \left. + \Delta(x', y) \gamma^{\lambda}_{\nu'}(x', r) \nabla_{\lambda}^{(r)} a(x'; r, \mathbf{k}) \right] \Big|_{\vec{w}=0, \vec{u}=0} \end{aligned}$$

or

$$\begin{aligned} -\frac{i}{2} \frac{\partial b}{\partial p_{\mu}}(x'; q, \mathbf{p}) g^{\nu'}_{\mu}(x', q) \left[\gamma^{\lambda}_{\nu'}(x', q) \nabla_{\lambda} \Delta(x', q) a(x'; q, \mathbf{p}) \right. \\ \left. + \Delta(x', q) \gamma^{\lambda}_{\nu'}(x', q) \nabla_{\lambda} a(x'; q, \mathbf{p}) \right] \end{aligned}$$

which is equal to

$$\frac{i}{2} \frac{\partial b}{\partial p_{\mu}}(q, \mathbf{p}) \nabla_{\mu} a(q, \mathbf{p}) \quad (6.81)$$

in the coincidence limit. For comparison the reader may refer to corresponding terms in the expansions (3.48) or (3.49).

3. $m = 2$

We have this one in three ways. First, $|\alpha| = |\beta'| = 2$, $|\theta| = |\delta'| = 0$. The quadruple sum obtained from (6.74) is

$$\frac{i^2}{2!} \frac{\partial^2}{\partial w^{\nu'} \partial w^{\lambda'}} \left[\Delta(x', y) \frac{\partial^2 a}{\partial k_\mu \partial k_\rho}(x'; r, \mathbf{k}) g^{\nu'}{}_\mu(x', r) g^{\lambda'}{}_\rho(x', r) b(x'; s, \mathbf{l}) \right]_{\vec{w}=0, \vec{u}=0}. \quad (6.82)$$

There will arise many terms in (6.82) but here we shall ignore all those that will vanish in the coincidence limit. These are the terms with the first derivatives of $\Delta(x', q)$ and $\gamma^{\kappa}{}_{\lambda'}(x', q)$. The remaining part is

$$\begin{aligned} & \frac{i^2}{2!} \frac{\partial^2 a}{\partial p_\mu \partial p_\rho}(x'; q, \mathbf{p}) g^{\nu'}{}_\mu(x', q) g^{\lambda'}{}_\rho(x', q) \\ & \quad \times \frac{1}{4} \left[\gamma^\theta{}_{\nu'}(x', q) \gamma^\kappa{}_{\lambda'}(x', q) \nabla_\theta^{(q)} \nabla_\kappa^{(q)} \Delta^{2\gamma-1}(x', q) b(x'; q, \mathbf{p}) \right. \\ & \quad \left. + \Delta^{2\gamma-1}(x', q) \gamma^\theta{}_{\nu'}(x', q) \gamma^\kappa{}_{\lambda'}(x', q) \nabla_\theta^{(q)} \nabla_\kappa^{(q)} b(x'; q, \mathbf{p}) \right] \quad (6.83) \end{aligned}$$

where we have now a curvature term due to $[\nabla_\alpha \nabla_\beta \Delta] = \frac{1}{3} R_{\alpha\beta}$. Taking the coincidence limit, we find

$$-\frac{1}{8} \frac{\partial^2 a}{\partial p_\mu \partial p_\rho}(q, \mathbf{p}) \left[\frac{1}{3} R_{\mu\rho}(q) b(q, \mathbf{p}) + \nabla_\mu \nabla_\rho b(q, \mathbf{p}) \right]. \quad (6.84)$$

The second way is $|\alpha| = |\beta'| = 0$, $|\theta| = |\delta'| = 2$. In this case the sum will be

$$\frac{i^2}{2!} \frac{\partial^2}{\partial u^{\nu'} \partial u^{\lambda'}} \left[\Delta(x', y) a(x'; r, \mathbf{k}) \frac{\partial^2 b}{\partial l_\mu \partial l_\rho}(x'; s, \mathbf{l}) g^{\nu'}{}_\mu(x', s) g^{\lambda'}{}_\rho(x', s) \right]_{\vec{w}=0, \vec{u}=0} \quad (6.85)$$

and the coincidence limit will be similar to (6.84):

$$-\frac{1}{8} \frac{\partial^2 b}{\partial p_\mu \partial p_\rho}(q, \mathbf{p}) \left[\frac{1}{3} R_{\mu\rho}(q) a(q, \mathbf{p}) + \nabla_\mu \nabla_\rho a(q, \mathbf{p}) \right]. \quad (6.86)$$

The third possibility is $|\alpha| = |\beta'| = 1$, $|\theta| = |\delta'| = 1$. Here we have derivatives with respect to both \vec{w} and \vec{u} :

$$i^2 \frac{\partial^2}{\partial w^{\nu'} \partial u^{\lambda'}} \left[\Delta(x', y) \frac{\partial a}{\partial k_\mu}(x'; r, \mathbf{k}) g^{\nu'}{}_\mu(x', r) \frac{\partial b}{\partial l_\rho}(x'; s, \mathbf{l}) g^{\lambda'}{}_\rho(x', s) \right]_{\vec{w}=0, \vec{u}=0} \quad (6.87)$$

and the result in the coincidence limit $x' \rightarrow q$ is

$$-\frac{1}{12} R_{\mu\rho}(q) \frac{\partial a}{\partial p_\mu}(q, \mathbf{p}) \frac{\partial b}{\partial p_\rho}(q, \mathbf{p}) + \frac{1}{4} \nabla_\mu \frac{\partial a}{\partial p_\rho}(q, \mathbf{p}) \nabla_\rho \frac{\partial b}{\partial p_\mu}(q, \mathbf{p}). \quad (6.88)$$

We will stop here and summarize. Using our results (6.76), (6.79), (6.81), (6.84), and (6.88), the expansion for $c(q, \mathbf{p})$ in terms of $a(q, \mathbf{p})$ and $b(q, \mathbf{p})$ is

$$\begin{aligned} c(q, \mathbf{p}) &= a(q, \mathbf{p})b(q, \mathbf{p}) - \frac{i}{2} \frac{\partial a}{\partial p_\mu}(q, \mathbf{p}) \nabla_\mu b(q, \mathbf{p}) + \frac{i}{2} \frac{\partial b}{\partial p_\mu}(q, \mathbf{p}) \nabla_\mu a(q, \mathbf{p}) \\ &\quad - \frac{1}{8} \frac{\partial^2 a}{\partial p_\mu \partial p_\rho}(q, \mathbf{p}) \left[\frac{1}{3} R_{\mu\rho}(q) b(q, \mathbf{p}) + \nabla_\mu \nabla_\rho b(q, \mathbf{p}) \right] \\ &\quad - \frac{1}{8} \frac{\partial^2 b}{\partial p_\mu \partial p_\rho}(q, \mathbf{p}) \left[\frac{1}{3} R_{\mu\rho}(q) a(q, \mathbf{p}) + \nabla_\mu \nabla_\rho a(q, \mathbf{p}) \right] \\ &\quad - \frac{1}{12} R_{\mu\rho}(q) \frac{\partial a}{\partial p_\mu}(q, \mathbf{p}) \frac{\partial b}{\partial p_\rho}(q, \mathbf{p}) + \frac{1}{4} \nabla_\mu \frac{\partial a}{\partial p_\rho}(q, \mathbf{p}) \nabla_\rho \frac{\partial b}{\partial p_\mu}(q, \mathbf{p}) \\ &\quad + \dots \end{aligned} \quad (6.89)$$

If the curvature terms are factored out, this becomes

$$\begin{aligned} c &= ab + \frac{i}{2} \left(\nabla_\mu a \frac{\partial b}{\partial p_\mu} - \frac{\partial a}{\partial p_\mu} \nabla_\mu b \right) \\ &\quad - \frac{1}{24} R_{\mu\nu} \left(\frac{\partial^2 a}{\partial p_\mu \partial p_\nu} b + a \frac{\partial^2 b}{\partial p_\mu \partial p_\nu} + 2 \frac{\partial a}{\partial p_\mu} \frac{\partial b}{\partial p_\nu} \right) \\ &\quad + \frac{1}{8} \left(2 \nabla_\mu \frac{\partial a}{\partial p_\nu} \nabla_\nu \frac{\partial b}{\partial p_\mu} - \frac{\partial^2 a}{\partial p_\mu \partial p_\nu} \nabla_\mu \nabla_\nu b - \nabla_\mu \nabla_\nu a \frac{\partial^2 b}{\partial p_\mu \partial p_\nu} \right) \\ &\quad + \dots, \end{aligned} \quad (6.90)$$

or

$$c = ab + \frac{i}{2} \left(\nabla_\mu a \frac{\partial b}{\partial p_\mu} - \frac{\partial a}{\partial p_\mu} \nabla_\mu b \right)$$

$$\begin{aligned}
& +\frac{1}{8}\left(2\nabla_{\mu}\frac{\partial a}{\partial p_{\nu}}\nabla_{\nu}\frac{\partial b}{\partial p_{\mu}}-\frac{\partial^2 a}{\partial p_{\mu}\partial p_{\nu}}\nabla_{\mu}\nabla_{\nu}b-\nabla_{\mu}\nabla_{\nu}a\frac{\partial^2 b}{\partial p_{\mu}\partial p_{\nu}}\right) \\
& -\frac{1}{24}R_{\mu\nu}\frac{\partial^2(ab)}{\partial p_{\mu}\partial p_{\nu}} \\
& +\dots
\end{aligned} \tag{6.91}$$

At this level it can be said that the only difference between the classical Weyl expansion and the covariant one, besides the fact that ordinary derivatives are replaced by covariant derivatives, is the additional curvature ($R_{\mu\nu}$) term .

CHAPTER VII

THE COVARIANT WIGNER FUNCTION AND EXAMPLES

We define the Wigner function in the covariant formalism of Chapter V and study the cases of a gauge field in flat space and a curved manifold (with no gauge field). The motivation for looking at Wigner functions for examples (but not Weyl symbols of nonpolynomial observables, for instance) is to have some results that are of physical interest. The first example is the problem of a charged particle in a constant magnetic field. The energy levels associated with this problem are known as the *Landau states* in the literature [64] [65] [66]. Gauge invariant results are obtained using a covariant definition. The second example is the Wigner function obtained from a test function on the 2-sphere. The covariant definition is not affected by coordinate transformations.

A. The Landau Problem

1. Equations of Motion

This is the problem of a charged particle of mass m and charge e moving in a magnetic field $\mathbf{B} = (0, 0, B)$ on the $x - y$ plane (the 3D problem reduces to the 2D one when the z -dependence is separated out). The Hamiltonian

$$\begin{aligned} \hat{H} &= \frac{1}{2m} \hat{\boldsymbol{\Pi}}^2 \\ &= \frac{1}{2m} \left[\left(\hat{P}_x - \frac{e}{c} A_x \right)^2 + \left(\hat{P}_y - \frac{e}{c} A_y \right)^2 + \left(\hat{P}_z - \frac{e}{c} A_z \right)^2 \right] \end{aligned} \quad (7.1)$$

is used to derive the equations of motion in the *Heisenberg picture*

$$\frac{d(\cdot)}{dt} = \frac{i}{\hbar} [\hat{H}, (\cdot)]. \quad (7.2)$$

Then,

$$\frac{d\hat{\Pi}_x}{dt} = -\omega\hat{\Pi}_y, \quad (7.3)$$

$$\frac{d\hat{\Pi}_y}{dt} = \omega\hat{\Pi}_x, \quad (7.4)$$

$$\frac{d\hat{\Pi}_z}{dt} = 0, \quad (7.5)$$

where $\omega \equiv -eB/mc$. Here one uses the fact that $\mathbf{B} = \nabla \times \mathbf{A}$ and $[\hat{\Pi}_x, \hat{\Pi}_y] = i\hbar eB/c$. Since $\hat{\mathbf{\Pi}}$ represents the kinetic momentum, (7.3) and (7.4) can be written as

$$\frac{d}{dt} \left(\hat{\Pi}_x + \omega m \hat{Y} \right) = 0, \quad (7.6)$$

and

$$\frac{d}{dt} \left(\hat{\Pi}_y - \omega m \hat{X} \right) = 0, \quad (7.7)$$

whence

$$\hat{X} = \frac{1}{m\omega} \hat{\Pi}_y - \hat{X}_0, \quad \hat{Y} = \hat{Y}_0 - \frac{1}{m\omega} \hat{\Pi}_x. \quad (7.8)$$

Due to the seemingly classical nature of these equations of motion, the operators (integration constants) (\hat{X}_0, \hat{Y}_0) can be identified as the center of the orbit. These operators do not commute with each other

$$[\hat{X}_0, \hat{Y}_0] = il^2, \quad (7.9)$$

where $l = \sqrt{-c\hbar/eB}$, but commute with the Hamiltonian creating an infinitely degenerate energy. Since the problem is formally identical with the one dimensional harmonic oscillator [65], the energy levels are given by

$$E_n = \frac{1}{2} \hbar \omega \left(n + \frac{1}{2} \right). \quad (7.10)$$

Practically any combination of \hat{X}_0 and \hat{Y}_0 can be used to get eigenstates for these energies; even for the ‘ground state’ there are infinitely many possibilities to choose from. Therefore the covariant Wigner function will be independent of the gauge chosen but will be a consequence of the particular state.

2. Gauge Dependent Solutions

There are two popular gauges for this problem, the *Landau gauge*,

$$\mathbf{A}^L = (0, Bx) \quad \text{or} \quad \mathbf{A}^L = (-By, 0), \quad (7.11)$$

and the *symmetric gauge*:

$$\mathbf{A}^S = \frac{B}{2}(-y, x); \quad (7.12)$$

note that we no longer use 3D notation, since the problem reduces to two dimensions. They both give the same magnetic field through $\mathbf{B} = \nabla \times \mathbf{A}$. These two are related by a gauge transformation

$$\mathbf{A}^L = \mathbf{A}^S + \nabla\Lambda \quad (7.13)$$

where $\Lambda = \frac{1}{2}Bxy$. Accordingly, the wave solutions in both gauges should be related also:

$$\psi^L = \psi^S e^{\frac{ie}{\hbar}\Lambda}. \quad (7.14)$$

Note that the gauges (7.11) and (7.12) are not unique, since one could add any constant vector to \mathbf{A} without essentially changing them. That amounts to changing the origin; the ‘popular’ gauges tacitly make the origin a preferred point. Textbooks which pick a certain gauge and find the solution in that particular gauge usually neglect to show this last point explicitly, for instance in the symmetric gauge the

ground state functions are given as

$$\psi_0^S(z, \bar{z}) \propto f(z)e^{z\bar{z}/4l^2} \quad (7.15)$$

where $f(z)$ is an arbitrary function of $z = x + iy$. On the other hand the ground state function in the Landau gauge is usually given as

$$\psi_{L,0}(x, y) \propto e^{-ix_0y/l^2} e^{-(x-x_0)^2/2l^2}. \quad (7.16)$$

It can easily be checked that (7.14) is not trivial for these two solutions. It is only in [66], that I could find a satisfactory answer. The solution is worked out in the symmetric gauge for the so-called ‘‘squeezed states’’:

$$\begin{aligned} \psi_{n=0;x_0,z}(x, y) &= \frac{1}{l\sqrt{2\pi}} e^{-y^2(1-\tanh z)/4l^2} e^{-ix_0y(1+\tanh z)/2l^2} \\ &\quad \times e^{-(x-x_0)^2(1+\tanh z)/4l^2} e^{2ixy \tanh z/4l^2} \end{aligned} \quad (7.17)$$

where z is a complex parameter. The Landau state can be recovered by choosing a real parameter, and letting $z \rightarrow \infty$. In this limit one obtains

$$\psi_{n=0;x_0,z}(x, y) = \frac{1}{(l\sqrt{\pi})^{1/2}} e^{-ix_0y/l^2} e^{-(x-x_0)^2/2l^2} e^{ixy/2l^2} \quad (7.18)$$

which is more suitable for demonstrating (7.14) than the rather vague form given in (7.15) because one can multiply (7.18) by

$$\exp\left\{-\frac{ixy}{2l^2}\right\} = \exp\left\{\frac{ie}{c\hbar}\left(\frac{1}{2}Bxy\right)\right\} \quad (7.19)$$

and get (7.16) as predicted by (7.14).

Finally, we need to consider what happens in the case of higher energy levels. The system is analogous to a simple harmonic oscillator, we can apply \hat{a}^\dagger many times and get the desired wave function. Higher harmonic oscillator states are given using

Hermite polynomials; the same applies for the Landau states. Using the appropriate normalization factors one can write the wave functions in both gauges as following:

a) symmetric gauge

$$\psi_{n;x_0}^S(x, y) = \frac{1}{(l\sqrt{\pi}2^n n!)^{1/2}} e^{-ix_0y/l^2} e^{-(x-x_0)^2/2l^2} e^{ixy/2l^2} H_n\left(\frac{x-x_0}{l}\right), \quad (7.20)$$

b) Landau gauge

$$\psi_{n;x_0}^L(x, y) = \frac{1}{(l\sqrt{\pi}2^n n!)^{1/2}} e^{-ix_0y/l^2} e^{-(x-x_0)^2/2l^2} H_n\left(\frac{x-x_0}{l}\right). \quad (7.21)$$

3. Gauge Invariant Wigner Function

Since the wave functions (7.20) and (7.21) are different, the ‘classical’ Wigner function (see [11] for the one-dimensional version)

$$W_c(\mathbf{r}, \mathbf{p}) = (\pi\hbar)^{-2} \int d^2\mathbf{r}' \psi^*(\mathbf{r} + \mathbf{r}') \psi(\mathbf{r} - \mathbf{r}') e^{2\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}'} \quad (7.22)$$

will have different forms in the Landau and symmetric gauges. We propose a new definition which is covariant under gauge and gravitational fields:

$$\begin{aligned} W(x'; q, \mathbf{k}) &= h^{-d} \int_{T_{x'}} d^d \xi^{\mu'} \sqrt{g(x')} \Delta^{-\gamma}(x', x) \Delta^{-\gamma}(x', z) \\ &\quad \times \exp(-i\tilde{k}_{\mu'} \xi^{\mu'} / \hbar) I(x'; q, x) \psi^*(x) \psi(z) I(x'; z, q) \end{aligned} \quad (7.23)$$

where

$$I(x'; q, x) \equiv \exp \left\{ \frac{ie}{c\hbar} \int_q^x \mathbf{A}(X) \cdot dX \right\} \quad (7.24)$$

$$X(s) \equiv \exp_{x'}[\hat{\sigma}^{\mu'}(x', q) + s \xi^{\mu'}] \quad (7.25)$$

and

$$X(-1/2) = z, \quad X(1/2) = x. \quad (7.26)$$

The momenta $\tilde{\mathbf{k}}$ and \mathbf{k} are related by the parallel transport

$$\tilde{k}_{\mu'} = g_{\mu'\nu}(x', q)k^\nu. \quad (7.27)$$

Now let us specialize to flat space and use this formula in the Landau problem. In flat space the VanVleck-Morette determinants are equal to 1.

$$W(x'; q, \mathbf{k}) = (2\pi\hbar)^{-2} \int_{-\infty}^{\infty} d\xi_1 \int_{-\infty}^{\infty} d\xi_2 e^{-i(k_1\xi_1 + k_2\xi_2)/\hbar} I(x'; q, x) \psi^*(x) \psi(z) I(x'; z, q) \quad (7.28)$$

Choose $x' = (0, 0)$, then $\mathbf{X} = (q_1 + s \xi_1, q_2 + s \xi_2)$ and pick the Landau gauge:

$$\mathbf{A} = (0, Bx),$$

then

$$\begin{aligned} I(x'; q, x) &= \exp \left\{ \frac{ie}{c\hbar} \int_0^{1/2} ds \mathbf{A}(\mathbf{X}(s)) \cdot \frac{d\mathbf{X}(s)}{ds} \right\} \\ &= \exp \left\{ \frac{ie}{c\hbar} \int_0^{1/2} ds (q_1 + s \xi_1) B \xi_2 \right\} \\ &= \exp \left\{ \frac{ie}{c\hbar} \left(\frac{1}{2} B q_1 \xi_2 + \frac{1}{8} B \xi_1 \xi_2 \right) \right\} \end{aligned} \quad (7.29)$$

and

$$\begin{aligned} I(x'; z, q) &= \exp \left\{ \frac{ie}{c\hbar} \int_{-1/2}^0 ds (q_1 + s \xi_1) B \xi_2 \right\} \\ &= \exp \left\{ \frac{ie}{c\hbar} \left(\frac{1}{2} B q_1 \xi_2 - \frac{1}{8} B \xi_1 \xi_2 \right) \right\}. \end{aligned} \quad (7.30)$$

These two give an exponential factor essentially equal to

$$\exp \left\{ \frac{ie}{c\hbar} (B q_1 \xi_2) \right\} = \exp \left\{ -i \frac{q_1 \xi_2}{l^2} \right\}, \quad (7.31)$$

and we can rewrite (7.28) as

$$\begin{aligned}
W(q, \mathbf{k}) &= (2\pi\hbar)^{-2} \int_{-\infty}^{\infty} d\xi_1 \int_{-\infty}^{\infty} d\xi_2 \psi^*(q_1 + \frac{\xi_1}{2}, q_2 + \frac{\xi_2}{2}) \psi(q_1 - \frac{\xi_1}{2}, q_2 - \frac{\xi_2}{2}) \\
&\quad \times \exp \left\{ -\frac{i}{\hbar}(k_1\xi_1 + k_2\xi_2) - i\frac{q_1\xi_2}{l^2} \right\}. \tag{7.32}
\end{aligned}$$

Then using the wave function (7.21)

$$\begin{aligned}
&\psi^*(q_1 + \frac{\xi_1}{2}, q_2 + \frac{\xi_2}{2}) \psi(q_1 - \frac{\xi_1}{2}, q_2 - \frac{\xi_2}{2}) \\
&= \frac{1}{l\sqrt{\pi}2^n n!} e^{iq_0(q_2 + \frac{\xi_2}{2})/l^2} e^{-(q_1 + \frac{\xi_1}{2} - q_0)^2/2l^2} e^{-iq_0(q_2 - \frac{\xi_2}{2})/l^2} \\
&\quad \times e^{-(q_1 - \frac{\xi_1}{2} - q_0)^2/2l^2} H_n\left(\frac{q_1 + \frac{\xi_1}{2} - q_0}{l}\right) H_n\left(\frac{q_1 - \frac{\xi_1}{2} - q_0}{l}\right).
\end{aligned}$$

Therefore,

$$\begin{aligned}
W(q_1, q_2, k_1, k_2) &= \frac{(2\pi\hbar)^{-2}}{l\sqrt{\pi}2^n n!} e^{-(q_1 - q_0)^2/l^2} \int d\xi_2 \exp\left(\frac{iq_0\xi_2}{l^2} - \frac{i}{\hbar}k_2\xi_2 - \frac{iq_1\xi_2}{l^2}\right) \\
&\quad \times \int d\xi_1 \exp\left(-\frac{\xi_1^2}{4l^2} - \frac{i}{\hbar}k_1\xi_1\right) H_n\left(\frac{q_1 - q_0 - \xi_1/2}{l}\right) H_n\left(\frac{q_1 - q_0 + \xi_1/2}{l}\right).
\end{aligned}$$

The first integral is equal to the Dirac delta function:

$$2\pi\delta\left(\frac{q_0}{l^2} + \frac{1}{\hbar}k_2 - \frac{q_1}{l^2}\right) = 2\pi l\delta\left(\frac{q_1 - q_0}{l} - \frac{k_2 l}{\hbar}\right). \tag{7.33}$$

This means we may replace $(q_0 - q_1)/l$ by $k_2 l/\hbar$ in the expression for the Wigner function. The wave function we use is not normalizable in the q_2 direction, this is why we encounter the Dirac delta. We don't need to keep it in the final result.

The second integral is not hard either. First write the exponent as

$$-\frac{1}{4l^2} \left[\left(\xi_1 - 2l^2 \frac{i}{\hbar} k_1\right)^2 - \left(2l^2 \frac{i}{\hbar} k_1\right)^2 \right] \tag{7.34}$$

and define a new variable z as

$$z = \frac{\xi_1}{2l} - \beta \tag{7.35}$$

where $\beta = -ilk_1/\hbar$. Then the integral becomes

$$2le^{\beta^2} \int dz e^{-z^2} H_n\left(\frac{q_1 - q_0}{l} - z - \beta\right) H_n\left(\frac{q_1 - q_0}{l} + z + \beta\right). \quad (7.36)$$

Using $H_n(-\zeta) = (-1)^n H_n(\zeta)$ and the result

$$\int dz e^{-z^2} H_n\left(-\frac{q_1 - q_0}{l} + z + \beta\right) H_n\left(\frac{q_1 - q_0}{l} + z + \beta\right) = 2^n \sqrt{\pi} n! L_n\left(2\left(\frac{q_1 - q_0}{l}\right)^2 - 2\beta^2\right)$$

(see [11]) where L_n is the n th the Laguerre polynomial, we get

$$\begin{aligned} W(q_1, q_2, k_1, k_2) &= \frac{(2\pi\hbar)^{-2}}{l\sqrt{\pi}2^n n!} e^{-(q_1 - q_0)^2/l^2} (2\pi l) \delta\left(\frac{q_1 - q_0}{l} - \frac{k_2 l}{\hbar}\right) \\ &\quad \times (2l) e^{-l^2 k_1^2/\hbar^2} (-1)^n 2^n \sqrt{\pi} n! L_n\left(2\left(\frac{q_1 - q_0}{l}\right)^2 + 2\frac{l^2 k_1^2}{\hbar^2}\right) \end{aligned} \quad (7.37)$$

or

$$W = \frac{(-1)^n l}{\pi \hbar^2} e^{-\frac{l^2}{\hbar^2}(k_1^2 + k_2^2)} L_n\left(\frac{(k_1^2 + k_2^2)}{\hbar^2/2l^2}\right). \quad (7.38)$$

This is a gauge invariant result and it is in accordance with the gauge invariant Wigner function for the squeezed states in the limit $|z| \rightarrow \infty$ [66]. The difference in our definition is the two-step parallel transport to the fiducial point. For this particular problem, the choice $x = (0, 0)$ worked fine, an arbitrary choice of x' can be separately analyzed, by calculating $W(x'; q, \mathbf{k})$ first and then taking the ‘coincidence limit’ $q \rightarrow x'$; this would correspond to shifting x' to the origin in flat space.

If one uses the symmetric gauge instead of the Landau gauge, then the parallel transport factors are

$$I(x'; q, x) = I(x'; z, q) = \exp\left[-\frac{i}{4l^2}(q_1 \xi_2 - q_2 \xi_1)\right], \quad (7.39)$$

and using (7.20), the Wigner function integral reduces to the form preceding (7.33).

Therefore, the gauge chosen does not affect the final answer.

B. Wigner Functions on the 2-Sphere

The formula we use for the Wigner function is

$$W(x'; q, \mathbf{p}) = h^{-2} \int_{T_{x'}} d^d \xi \sqrt{g(x')} \Delta^{-1}(x', x) \Delta^{-1}(x', z) e^{-i\tilde{p}_{\mu'} \xi^{\mu'} / \hbar} \psi^*(x) \psi(z) \quad (7.40)$$

where points x and z are defined as

$$x = \exp_{x'}[\hat{\sigma}^{\mu'}(x', q) + \frac{1}{2}\xi^{\mu'}] \quad (7.41)$$

and

$$z = \exp_{x'}[\hat{\sigma}^{\mu'}(x', q) - \frac{1}{2}\xi^{\mu'}]. \quad (7.42)$$

Here $\hat{\sigma}^{\mu'}(x', q)$ is the tangent vector at x' pointing in the direction of q (the inverse exponential map):

$$\hat{\sigma}^{\mu'}(x', q) \equiv \exp_{x'}^{-1} q. \quad (7.43)$$

The one-half-square of the geodetic distance s between x' and q is known as the Synge-deWitt world function,

$$\sigma(x', q) = \frac{1}{2}s^2 \quad (7.44)$$

and its covariant derivative with respect to x' is equal to this tangent vector up to a minus sign:

$$\begin{aligned} \hat{\sigma}^{\mu'}(x', q) &\equiv -\sigma^{\mu'}(x', q) \\ &\equiv -g^{\mu'\nu'}(x') \nabla_{\nu'} \sigma(x', q). \end{aligned} \quad (7.45)$$

Another useful object that could be obtained from this $\sigma(x', q)$ is the VanVleck-Morette determinant:

$$\Delta(x', q) \equiv -g^{-1/2}(x') \det[-\nabla_{\nu'} \nabla_{\mu'} \sigma(x', q)] g^{-1/2}(q). \quad (7.46)$$

Here the derivative with respect to a nonprimed index refers to a derivative at point q and g is the determinant of the metric.

The parallel transport of momentum co-vector \mathbf{p} from q to x' is done by the matrix $g_{\mu'}{}^{\nu}(x', q)$:

$$\tilde{p}_{\mu'} = g_{\mu'}{}^{\nu} p_{\nu}. \quad (7.47)$$

1. The Sphere

The sphere is a good example to demonstrate the details of this calculation since the world function is easy to find. The geodesics on the 2-sphere are the segments of the great circles and the arc length on such a great circle on a sphere of radius R is $s = R\alpha$, where α is the angle between two radii. Let the two end points be given by $\mathbf{r}' = (\theta', \phi')$ and $\mathbf{r} = (\theta, \phi)$ (these are the usual spherical coordinates $0 \leq \theta \leq \pi$, $0 \leq \phi \leq \pi/2$). The 2-sphere is embedded in three dimensional space with the cartesian coordinates

$$\begin{aligned} x &= R \sin \theta \cos \phi, \\ y &= R \sin \theta \sin \phi, \\ z &= R \cos \theta. \end{aligned} \quad (7.48)$$

Then

$$\begin{aligned} \cos \alpha &= \frac{\mathbf{r}' \cdot \mathbf{r}}{R^2} \\ &= \sin \theta' \sin \theta \cos(\phi - \phi') + \cos \theta' \cos \theta \end{aligned} \quad (7.49)$$

and therefore

$$s = R \cos^{-1} [\sin \theta' \sin \theta \cos(\phi - \phi') + \cos \theta' \cos \theta]. \quad (7.50)$$

Now we can write the world function (7.44) as

$$\sigma(\mathbf{r}', \mathbf{r}) = \frac{1}{2} \left(R \cos^{-1} [\sin \theta' \sin \theta \cos(\phi - \phi') + \cos \theta' \cos \theta] \right)^2 \quad (7.51)$$

Now in order to find the tangent vectors (defined in (7.43)) we need the covariant derivatives of this with respect to θ' and ϕ' . Since σ is a scalar, these are equal to the ordinary partial derivatives

$$\begin{aligned} \frac{\partial \sigma}{\partial \theta'} &= [\cos \theta \sin \theta' - \cos(\phi - \phi') \cos \theta' \sin \theta] h^{-1} R^2 \\ \frac{\partial \sigma}{\partial \phi'} &= -h^{-1} R^2 \sin \theta' \sin(\phi - \phi') \sin \theta \end{aligned} \quad (7.52)$$

where $h = \sin \alpha / \alpha$. These are $\nabla_{\theta'} \sigma$ and $\nabla_{\phi'} \sigma$, respectively; but we need the form given in (7.45). The metric can easily be found from the line element on the sphere:

$$d\mathbf{l}^2 = R^2 d\theta^2 + R^2 \sin^2 \theta d\phi^2 \quad (7.53)$$

$$(g_{\mu\nu}) = \begin{pmatrix} R^2 & 0 \\ 0 & R^2 \sin^2 \theta \end{pmatrix}, \quad (7.54)$$

therefore

$$\hat{\sigma}^{\theta'} = -[\cos \theta \sin \theta' - \cos(\phi - \phi') \cos \theta' \sin \theta] h^{-1} \quad (7.55)$$

$$\hat{\sigma}^{\phi'} = h^{-1} \csc \theta' \sin(\phi - \phi') \sin \theta. \quad (7.56)$$

The calculation of the VanVleck-Morette determinant also does not involve any Christoffel symbols since the \mathbf{r}' and \mathbf{r} derivatives are independent. We get

$$\Delta(\mathbf{r}', \mathbf{r}) = \frac{1}{R^4 \sin \theta' \sin \theta} \begin{vmatrix} \frac{\partial^2 \sigma}{\partial \theta' \partial \theta} & \frac{\partial^2 \sigma}{\partial \theta' \partial \phi} \\ \frac{\partial^2 \sigma}{\partial \phi' \partial \theta} & \frac{\partial^2 \sigma}{\partial \phi' \partial \phi} \end{vmatrix}. \quad (7.57)$$

The result is rather lengthy so let's not include it here but instead see what happens when we pick a certain (θ', ϕ') pair. A point on the equator ($\theta' = \pi/2$) should work

just fine. Let the longitudinal angle be $\phi' = \pi/2$ (obviously the poles are not good because ϕ' is undefined there).

When $\theta' = \pi/2$ and $\phi' = \pi/2$, (7.57) which is now only a function of θ and ϕ becomes

$$\Delta(\theta, \phi) = \frac{4 \cos^{-1}[\sin \phi \sin \theta] \sqrt{1 - \sin^2 \theta \sin^2 \phi}}{3 + \cos 2\theta + 2 \cos 2\phi \sin^2 \theta}. \quad (7.58)$$

Let's define $A \equiv \hat{\sigma}^{\theta'}|_{(\theta'=\pi/2, \phi'=\pi/2)}$ and $B \equiv \hat{\sigma}^{\phi'}|_{(\theta'=\pi/2, \phi'=\pi/2)}$. Then (7.55) and (7.56) become

$$A = -\frac{\cos^{-1}[\cos \phi \sin \theta] \cos \theta}{\sqrt{1 - \sin^2 \phi \sin^2 \theta}}, \quad (7.59)$$

$$B = -\frac{\cos^{-1}[\sin \phi \sin \theta] \cos \phi \sin \theta}{\sqrt{1 - \sin^2 \phi \sin^2 \theta}}. \quad (7.60)$$

These are the components of the tangent vector pointing in the direction of any (θ, ϕ) on the sphere. We also need the expressions for θ and ϕ in terms of A and B . Define β as

$$\cos \beta \equiv \sin \phi \sin \theta, \quad (7.61)$$

then

$$A = -\frac{\beta \cos \theta}{\sin \beta}, \quad (7.62)$$

$$B = -\frac{\beta \cos \phi \sin \theta}{\sin \beta}. \quad (7.63)$$

Now from above

$$(A^2 + B^2) \frac{\sin^2 \beta}{\beta^2} = \cos^2 \theta + \cos^2 \phi \sin^2 \theta \quad (7.64)$$

and adding $\cos^2 \beta$ to both sides,

$$\begin{aligned} (A^2 + B^2) \frac{\sin^2 \beta}{\beta^2} + \cos^2 \beta &= \cos^2 \theta + \cos^2 \phi \sin^2 \theta + \sin^2 \theta \sin^2 \phi \\ &= \cos^2 \theta + \sin^2 \theta \end{aligned}$$

$$\begin{aligned}
&= 1 \\
&= \cos^2 \beta + \sin^2 \beta
\end{aligned} \tag{7.65}$$

from which it follows that

$$2(A^2 + B^2) \frac{\sin^2 \beta}{\beta^2} = 2 \sin^2 \beta \tag{7.66}$$

and hence

$$\beta = \sqrt{A^2 + B^2} \tag{7.67}$$

(ignoring the negative solution). From (7.62),

$$\begin{aligned}
\theta &= \cos^{-1} \left(-\frac{A \sin \beta}{\beta} \right) \\
&= \cos^{-1} \left(-\frac{A \sin \sqrt{A^2 + B^2}}{\sqrt{A^2 + B^2}} \right)
\end{aligned} \tag{7.68}$$

and from (7.63),

$$\phi = \cos^{-1} \left(-\frac{B \sin \beta}{\beta \sin \theta} \right). \tag{7.69}$$

Now

$$\begin{aligned}
\sin^2 \theta &= 1 - \cos^2 \theta \\
&= 1 - \frac{A^2 \sin^2 \beta}{A^2 + B^2} \\
&= \frac{B^2 + A^2(1 - \sin^2 \beta)}{\beta^2}
\end{aligned} \tag{7.70}$$

and hence

$$\beta \sin \theta = \sqrt{B^2 + A^2 \cos^2 \beta}. \tag{7.71}$$

Therefore

$$\phi = \cos^{-1} \left(-\frac{B \sin \sqrt{A^2 + B^2}}{\sqrt{B^2 + A^2 \cos^2 \sqrt{A^2 + B^2}}} \right). \tag{7.72}$$

Now we can actually analyze the integrals in the Wigner function formula given

in (7.40). For notational consistency we define

$$\vec{\xi} = (A, B), \quad (7.73)$$

$$\hat{\sigma}^{\mu'}(x', q) = (A_q, B_q), \quad (7.74)$$

$$\hat{\sigma}^{\mu'}(x', x) = (A_x, B_x), \quad (7.75)$$

$$\hat{\sigma}^{\mu'}(x', z) = (A_z, B_z), \quad (7.76)$$

and

$$q = (\theta_q, \phi_q), \quad (7.77)$$

$$x = (\theta_x, \phi_x), \quad (7.78)$$

$$z = (\theta_z, \phi_z). \quad (7.79)$$

In this calculation the independent variables will be θ_q , ϕ_q , A and B . The rest can be written in terms of these as follows:

$$A_q = -\frac{\cos^{-1}[\sin \phi_q \sin \theta_q] \cos \theta_q}{\sqrt{1 - \sin^2 \phi_q \sin^2 \theta_q}}, \quad (7.80)$$

$$B_q = -\frac{\cos^{-1}[\sin \phi_q \sin \theta_q] \cos \phi_q \sin \theta_q}{\sqrt{1 - \sin^2 \phi_q \sin^2 \theta_q}}, \quad (7.81)$$

$$A_x = A_q + \frac{A}{2}, \quad (7.82)$$

$$A_z = A_q - \frac{A}{2}, \quad (7.83)$$

$$B_x = B_q + \frac{B}{2}, \quad (7.84)$$

$$B_z = B_q - \frac{B}{2}, \quad (7.85)$$

$$\theta_x = \cos^{-1} \left(-\frac{A_x \sin \sqrt{A_x^2 + B_x^2}}{\sqrt{A_x^2 + B_x^2}} \right), \quad (7.86)$$

$$\theta_z = \cos^{-1} \left(-\frac{A_z \sin \sqrt{A_z^2 + B_z^2}}{\sqrt{A_z^2 + B_z^2}} \right), \quad (7.87)$$

$$\phi_x = \sin^{-1} \left(- \frac{B_x \sin \sqrt{A_x^2 + B_x^2}}{\sqrt{B_x^2 + A_x^2 \cos^2 \sqrt{A_x^2 + B_x^2}}} \right), \quad (7.88)$$

$$\phi_z = \sin^{-1} \left(- \frac{B_z \sin \sqrt{A_z^2 + B_z^2}}{\sqrt{B_z^2 + A_z^2 \cos^2 \sqrt{A_z^2 + B_z^2}}} \right). \quad (7.89)$$

An ideal test function ψ for this analysis should be localized around (θ', ϕ') and decay fast enough so that there wont be any problems around caustics. We will consider a fixed momentum and try to obtain a Wigner function $W(\theta_q, \phi_q)$. Let the test function be of the form

$$\psi(\theta, \phi) = \frac{1 - \zeta(\theta, \phi)}{1 - b\zeta(\theta, \phi)} e^{-c(\theta - \theta_0)^2} \quad (7.90)$$

where

$$\zeta(\theta, \phi) = [\tan^{-1} a(\phi - \phi_0)]^2. \quad (7.91)$$

In our numeric calculations $a = 5$, $b = 0.96$, $c = 40$ and $\phi_0 = \theta_0 = \pi/2$. The function viewed from the $+\hat{y}$ direction in the form of a contour plot is given in Fig. 8. Note the symmetry here (a rotation of π about the \hat{y} axis should preserve this symmetry). A $\pi/2$ rotation can be done by swapping z and x . In spherical coordinates this is done by the transformations

$$\theta \rightarrow \cos^{-1}(\sin \theta \cos \phi), \quad (7.92)$$

$$\phi \rightarrow \tan^{-1}(\tan \theta \sin \phi). \quad (7.93)$$

2. The Non-covariant Wigner Function

What does one get when he uses the classical definition? Here we have no way to plot the four-variable function

$$W \sim \int du \int dv e^{-i(p_\theta u + p_\phi v)} \psi^*(\theta + u/2, \phi + v/2) \psi(\theta - u/2, \phi - v/2) \quad (7.94)$$

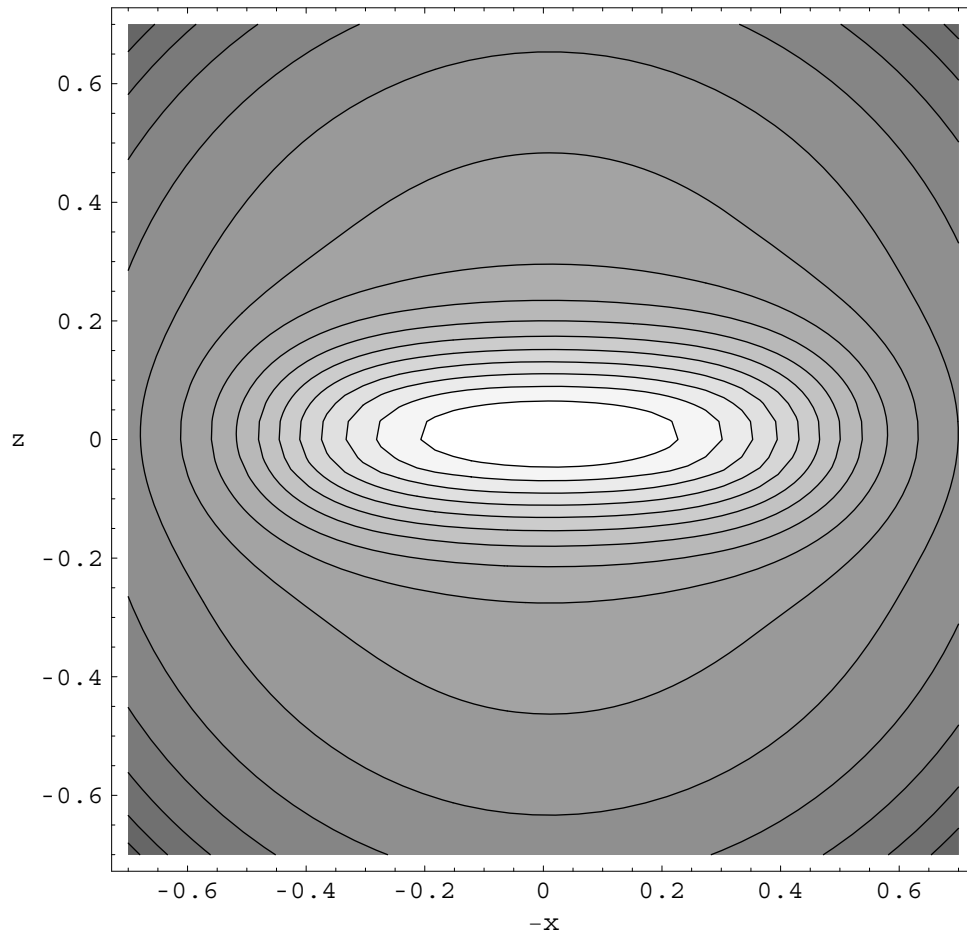


Fig. 8. Contour plot of the test function.

so we will assume the momentum is constant and plot the coordinate part of the Wigner function. Remember, our goal is to see whether this function is invariant under rotations. The answer is no. A numerical analysis shows that the Wigner function calculated using the definition above (Fig. 9) is distorted when a rotation is performed on ϕ and θ (Fig. 10).

3. The Covariant Wigner Function on the 2-Sphere

Now it is time to employ the covariant function defined in the beginning. The integral is very complicated and it is impossible to obtain an analytical result, therefore the numerical integration will be done at each point on a 70×70 mesh. The integration method is quasi Monte-Carlo in *Mathematica* with an iteration of 2000. The real part of the integrand is used in the evaluation and the momenta are equal to 10. The covariant Wigner function (Fig. 11) in this case preserves its symmetry under a rotation of ψ . Note that this is an *active* transformation of the function; it is expected that the Wigner function will reorient itself (Fig 12). What we mean by covariance here is that the shape of the result should also be rotated by $\pi/2$ without any distortion.

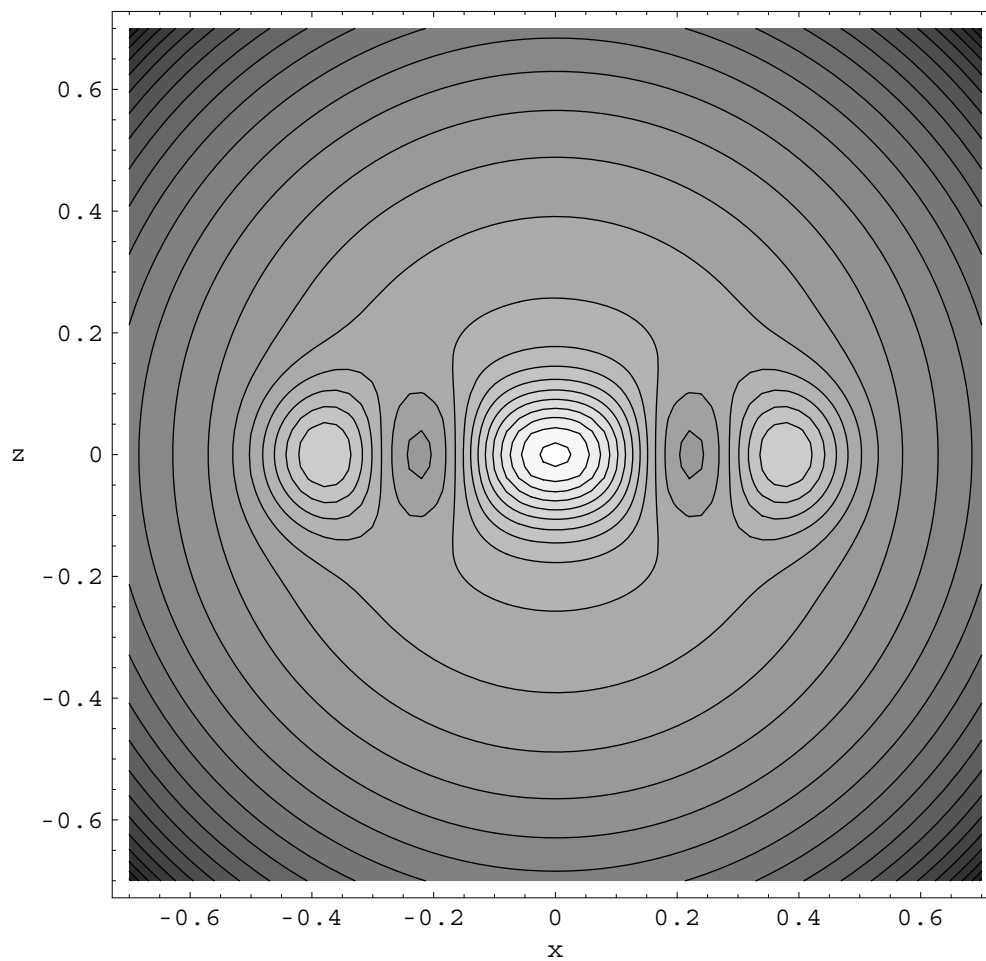


Fig. 9. Contour plot of the non-covariant Wigner function ($p_\theta=p_\phi=10$, $-\pi/2 < u < \pi/2$, $-\pi < v < \pi$).

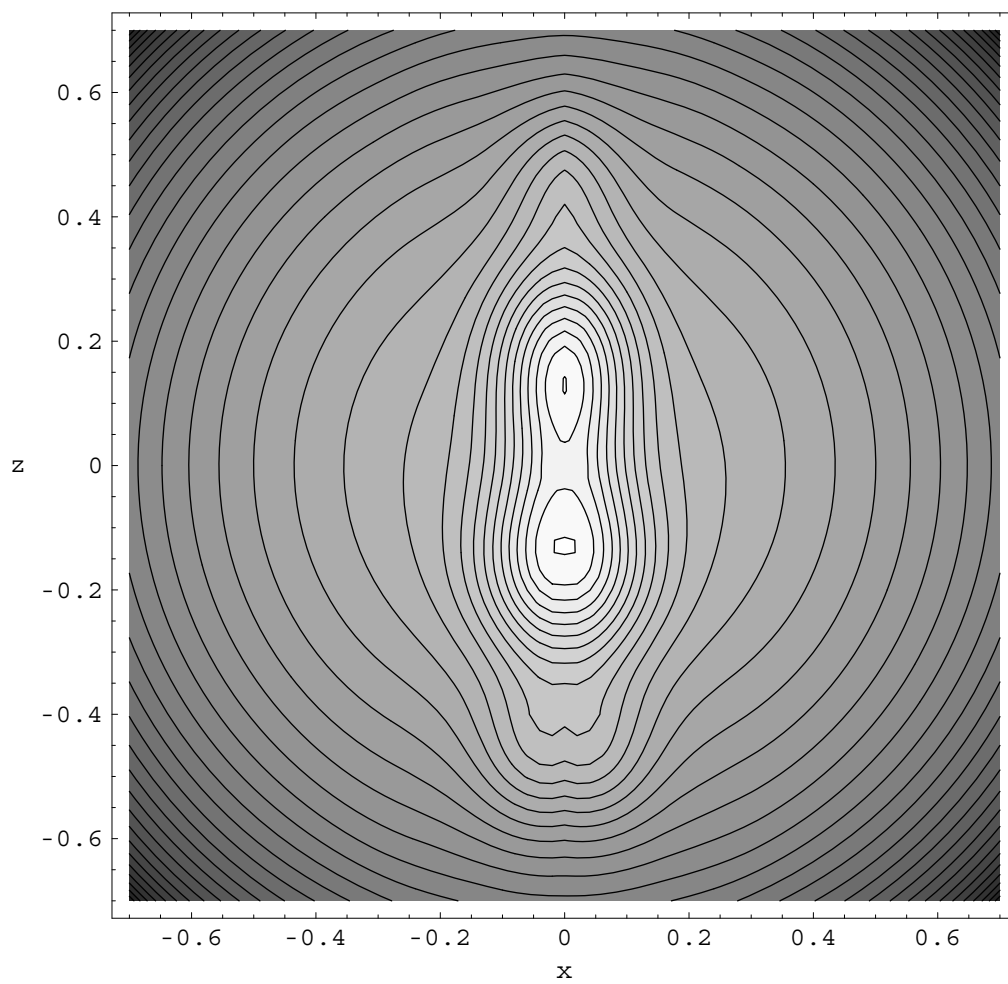


Fig. 10. Contour plot of the non-covariant Wigner function after the coordinate transformation.

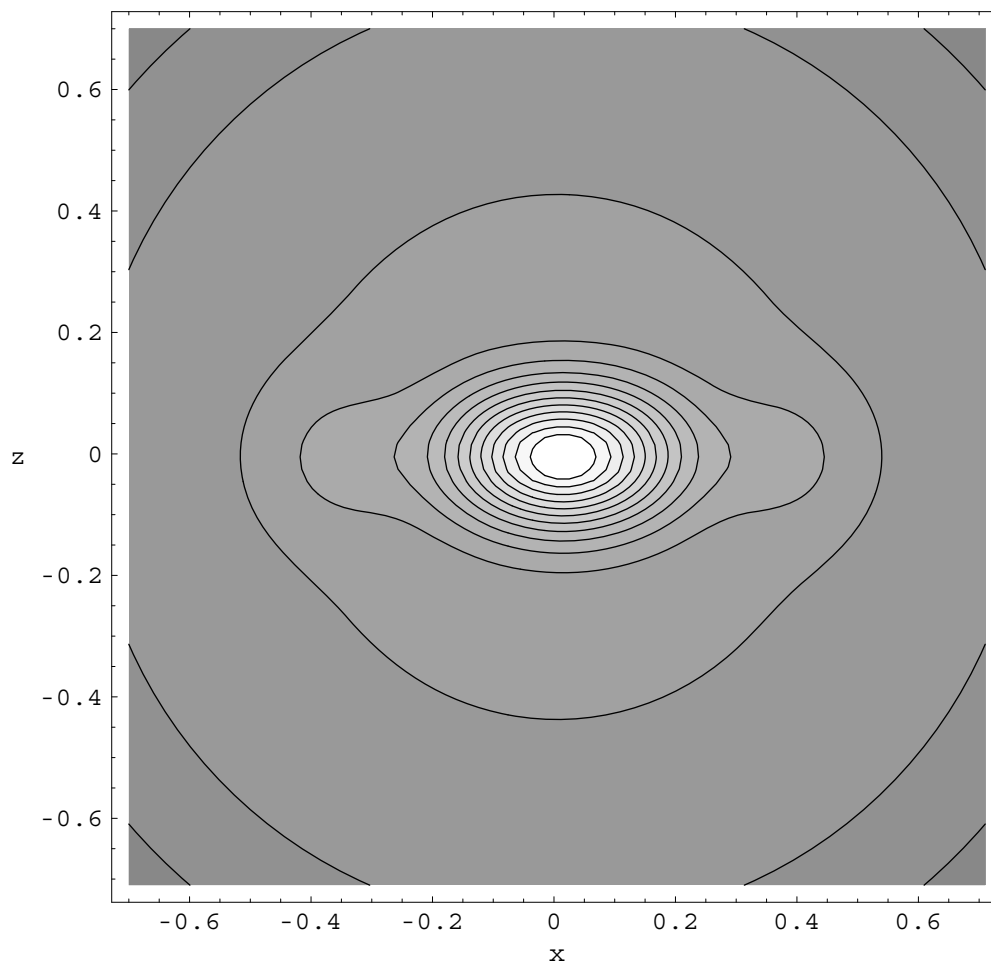


Fig. 11. Covariant Wigner function of the state ψ .

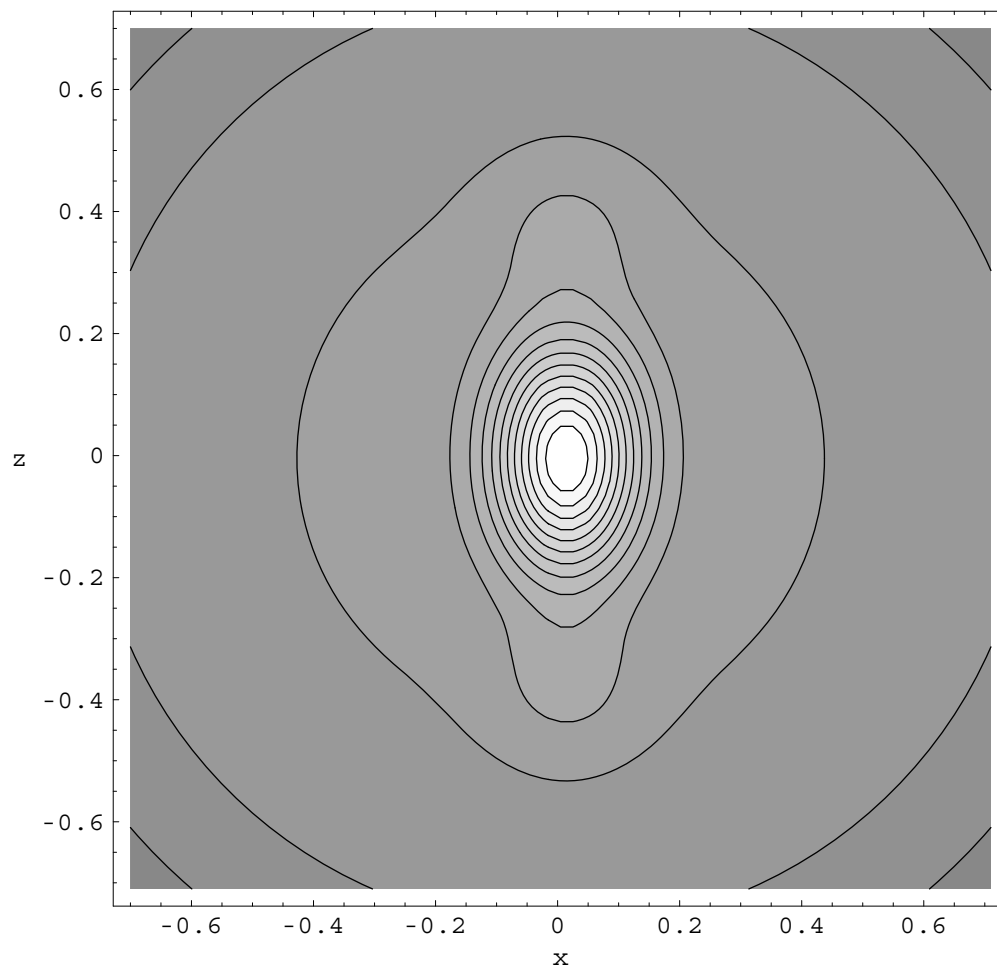


Fig. 12. Covariant Wigner function after ψ rotated by $\pi/2$.

CHAPTER VIII

CONCLUSION

The application of the gauge-invariant Wigner function in flat space to the Landau problem was relatively easier than exploring the covariant Wigner function on the manifold. The spherical symmetry did help in constructing the world function analytically, but a numerical analysis was inescapable considering the complexity of the integral defining the Wigner function. The study of arbitrary manifolds in this context needs more work due to the fact that the geodesic distance should also be calculated numerically.

The new quantization scheme introduced in Chapter V is only a definition. As Prof. Fulling wrote, “A definition is not true or false. On the other hand, some definitions are more useful or more elegant than others” [6]. Finding a ‘tasteful richness of design’ or ‘scientific neatness and simplicity’ in (5.2)–(5.9) is a subjective matter yet the definitions proved to be useful in obtaining the asymptotic product formula of Chapter VI. On the other hand, the cumbersome task of getting (6.73) and the lack of simplicity of the final formula itself were practical barriers to find asymptotic expressions for the symbols of operators such as $e^{\hat{A}}$.

According to Sigurdsson, “Weyl wanted to understand and not merely to produce mechanically like a factory worker” [2].

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APPENDIX A

DERIVATION OF THE COINCIDENCE LIMITS USED IN THIS
DISSERTATION

One starts with the basic equation

$$\sigma = \frac{1}{2}\sigma_\mu\sigma^\mu \quad (\text{A.1})$$

and the boundary conditions

$$[\sigma] = 0 \quad \text{and} \quad [\sigma_\mu] = 0. \quad (\text{A.2})$$

Then

$$\begin{aligned} \sigma_\nu &= \frac{1}{2}(\nabla_\nu\sigma_\mu)\sigma^\mu + \frac{1}{2}\sigma_\mu\nabla_\nu\sigma^\mu \\ &= \sigma_\mu\nabla_\nu\sigma^\mu \end{aligned} \quad (\text{A.3})$$

and

$$\nabla_\alpha\sigma_\nu = (\nabla_\alpha\sigma_\mu)\nabla_\nu\sigma^\mu + \sigma_\mu\nabla_\alpha\nabla_\nu\sigma^\mu. \quad (\text{A.4})$$

At the coincidence limit,

$$[\nabla_\alpha\sigma_\nu] = [\nabla_\alpha\sigma_\mu][\nabla_\nu\sigma^\mu] + [\sigma_\mu][\nabla_\alpha\nabla_\nu\sigma^\mu]; \quad (\text{A.5})$$

the rightmost term vanishes according to (A.2). Therefore,

$$[\nabla_\nu\sigma^\mu] = \delta^\mu_\nu \quad (\text{A.6})$$

or, equivalently,

$$[\nabla_\nu\sigma_\mu] = g_{\mu\nu}. \quad (\text{A.7})$$

The derivative of (A.4) is

$$\nabla_\beta \nabla_\alpha \sigma_\nu = (\nabla_\beta \nabla_\alpha \sigma_\mu) \nabla_\nu \sigma^\mu + (\nabla_\alpha \sigma_\mu) \nabla_\beta \nabla_\nu \sigma^\mu + (\nabla_\beta \sigma_\mu) \nabla_\alpha \nabla_\nu \sigma^\mu + \sigma_\mu \nabla_\beta \nabla_\alpha \nabla_\nu \sigma^\mu, \quad (\text{A.8})$$

which at the coincidence limit reads

$$[\nabla_\beta \nabla_\alpha \sigma_\nu] = [\nabla_\beta \nabla_\alpha \sigma_\mu] \delta^\mu{}_\nu + g_{\mu\alpha} [\nabla_\beta \nabla_\nu \sigma^\mu] + g_{\mu\beta} [\nabla_\alpha \nabla_\nu \sigma^\mu], \quad (\text{A.9})$$

or

$$[\nabla_\beta \nabla_\nu \sigma_\alpha] + [\nabla_\alpha \nabla_\nu \sigma_\beta] = 0. \quad (\text{A.10})$$

Since $\sigma(x', x)$ is a bi-scalar,

$$\nabla_\nu \sigma_\beta = \nabla_\nu \nabla_\beta \sigma = \nabla_\beta \sigma_\nu \quad (\text{A.11})$$

and (A.10) can be written as

$$[\nabla_\beta \nabla_\alpha \sigma_\nu] + [\nabla_\alpha \nabla_\beta \sigma_\nu] = 0. \quad (\text{A.12})$$

In a torsion-free space

$$\nabla_\alpha \nabla_\beta \sigma_\nu = \nabla_\beta \nabla_\alpha \sigma_\nu + R_{\nu\lambda\alpha\beta} \sigma^\lambda, \quad (\text{A.13})$$

which one uses to find

$$[\nabla_\beta \nabla_\alpha \sigma_\nu] = 0. \quad (\text{A.14})$$

The derivative of (A.8) and the coincidence limits derived so far can be used to get the following:

$$[\nabla_\delta \nabla_\beta \nabla_\nu \sigma_\alpha] + [\nabla_\delta \nabla_\alpha \nabla_\nu \sigma_\beta] + [\nabla_\beta \nabla_\alpha \nabla_\nu \sigma_\delta] = 0. \quad (\text{A.15})$$

Using (A.13) one gets

$$\nabla_\delta \nabla_\alpha \nabla_\beta \sigma_\nu = \nabla_\delta \nabla_\beta \nabla_\alpha \sigma_\nu + \nabla_\delta (R_{\nu\lambda\alpha\beta} \sigma^\lambda), \quad (\text{A.16})$$

and hence

$$[\nabla_\delta \nabla_\alpha \nabla_\beta \sigma_\nu] = [\nabla_\delta \nabla_\beta \nabla_\alpha \sigma_\nu] + R_{\nu\delta\alpha\beta}. \quad (\text{A.17})$$

Then

$$2[\nabla_\delta \nabla_\beta \nabla_\alpha \sigma_\nu] + R_{\nu\delta\alpha\beta} + [\nabla_\beta \nabla_\alpha \nabla_\delta \sigma_\nu] = 0. \quad (\text{A.18})$$

Similarly, using

$$[\nabla_\beta \nabla_\alpha \nabla_\delta \sigma_\nu] = [\nabla_\beta \nabla_\delta \nabla_\alpha \sigma_\nu] + R_{\nu\beta\alpha\delta} \quad (\text{A.19})$$

and

$$[\nabla_\beta \nabla_\delta \nabla_\alpha \sigma_\nu] = [\nabla_\delta \nabla_\beta \nabla_\alpha \sigma_\nu] + R_{\alpha\nu\delta\beta} + R_{\nu\alpha\delta\beta} \quad (\text{A.20})$$

one finds

$$3[\nabla_\delta \nabla_\beta \nabla_\alpha \sigma_\nu] + R_{\nu\delta\alpha\beta} + R_{\nu\beta\alpha\delta} + R_{\alpha\nu\delta\beta} + R_{\nu\alpha\delta\beta} = 0. \quad (\text{A.21})$$

Finally, since $R_{\alpha\nu\delta\beta} = -R_{\nu\alpha\delta\beta}$,

$$[\nabla_\delta \nabla_\beta \nabla_\alpha \sigma_\nu] = -\frac{1}{3}(R_{\nu\delta\alpha\beta} + R_{\nu\beta\alpha\delta}). \quad (\text{A.22})$$

The coincidence limit of $\nabla_\lambda \nabla_\beta g^{\nu'}{}_\alpha$ can be found in a similar manner. One starts with

$$\sigma^\mu \nabla_\mu g^{\nu'}{}_\alpha = 0 \quad (\text{A.23})$$

and differentiates twice to get

$$\begin{aligned} & (\nabla_\lambda \nabla_\beta \sigma^\mu) \nabla_\mu g^{\nu'}{}_\alpha + (\nabla_\beta \sigma^\mu) \nabla_\lambda \nabla_\mu g^{\nu'}{}_\alpha \\ & + (\nabla_\lambda \sigma^\mu) \nabla_\beta \nabla_\mu g^{\nu'}{}_\alpha + \sigma^\mu \nabla_\lambda \nabla_\beta \nabla_\mu g^{\nu'}{}_\alpha = 0. \end{aligned} \quad (\text{A.24})$$

Taking the coincidence limit one finds that

$$[\nabla_\lambda \nabla_\beta g^{\nu'}{}_\alpha] + [\nabla_\beta \nabla_\lambda g^{\nu'}{}_\alpha] = 0. \quad (\text{A.25})$$

Using

$$\nabla_\beta \nabla_\lambda g^{\nu'}{}_\alpha = \nabla_\lambda \nabla_\beta g^{\nu'}{}_\alpha + R_{\alpha\rho\beta\lambda} g^{\nu'}{}_\rho \quad (\text{A.26})$$

and

$$[g^{\nu'}{}_\rho] = \delta^\nu{}_\rho, \quad (\text{A.27})$$

(A.25) can be written as

$$[\nabla_\lambda \nabla_\beta g^{\nu'}{}_\alpha] = \frac{1}{2} R^\nu{}_{\alpha\beta\lambda}. \quad (\text{A.28})$$

In order to find the coincidence limits of derivatives of the VanVleck-Morette determinant, one uses

$$\Delta^{-1} \nabla_\mu (\Delta \sigma^\mu) = d, \quad (\text{A.29})$$

or

$$d\Delta = (\nabla_\mu \Delta) \sigma^\mu + \Delta \nabla_\mu \sigma^\mu. \quad (\text{A.30})$$

in d -dimensions. Differentiating twice:

$$\begin{aligned} d\nabla_\beta \nabla_\alpha \Delta &= (\nabla_\beta \nabla_\alpha \nabla_\mu \Delta) \sigma^\mu + (\nabla_\alpha \nabla_\mu \Delta) \nabla_\beta \sigma^\mu + (\nabla_\beta \nabla_\mu \Delta) \nabla_\alpha \sigma^\mu \\ &\quad + (\nabla_\mu \Delta) \nabla_\beta \nabla_\alpha \sigma^\mu + (\nabla_\beta \nabla_\alpha \Delta) \nabla_\mu \sigma^\mu + (\nabla_\alpha \Delta) \nabla_\beta \nabla_\mu \sigma^\mu \\ &\quad + (\nabla_\beta \Delta) \nabla_\alpha \nabla_\mu \sigma^\mu + \Delta \nabla_\beta \nabla_\alpha \nabla_\mu \sigma^\mu. \end{aligned} \quad (\text{A.31})$$

In the coincidence limit, (A.31) becomes

$$\begin{aligned} d[\nabla_\beta \nabla_\alpha \Delta] &= [\nabla_\alpha \nabla_\mu \Delta] \delta^\mu{}_\beta + [\nabla_\beta \nabla_\mu \Delta] \delta^\mu{}_\alpha + d[\nabla_\beta \nabla_\alpha \Delta] \\ &\quad - \frac{1}{3} (R^\mu{}_{\beta\mu\alpha} + R^\mu{}_{\alpha\mu\beta}), \end{aligned} \quad (\text{A.32})$$

or

$$[\nabla_\alpha \nabla_\beta \Delta] + [\nabla_\beta \nabla_\alpha \Delta] - \frac{1}{3} (R_{\beta\alpha} + R_{\alpha\beta}) = 0; \quad (\text{A.33})$$

therefore,

$$[\nabla_\alpha \nabla_\beta \Delta] = \frac{1}{3} R_{\beta\alpha}. \quad (\text{A.34})$$

Rewriting (A.29) as

$$\Delta^{-1/2}\nabla_\mu(\Delta^{1/2}\Delta^{1/2}\sigma^\mu) = \Delta^{1/2}d, \quad (\text{A.35})$$

differentiating repeatedly and taking the coincidence limits, one finds

$$[\nabla_\beta\nabla_\alpha\Delta^{1/2}] = \frac{1}{6}R_{\alpha\beta}. \quad (\text{A.36})$$

VITA

- Kamil Serkan Güntürk.
- Place of Birth: Ankara, Turkey.
- Country of Citizenship: Turkey.
- Address: c/o Dr. Stephen A. Fulling
Department of Mathematics
Texas A&M University
College Station, TX 77843-3368
- E-mail: serkan_gunturk@yahoo.com
- Education:
 - Istanbul Technical University B.S. in Physics, 1995
 - Boğaziçi University M.S. in Physics, 1998
 - Texas A&M University Ph.D. in Physics, 2006