# MULTICOMPONENT WKB AND QUANTIZATION*

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A geometric approach for the formulation of the WKB expansion of multicomponent wave equations is formulated for arbitrary symplectic manifolds. The problem is reduced as much as possible to one component equations. Essential use is made of Fedosov's star product. Obstructions against the existence of global WKB amplitudes may arise.

PACS numbers: 03.65. Sq

## 1. Introduction

Hamiltonians whose symbols are not simply real valued, but matrix or, more generally, endomorphism valued functions appear in many places in physics, examples being the Dirac equation, multicomponent wave equations like electrodynamics in media, and Yang–Mills theories, and the Born–Oppenheimer approximation in molecular physics.

Whereas the semiclassical and WKB approximation of scalar systems is well understood, this is not the case to the same extent for Hamiltonians with matrix valued symbols. In particular, semiclassical states in the scalar case have a nice geometric interpretation as half densities on Lagrangean submanifolds invariant under the Hamiltonian flow, and discrete spectra may be computed using the Bohr–Sommerfeld condition, taking into account the Maslov correction [14, 1, 7, 10]. In the multicomponent case, the analogous structures are not known. The usual WKB ansatz

$$\Psi(x) = a(x, \hbar) \exp(iS(x)/\hbar)$$

with $a(x, \hbar) = a_0(x) + a_1(x)\hbar + ...$ being a power series in $\hbar$ with vector valued coefficients is still possible [9, 12, 14, 5] in this situation, but it is

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in general defined only locally and leads to equations which don't have an obvious geometrical interpretation.

The aim of this paper is to give a completely geometric approach to this problems, and to reduce the problem "as far as possible" to the scalar case. As observed in [13] the use of a star-product formulation of quantum mechanics proves to be particularly useful in this context. However, whereas [13] restrict themselves to the use of the Moyal product and thus to the study of trivial bundles (or local trivializations) over $\mathbb{R}^{2n}$, we will consider general bundles over arbitrary symplectic manifolds. Here, Fedosov's construction [8] will be the adequate tool, since it gives an explicit construction for star products in this general setting.

## 2. WKB on $\mathbb{R}^{2n}$

In this section, we give a short overview of some well known results on WKB for multicomponent systems:

Multicomponent WKB deals with equations of the form

$$(\hat{H} - E)\psi = 0 \,,$$

where $\hat{H}$ is an $(N \times N)$-matrix-valued differential operator, or equivalently, an $(N \times N)$-matrix of differential operators. The WKB-ansatz for a solution is:

$$\psi = ae^{\frac{i}{\hbar}S}, \quad a = a_0 + \hbar a_1 + \dots .$$

At zeroth order, this yields:

$$(H_0(q, dS) - E)a_0 = 0 \,,$$

where $H_0$ is the principal symbol of $\hat{H}$, i.e. the zeroth order part of the symbol of $\hat{H}$. In the scalar case ($N = 1$) this simply is the Hamilton-Jacobi-equation for the scalar Hamiltonian $H_0(q, p)$.

For $N > 1$, this equation has two implications: Firstly, $S$ has to be a solution of a Hamilton-Jacobi-equation

$$\lambda_\alpha(q, dS) = E \,,$$

where $\lambda_\alpha(q, p)$ is an eigenvalue of $H_0(q, p)$. (Here, we need the fact that — at least locally — the degeneracies of the eigenvalues do not change in order to define the *function* $\lambda_\alpha$.) Secondly, $a_0(q, p)$ has to be an eigenvector of $H_0(q, p)$ with eigenvalue $E$.

Solutions of the Hamilton-Jacobi-equation define *Lagrangean submanifold* $\Lambda_\alpha$ of $\mathbb{R}^{2n}$ and we may interpret

$$ae^{\frac{i}{\hbar}S}\sqrt{d\mu}$$

as a *half-density on* $\Lambda$ with values in $\mathbb{R}^N$. (strictly speaking, it has to be tensorized with a section of the Maslov bundle).

To study the next order in the WKB approximation, we introduce the projector $\pi_\alpha^0$ on the $\alpha$th eigenspace of $H_0$. We make the assumptions that the multiplicity of $\lambda_\alpha$ is constant on a neighborhood of $\Lambda$, and that kernel and range of $H - \lambda_\alpha$ are complementary (which is in particular fulfilled for hermitian $H$).

Then, the first order equation, which is a "transport equation" for $u = a \otimes \sqrt{d\mu}$, may be written as [15]:

$$a \otimes \mathcal{L}_{X_{\lambda_\alpha}} \sqrt{d\mu} + D_{X_{\lambda_\alpha}} a \otimes \sqrt{d\mu}$$
$$+ \left[ -\tfrac{1}{2}\pi_\alpha^0 \{\pi_\alpha^0, H_0 - \lambda_\alpha \mathbb{I}\}\pi_\alpha^0 + i\pi_\alpha^0 H_1 \pi_\alpha^0 \right] a \otimes \sqrt{d\mu} = 0\,.$$

As compared to the scalar case, there are two additional terms for $N > 1$:

1. "Berry term" for Berry-connection [3, 13, 15]

$$Da = \sum_\alpha \pi_\alpha^0 d\pi_\alpha^0 a\,.$$

2. "Curvature term", involves the curvature $F$ and second fundamental forms $S, S^*$ of the Berry-connection. With

$$S\xi \stackrel{\text{def}}{=} (1 - \pi_\alpha^0)(d\pi_\alpha^0)\xi, \quad S^*\eta \stackrel{\text{def}}{=} -\pi_\alpha^0(d(1 - \pi_\alpha^0))\eta$$

this term may be rewritten as [15]

$$\lambda_\alpha < \Pi, F > - < \Pi, S^* \wedge (H_0 - \lambda_\alpha \pi_\alpha^0)S >\,,$$

where $\Pi$ is the Poisson tensor.

## 3. Star products and geometrization

As mentioned earlier, the star product approach to quantization is particularly adapted to our problem: Firstly, its structure allows us to deal with the expansion in $\hbar$ in a simple way, and secondly, it is the only known general quantization scheme which allows the quantization of any symplectic manifold, and which is not restricted to just of a small subclass of observables (as, *e.g.* geometric quantization). The idea of star product quantization is to pull back the operator product, which is defined on operators on Hilbert space $\mathcal{H}$, to an associative, non-commutative product on the functions on

phase space, via a suitable symbol calculus [2]: Assuming that we we are given a quantization procedure

$$Q : \mathcal{C}^\infty(M) \otimes \mathbb{C}[[\hbar]] \to End\mathcal{H}$$

we may define a star product on $\mathcal{C}^\infty(M) \otimes \mathbb{C}[[\hbar]]$ by:

$$a * b = Q^{-1}(Q(a)Q(b)) .$$

The simplest example for such a star product is the case $M = \mathbb{R}^{2n}$ and $Q$ being Weyl-ordering, which leads to the well known Weyl-Moyal product. It is explictly given by:

$$(a \diamond b)(x) = (e^{\frac{i\hbar}{2} \omega^{ij} \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial y^j}} a(x)b(y))|_{x=y} ,$$

where $\omega_{ij}$ are the components of the standard symplectic form on $\mathbb{R}^{2n}$. Although we have only considered scalar valued observables so far, the matrix generalization is obvious in this simple example: In the matrix product, one simply has to replace the ordinary pointwise product of the matrix elements by the Moyal product.

The formal definition is as follows:

**Definition 3.1.** *A star product on a symplectic manifold $M$ is an associatiative product on $\mathcal{C}^\infty(M) \otimes \mathbb{C}[[\hbar]]$ with*

1. $a * b = ab + O(\hbar)$
2. $a * b - b * a = i\hbar\{a, b\}$
3. $a * 1 = 1 * a = a$
4. $\underline{supp(a * b)} \subset supp(a) \cap supp(b)$
5. $\overline{a * b} = \bar{b} * \bar{a}$

Star products exist for every symplectic manifold $M$ [6, 8]. Given a star product and a differential operator $W = W_0 + \hbar W_1 + \ldots$ on $\mathcal{C}^\infty(M) \otimes \mathbb{C}[[\hbar]]$ with $W1 = 0$, we may define a new star product:

$$a *_W b = e^{-\hbar W}(e^{\hbar W} a * e^{\hbar W} b) .$$

$*$ and $*_W$ are called *equivalent*. The importance of this notion is that "physics remains unchanged", if the change of $*$ to $*_W$ is accompanied by the application of the isomorphism $e^{\hbar W}$ to the observables: Heuristically, this means that if we change the ordering prescription and at the same time the symbol calculus in such a way that the operators on Hilbert space remain unchanged, then physics remains unchanged. We shall exploit this freedom later on.

## 4. Fedosov's star product

In this section, we give a short overview of Fedosov's explicit construction of a star product on endomorphism bundles of vector bundles over a symplectic manifold. The arena is as follows: We consider an Hermitean vector bundle $V$ over a symplectic manifold $M$. Denoting by $\mathbb{C}[[\hbar]]$ the set of formal power series in $\hbar$ with coefficients in $\mathbb{C}$, we construct from these data the bundles $V[[\hbar]] \overset{\text{def}}{=} V \otimes \mathbb{C}[[\hbar]]$, $E[[\hbar]] = \cup_{m \in M} End(V_m) \otimes \mathbb{C}[[\hbar]]$, and the algebra $\mathcal{A} = \Gamma(E[[\hbar]] \otimes W)$, where $W$ denotes the Weyl-bundle over $M$, the bundle whose fibres $W_q$ are the Weyl algebras over $T_q M$.

Finally we consider the algebra: $\Omega(M) \otimes \mathcal{A}$, with $\Omega(M)$ being the algebra of differential forms on $M$. On this algebra, we define two globally defined operators $\delta, \delta^{-1} : \Omega(M) \otimes \mathcal{A} \to \Omega(M) \otimes \mathcal{A}$ whose coordinate expressions are given by

$$\delta \hat{a} = dx^i \wedge \frac{\partial}{\partial y^i} \hat{a}, \quad \delta^{-1} \hat{a} = \frac{1}{p+q} i_{y^i \frac{\partial}{\partial x^i}} \hat{a}$$

for a $q$-form $\hat{a}$ with values in the homogeneous polynomials in $y$ of degree $p$. Here, $x^i$ are coordinates on $M$, and $y^i$ the induced coordinates on $T_q M$.

To construct a unique star product on $E[[\hbar]]$ two additional data are required: a Hermitian connection $\nabla$ on $V$ (inducing a connection on $E[[\hbar]]$) and a symplectic connection $\partial_s$ on $M$. From these we can construct a connection $\partial = 1 \otimes \partial_s + \nabla \otimes 1$ on $E[[\hbar]] \otimes W$. Now, these data given, the main step of Fedosov's construction consists in finding by a recursive procedure a covariant exterior derivative

$$D = -\delta + \partial + [\frac{i}{\hbar} r, \cdot]$$

with $r \in \Omega^1(M) \otimes \mathcal{A}$ such that

1. $D^2 = 0$, i.e., $D$ is a flat connection.
2. Covariantly constant elements in $\Omega_0(M) \otimes \mathcal{A}$ are in linear one-to-one correspondence to $\Gamma(E[[\hbar]])$
3. $D$ is a derivation on $\Omega(M) \otimes \mathcal{A}$ (hence, covariantly constant sections form a subalgebra)

If we denote the isomorphism in 2., which maps $a \in \Gamma E[[\hbar]]$ to its covariantly constant continuation in $\Omega_0(M) \otimes \mathcal{A}$, by $Q$, it is given by the solution of

$$Q(a) = a + \delta^{-1}(\partial Q(a) + [\frac{i}{\hbar} r, Q(a)]),$$

which may be solved iteratively.

With these notions, Fedosov's star product is simply given by

$$a * b = Q^{-1}(Q(a) \diamond Q(b)),$$

where $\diamond$ is the fibrewise Moyal product.

Different choices of $\nabla$ (and $\partial_s$) lead to different star products. However, the star products obtained in this way are equivalent:

**Theorem 4.1.** *Let $D^{(1,2)}$ be the Fedosov connections associated to $\nabla^{(1,2)}$, $\partial^{(1,2)}$. Then there is $A_{(1,2)} \in \mathcal{A}$ and*

$$U_{(1,2)} = exp_\diamond(\frac{i}{\hbar} A_{(1,2)})$$

*such that*

$$D^{(1)}\hat{a} = 0 \Leftrightarrow D^{(2)}(U_{(1,2)} \diamond \hat{a} \diamond U_{(1,2)}^{-1}) = 0$$

*and*

$$\phi(a) \stackrel{\text{def}}{=} Q^{(2)^{-1}}(U_{(1,2)} \diamond Q^{(1)}(a) \diamond U_{(1,2)}^{-1})$$

*is an isomorphism of the products $*^{(1)}$ and $*^{(2)}$.*

$$\nabla^{(1)} - \nabla^{(2)} = O(\hbar^m)$$

$$\Rightarrow Q^{(2)^{-1}}(U_{(1,2)} \diamond \hat{a} \diamond U_{(1,2)}^{-1}) - Q^{(1)^{-1}}(\hat{a}) = O(\hbar^{m+1})$$

*for every $\hat{a}$ with $D^{(1)}\hat{a} = 0$.*

## 5. Application to WKB

We are now ready to apply the above techniques to multicomponent WKB. Let

$$H = H_0 + \hbar H_1 + \ldots$$

be a section of $E[[\hbar]]$, $\pi_\alpha^0(x)$ the projection on the (regular) eigenspace belonging to $\lambda_\alpha(x)$. Now, the main problem in WKB, which prevents us from naively reducing the problem to a scalar problem on each bundle of eigenspaces, is the fact that, due to quantum corrections, WKB states are not sections in these bundles, but have higher order corrections. In the star product approach this is related to the fact that the star commutator of the Hamiltonian with an observable commuting with $\pi_\alpha^0(x)$ does not commute with $\pi_\alpha^0(x)$, hence a reduction to the bundles of eigenspaces is not possible. Thus, we have to find a kind of "quantum diagonalization procedure".

The formal reason for this problem in Fedosov's approach to star products is the fact that the projections are not covariantly constant under the hermitian connection which defines the star product. Our strategy for solving this problem is to use the freedom to change $\nabla$ when applying the corresponding star product isomorphism at the same time to preserve physics. This is possible indeed, as expressed by the following theorem:

**Theorem 5.1.** *There exists a formally orthogonal decomposition* $V[[\hbar]] = \oplus_\alpha V_\alpha$, $\dim V_\alpha = m_\alpha$ *with corresponding quantum projections* $\pi_\alpha^{(\infty)}$ *and a hermitian connection* $\nabla^{(\infty)}$ *with*

$$\nabla^{(\infty)} \pi_\alpha^{(\infty)} = 0$$

*such that the corrected Hamiltonian (obtained by applying the corresponding isomorphism* $\phi^{(\infty)}$ *):*

$$H^{(\infty)} = \phi^{(\infty)}(H)$$

*preserves the decomposition:*

$$[H^{(\infty)}, \pi_\alpha^{(\infty)}]_{*_\infty} = 0 \quad \forall \alpha \,,$$

*where* $*_\infty$ *is the Fedosov star product defined by* $\nabla^{(\infty)}$

*Proof:*

The proof is by induction: To start we set $\pi_\alpha^{(1)} = \pi_\alpha^{(0)}$ *and define* $\nabla^{(1)}$ *by* $\nabla^{(1)}\psi = \sum_\alpha \pi_\alpha^{(1)} \nabla \pi_\alpha^{(1)} \psi$. *With* $H^{(1)} = \phi^{(1)}(H)$, *we have*

$$\nabla^{(1)} \pi_\alpha^{(1)} = 0, \quad [\pi^{(1)}, H^{(1)}]_{*_1} = O(\hbar) \,.$$

*Now assume we have found* $\pi_\alpha^{(k)}, \nabla^{(k)} = \sum_\alpha \pi_\alpha^{(k)} \nabla \pi_\alpha^{(k)}$, $H^{(k)} = \phi^{(k)}(H)$ *such that*

$$\nabla^{(k)} \pi_\alpha^{(k)} = 0, \quad [\pi^{(k)}, H^{(k)}]_{*_k} = O(\hbar^k) \,.$$

*We construct* $\pi_\alpha^{(k+1)}$ *with*

$$[\pi_\alpha^{(k+1)}, H^{(k)}]_{*_k} = O(\hbar^{(k+1)})$$

*using the ansatz*

$$\pi_\alpha^{(k+1)} = e^{i\hbar^k A} *_k \pi_\alpha^{(k)} *_k e^{-i\hbar^k A} \,,$$

*which has a solution*

$$A = \sum_{\alpha \neq \beta} \frac{\pi_\alpha^{(k)} W \pi_\beta^{(k)}}{\lambda_\alpha - \lambda_\beta} \,,$$

*where $W$ is defined by*

$$H^{(k)} = \sum_\alpha \pi_\alpha^{(k)} *_k H^{(k)} *_k \pi_\alpha^{(k)} + \hbar^k W \,.$$

*Now, setting $\nabla^{(k+1)} = \sum_\alpha \pi_\alpha^{(k+1)} \nabla \pi_\alpha^{(k+1)} \psi$ and using lemma 4.2., the theorem follows.*

$\square$

## 6. Compatibility

Now, we are ready to address the issue of compatibility of observables, *i.e.*, the question which observables preserve the quantum decomposition found above. The results may be considered generalizations of results found in [4] for the Dirac equation. In physics language, we find an answer to the question which observables are "slow" in the sense that their time evolution is analytic in $\hbar$, and hence does not depend on inverse powers of $\hbar$.

Take $a, b \in \Gamma(E[[\hbar]])$ such that

$$[\pi_\alpha^{(\infty)}, a]_{*_\infty} = [\pi_\alpha^{(\infty)}, b]_{*_\infty} = 0$$

then

$$[\pi_\alpha^{(\infty)}, a *_\infty b]_{*_\infty} = 0 \,.$$

Compatible elements form a $*_\infty$-subalgebra $\tilde{\mathcal{O}}$. In particular, for $b = H^{(\infty)}$ we see that the star commutator of observables in $\tilde{\mathcal{O}}$ with the corrected Hamiltonian is in $\tilde{\mathcal{O}}$ again.

**Theorem 6.1.** *Let $\phi^{(\infty)}$ be the isomorphism between the star products $*$ and $*_\infty$. For every $a$ in the subalgebra $\mathcal{O} = \phi^{\infty -1}(\tilde{\mathcal{O}})$ the Heisenberg evolution equation*

$$\dot{a} = \frac{1}{i\hbar}[H, a]_*$$

*is a well defined differential equation in $\mathcal{O}$ (i.e., there are no inverse powers of $\hbar$ on the right hand side).*

## 7. $O(\hbar)$-correction

In the formalism developped so far, it is straightforward to compute the correction of order $\hbar$: We have

$$H^{(\infty)} = \sum_\alpha \pi_\alpha^{(2)} *_1 H^{(1)} *_1 \pi_\alpha^{(2)} + O(\hbar^2)$$

$$= e^{i\hbar A} * \pi_\alpha^{(0)} * H^{(1)} * \pi_\alpha^{(0)} * e^{-i\hbar A} + O(\hbar^2) \,.$$

A straightforward calculation, using the explicit formula for $U$ leads to [16]

$$\pi_\alpha^{(0)} *_1 H^{(1)} *_1 \pi_\alpha^{(0)} = \pi_\alpha^{(0)} H^{(0)} \pi_\alpha^{(0)} + \frac{i\hbar}{2} \omega^{il} \sum_\gamma \pi_\alpha^{(0)} (\nabla_i \pi_\gamma^0) \nabla_l \pi_\alpha^{(0)} .$$

With the curvature of the "Berry connection"

$$F^B \psi = \sum_\alpha \pi_\alpha^{(0)} \circ \nabla \circ \pi_\alpha^{(0)} \nabla \pi_\alpha^{(0)} \psi = \sum_\alpha \pi_\alpha^{(0)} F^0 \pi_\alpha^{(0)} + \sum_\alpha \pi_\alpha^{(0)} (\nabla \pi_\gamma^0)(\nabla \pi_\alpha^{(0)})$$

and the "Second fundamental form"

$$S^{\beta\alpha}(X)\psi = (\pi_\beta^{(0)} \circ \nabla_X \circ \pi_\alpha^{(0)})\psi \quad (\beta \neq \alpha) ,$$

we finally get:

$$\pi_\alpha^{(0)} * H^{(1)} * \pi_\alpha^{(0)} = \frac{i\hbar}{2} \lambda_\alpha \langle \Pi, \pi_\alpha^0 (F^B - F^0) \pi_\alpha^0 \rangle + \frac{i\hbar}{2} \sum_{\gamma \neq \alpha} \lambda_\gamma \langle \Pi, S^{\gamma\alpha} S^{\alpha\gamma} \rangle .$$

This result is a generalization of our results in [15]: There, the starting point was the Moyal product on $\mathbb{R}^{2n}$, which is a Fedosov star product for a flat connection. Hence, the curvature $F^0$ of $\nabla$ was missing there.

## 8. Change of compatible connection

In the constructions above we have made explicit use of Berry type connections. Nevertheless, we are not really forced to do so, but it is just a convenient choice for the proof. Hence, the question arises whether the correction terms computed above are just a consequence of the choice of our connection, or whether they are really "physical".

To answer this question, take another compatible connection $\tilde{\nabla}$. With

$$\nabla^{(1)} - \tilde{\nabla}^{(1)} = \Delta\Gamma$$

we obtain

$$\pi_\alpha^0 * \tilde{H}^{(1)} * \pi_\alpha^0 = \pi_\alpha^0 * H^{(1)} * \pi_\alpha^0 + i\hbar\pi_\alpha^0 \underbrace{\Delta\Gamma(X_{\lambda_\alpha})}_{\text{"Berry phase" term}} \pi_\alpha^0 .$$

Hence, the only difference is the appearence of an additional Berry phase, which was so far hidden in the explicit use of a non-flat connection. However, the curvature term remains and it still is constructed from the

curvature of the Berry connection, *not* from the curvature of the chosen connection.

*The correction terms involving the curvature and the second fundamental form of the Berry connection have intrisic meaning.*

## 9. Problems

In this section, we just mention a few open problems which are discussed in more detail in [16].

1. Nontrivial holonomy of compatible connections may give an obstruction to the existence of WKB states: only projectors exist because of a $U(n)$ holonomy. Solution are known only for $m_\alpha = 1$(no degeneracy) or $\dim M = 2$ [11, 16].

2. A Maslov-correction has to be implemented. This is straightforward if the problem can really be reduced to a scalar problem, *e.g.* for $m_\alpha = 1$.

3. Level crossings appear in many physical applications. These have been excluded by our regularity conditions. Nevertheless, our approach is still applicable to the open submanifold where the degeneracies are constant. The level crossing points have to be studied in a second step.

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